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(54)名稱

雙液晶原化合物

BIMESOGENIC COMPOUNDS

(57)摘要

本發明係關於式 I 之雙液晶原化合物 $R^1-MG^1-Sp-MG^2-R^2$ I 其中 R^1 、 R^2 、 MG^1 、 MG^2 及 Sp 具有技術方案 1 中所給出之含義；式 I 之雙液晶原化合物在液晶介質中之用途；尤其是有關包括本發明之液晶介質之撓變電子液晶裝置。

另外，本發明係關於在向列混合物中誘導第二向列相之式 I 之雙液晶原化合物，該向列混合物在不含式 I 化合物之情形下並不展現此額外相。

The invention relates to bimesogenic compounds of formula I $R^1-MG^1-Sp-MG^2-R^2$ I wherein R^1 , R^2 , MG^1 , MG^2 and Sp have the meaning given in claim 1, to the use of bimesogenic compounds of formula I in liquid crystal media and particular to flexoelectric liquid crystal devices comprising a liquid crystal medium according to the present invention.

Furthermore the invention relates to bimesogenic compounds of formula I inducing a second nematic phase in nematic mixtures that do not show this additional phase without compounds of formula I.

特徵化學式：

發明專利說明書

(本說明書格式、順序及粗體字，請勿任意更動，※記號部分請勿填寫)

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一、發明名稱：(中文/英文)

雙液晶原化合物

BIMESOGENIC COMPOUNDS

二、中文發明摘要：

本發明係關於式I之雙液晶原化合物

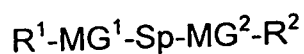


其中 R^1 、 R^2 、 MG^1 、 MG^2 及 Sp 具有技術方案1中所給出之含義；式I之雙液晶原化合物在液晶介質中之用途；尤其是有關包括本發明之液晶介質之撓變電子液晶裝置。

另外，本發明係關於在向列混合物中誘導第二向列相之式I之雙液晶原化合物，該向列混合物在不含式I化合物之情形下並不展現此額外相。

三、英文發明摘要：

The invention relates to bimesogenic compounds of formula I



wherein R^1 , R^2 , MG^1 , MG^2 and Sp have the meaning given in claim 1, to the use of bimesogenic compounds of formula I in liquid crystal media and particular to flexoelectric liquid crystal devices comprising a liquid crystal medium according to the present invention.

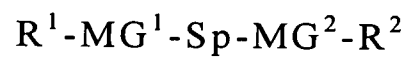
Furthermore the invention relates to bimesogenic compounds of formula I inducing a second nematic phase in nematic mixtures that do not show this additional phase without compounds of formula I.

四、指定代表圖：

(一)本案指定代表圖為：(無)

(二)本代表圖之元件符號簡單說明：

五、本案若有化學式時，請揭示最能顯示發明特徵的化學式：



六、發明說明：

【發明所屬之技術領域】

本發明係關於式I之雙液晶原化合物



其中 R^1 、 R^2 、 MG^1 、 MG^2 及 Sp 具有技術方案1中所給出之含義；式I之雙液晶原化合物在液晶介質中之用途及特定而言包括本發明之液晶介質之撓變電子液晶裝置。

另外，本發明係關於在向列混合物中誘導第二向列相之式I之雙液晶原化合物，該向列混合物在不含式I化合物之情形下並不展現此額外相。

【先前技術】

液晶顯示器(LCD)廣泛地用於顯示資訊。LCD用於直視顯示器以及投影型顯示器。用於大部分顯示器中之光電模式仍係扭轉向列(TN)模式以及其各種修改形式。除此模式外，已逐漸使用超扭轉向列(STN)模式及最近之光學補償彎曲(OCB)模式及電控雙折射(ECB)模式以及其各種修改形式(例如垂直配向向列(VAN)、圖案化ITO垂直配向向列(PVA)、聚合物穩定垂直配向向列(PSVA)模式及多域垂直配向向列(MVA)模式以及其他模式)。所有該等模式皆使用與基板、(個別地)液晶層實質上垂直之電場。除該等模式外，亦存在採用與基板、(個別地)液晶層實質上平行之電場之光電模式，例如平面內切換(短IPS)模式(例如在DE 40 00 451及EP 0 588 568中所揭示)及邊緣場切換(FFS)模式。尤其而言，後一光電模式(其具有良好視角性質及改

良之反應時間)逐漸用於現代桌上型監視器所用之LCD中且甚至用於TV及多媒體應用所用之顯示器中，且由此與TN-LCD進行競爭。

除該等顯示器外，在利用所謂的「撓變電子」效應之顯示器中，提出使用利用具有相對較短膽固醇節距之膽固醇液晶之新顯示模式。術語「液晶」、「液晶態化合物(mesomorphic compound)」或「液晶原化合物」(亦簡稱為「液晶原」)意指在適宜溫度、壓力及濃度條件下可作為中間相(向列相、層列相等)或具體而言作為LC相存在之化合物。非兩親性液晶原化合物包括(例如)一或多個桿條狀、香蕉形或盤狀液晶原基團。

在先前技術中已知撓變電子液晶材料。撓變電子效應尤其闡述於Chandrasekhar, 「Liquid Crystals」, 第2版, Cambridge University Press (1992)及P.G. deGennes等人, 「The Physics of Liquid Crystals」, 第2版, Oxford Science Publications (1995)中。

在該等顯示器中，膽固醇液晶以「均勻臥式螺旋」配置(ULH)進行定向，此顯示模式亦以此命名。出於此目的，與向列材料混合之對掌性物質誘導該材料發生螺旋扭轉而轉變成等效於膽固醇材料之對掌性向列材料。一般而言，術語「對掌性」用於闡述與其鏡像不可疊合之物體。「非對掌性(無對掌性)」物體係與其鏡像相同之物體。除非另外明確闡述，否則術語對掌性向列及膽固醇在本申請案中同義使用。在第一近似法中，由對掌性物質誘導之節距

(P_0)與所用對掌性材料之濃度(c)成反比。此相關性之比例常數稱為對掌性物質之螺旋扭轉力(HTP)且由等式(1)加以定義：

$$\text{HTP} \equiv 1/(c \cdot P_0) \quad (1)$$

其中

c 係對掌性化合物之濃度。

使用具有短節距(通常介於 $0.2 \mu\text{m}$ 至 $1 \mu\text{m}$ 之間、較佳地 $1.0 \mu\text{m}$ 或更小、特定而言 $0.5 \mu\text{m}$ 或更小)之對掌性向列液晶來實現均勻臥式螺旋結構，該對掌性向列液晶與液晶單元中平行於基板(例如玻璃片)之其螺旋軸單向配向。在此組態中，對掌性向列液晶之螺旋軸等效於雙折射片之光軸。

若垂直於螺旋軸向此組態施加電場，則光軸在單元之平面中旋轉，此類似於鐵電液晶之指向矢在表面穩定鐵電液晶顯示器中旋轉。撓變電子效應之特徵在於通常介於 $6 \mu\text{s}$ 至 $100 \mu\text{s}$ 之間之快速反應時間。其進一步描述極佳之灰度能力。

電場在適於在光軸中傾斜之指向矢中誘導延展彎曲結構。在第一近似法中，軸之旋轉角度與電場強度成正比且呈線性比例。在將液晶單元置於交叉偏振器之間且呈無動力狀態之光軸與一個偏振器之吸收軸成 22.5° 角時，看到最佳光學效應。此 22.5° 角亦係電場旋轉之理想角度，因此藉由使電場反轉光軸旋轉 45° ，且藉由適當選擇螺旋軸之較佳方向、偏振器之吸收軸及電場方向之相對定向，光軸可自平行於一個偏振器切換至偏振器之間之中心角度。在光

軸之總切換角度為 45° 時，則達成最佳對比度。在該情形下，該配置可用作可切換四分之一波片，前提係光學延遲（亦即液晶之有效雙折射率與單元間隙之乘積）選擇為波長之四分之一。在此背景下，除非另外明確闡述，否則提及 550 nm 之波長，在該波長下人眼之敏感性最高。

藉由式(2)給出光軸之旋轉角度(Φ)之良好近似值

$$\tan\Phi = \bar{e}P_0E / (2\pi K) \quad (2)$$

其中

P_0 係膽固醇液晶之未受擾節距，

\bar{e} 係延展撓變電子係數($e_{\text{延展}}$)及彎曲撓變電子係數($e_{\text{彎曲}}$)之平均值 [$\bar{e} = \frac{1}{2}(e_{\text{延展}} + e_{\text{彎曲}})$]，

E 係電場強度且

K 係延展彈性常數(k_{11})及彎曲彈性常數(K_{33})之平均值 [$K = \frac{1}{2}(k_{11} + k_{33})$]

且其中

\bar{e}/K 稱為撓性-彈性比。

此旋轉角度係撓變電子切換元件中之切換角度之一半。

藉由式(3)給出此光電效應之反應時間(τ)之良好近似值

$$\tau = [P_0 / (2\pi)]^2 \cdot \gamma / K \quad (3)$$

其中

γ 係與螺旋之扭曲有關之有效黏度係數。

存在解開螺旋之臨界場(E_c)，其可自等式(4)獲得

$$E_c = (\pi^2 / P_0) \cdot [k_{22} / (\epsilon_0 \Delta\epsilon)]^{1/2} \quad (4)$$

其中

k_{22} 係扭轉彈性常數，

ϵ_0 係真空之電容率且

$\Delta\epsilon$ 係液晶之介電各向異性。

然而，在此模式中，若干問題仍必須解決，該等問題尤其係：難以獲得所需均勻定向、需要解決不利之高電壓（其與常用驅動電子元件不相容）、「關態」並非真黑（dark）（其使對比度劣化）及（最後，但並非最不important）光電特性中之顯著滯後。

相對較新顯示模式-所謂的均勻豎立螺旋（USH）模式可視為接替IPS之替代性模式，此乃因其可展現改良之黑階，即使在與其他提供寬視角之顯示模式（例如IPS、VA等）相比時亦如此。

對於USH模式而言，如同ULH模式，已提出使用雙液晶原液晶材料之撓變電子切換。雙液晶原化合物在先前技術中通常已眾所周知（亦參照Hori, K., Iimuro, M., Nakao, A., Toriumi, H., *J. Mol. Struc.* 2004, 699, 23-29）。術語「雙液晶原化合物」係關於在分子中包括兩個液晶原基團之化合物。與正常液晶原一樣，其端視其結構可形成許多中間相。特定而言，在添加至向列液晶介質中時，式I化合物誘導第二向列相。

在此上下文中，術語「液晶原基團」意指能夠誘導液晶（LC）相行為之基團包括液晶原基團之化合物自身並不一定必須展現LC相。其亦可僅在與其他化合物之混合物中展現

LC相行為。為簡明起見，術語「液晶」在下文中用於液晶原材料及LC材料二者。

然而，因所需之不利之高驅動電壓、對掌性向列材料之相對較窄相範圍及其不可逆切換性質，來自先前技術之材料並不適應於當前之LCD驅動方案。

對於USH及ULH模式之顯示器而言，需要具有改良性質之新液晶介質。尤其而言，應針對光學模式優化雙折射率(Δn)。本文中之雙折射率 Δn 定義於等式(5)中

$$\Delta n = n_e - n_o \quad (5)$$

其中 n_e 係非尋常折射率且 n_o 係尋常折射率，且平均折射率 n_{av} 由下列等式(6)給出。

$$n_{av} = [(2n_o^2 + n_e^2)/3]^{1/2} \quad (6)$$

可使用Abbe折射計量測非尋常折射率 n_e 及尋常折射率 n_o 。然後可自等式(5)計算 Δn 。

另外，對於利用USH或ULH模式之顯示器而言，液晶介質之光學延遲 $d \cdot \Delta n$ (有效)較佳地應使得滿足等式(7)

$$\sin 2(\pi \cdot d \cdot \Delta n / \lambda) = 1 \quad (7)$$

其中

d 係單元間隙且

λ 係光之波長

等式(7)之右手側之容許偏差為 $\pm 3\%$ 。

除非另外明確指定，否則在本申請案中通常提及之光之波長為550 nm。

單元之單元間隙較佳地在1 μm 至20 μm 範圍內，特定而言在2.0 μm 至10 μm 範圍內。

對於ULH/USH模式而言，介電各向異性($\Delta\epsilon$)應盡可能小以防止在施加定址電壓後解開螺旋。較佳地， $\Delta\epsilon$ 應略高於0及極佳地0.1或更高、但較佳地10或更小、更佳地7或更小及最佳地5或更小。在本申請案中，術語「介電正性」係用於 $\Delta\epsilon > 3.0$ 之化合物或組份，「介電中性」係用於 $-1.5 \leq \Delta\epsilon \leq 3.0$ 之化合物或組份，且「介電負性」係用於 $\Delta\epsilon < -1.5$ 之化合物或組份。 $\Delta\epsilon$ 係在1 kHz頻率及20°C下測得。各別化合物之介電各向異性係根據向列相主體混合物中相應個別化合物之10%溶液的結果來確定。在主體介質中之各別化合物之溶解度小於10%之情形下，將其濃度減小至先前之1/2直至所得介質足夠穩定以至少容許測定其性質為止。然而，較佳地，將濃度至少保持於5%以保持盡可能高之結果顯著性。測試混合物之電容係在具有垂直及均勻配向兩種單元中測得。該兩種類型單元之單元間隙係大約20微米。所施加電壓係頻率為1 kHz之矩形波且均方根值通常為0.5伏至1.0伏，然而其始終經選擇以低於各別測試混合物之電容臨限值。

$\Delta\epsilon$ 定義為 $(\epsilon_{\parallel} - \epsilon_{\perp})$ ，而 ϵ_{av} 為 $(\epsilon_{\parallel} + 2\epsilon_{\perp})/3$ 。自在添加所關注化合物後主體介質之各別值之變化來測定化合物之介電電容率。將該等值外推至100%之所關注化合物之濃度。主體混合物揭示於H.J. Coles等人，J. Appl. Phys. 2006, 99, 034104中且具有表1中所給出之組成。

化合物	濃度
F-PGI-ZI-9-ZGP-F	25%
F-PGI-ZI-11-ZGP-F	25%
FPGI-O-5-O-PP-N	9.5%
FPGI-O-7-O-PP-N	39%
CD-1	1.5%

表 1：主體混合物組成

除上述參數外，介質必須展現適宜寬範圍之向列相、極小旋轉黏度及至少適當高之比電阻率。

用於撓變電子裝置之具有短膽固醇節距之類似液晶組合物可自 EP 0 971 016、GB 2 356 629 及 Coles, H.J., Musgrave, B., Coles, M.J., 及 Willmott, J., J. Mater. Chem., 11, 第 2709-2716 頁 (2001) 獲知。EP 0 971 016 報導液晶原雌二醇，其由此具有高撓變電子係數。GB 2 356 629 建議在撓變電子裝置中使用雙液晶原化合物。迄今為止，已在純膽固醇液晶化合物中及僅均勻化合物之混合物中研究本文之撓變電子效應。大部分該等化合物係用於由對掌性添加劑及向列液晶材料組成之二元混合物中，該向列液晶材料係簡單之習用單液晶原材料或雙液晶原材料。該等材料在實踐應用中具有若干缺點，例如對掌性向列-或膽固醇相之不夠寬之溫度範圍、過小之撓變電子比率、較小旋轉角度。

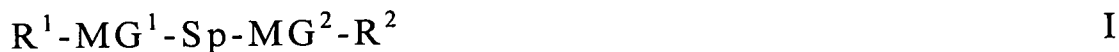
本發明之一目的係提供展現高切換角度及快速反應時間之改良撓變電子裝置。另一目的係提供具有有利性質之特定而言用於撓變電子顯示器中之如下液晶材料：其能夠在不使用機械剪切過程之情形下在顯示單元之整個區域中獲

得良好均勻配向且具有良好對比度、高切換角度及快速反應時間(在低溫下亦如此)。液晶材料應展現低熔點、寬對掌性向列相範圍、短溫度獨立性節距長度及高撓變電子係數。熟習此項技術者可自下列實施方式即刻明瞭本發明之其他目的。

本發明者已發現，可令人吃驚地藉由提供本發明之雙液晶原化合物來達成上述目的。在用於對掌性向列液晶混合物中時，該等化合物產生低熔點、寬對掌性向列相。特定而言，其展現彈性常數 k_{11} 之相對較高值、彎曲彈性常數 k_{33} 之較低值及較高撓變電子係數。

【發明內容】

因此，本發明係關於式I之雙液晶原化合物



其中

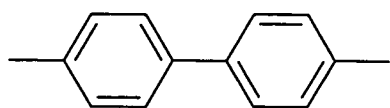
R^1 及 R^2 各自獨立地係H、F、Cl、CN、NCS或具有1至25個C原子之直鏈或具支鏈烷基，該烷基可未經取代、經鹵素或CN單-或多取代，其一或多個非毗鄰 CH_2 基團亦可在每次出現時彼此獨立地由-O-、-S-、-NH-、-N(CH₃)-、-CO-、-COO-、-OCO-、-O-CO-O-、-S-CO-、-CO-S-、-CH=CH-、-CH=CF-、-CF=CF-或-C≡C-以氧原子並不彼此直接連接之方式代替，

MG^1 及 MG^2 各自獨立地係液晶原基團且

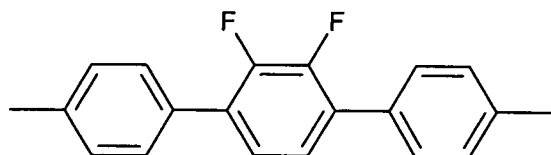
Sp 係包括 5 至 40 個 C 原子之間隔基團，其中一或多個非毗鄰之非末端 CH_2 基團亦可由 $-\text{O}-$ 、 $-\text{S}-$ 、 $-\text{NH}-$ 、 $-\text{N}(\text{CH}_3)-$ 、 $-\text{CO}-$ 、 $-\text{O}-\text{CO}-$ 、 $-\text{S}-\text{CO}-$ 、 $-\text{O}-\text{COO}-$ 、 $-\text{CO}-\text{S}-$ 、 $-\text{CO}-\text{O}-$ 、 $-\text{CH}(\text{鹵素})-$ 、 $-\text{CH}(\text{CN})-$ 、 $-\text{CH}=\text{CH}-$ 或 $-\text{C}\equiv\text{C}-$ 代替，

前提係若 R^1 及 R^2 皆係 $-\text{CN}$ ，則

MG^1 及 MG^2 不會同時為



且若 MG^1 及 MG^2 皆係

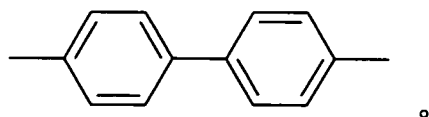


，則 R^1 及 R^2 不會同時為直鏈烷基。

較佳係式 I 化合物，其中

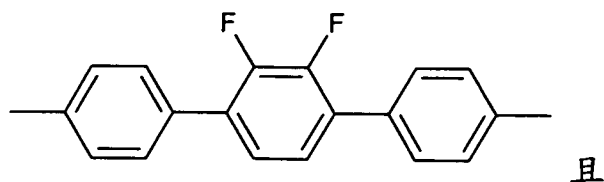
R^1 及 R^2 皆係 $-\text{CN}$ 且

MG^1 及 MG^2 皆不係



其他較佳者係式 I 化合物，其中

MG^1 及 MG^2 皆係



且

R^1 及 R^2 皆不係直鏈烷基。

液晶原基團 MG^1 及 MG^2 較佳地彼此獨立地選自式II



其中

Z^1 係 -COO-、-OCO-、-O-CO-O-、-OCH₂-、-CH₂O-、
-CH₂CH₂-、-(CH₂)₄-、-CF₂CF₂-、-CH=CH-、
-CF=CF-、-CH=CH-COO-、-OCO-CH=CH-、-C≡C-
或單鍵，

A^1 及 A^2 在每次出現時各自獨立地係1,4-伸苯基(另外，其中一或多個CH基團可由N代替)、反式-1,4-環-伸己基(另外，其中一或兩個非毗鄰CH₂基團可由O及/或S代替)、1,4-伸環己烯基、1,4-雙環-(2,2,2)-伸辛基、六氫吡啶-1,4-二基、萘-2,6-二基、十氫-萘-2,6-二基、1,2,3,4-四氫-萘-2,6-二基、環丁烷-1,3-二基、螺[3.3]庚烷-2,6-二基或二螺[3.1.3.1]癸烷-2,8-二基，所有該等基團皆可未經取代、經以下基團單-、二-、三-或四取代：F、Cl、CN或具有1至7個C原子之烷基、烷氧基、烷基羰基或烷氧基羰基，其中一或多個H原子可經F或Cl取代，

m 為0、1、2或3。

尤佳者係如下之式I化合物：其中液晶原基團 MG^1 及 MG^2 在每次出現時彼此獨立地包括一個、兩個或三個6員環、較佳地兩個或三個6員環。

【實施方式】

式II之較佳液晶原基團之較小群列示於下文中。出於簡明之原因，該等基團中之Phe係1,4-伸苯基，PheL係經1至4個基團L取代之1,4-伸苯基，其中L較佳係F、Cl、CN、OH、NO₂或具有1至7個C原子之視情況氟化之烷基、烷氧基或烷醯基，極佳係F、Cl、CN、OH、NO₂、CH₃、C₂H₅、OCH₃、OC₂H₅、COCH₃、COC₂H₅、COOCH₃、COOC₂H₅、CF₃、OCF₃、OCHF₂、OC₂F₅，特定而言係F、Cl、CN、CH₃、C₂H₅、OCH₃、COCH₃及OCF₃，最佳係F、Cl、CH₃、OCH₃及COCH₃，且Cyc係1,4-伸環己基。此列表包括下文所展示之子式以及其鏡像

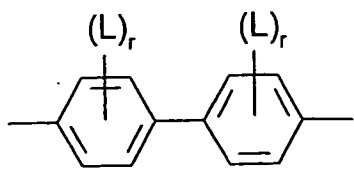
-Phe-Z-Phe-	II-1
-Phe-Z-Cyc-	II-2
-Cyc-Z-Cyc-	II-3
-PheL-Z-Phe-	II-4
-PheL-Z-Cyc-	II-5
-PheL-Z-PheL-	II-6
-Phe-Z-Phe-Z-Phe-	II-7
-Phe-Z-Phe-Z-Cyc-	II-8
-Phe-Z-Cyc-Z-Phe-	II-9
-Cyc-Z-Phe-Z-Cyc-	II-10
-Phe-Z-Cyc-Z-Cyc-	II-11
-Cyc-Z-Cyc-Z-Cyc-	II-12
-Phe-Z-Phe-Z-PheL-	II-13

-Phe-Z-PheL-Z-Phe-	II-14
-PheL-Z-Phe-Z-Phe-	II-15
-PheL-Z-Phe-Z-PheL-	II-16
-PheL-Z-PheL-Z-Phe-	II-17
-PheL-Z-PheL-Z-PheL-	II-18
-Phe-Z-PheL-Z-Cyc-	II-19
-Phe-Z-Cyc-Z-PheL-	II-20
-Cyc-Z-Phe-Z-PheL-	II-21
-PheL-Z-Cyc-Z-PheL-	II-22
-PheL-Z-PheL-Z-Cyc-	II-23
-PheL-Z-Cyc-Z-Cyc-	II-24
-Cyc-Z-PheL-Z-Cyc-	II-25

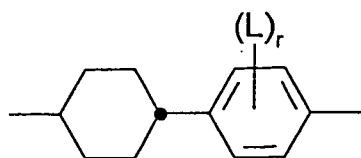
尤佳者係子式 II-1、II-4、II-6、II-7、II-13、II-14、II-15、II-16、II-17 及 II-18。

在該等較佳基團中，每一情形中之 Z 獨立地具有如式 II 中所給出 Z¹ 之含義中之一者。較佳地，Z 係 -COO-、-OCO-、-CH₂CH₂-、-C≡C- 或單鍵，尤佳係單鍵。

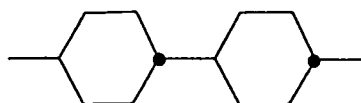
極佳地，液晶原基團 MG¹ 及 MG² 各自且獨立地選自下列式及其鏡像



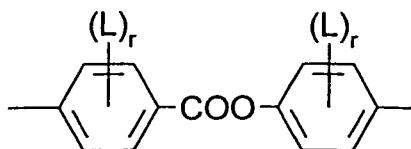
IIa



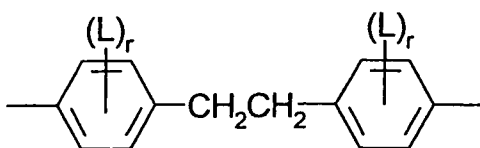
IIb



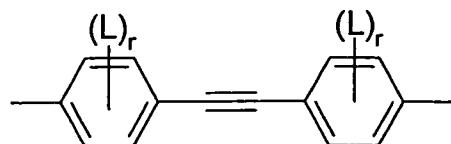
IIc



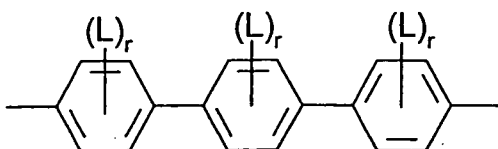
IIId



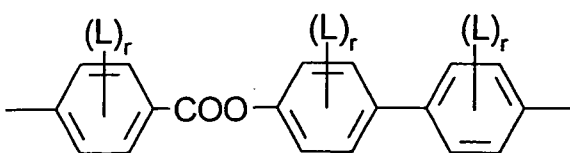
IIe



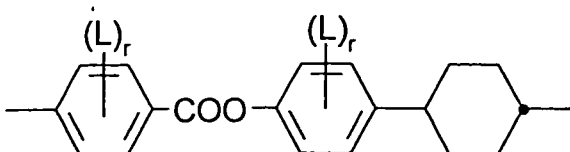
IIIf



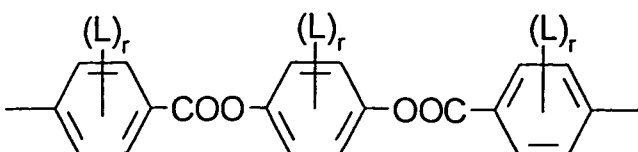
IIg



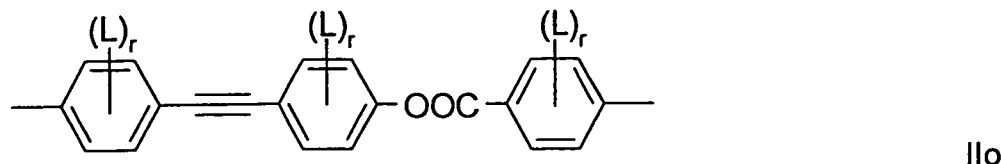
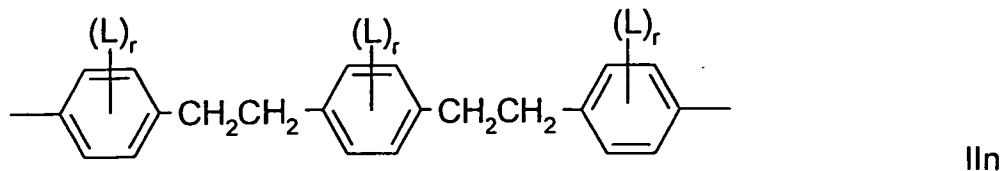
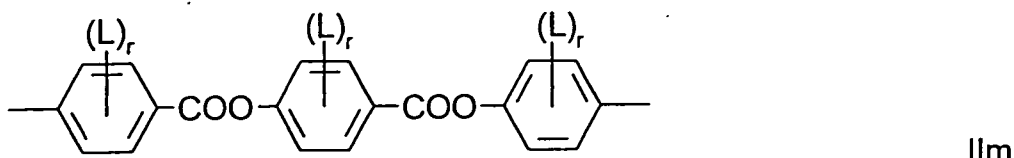
IIh



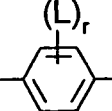
IIi

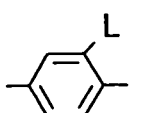
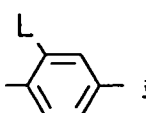
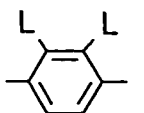
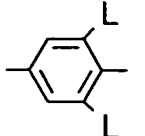


IIk



其中L在每次出現時較佳地彼此獨立地係F、Cl、CN、OH、NO₂或具有1至7個C原子之視情況氟化之烷基、烷氧基或烷醯基，極佳係F、Cl、CN、OH、NO₂、CH₃、C₂H₅、OCH₃、OC₂H₅、COCH₃、COC₂H₅、COOCH₃、COOC₂H₅、CF₃、OCF₃、OCHF₂、OC₂F₅，特定而言係F、Cl、CN、CH₃、C₂H₅、OCH₃、COCH₃及OCF₃，最佳係F、Cl、CH₃、OCH₃及COCH₃，且r在每次出現時彼此獨立地係0、1、2、3或4，較佳係0、1或2。

該等較佳式中之基團  極佳地

表示 ,  或 , 另外表示 , L在

每次出現時較佳地彼此獨立地係F、Cl、CN、OH、NO₂或具有1至7個C原子之視情況氟化之烷基、烷氧基或烷醯基，極佳係F、Cl、CN、OH、NO₂、CH₃、C₂H₅、OCH₃、OC₂H₅、COCH₃、COC₂H₅、COOCH₃、COOC₂H₅、CF₃、

OCF₃、OCHF₂、OC₂F₅，特定而言係F、Cl、CN、CH₃、C₂H₅、OCH₃、COCH₃及OCF₃，最佳係F、Cl、CH₃、OCH₃及COCH₃。

尤佳者係子式IIa、II d、IIg、IIh、IIi、IIk及IIo，特定而言係子式IIa及IIg。

在具有非極性極性基團之化合物之情形下，R¹及R²較佳係具有至多15個C原子之烷基或具有2至15個C原子之烷氧基。

若R¹或R²係烷基或烷氧基(亦即，其中末端CH₂基團由-O-代替)，則其可係直鏈或具支鏈基團。其較佳為直鏈，具有2、3、4、5、6、7或8個碳原子，且因此較佳為乙基、丙基、丁基、戊基、己基、庚基、辛基、乙氧基、丙氧基、丁氧基、戊氧基、己氧基、庚氧基或辛氧基，其亦可為(例如)甲基、壬基、癸基、十一烷基、十二烷基、十三烷基、十四烷基、十五烷基、壬氧基、癸氧基、十一烷氧基、十二烷氧基、十三烷氧基或十四烷氧基。

氧雜烷基(亦即，其中一個CH₂基團由-O-代替)較佳係(例如)直鏈2-氧雜丙基(=甲氧基甲基)、2-氧雜丁基(=乙氧基甲基)或3-氧雜丁基(=2-甲氧基乙基)、2-、3-或4-氧雜戊基、2-、3-、4-或5-氧雜己基、2-、3-、4-、5-或6-氧雜庚基、2-、3-、4-、5-、6-或7-氧雜辛基、2-、3-、4-、5-、6-、7-或8-氧雜壬基或2-、3-、4-、5-、6-、7-、8-或9-氧雜癸基。

在具有末端極性基團之化合物之情形下， R^1 及 R^2 係選自CN、 NO_2 、鹵素、 OCH_3 、 OCN 、 SCN 、 COR^x 、 $COOR^x$ 或具有1至4個C原子之單-、寡-或多氟化烷基或烷氧基。 R^x 係具有1至4個、較佳地1至3個C原子之視情況氟化之烷基。鹵素較佳地係F或Cl。

尤佳地，式I中之 R^1 及 R^2 係選自H、F、Cl、CN、 NO_2 、 OCH_3 、 $COCH_3$ 、 COC_2H_5 、 $COOCH_3$ 、 $COOC_2H_5$ 、 CF_3 、 C_2F_5 、 OCF_3 、 $OCHF_2$ 及 OC_2F_5 ，特定而言係H、F、Cl、CN、 OCH_3 及 OCF_3 ，尤其係H、F、CN及 OCF_3 。

此外，含有非對掌性具支鏈基團 R^1 及/或 R^2 之式I化合物有時可較為重要，此乃因(例如)發生結晶之趨勢減小。此類型之具支鏈基團通常不含超過一條之支鏈。較佳非對掌性具支鏈基團係異丙基、異丁基(=甲基丙基)、異戊基(=3-甲基丁基)、異丙氧基、2-甲基-丙氧基及3-甲基丁氧基。

間隔基團Sp較佳係具有5至40個C原子、特定而言5至25個C原子、極佳地5至15個C原子之直鏈或具支鏈伸烷基，此外，其中一或多個非毗鄰之非末端 CH_2 基團可由-O-、-S-、-NH-、-N(CH_3)-、-CO-、-O-CO-、-S-CO-、-O-COO-、-CO-S-、-CO-O-、-CH(鹵素)-、-CH(CN)-、-CH=CH-或-C≡C-代替。

「末端」 CH_2 基團係彼等直接鍵結至液晶原基團上者。因此，「非末端」 CH_2 基團並不直接鍵結至液晶原基團 MG^1 及 MG^2 。

典型間隔基團係(例如) $-(\text{CH}_2)_o-$ 、 $-(\text{CH}_2\text{CH}_2\text{O})_p-\text{CH}_2\text{CH}_2-$ ，其中 o 為5至40、特定而言5至25、極佳地5至15之整數，且 p 為1至8、特定而言1、2、3或4之整數。

較佳間隔基團係(例如)伸戊基、伸己基、伸庚基、伸辛基、伸壬基、伸癸基、伸十一烷基、伸十二烷基、伸十八烷基、二伸乙基氧基伸乙基、二亞甲基氧基伸丁基、伸戊烯基、伸庚烯基、伸壬烯基及伸十一烯基。

尤佳者係 Sp 表示具有5至15個C原子之伸烷基之式I之發明性化合物。尤佳者係直鏈伸烷基。

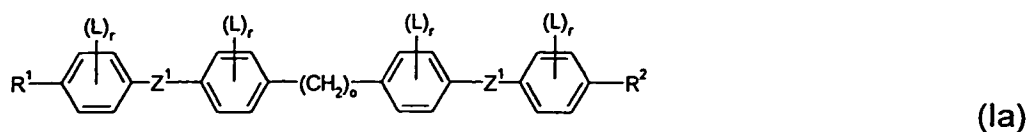
較佳者係具有偶數個具有6、8、10、12及14個C原子之直鏈伸烷基之間隔基團。

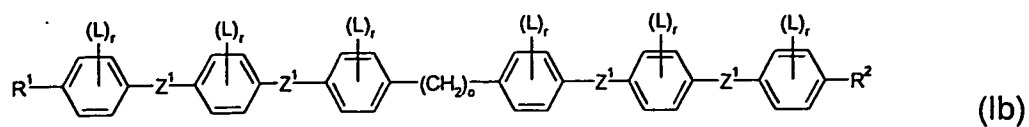
本發明之另一實施例係較佳地具有奇數個具有5、7、9、11、13及15個C原子之直鏈伸烷基之間隔基團。極佳者係具有7、9及11個C原子之直鏈伸烷基間隔基團。

尤佳者係 Sp 表示具有5至15個C原子之完全氙化之伸烷基之式I之發明性化合物。極佳者係氙化直鏈伸烷基。最佳者係部分氙化之直鏈伸烷基。

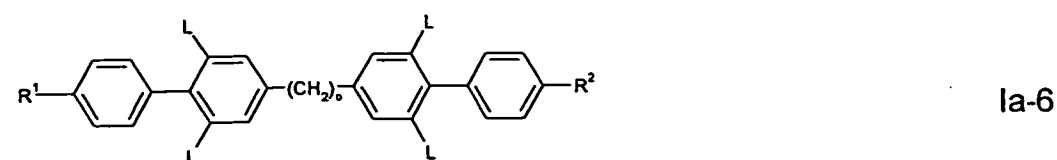
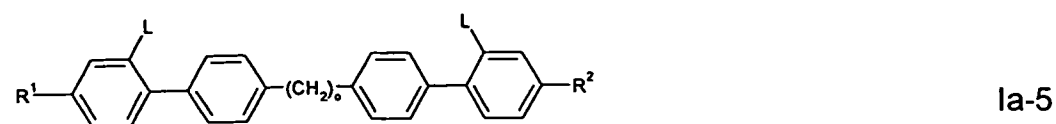
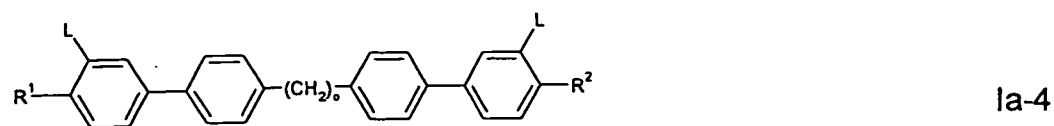
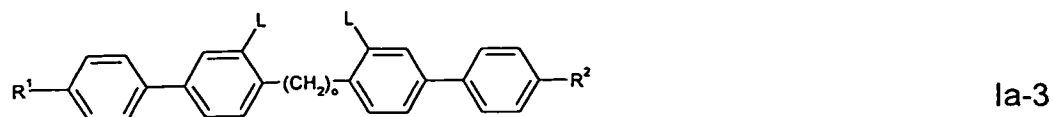
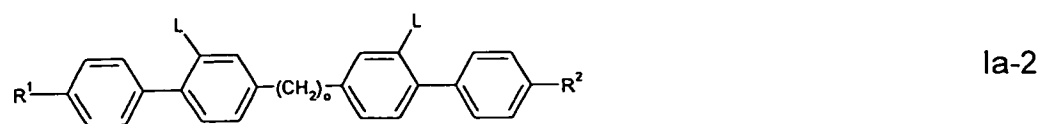
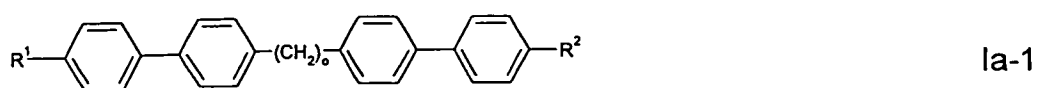
較佳者係液晶原基團 R^1-MG^1- 及 R^2-MG^2- 不同之式I化合物。尤佳者係式I中之 R^1-MG^1- 及 R^2-MG^2- 相同之式I化合物。

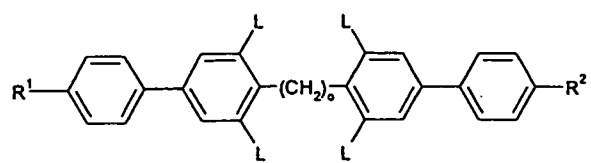
尤佳者係選自式Ia及Ib之下列化合物：



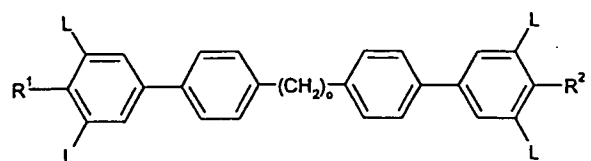


其中 R^1 及 R^2 、 Z^1 、 o 及 r 在每次出現時彼此獨立地如上文所定義，包含該等基團之較佳含義且其中 L 在每次出現時彼此獨立地較佳地係 F 、 Cl 、 CN 、 OH 、 NO_2 或具有 1 至 7 個 C 原子之視情況氟化之烷基、烷氧基或烷醯基，極佳係 F 、 Cl 、 CN 、 OH 、 NO_2 、 CH_3 、 C_2H_5 、 OCH_3 、 OC_2H_5 、 $COCH_3$ 、 COC_2H_5 、 $COOCH_3$ 、 $COOC_2H_5$ 、 CF_3 、 OCF_3 、 $OCHF_2$ 、 OC_2F_5 ，特定而言係 F 、 Cl 、 CN 、 CH_3 、 C_2H_5 、 OCH_3 、 $COCH_3$ 及 OCF_3 ，最佳係 F 、 Cl 、 CH_3 、 OCH_3 及 $COCH_3$ 。式 Ia 及 Ib 之較佳化合物如下文所指示：

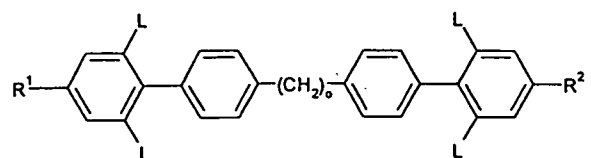




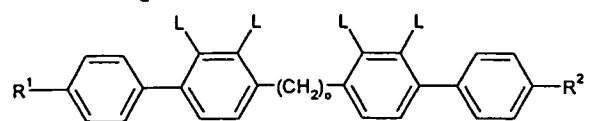
Ia-7



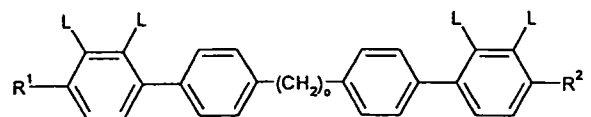
Ia-8



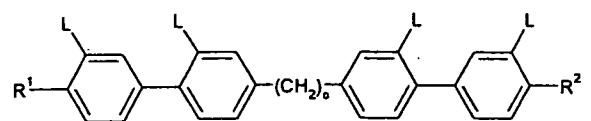
Ia-9



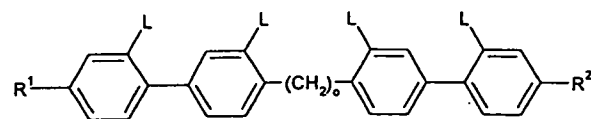
Ia-10



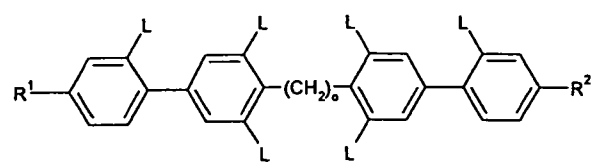
Ia-11



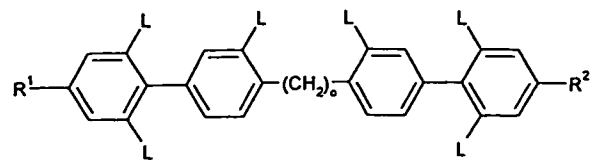
Ia-12



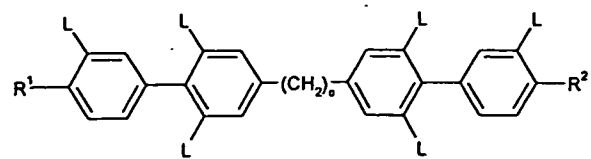
Ia-13



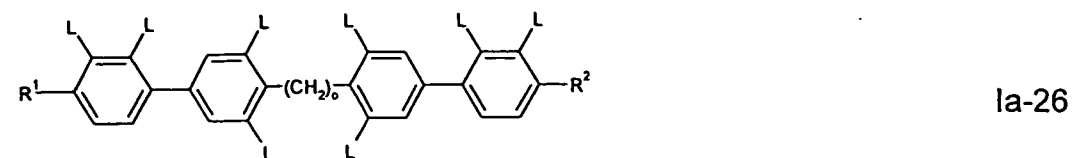
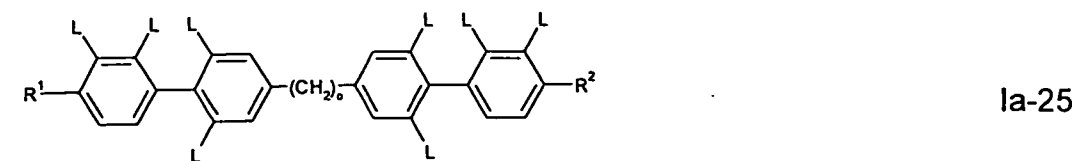
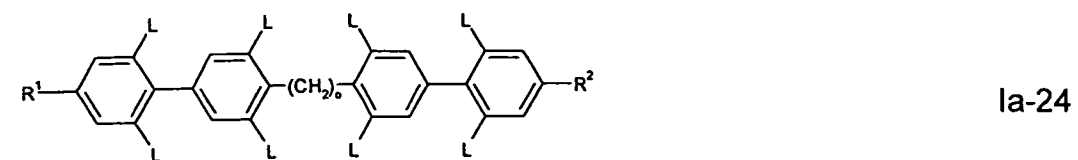
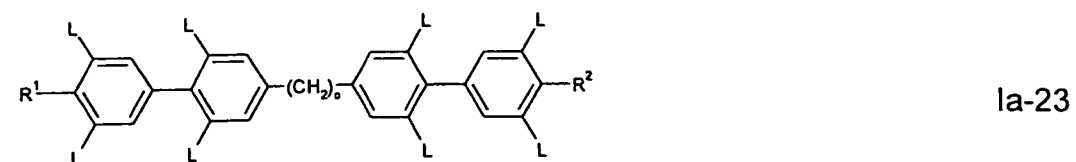
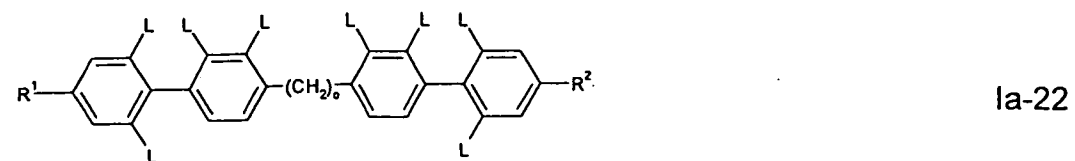
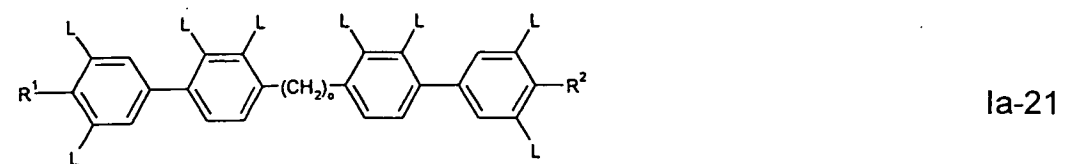
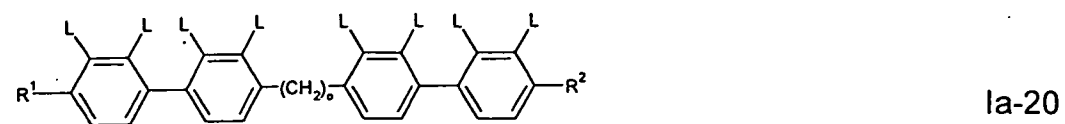
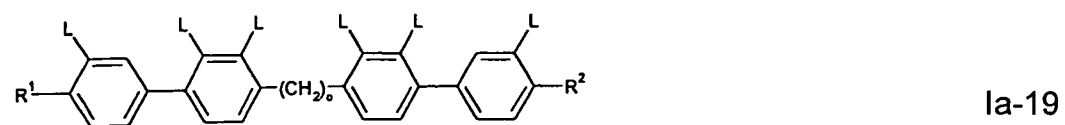
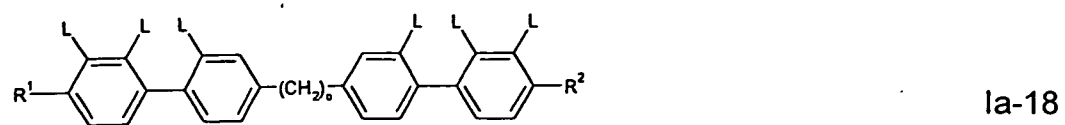
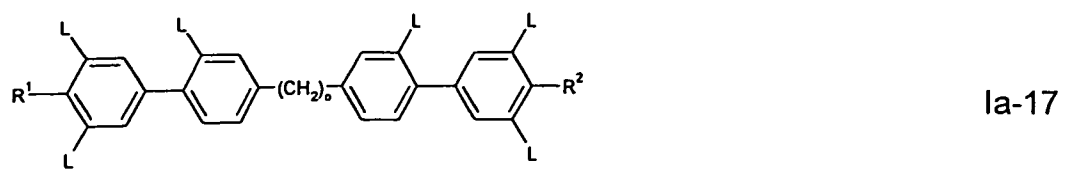
Ia-14

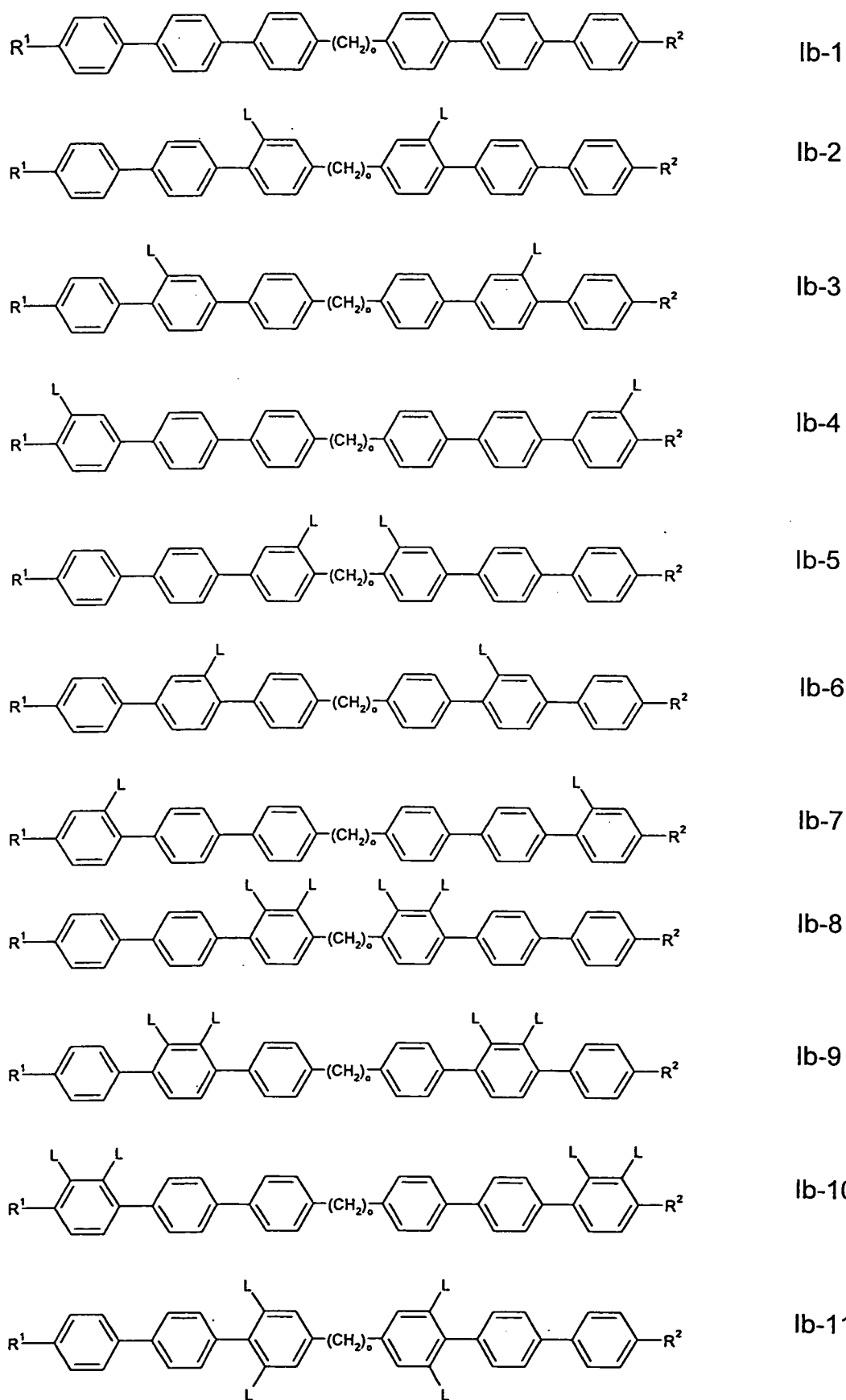


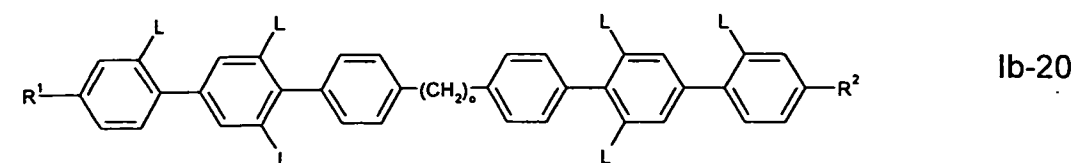
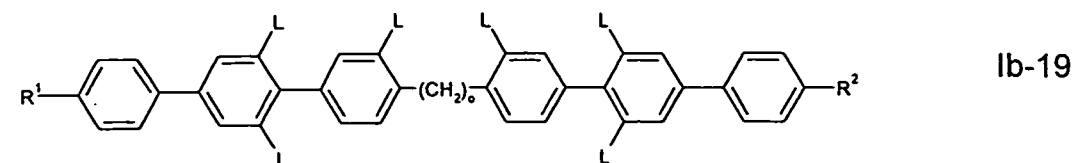
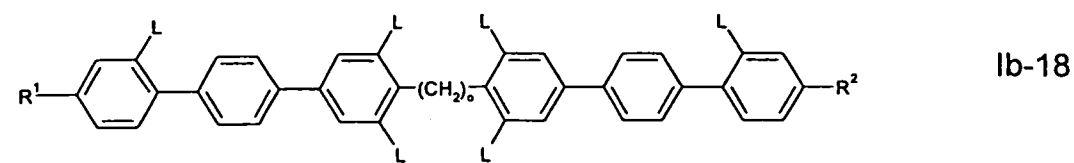
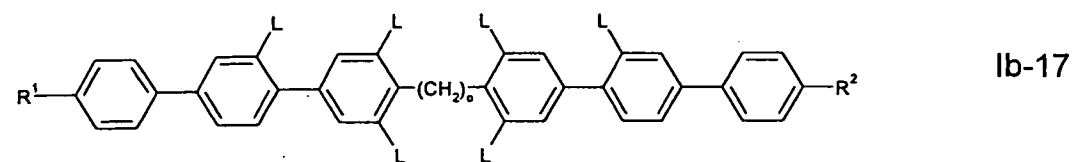
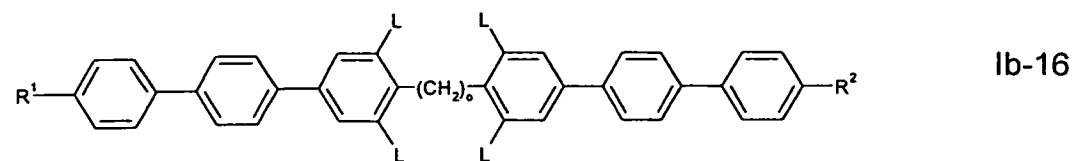
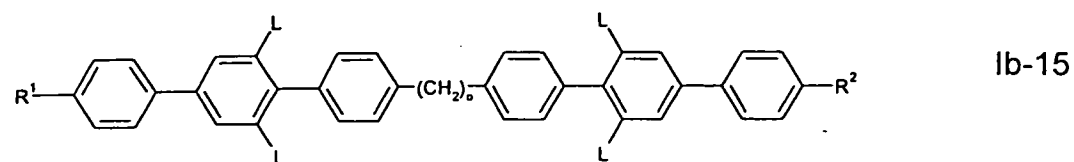
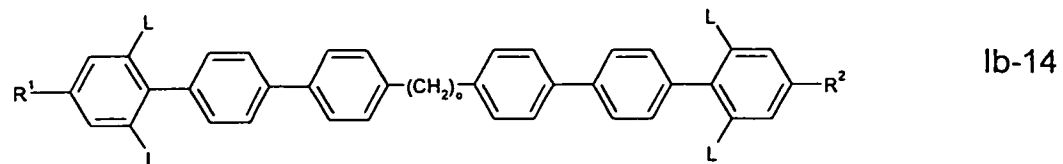
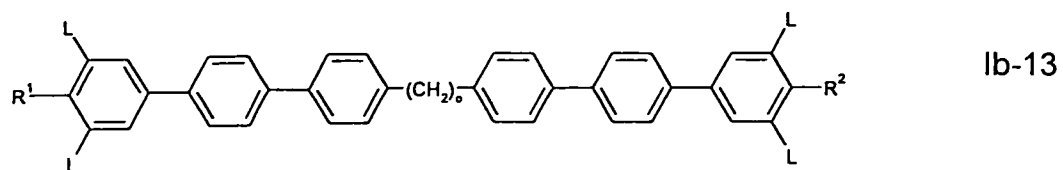
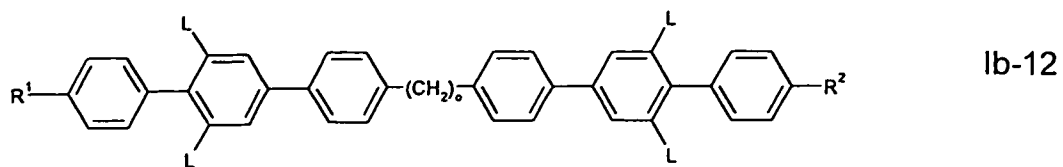
Ia-15

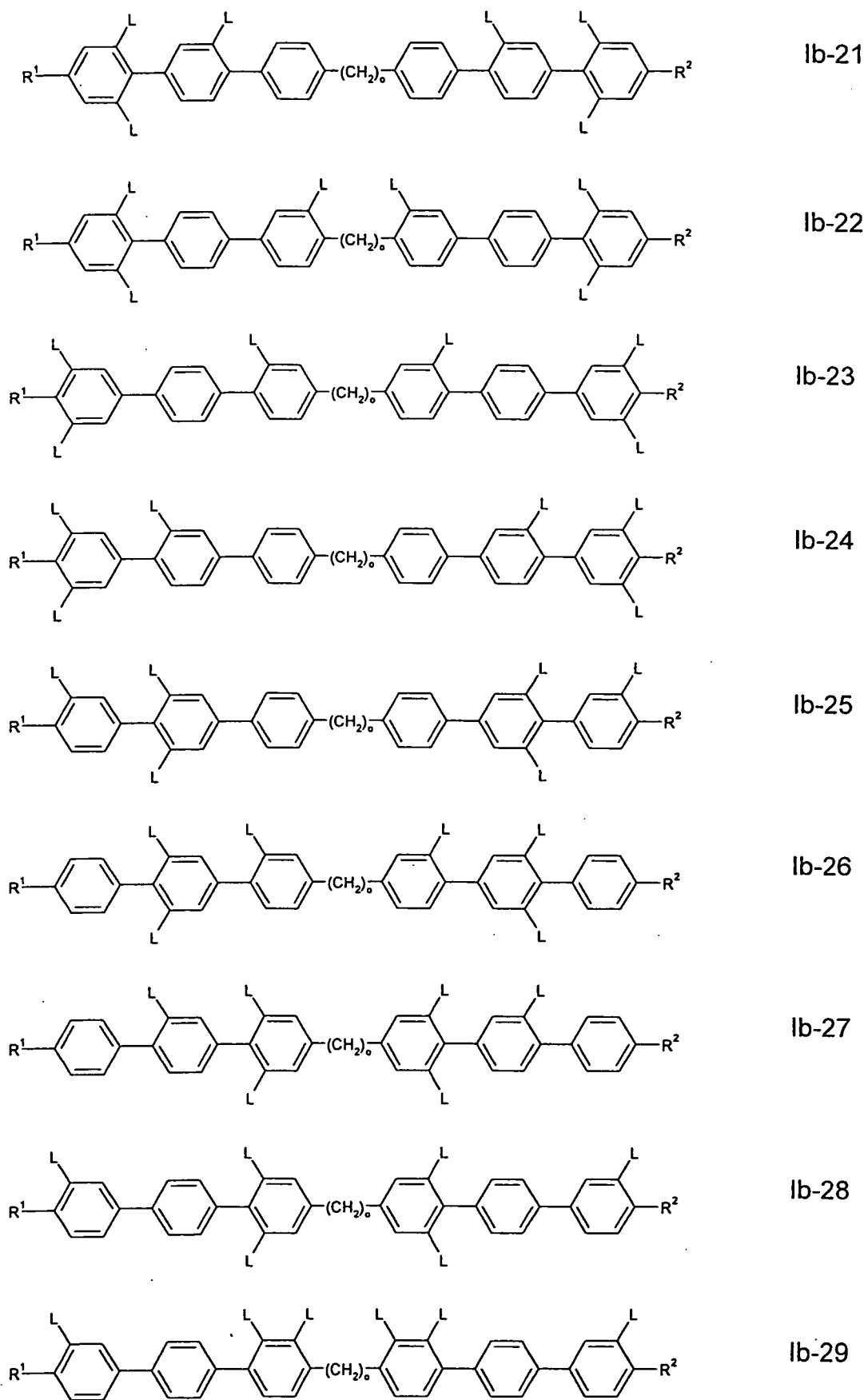


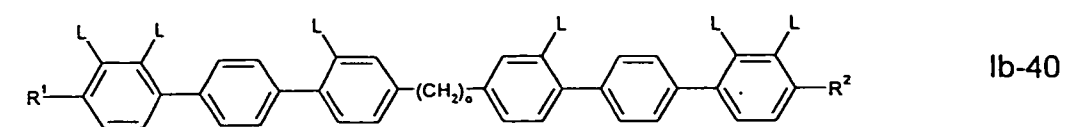
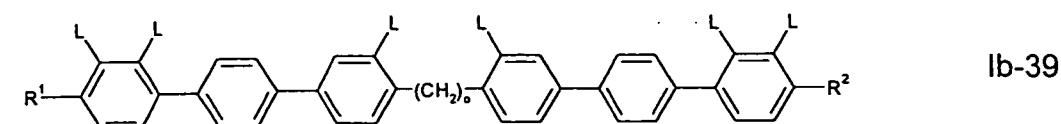
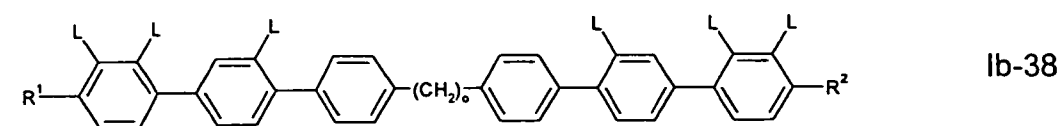
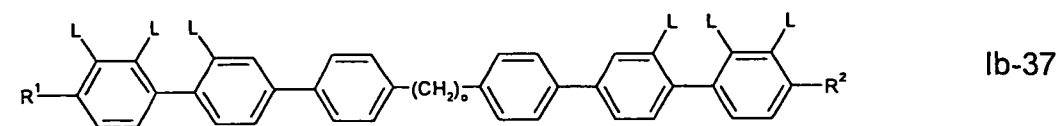
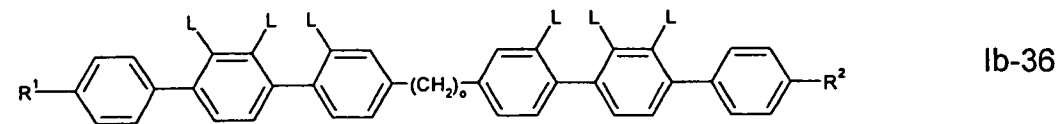
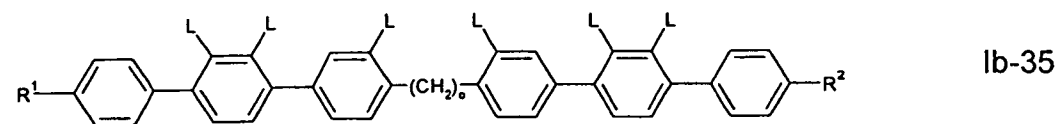
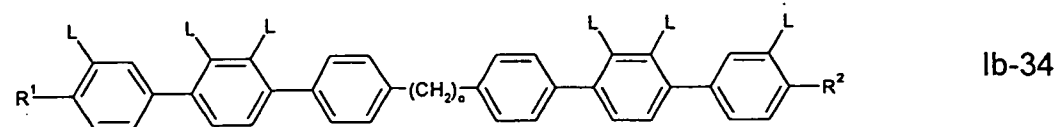
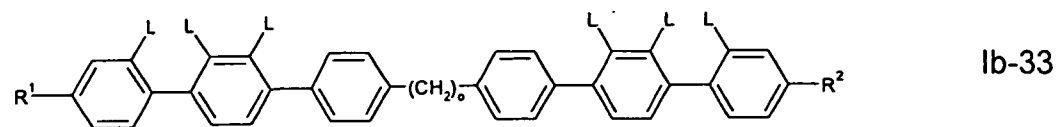
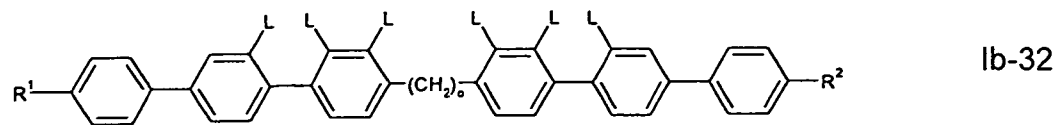
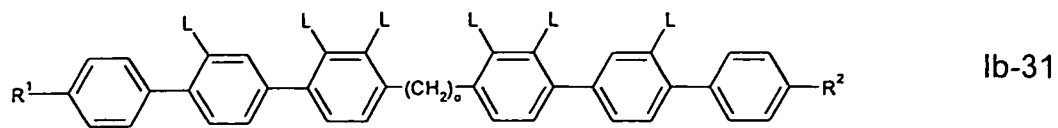
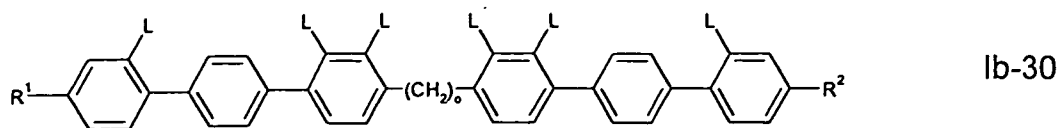
Ia-16

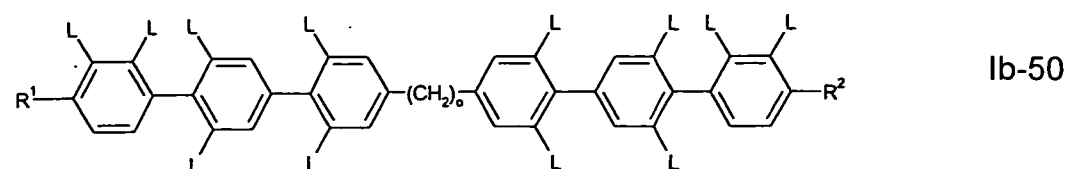
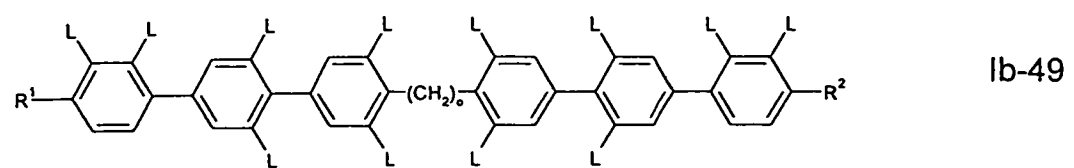
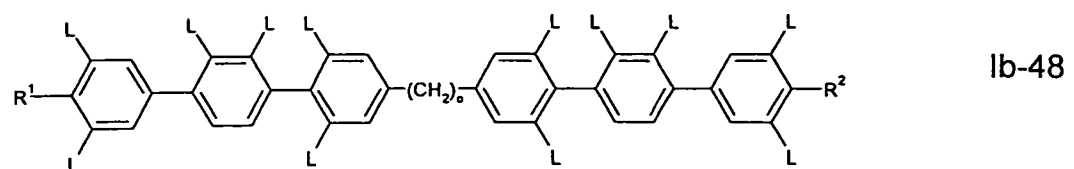
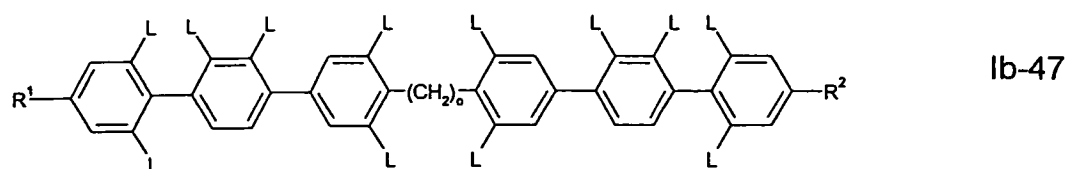
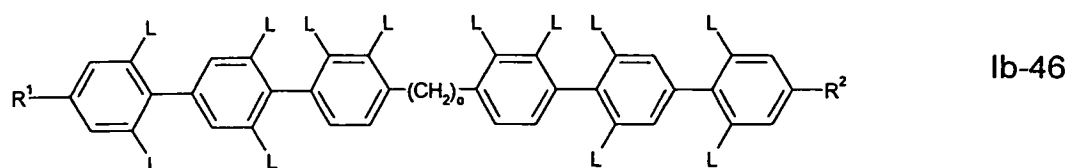
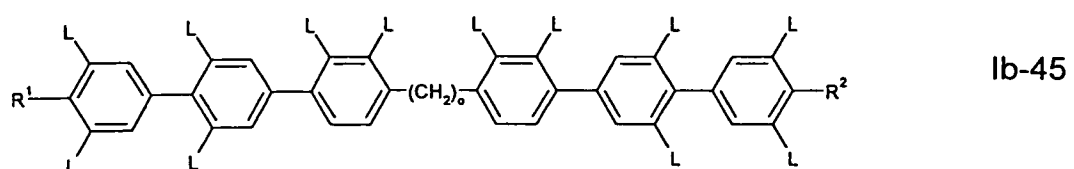
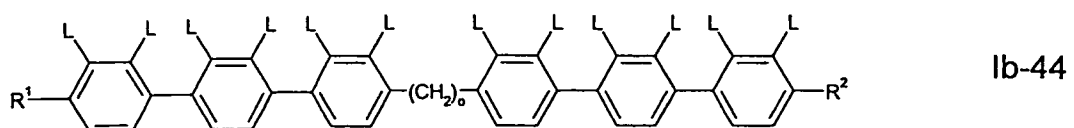
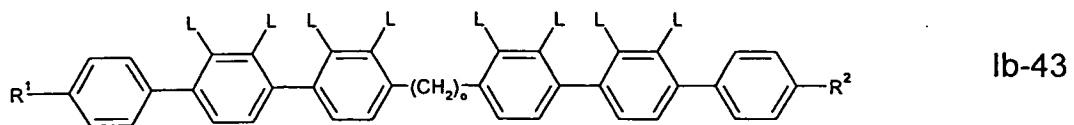
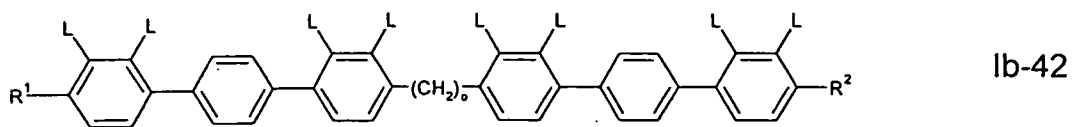
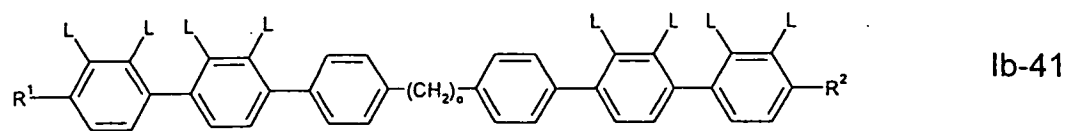


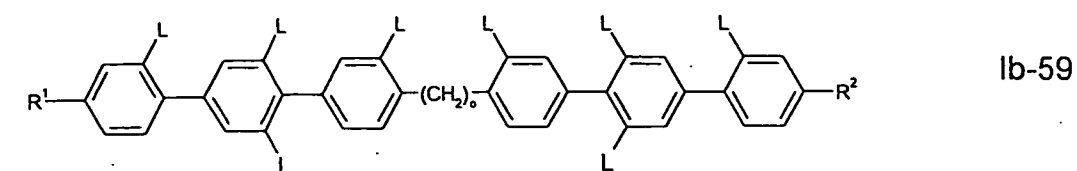
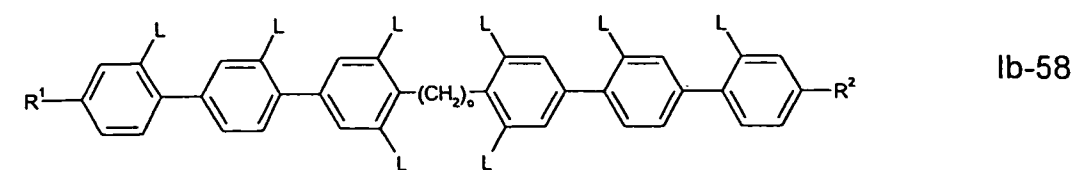
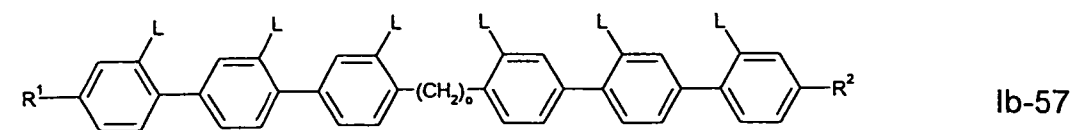
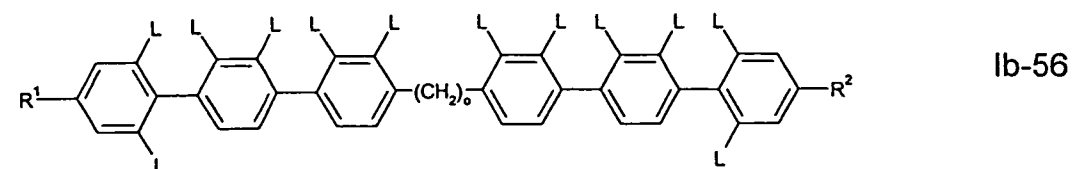
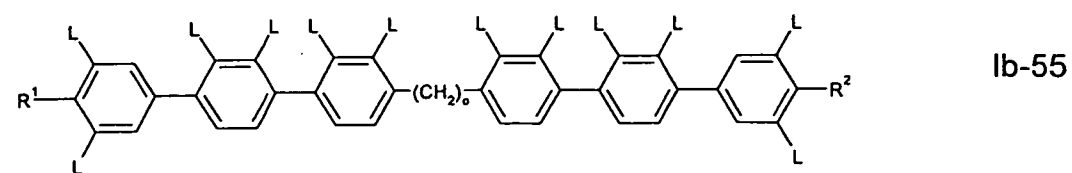
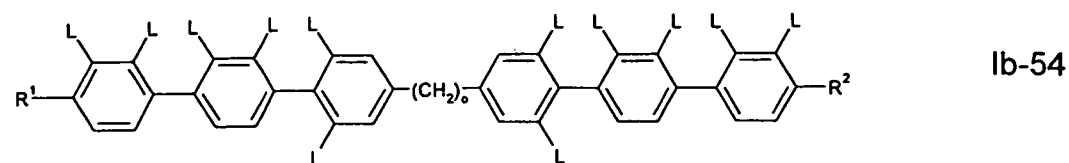
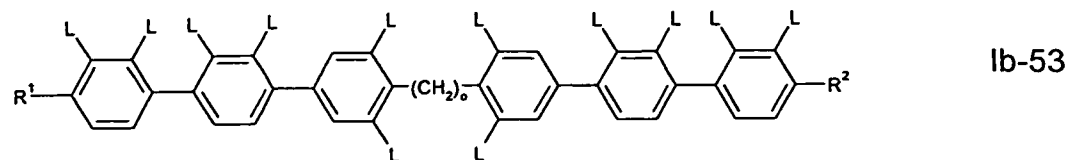
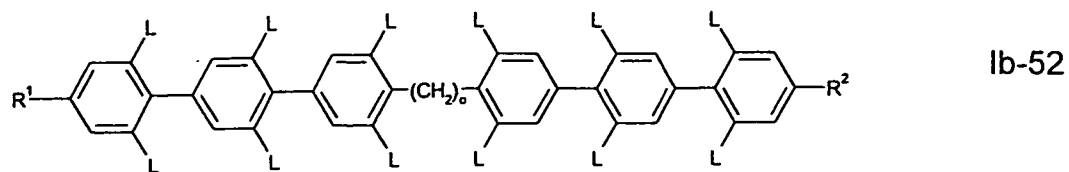
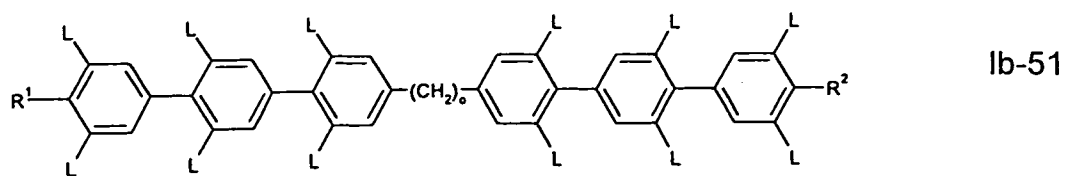


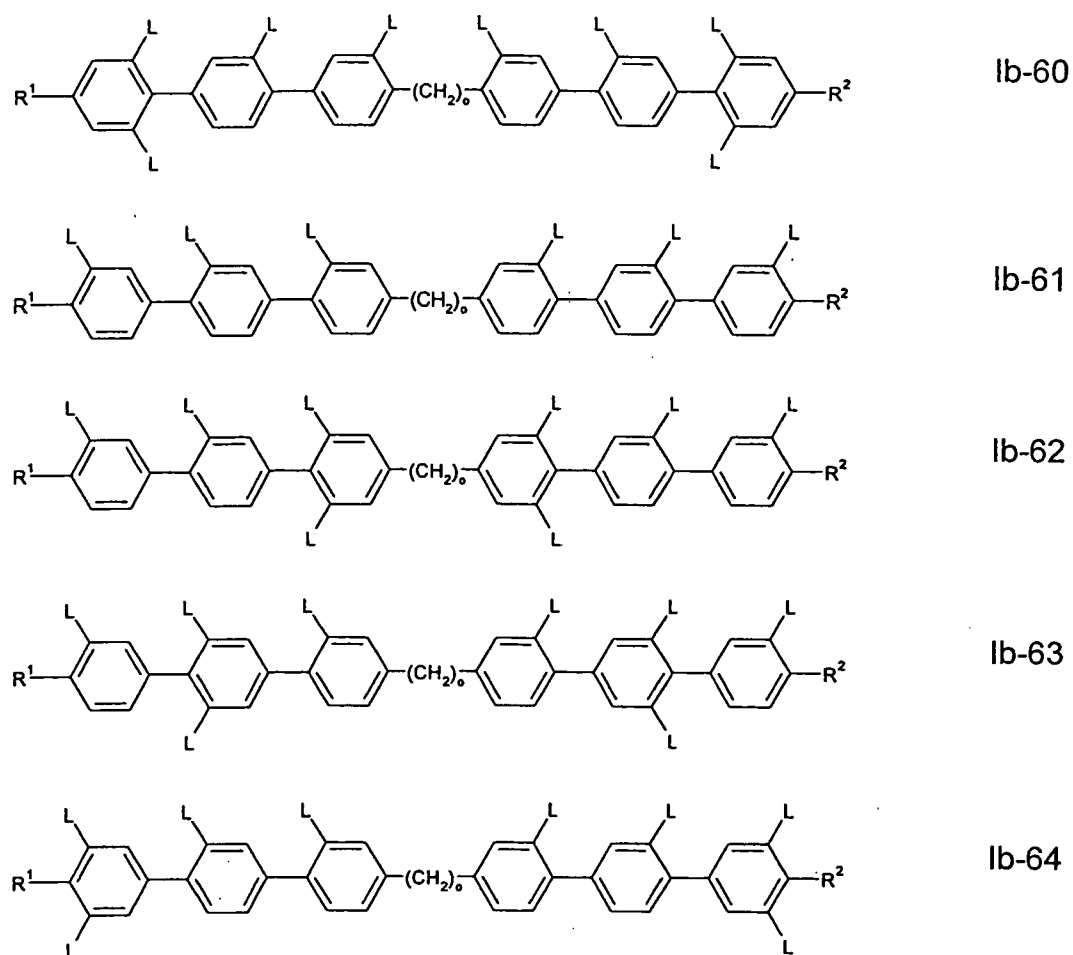










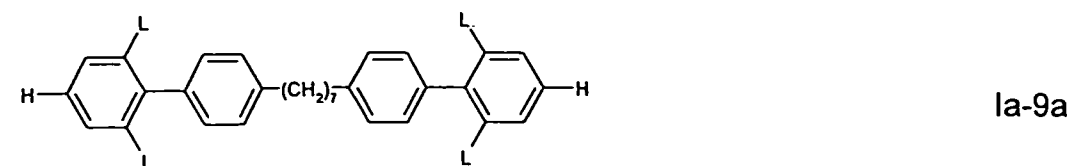
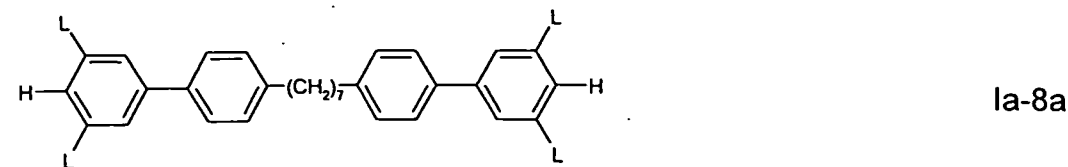
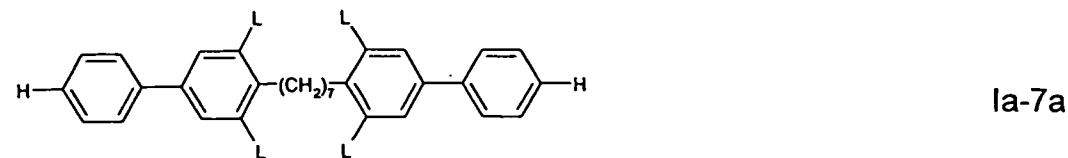
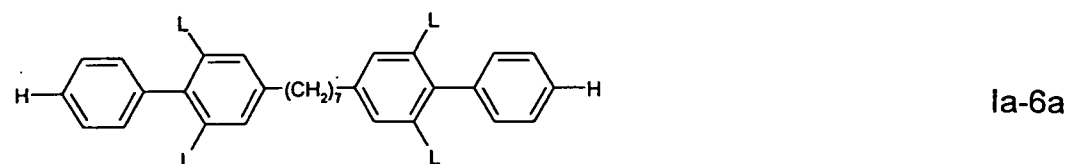
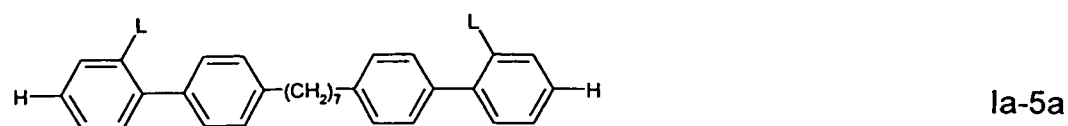
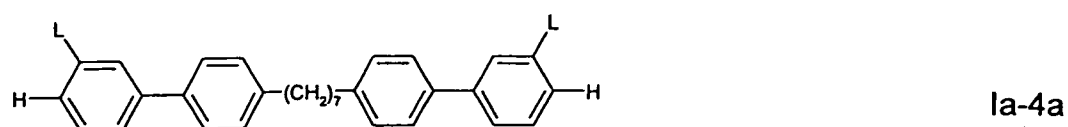
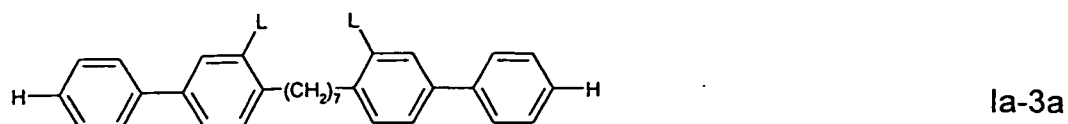
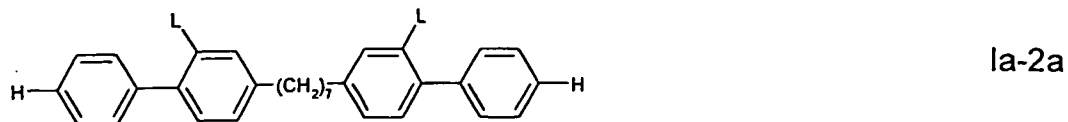
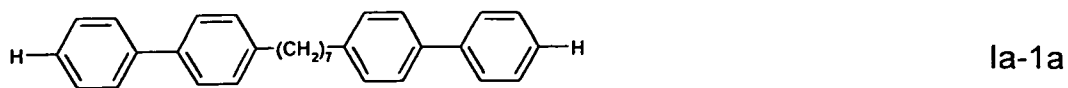


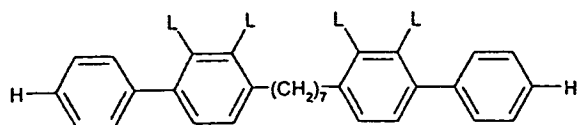
其中 R^1 及 R^2 、及 o 在每次出現時彼此獨立地如上文所定義，包含該等基團之較佳含義且其中 L 在每次出現時彼此獨立地較佳地係 F 、 Cl 、 CN 、 OH 、 NO_2 或具有 1 至 7 個 C 原子之視情況氟化之烷基、烷氧基或烷醯基，極佳係 F 、 Cl 、 CN 、 OH 、 NO_2 、 CH_3 、 C_2H_5 、 OCH_3 、 OC_2H_5 、 $COCH_3$ 、 COC_2H_5 、 $COOCH_3$ 、 $COOC_2H_5$ 、 CF_3 、 OCF_3 、 $OCHF_2$ 、 OC_2F_5 ，特定而言係 F 、 Cl 、 CN 、 CH_3 、 C_2H_5 、 OCH_3 、 $COCH_3$ 及 OCF_3 ，最佳係 F 、 Cl 、 CH_3 、 OCH_3 及 $COCH_3$ 。

尤佳者係式 Ia-1、Ia-2、Ia-3, Ia-6、Ia-8、Ia-12、Ia-17、Ia-23、Ib-61 及 Ib-63 之化合物。

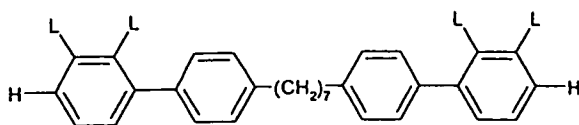
式 Ia-1 至 Ia-26 及 Ib-1 至 Ib-56 之極佳化合物如下文所指

示：

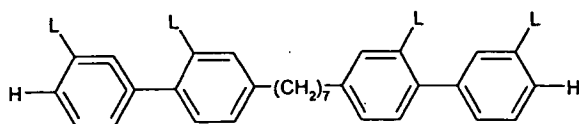




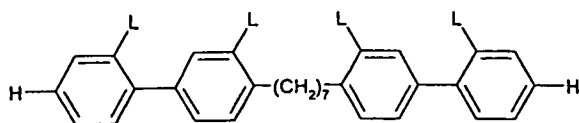
1a-10a



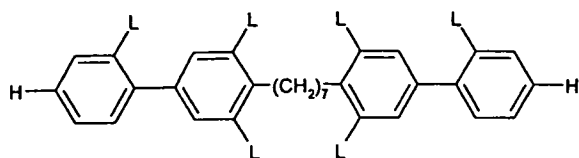
1a-11a



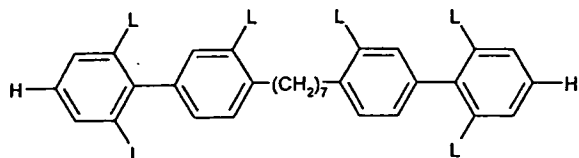
1a-12a



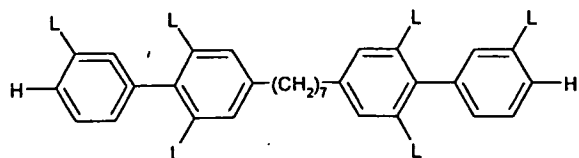
1a-13a



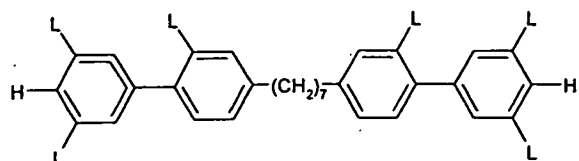
1a-14a



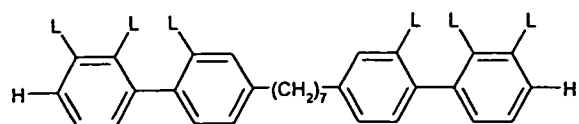
1a-15a



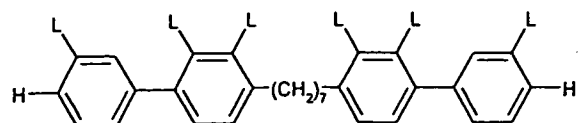
1a-16a



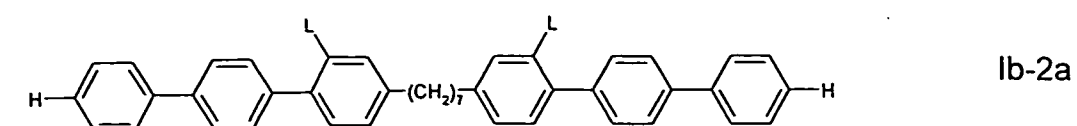
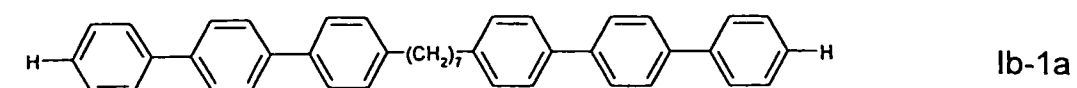
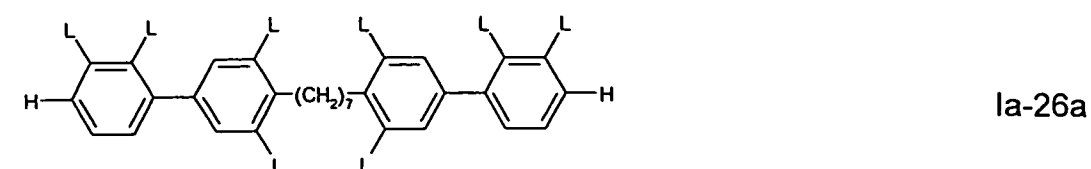
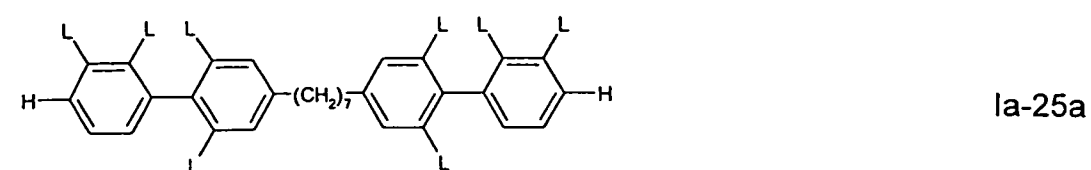
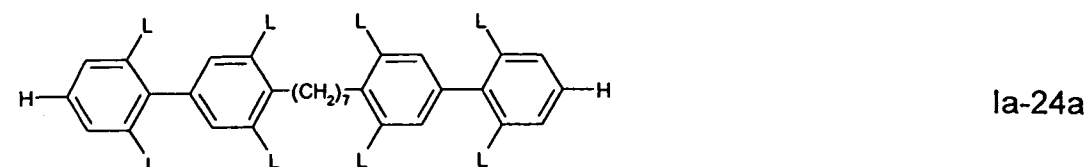
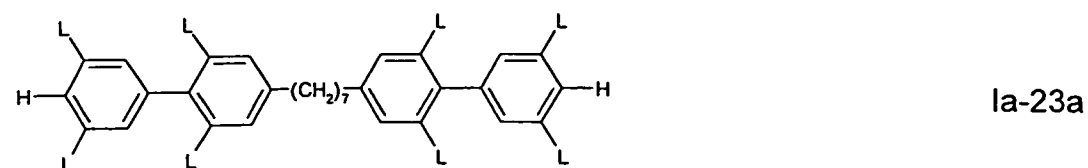
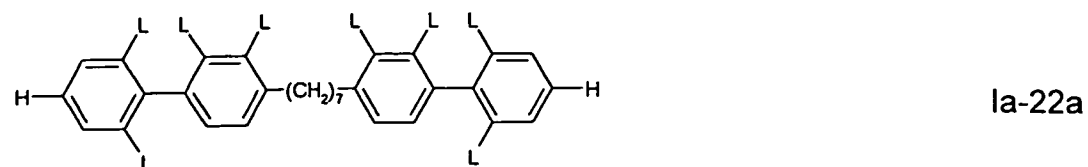
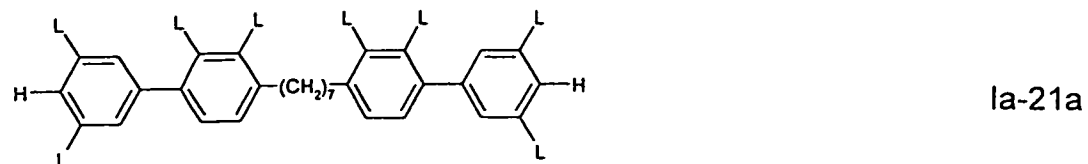
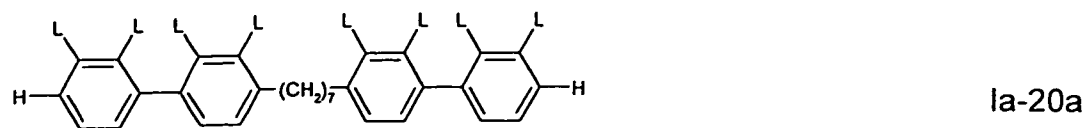
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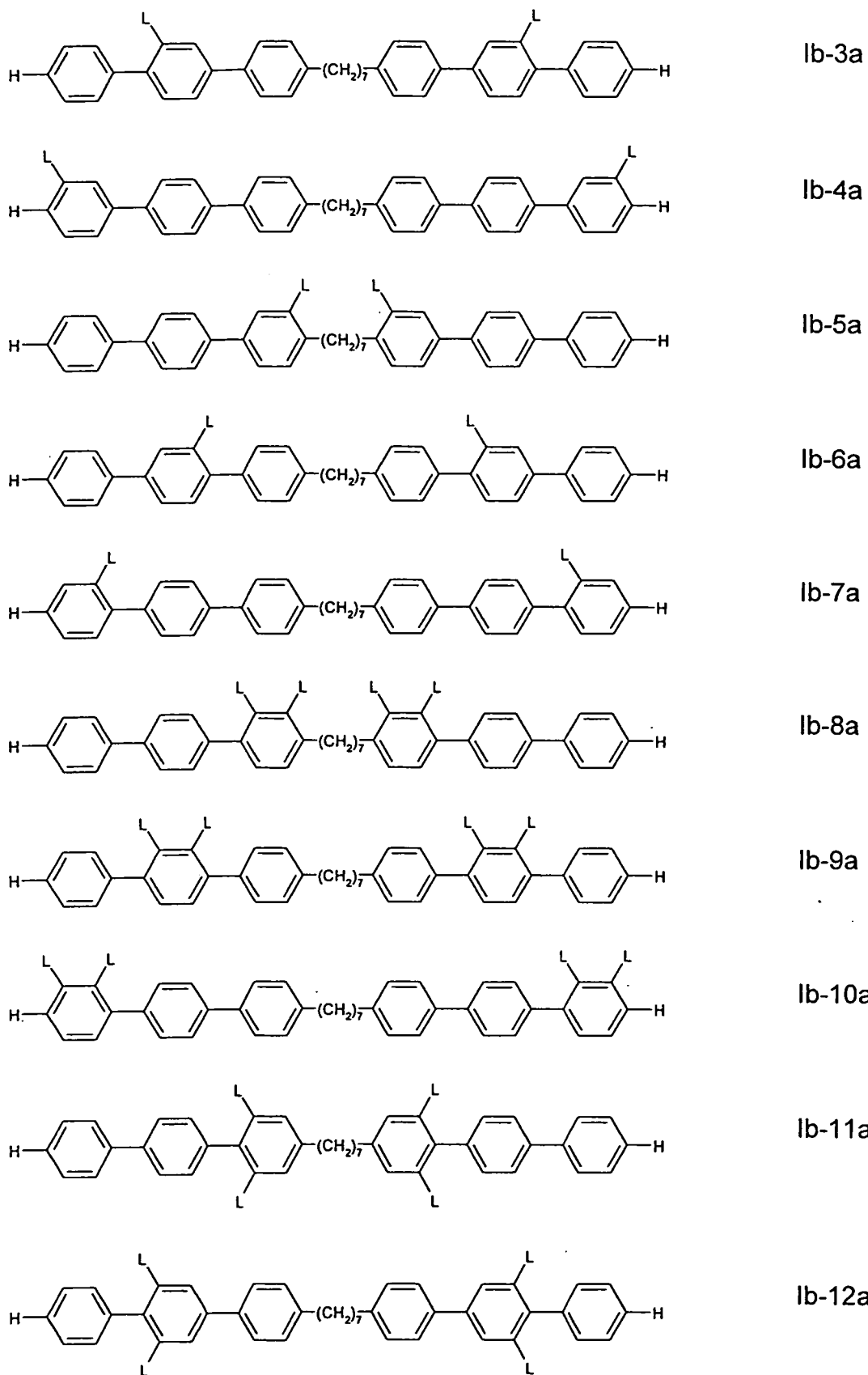


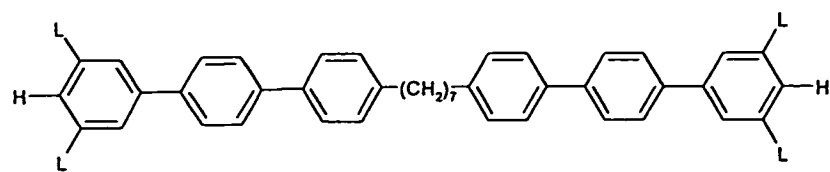
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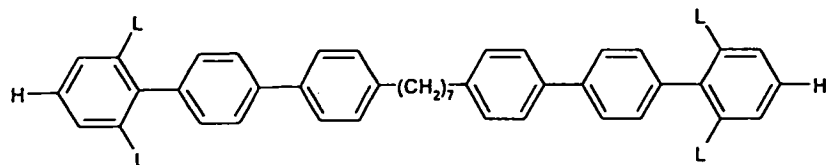
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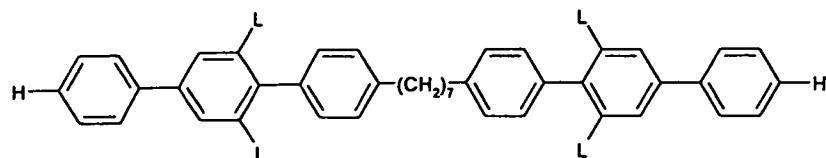




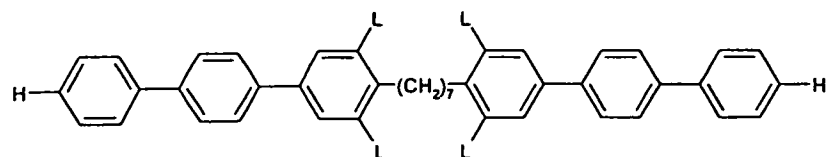
Ib-13a



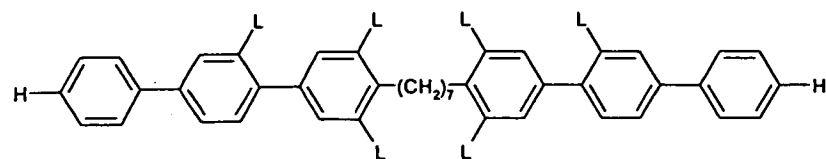
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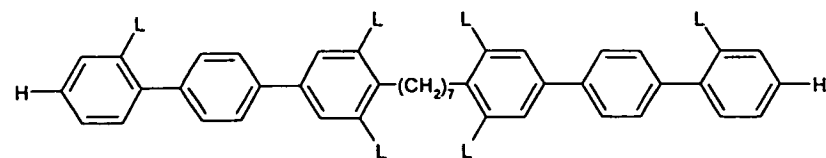
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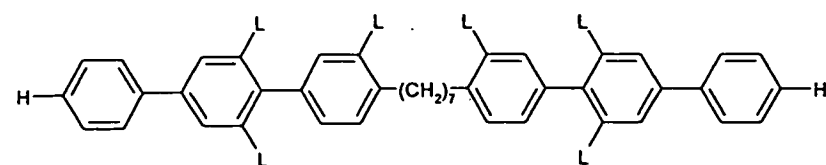
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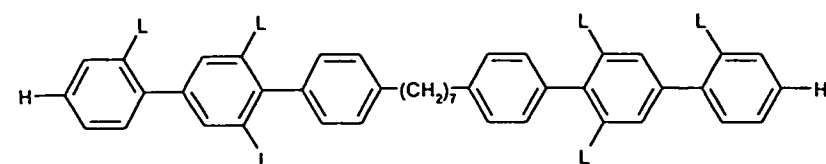
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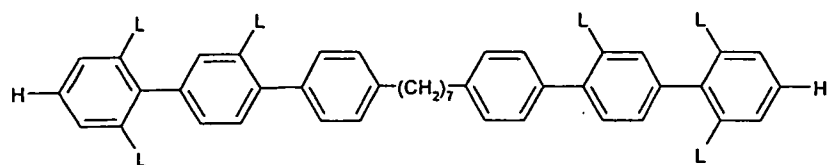
Ib-18a



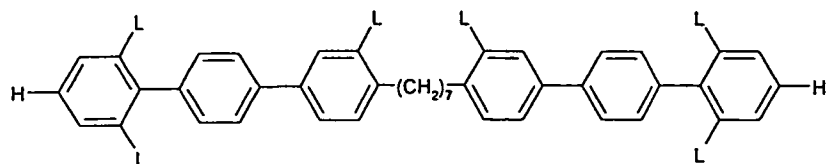
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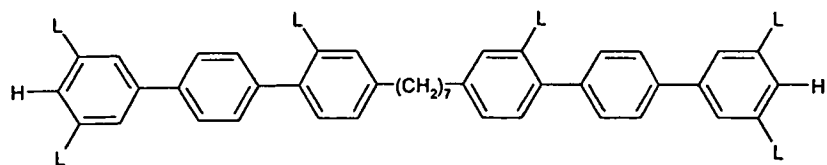
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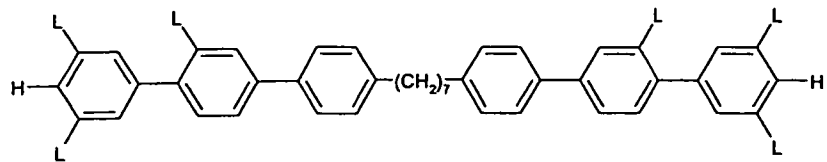
Ib-21a



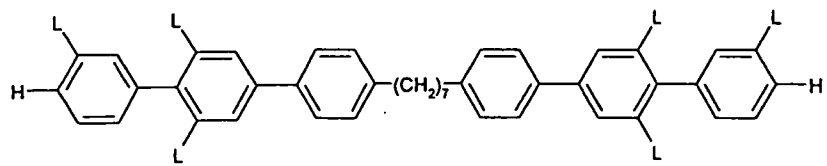
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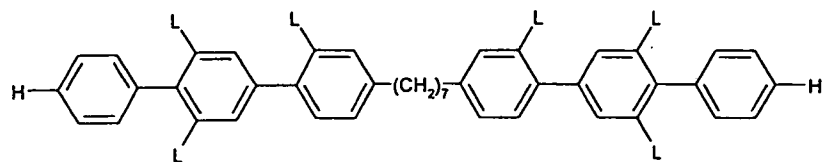
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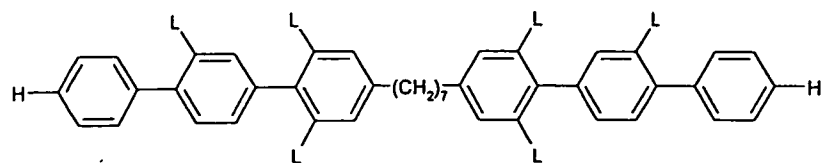
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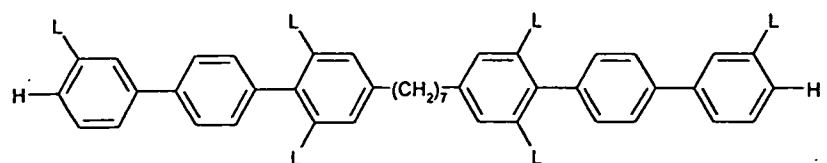
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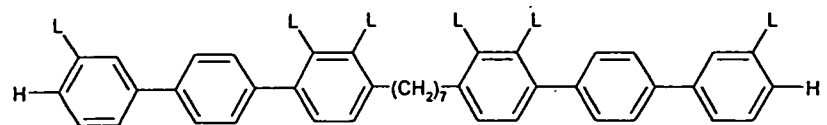
Ib-26a



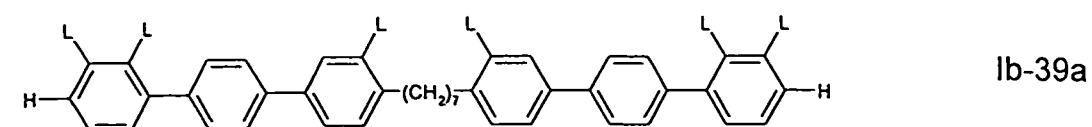
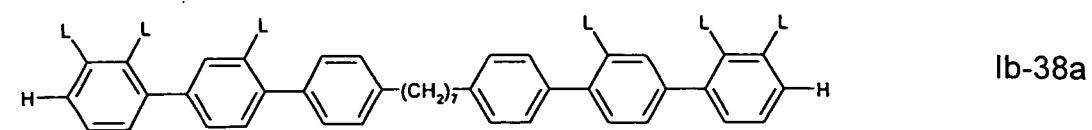
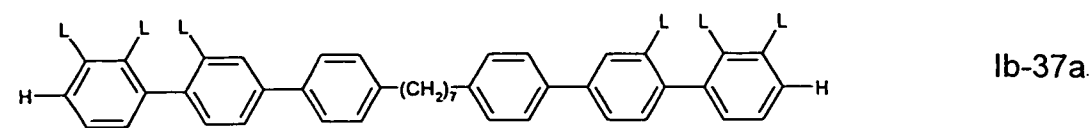
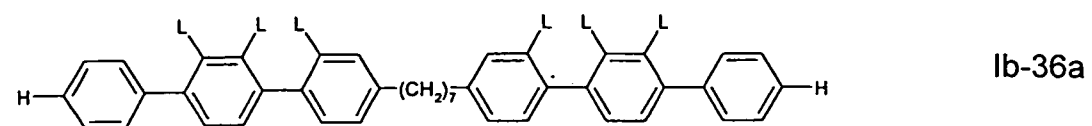
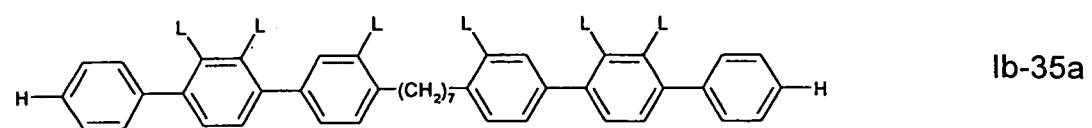
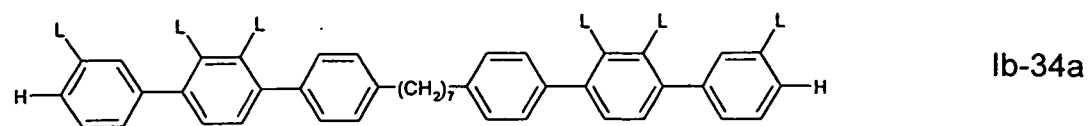
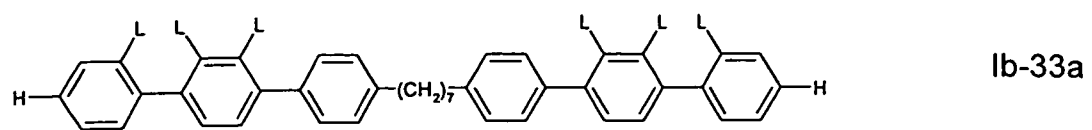
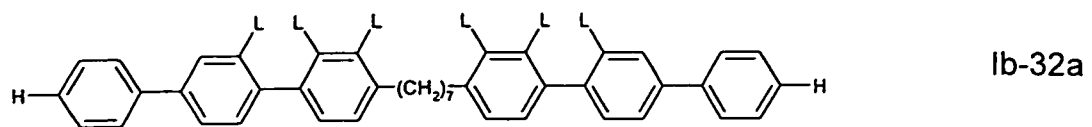
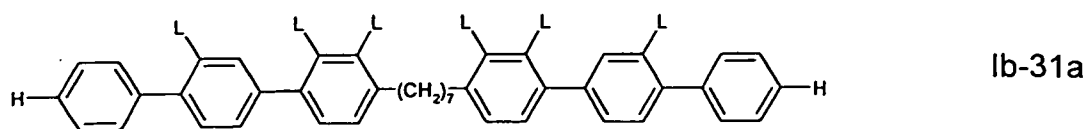
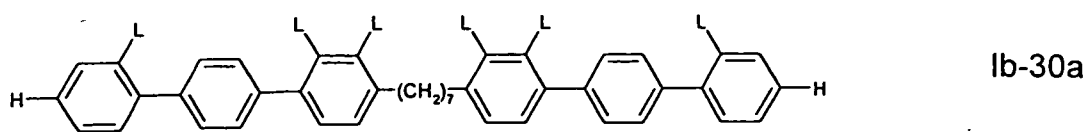
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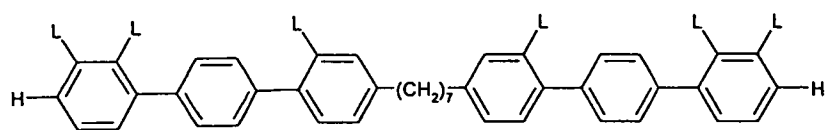


Ib-28a

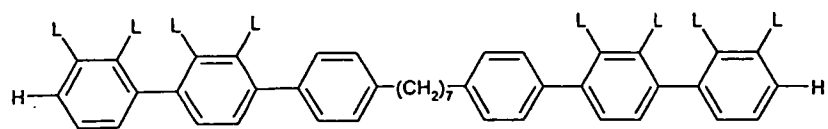


Ib-29a

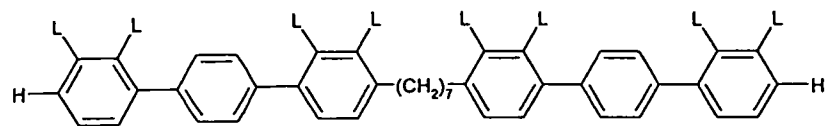




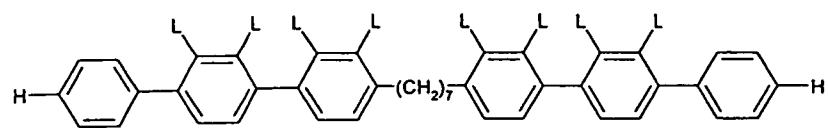
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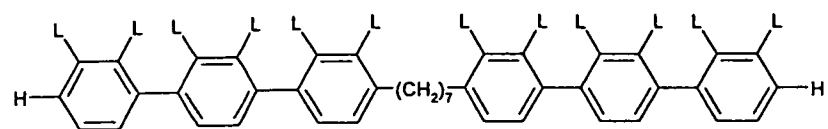
Ib-41a



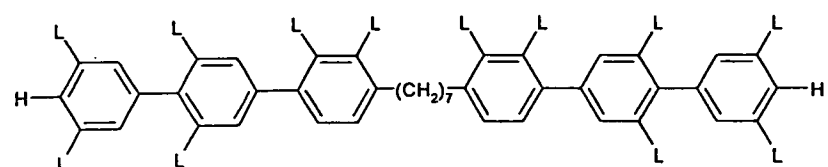
Ib-42a



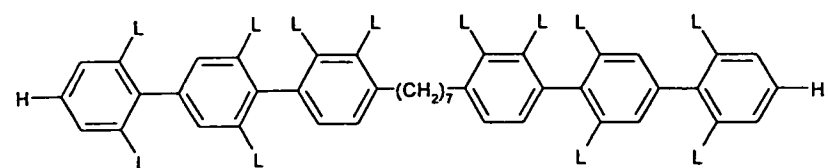
Ib-43a



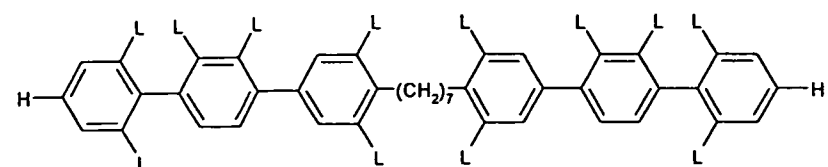
Ib-44a



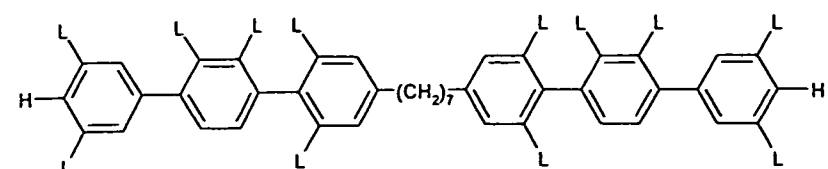
Ib-45a



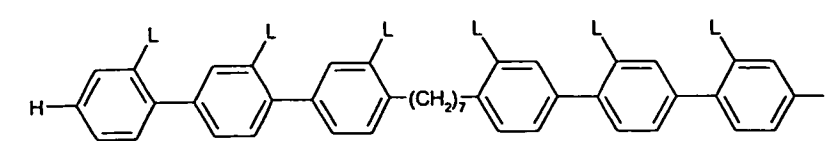
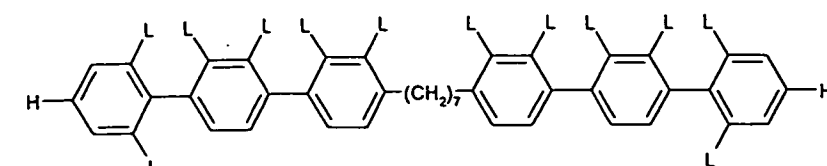
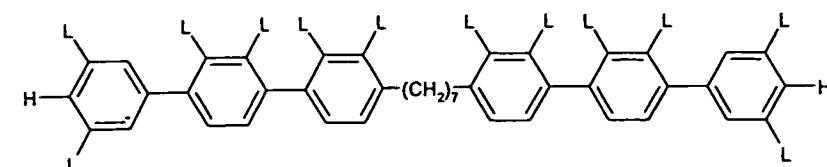
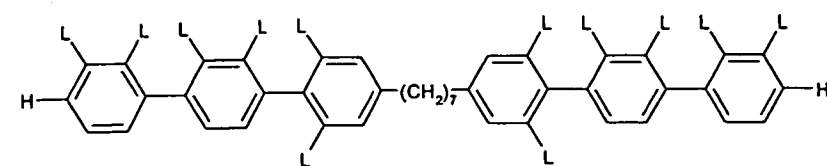
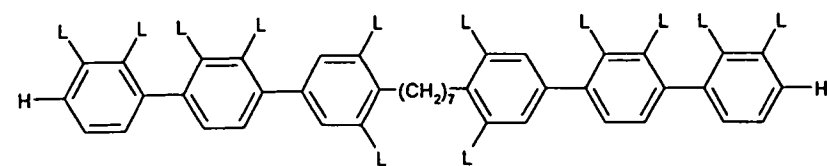
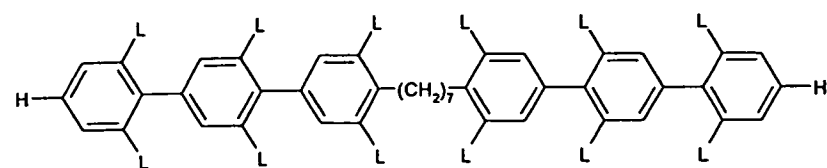
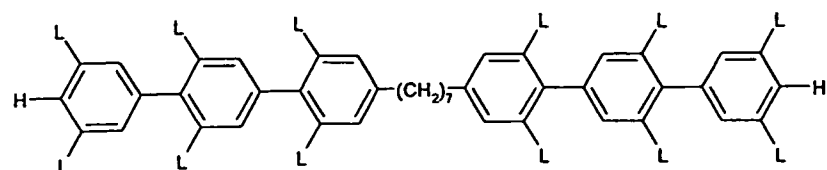
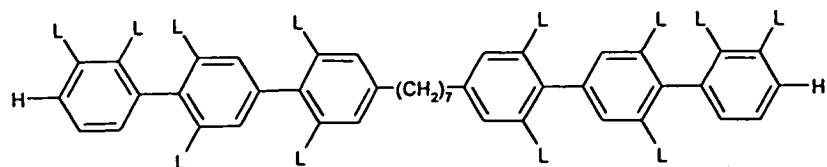
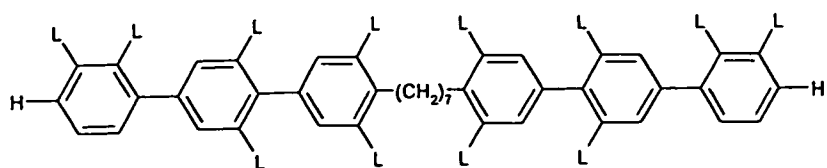
Ib-46a

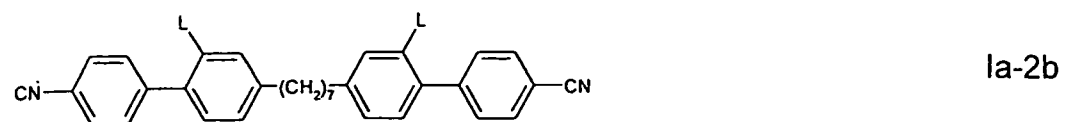
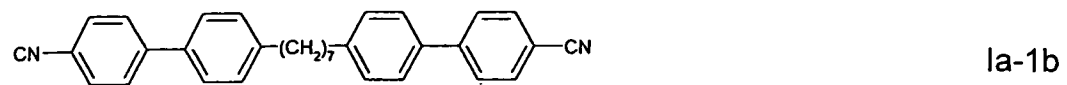
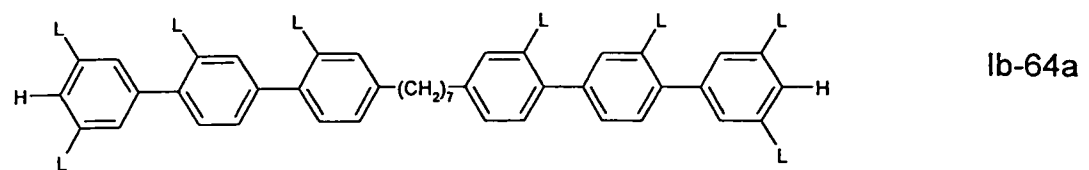
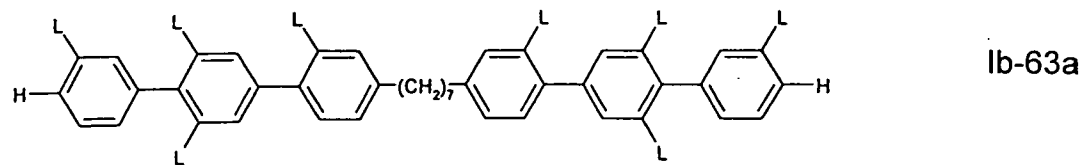
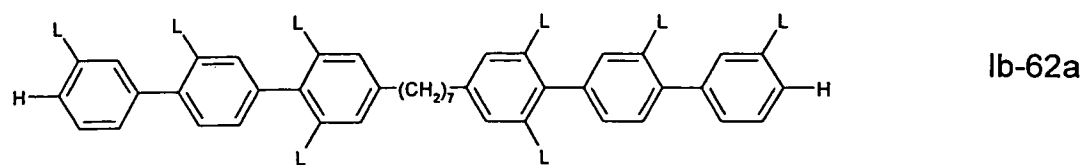
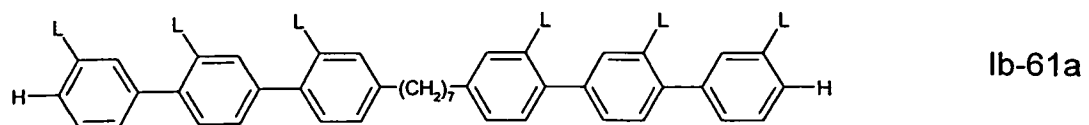
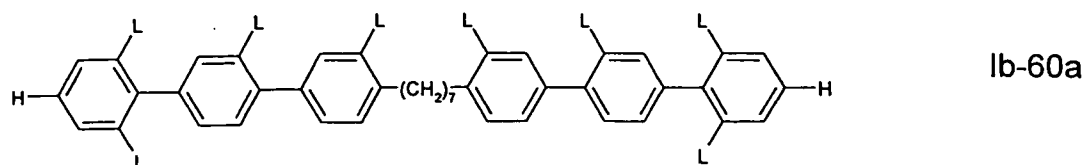
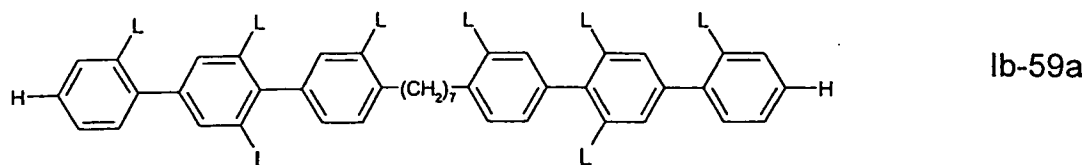
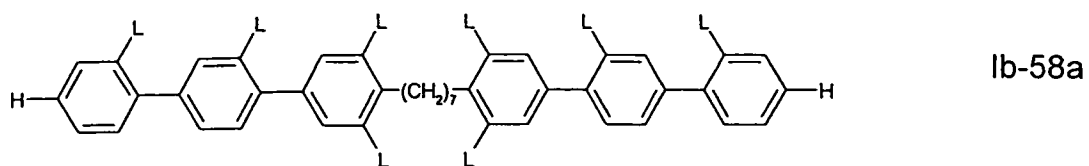


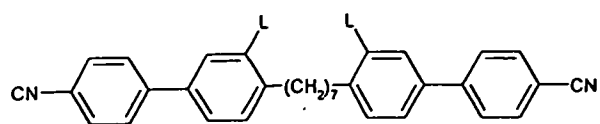
Ib-47a



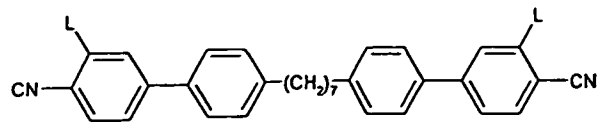
Ib-48a



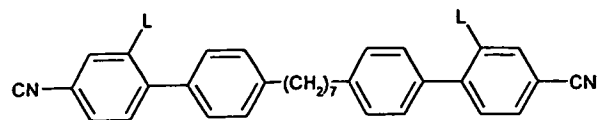




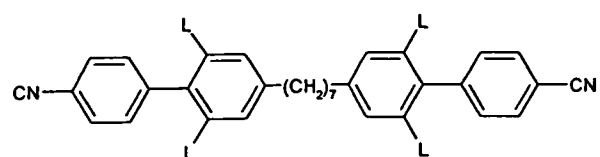
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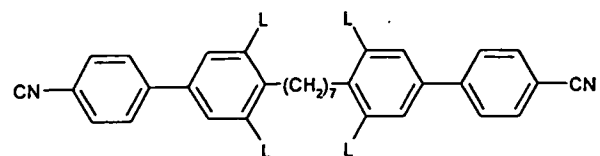
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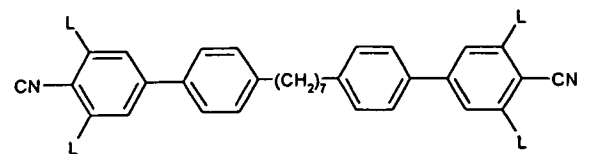
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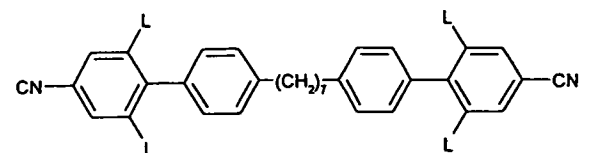
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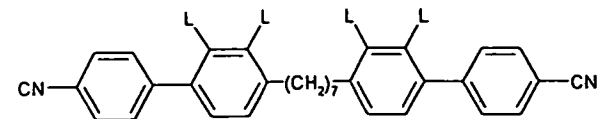
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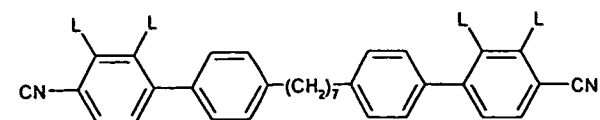
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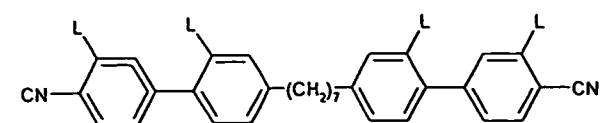
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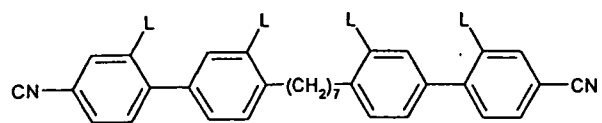
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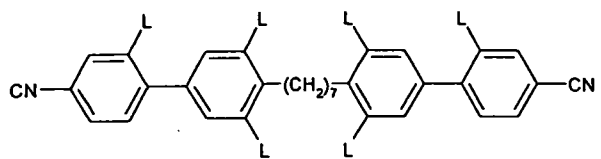
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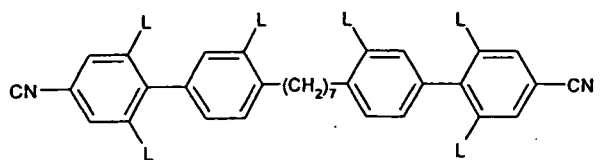
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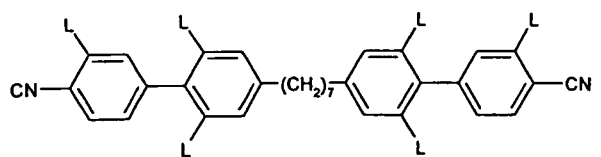
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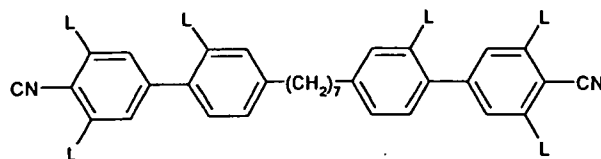
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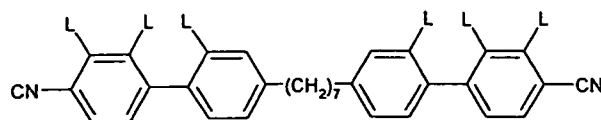
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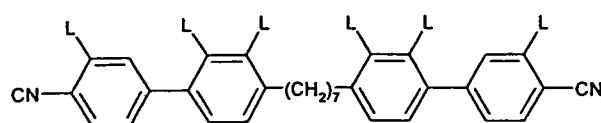
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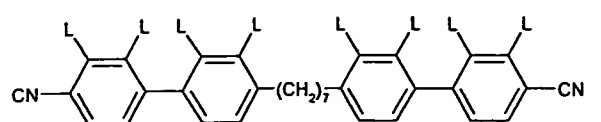
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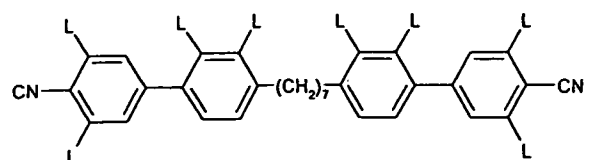
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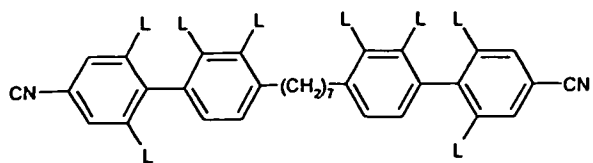
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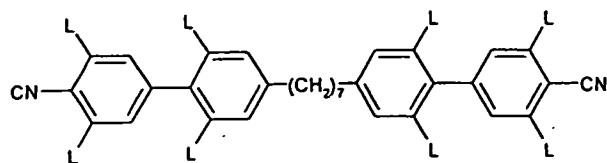
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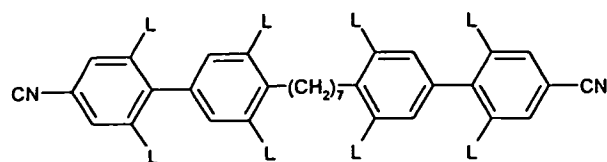
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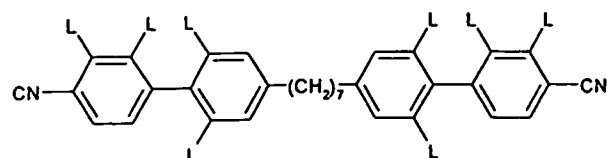
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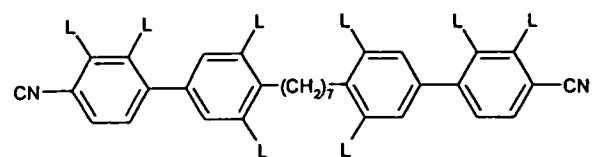
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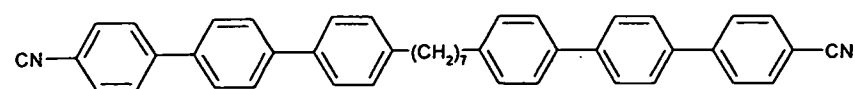
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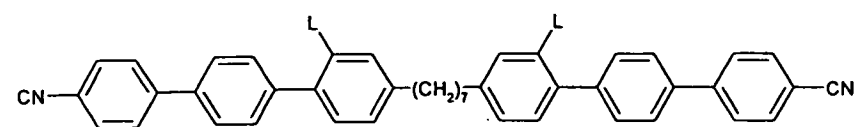
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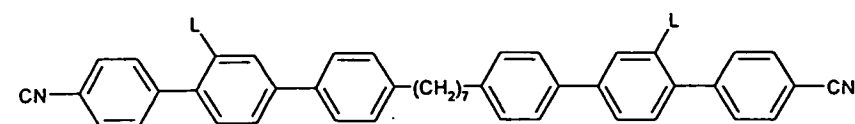
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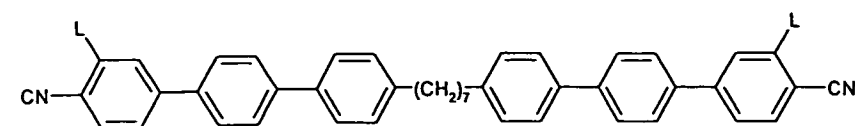
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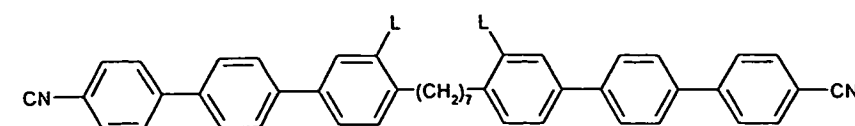
1b-2b



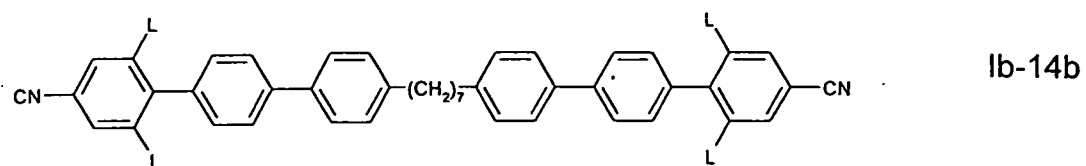
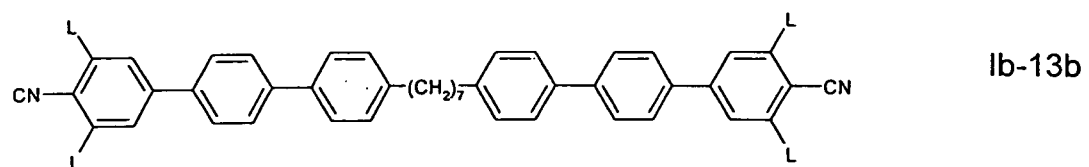
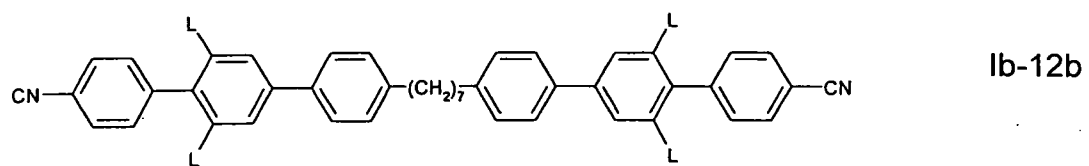
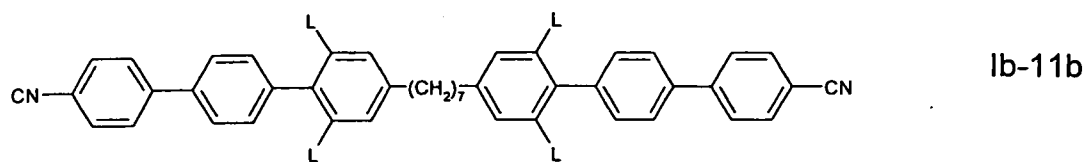
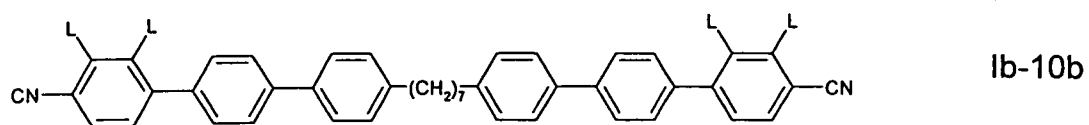
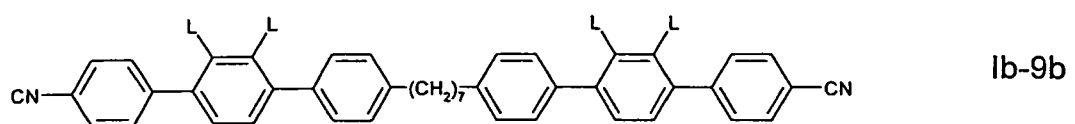
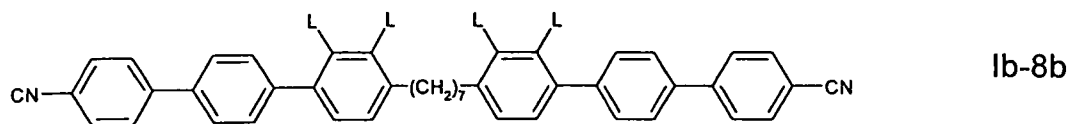
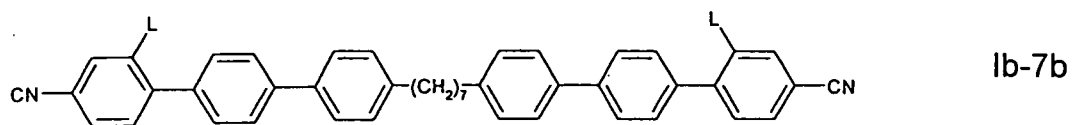
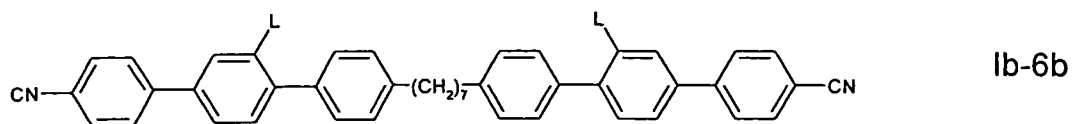
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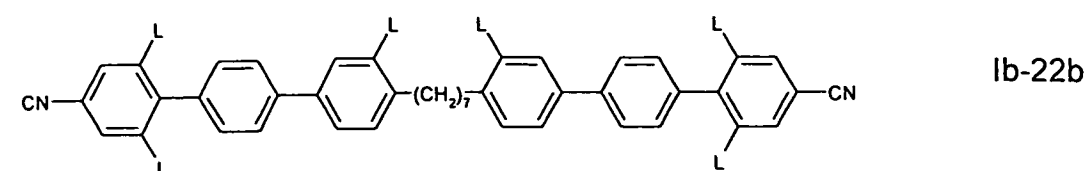
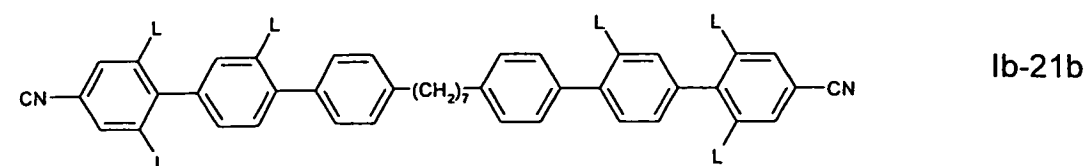
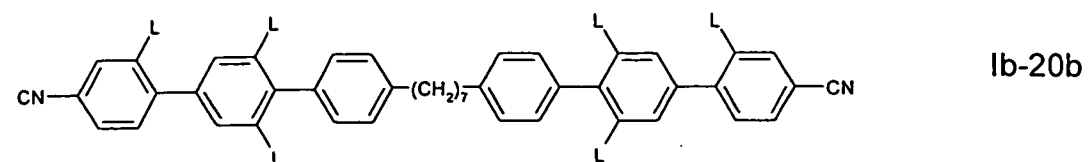
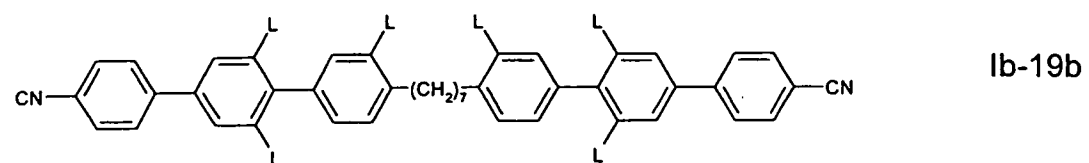
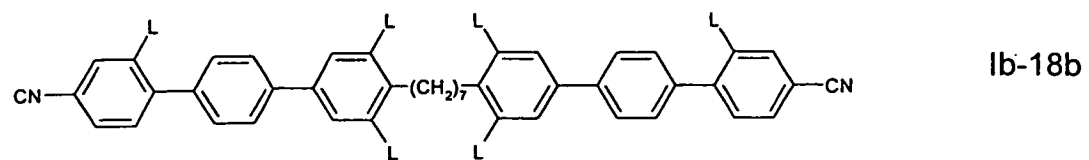
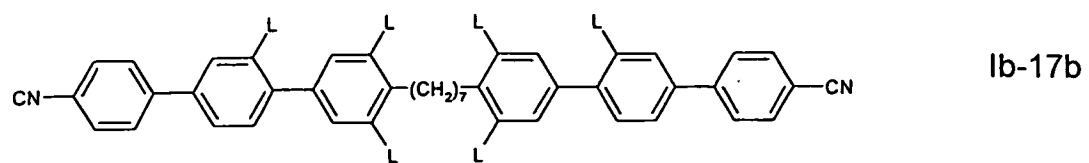
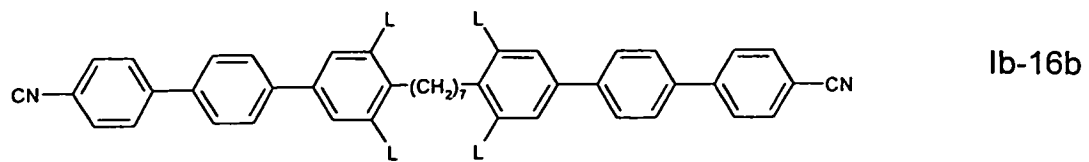
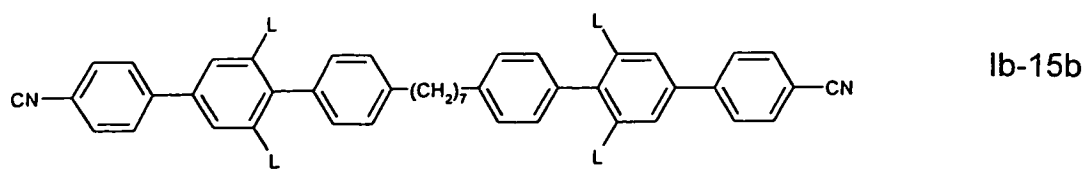


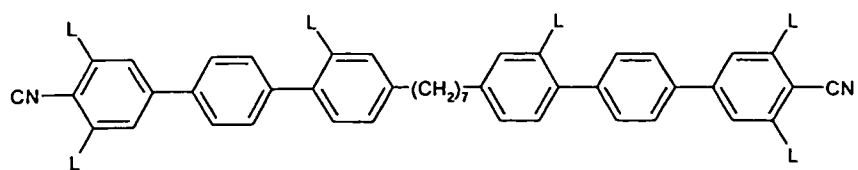
1b-4b



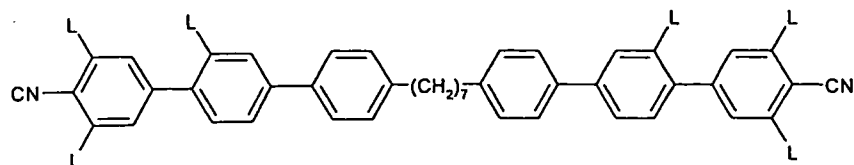
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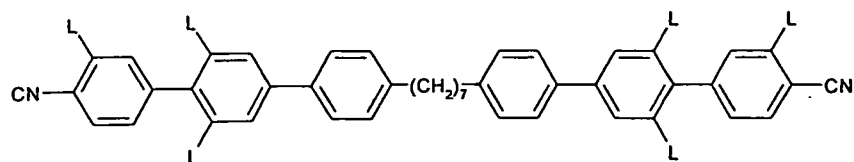




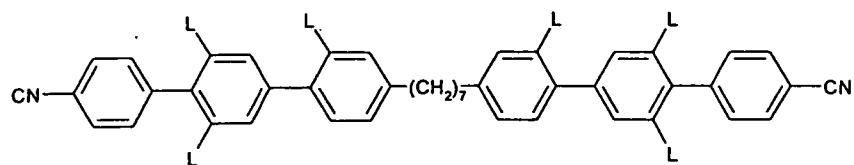
Ib-23b



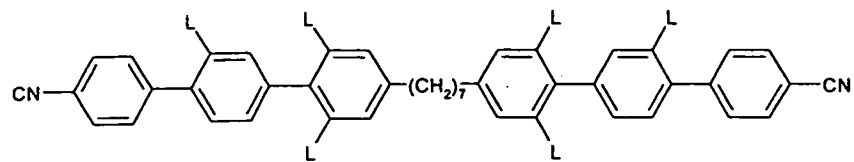
Ib-24b



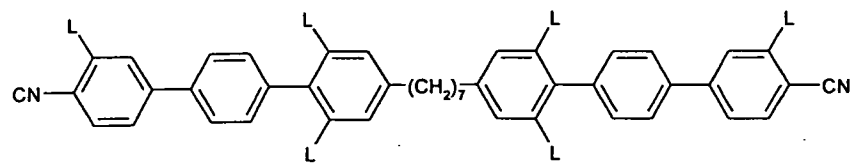
Ib-25b



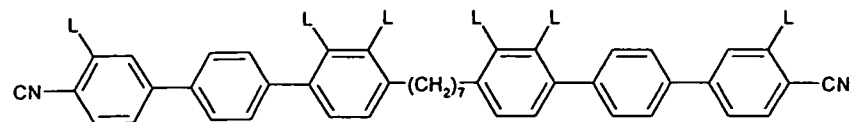
Ib-26b



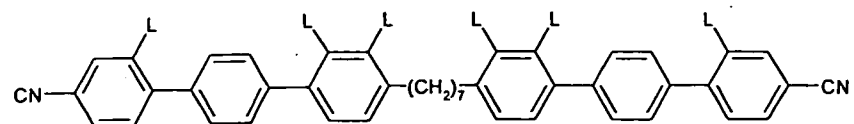
Ib-27b



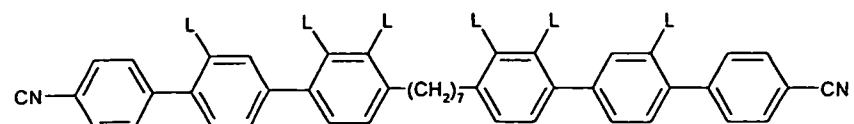
Ib-28b



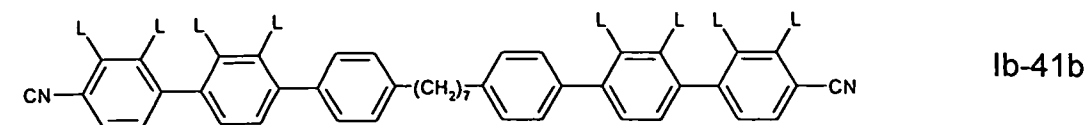
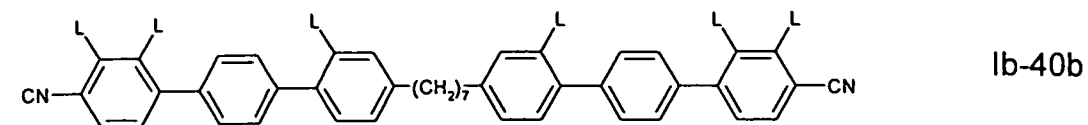
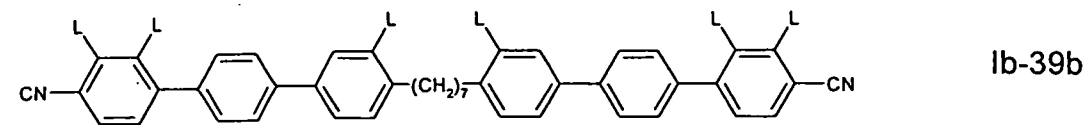
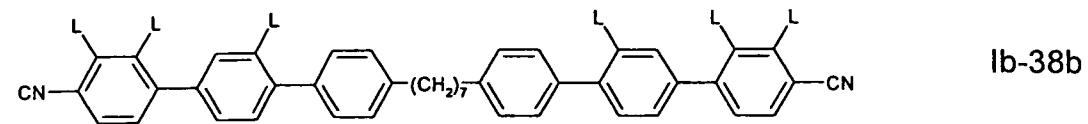
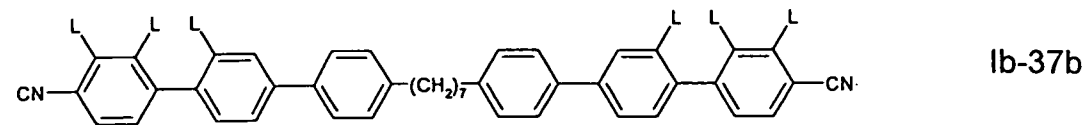
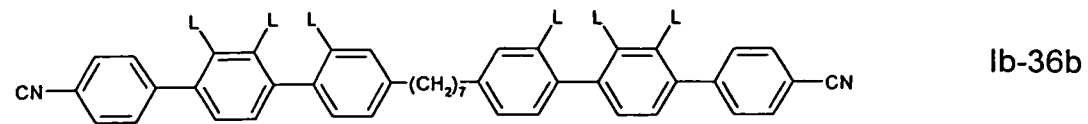
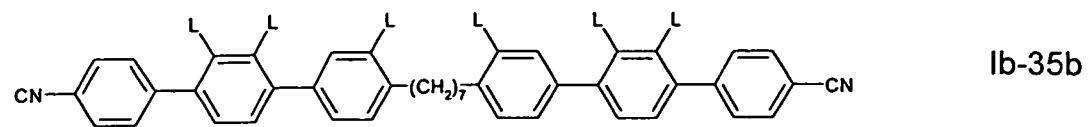
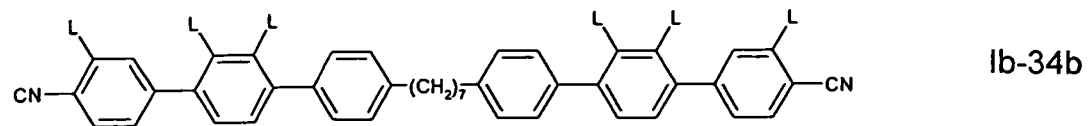
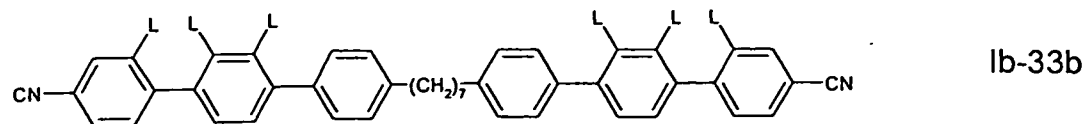
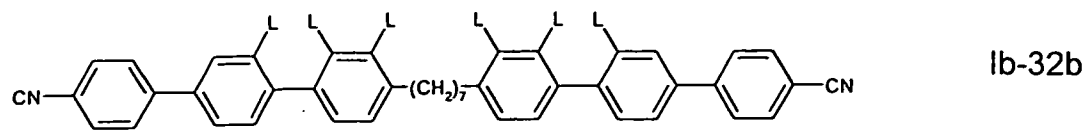
Ib-29b

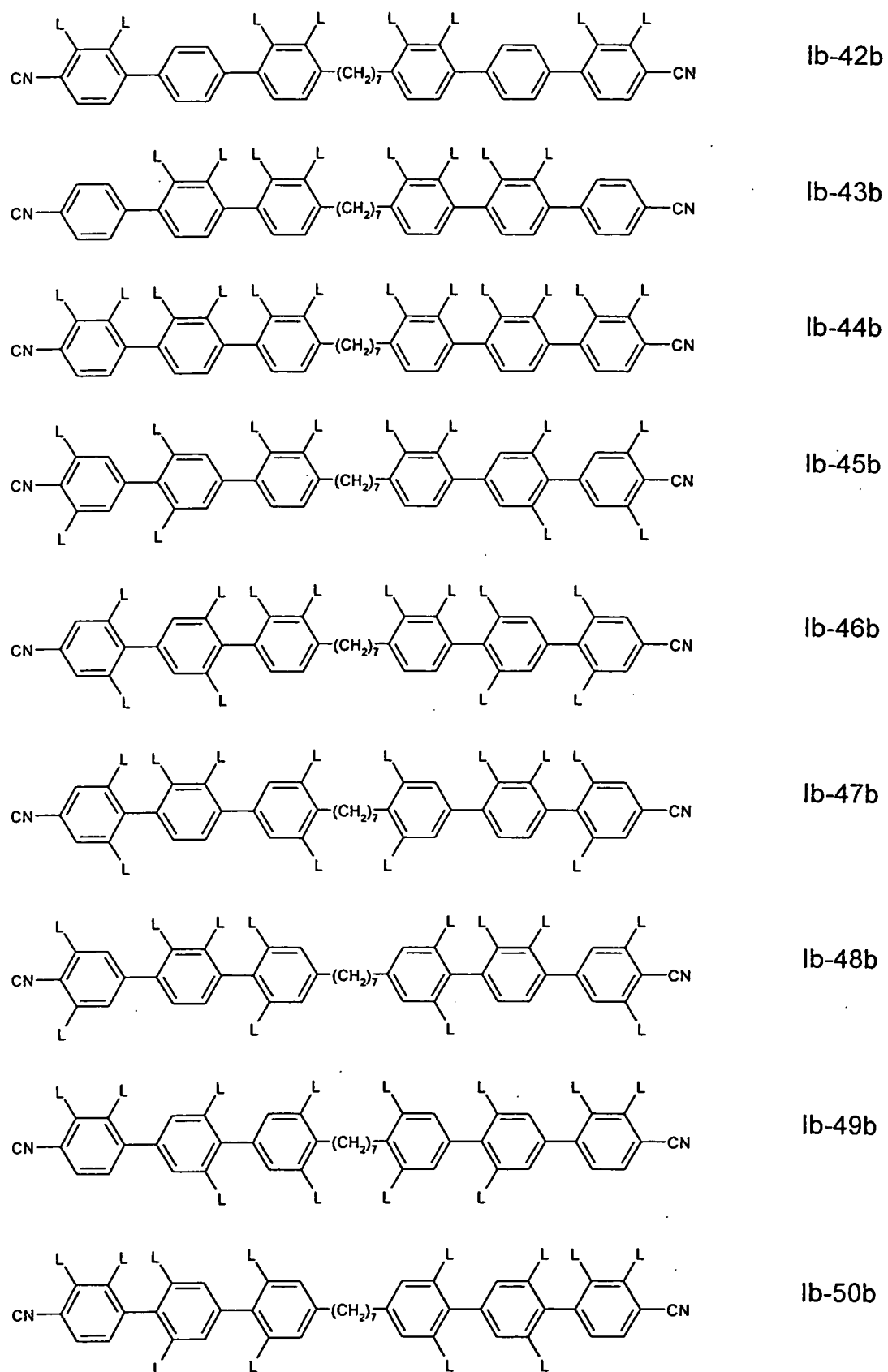


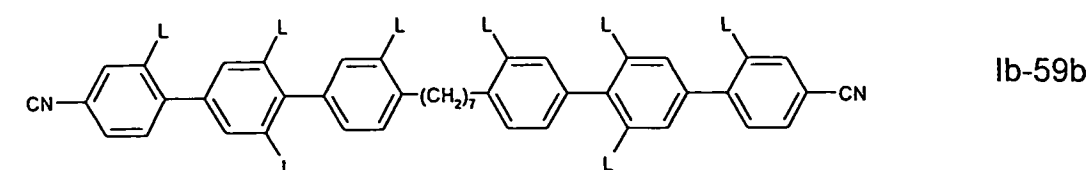
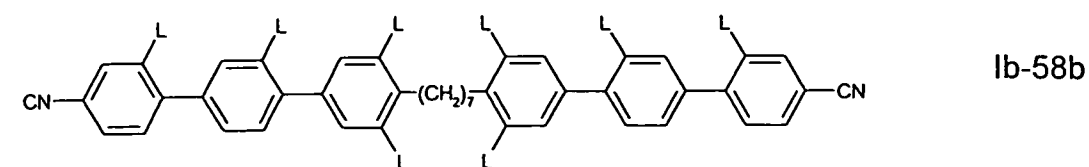
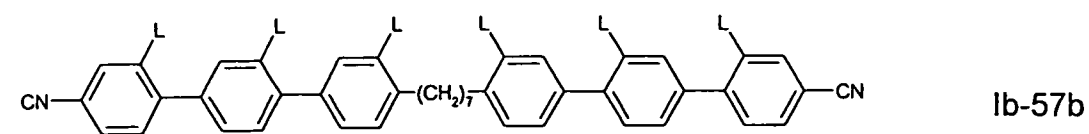
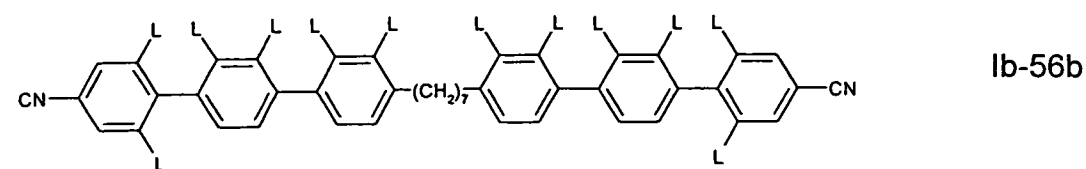
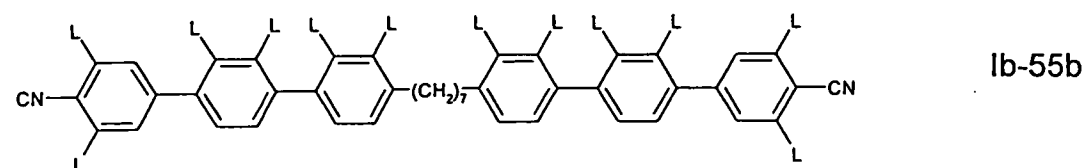
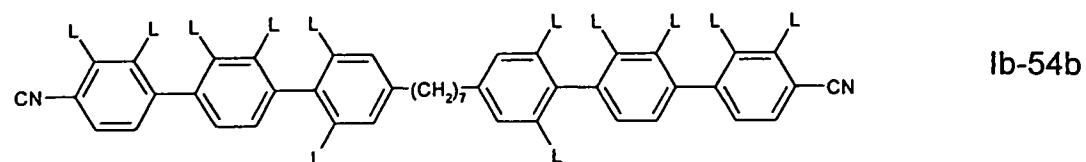
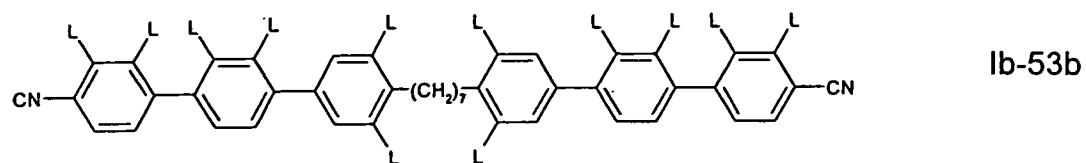
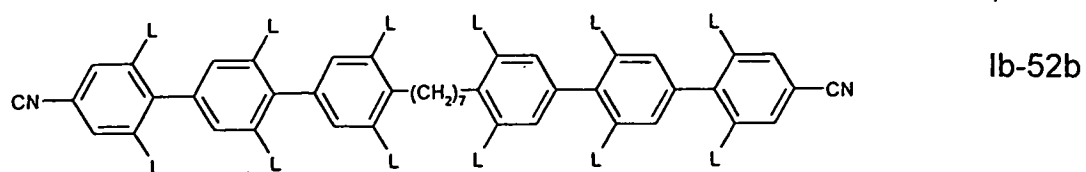
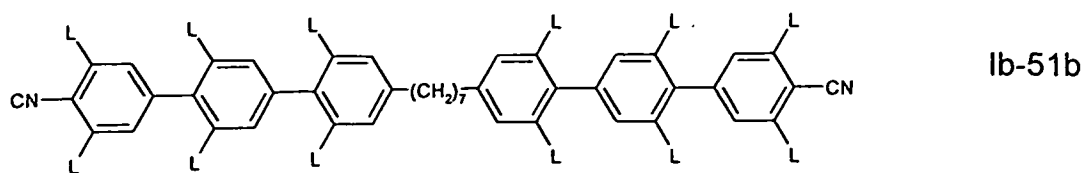
Ib-30b

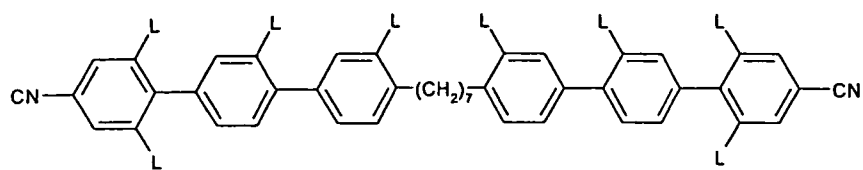


Ib-31b

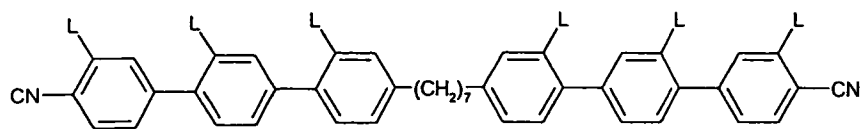




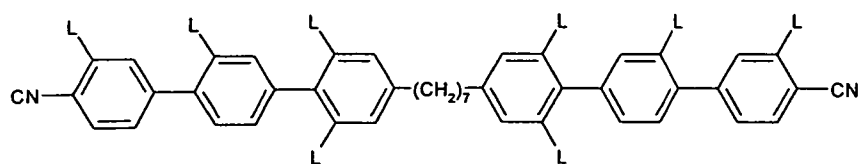




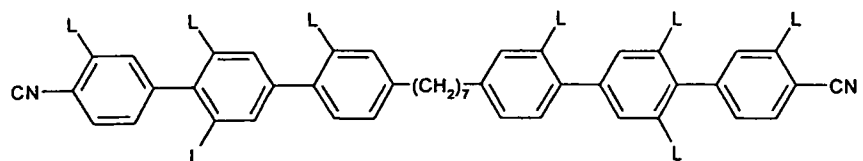
Ib-60b



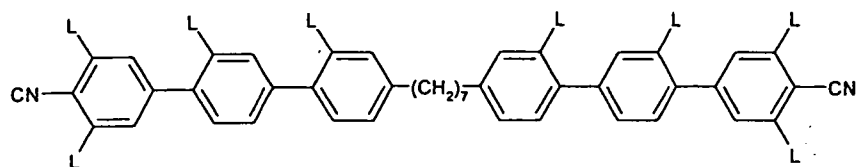
Ib-61b



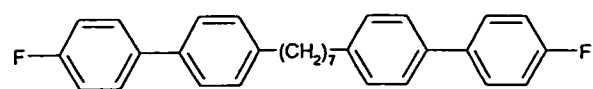
Ib-62b



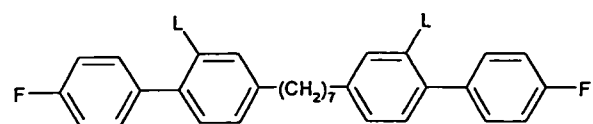
Ib-63b



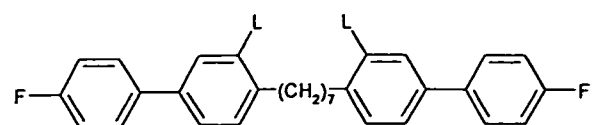
Ib-64b



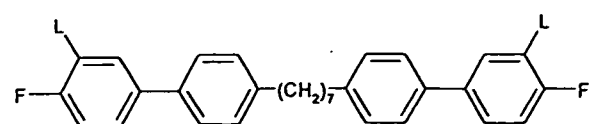
Ia-1c



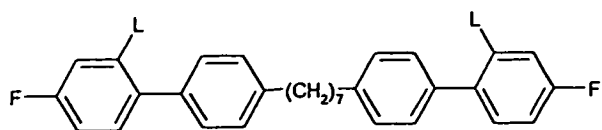
Ia-2c



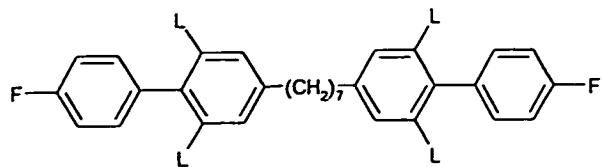
Ia-3c



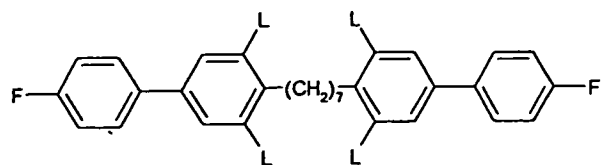
Ia-4c



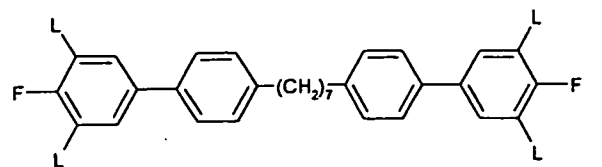
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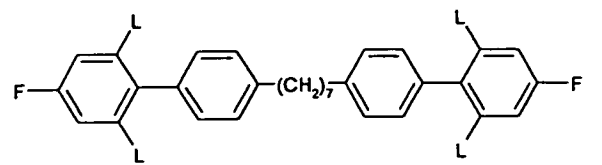
1a-6c



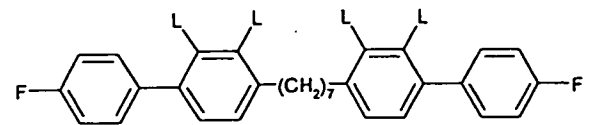
1a-7c



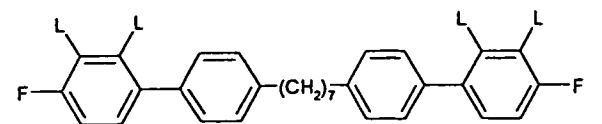
1a-8c



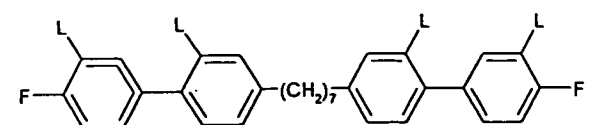
1a-9c



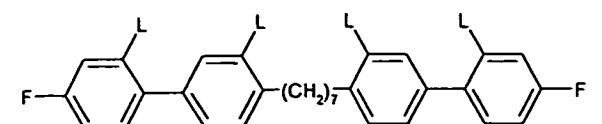
1a-10c



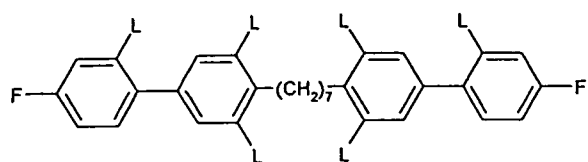
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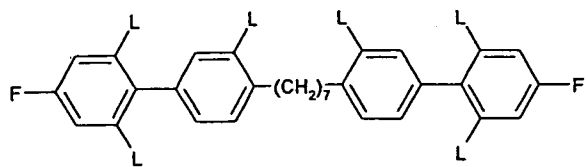
1a-12c



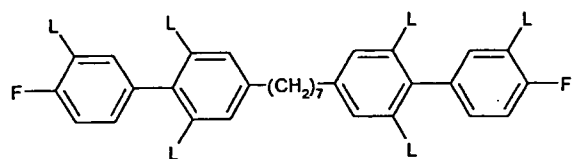
1a-13c



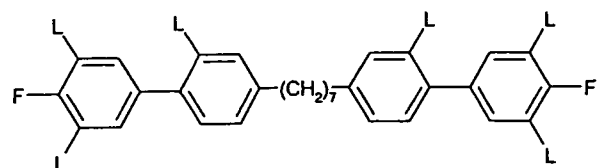
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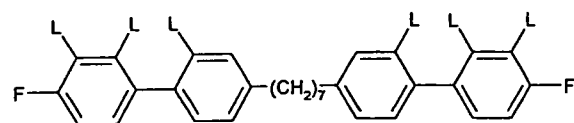
1a-15c



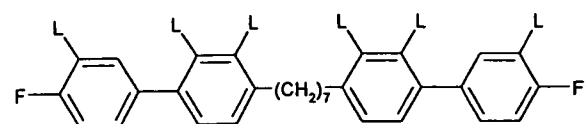
1a-16c



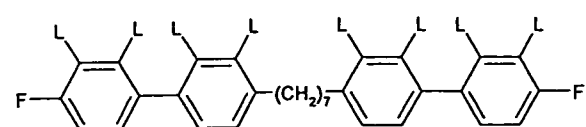
1a-17c



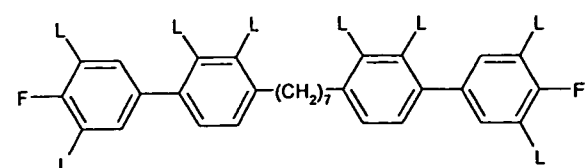
1a-18c



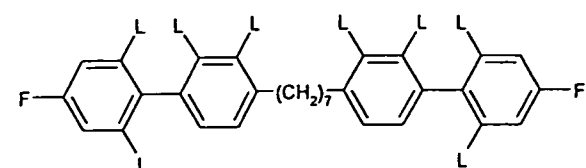
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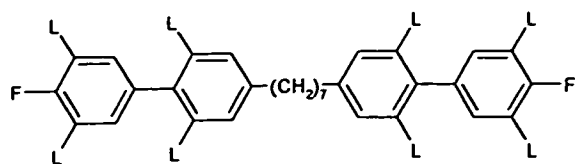
1a-20c



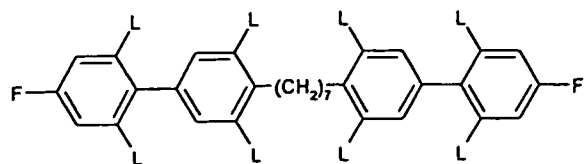
1a-21c



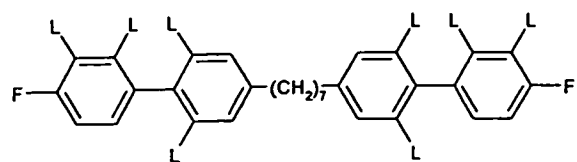
1a-22c



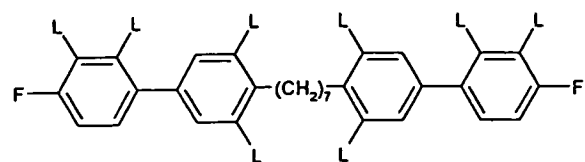
Ia-23c



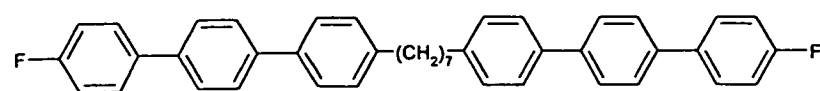
Ia-24c



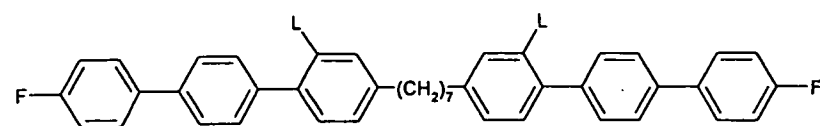
Ia-25c



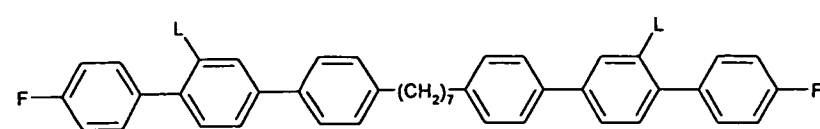
Ia-26c



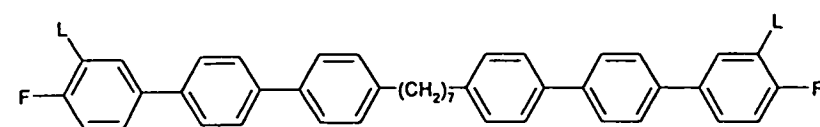
Ib-1c



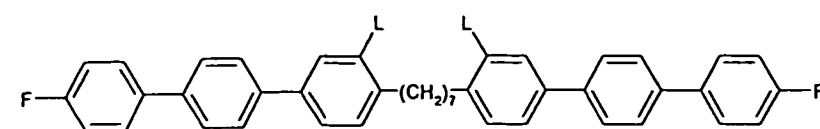
Ib-2c



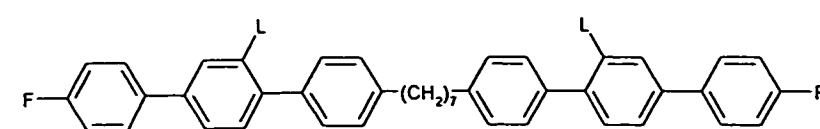
Ib-3c



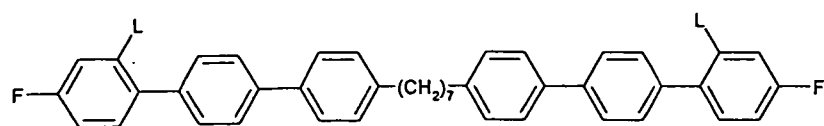
Ib-4c



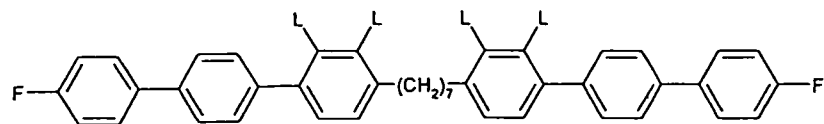
Ib-5c



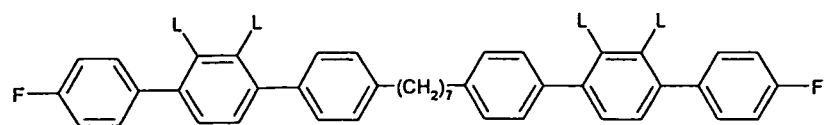
Ib-6c



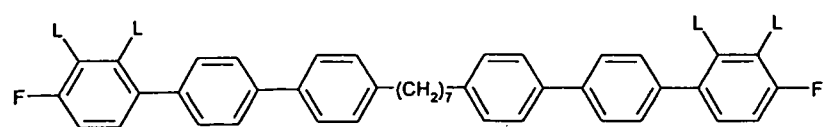
Ib-7c



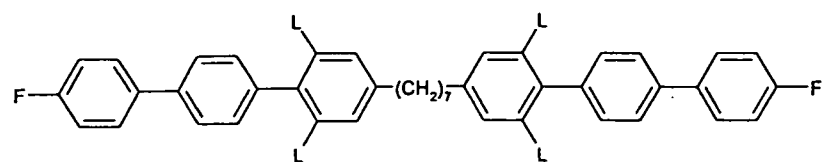
Ib-8c



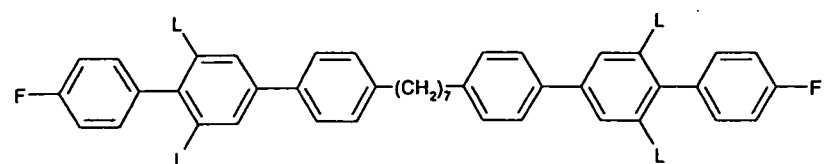
Ib-9c



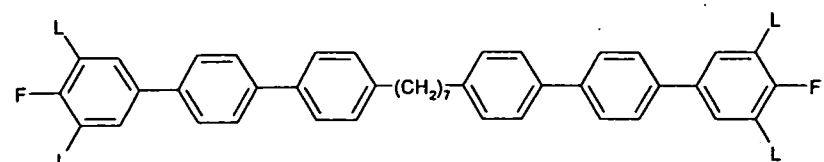
Ib-10c



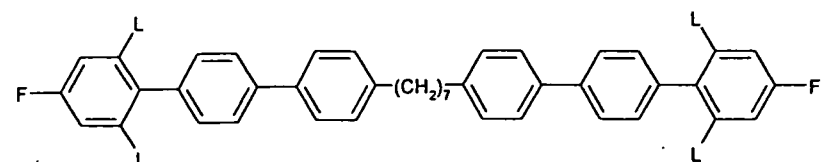
Ib-11c



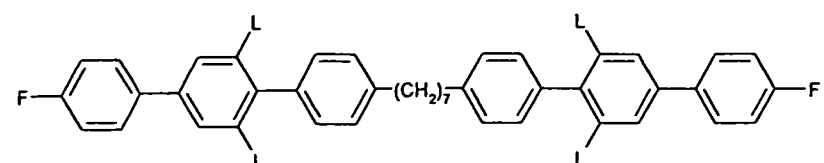
Ib-12c



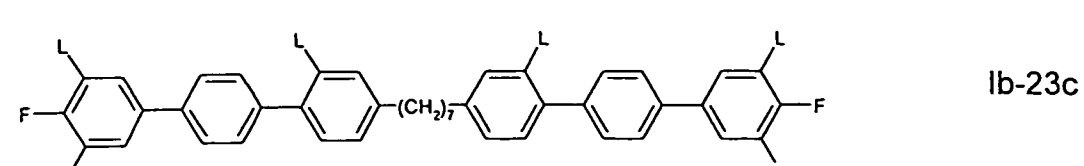
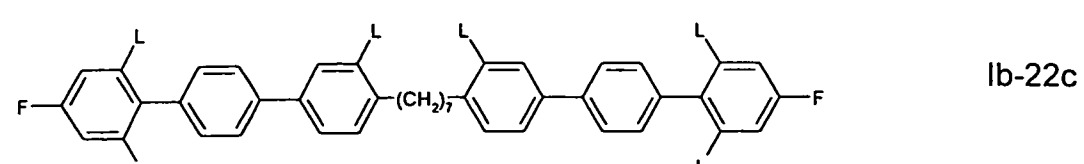
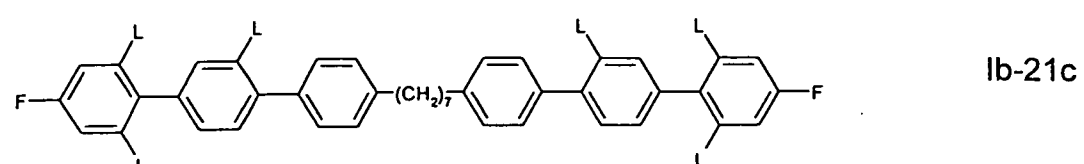
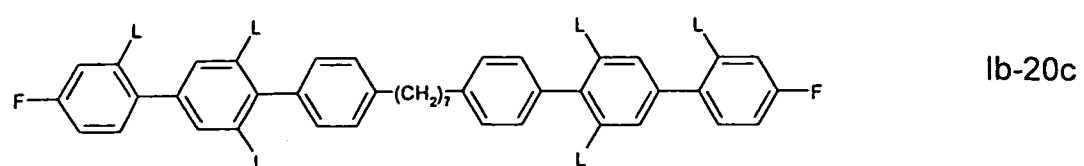
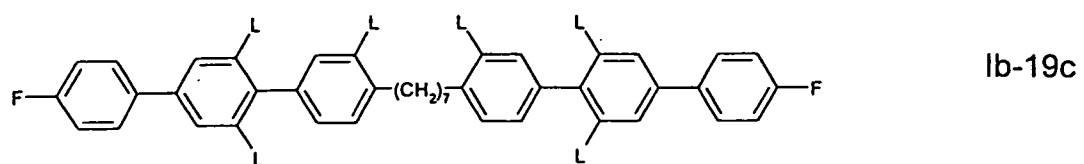
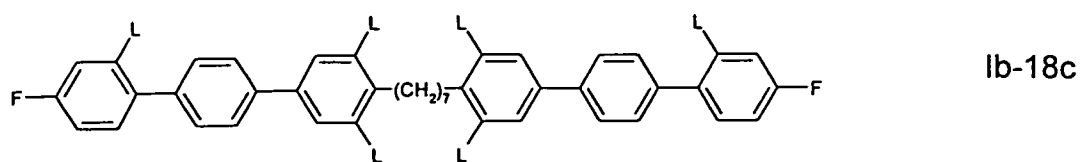
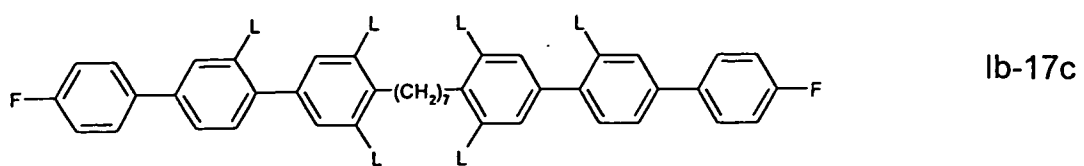
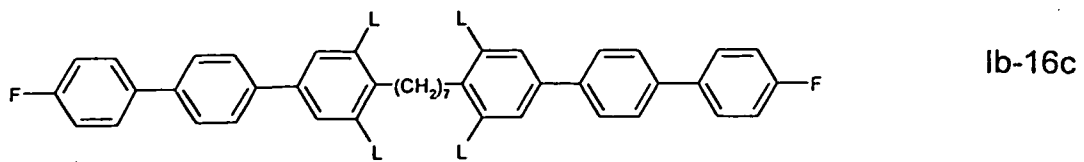
Ib-13c

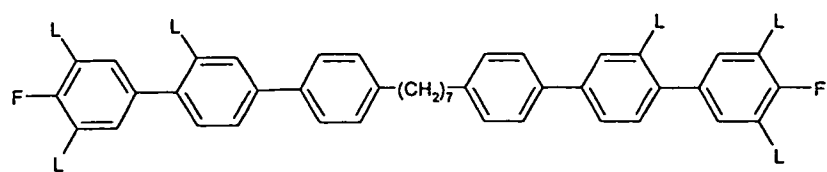


Ib-14c

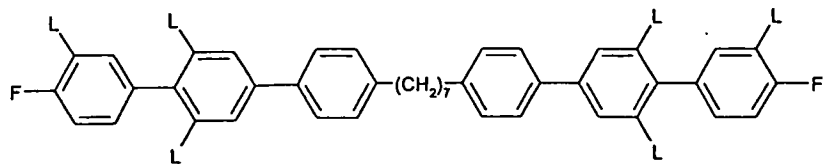


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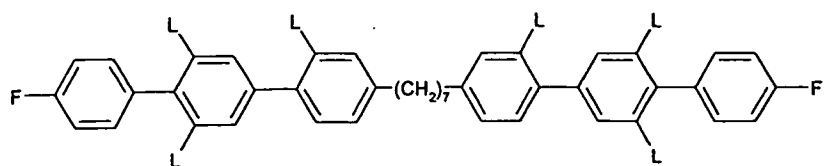




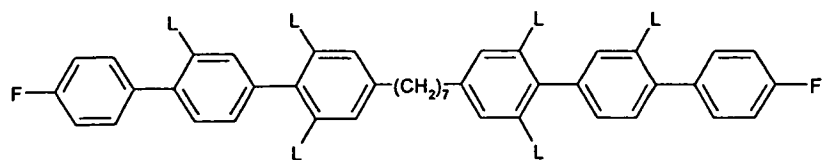
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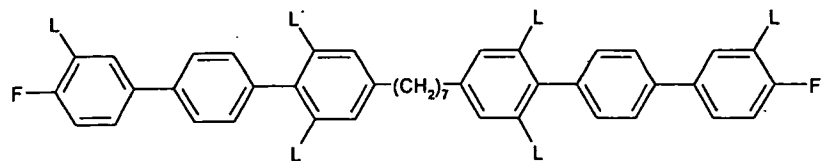
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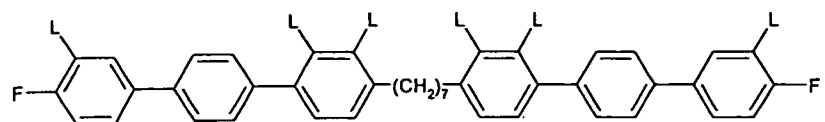
Ib-26c



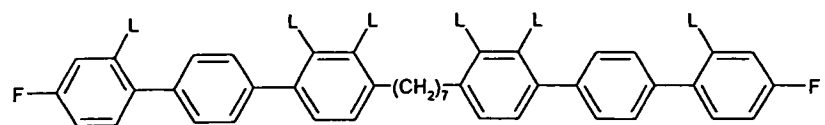
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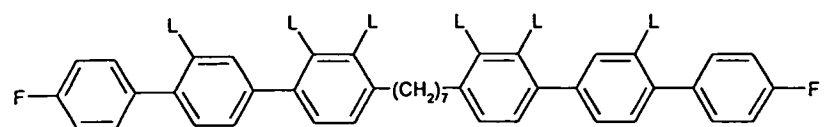
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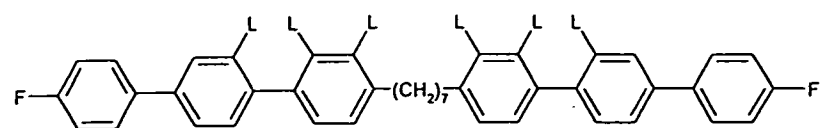
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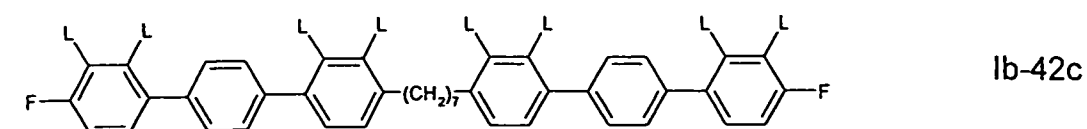
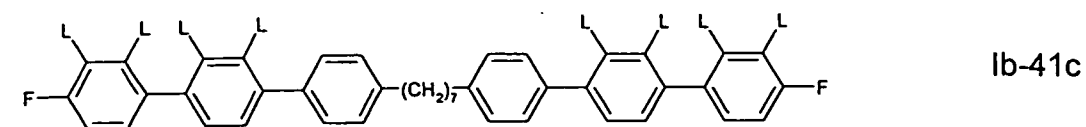
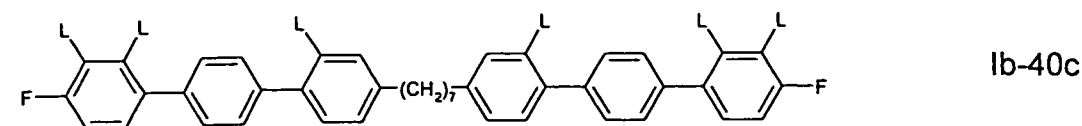
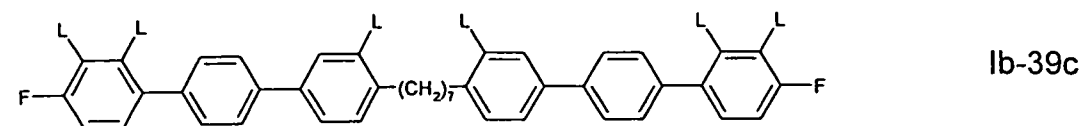
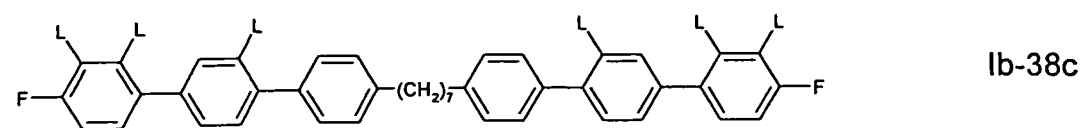
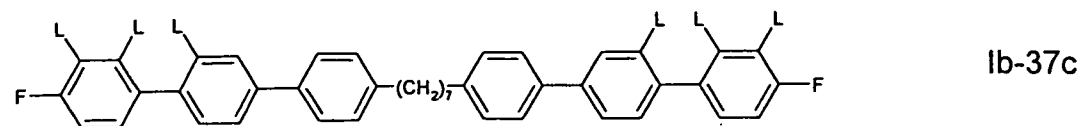
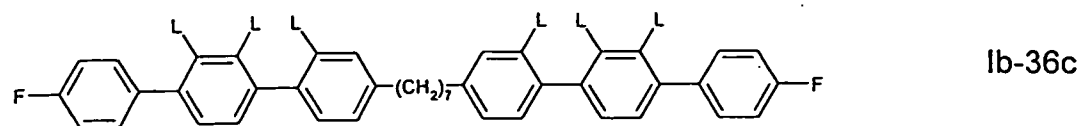
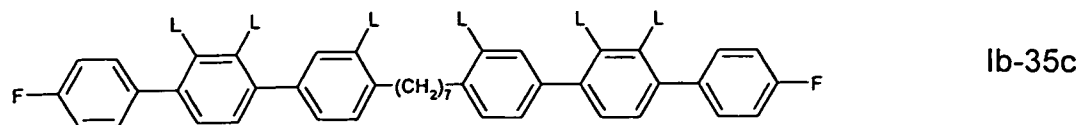
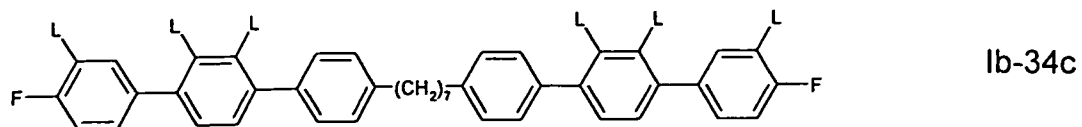
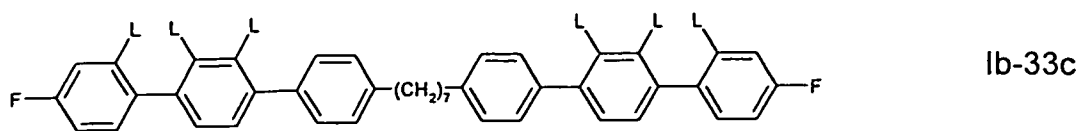
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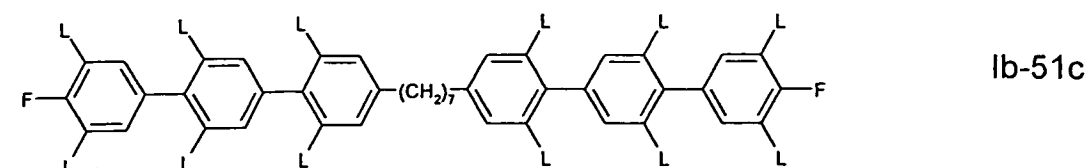
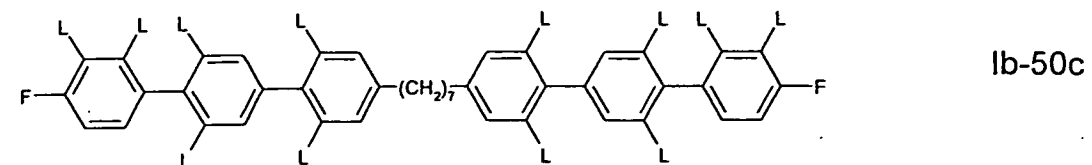
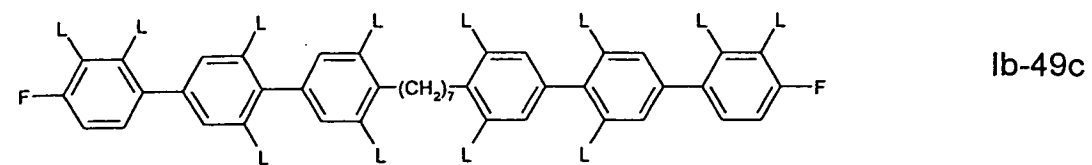
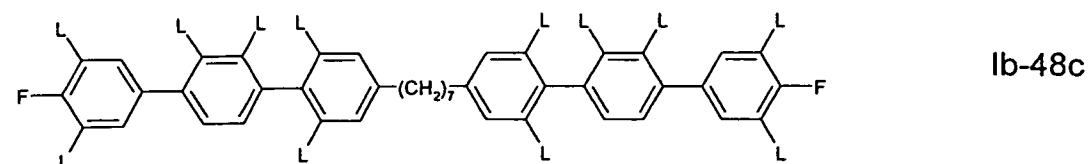
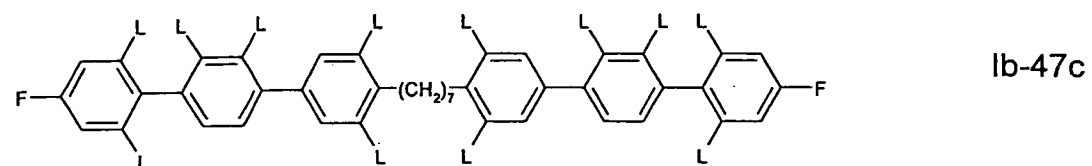
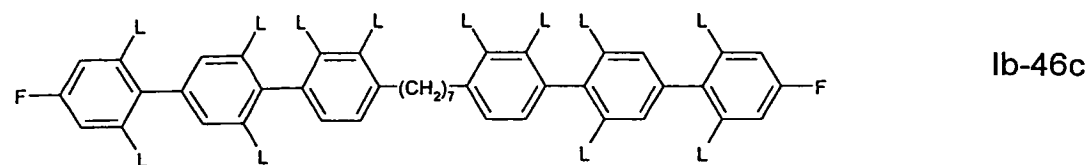
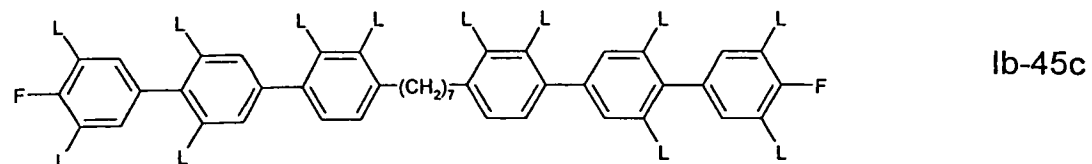
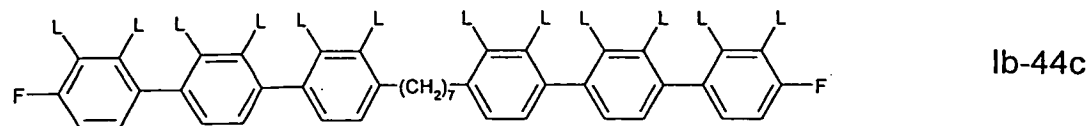
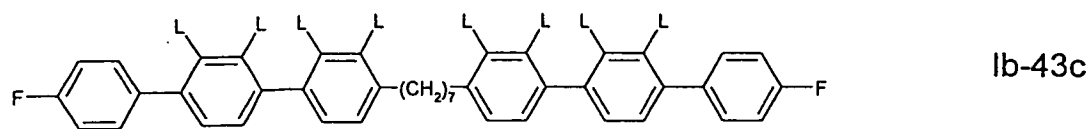


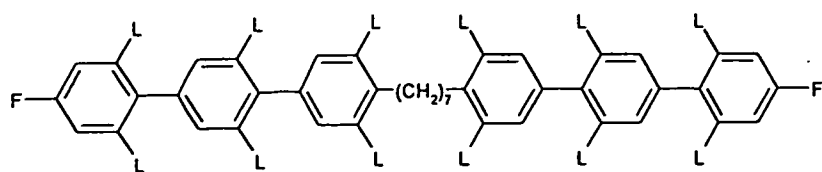
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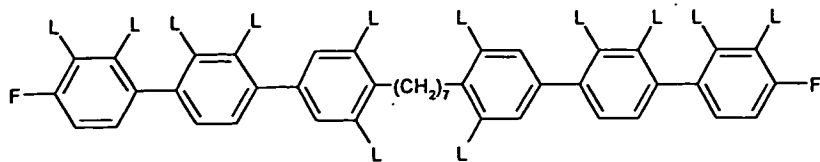
Ib-32c



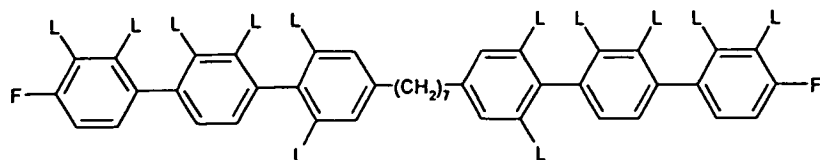




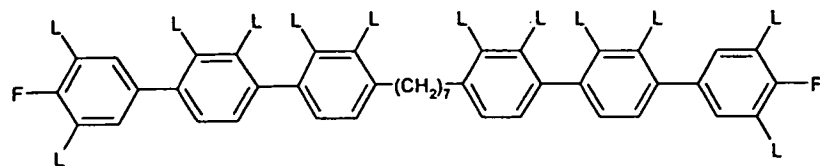
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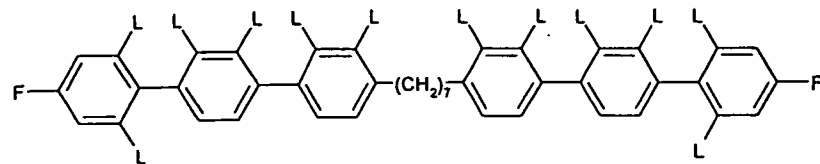
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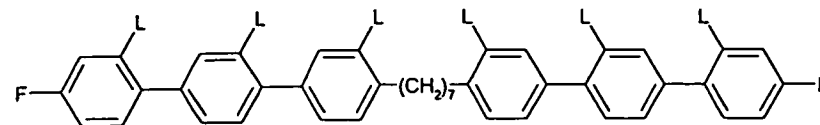
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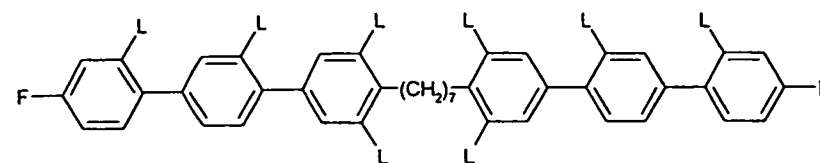
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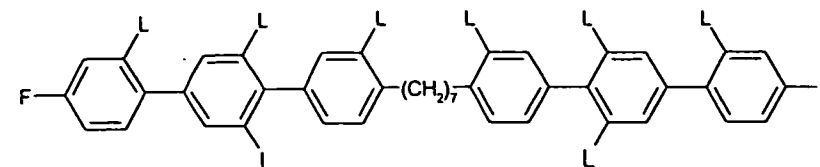
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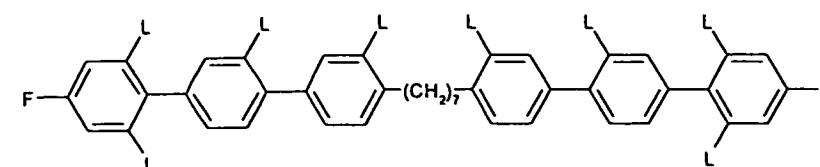
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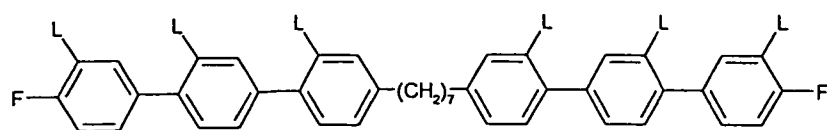
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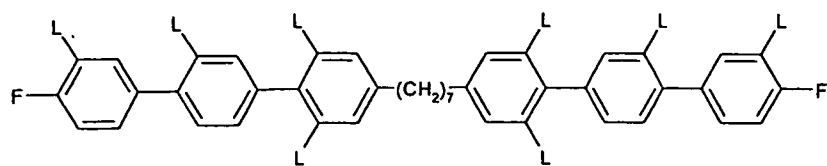
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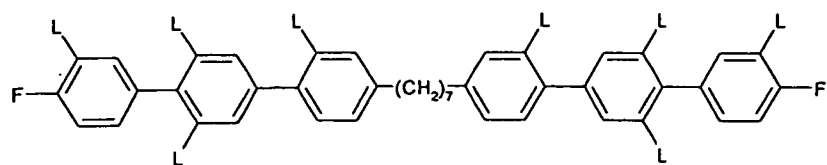
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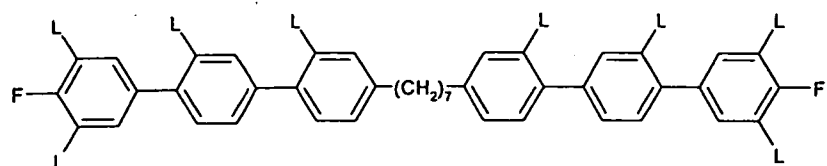
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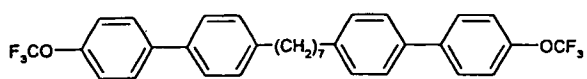
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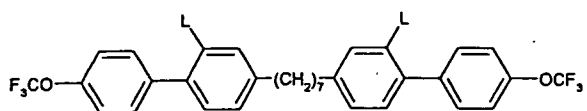
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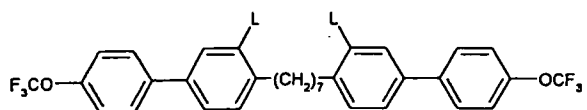
Ib-64c



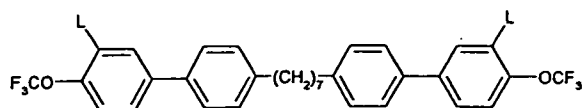
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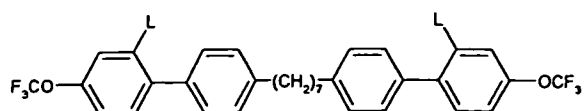
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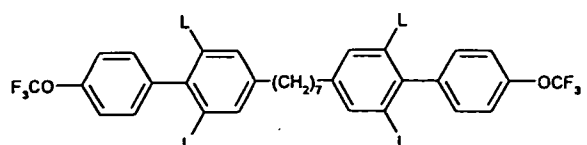
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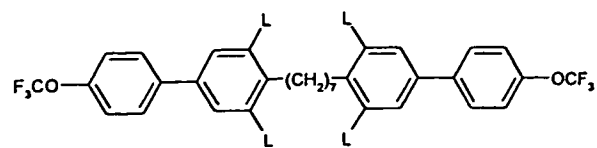
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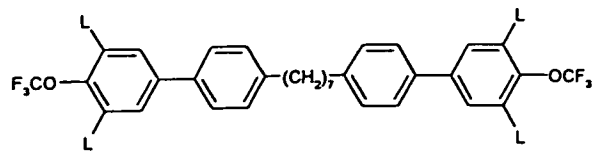
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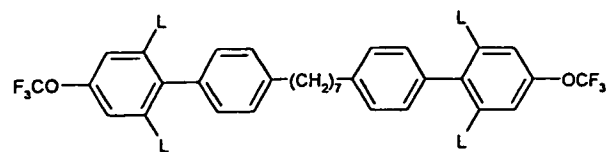
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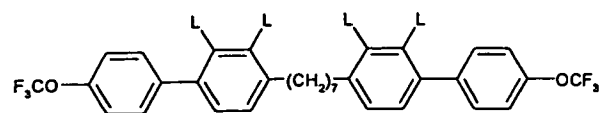
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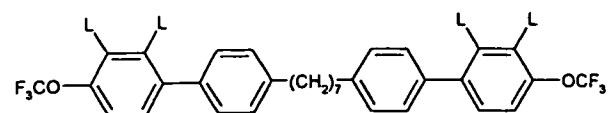
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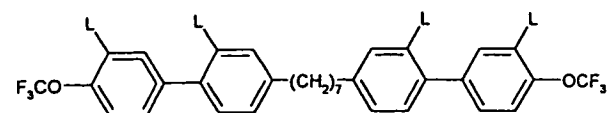
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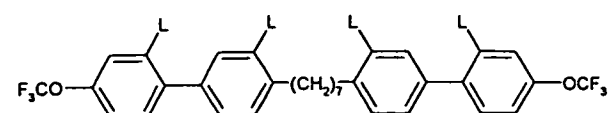
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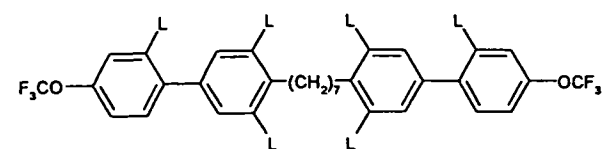
la-11d



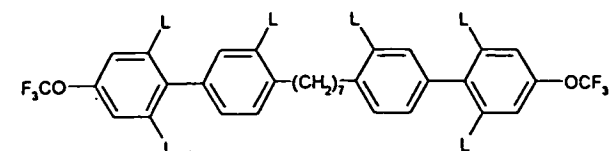
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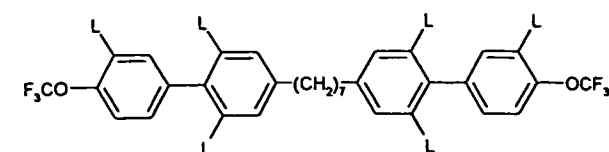
la-13d



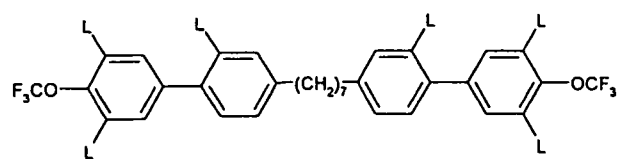
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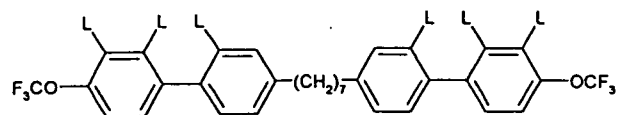
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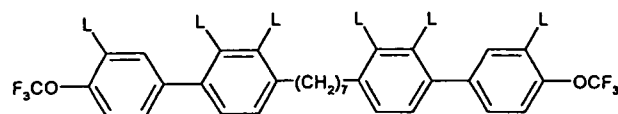
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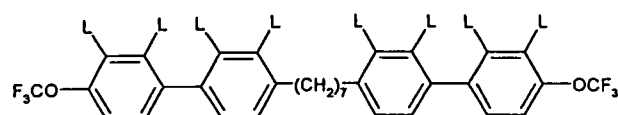
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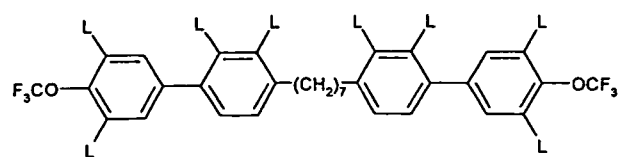
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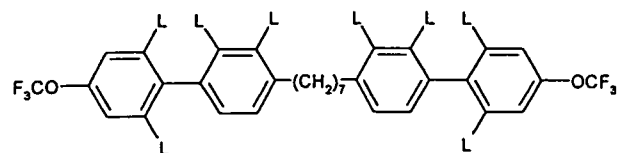
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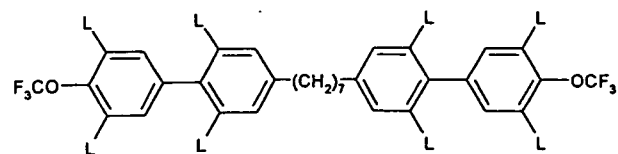
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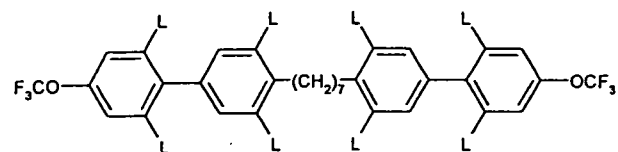
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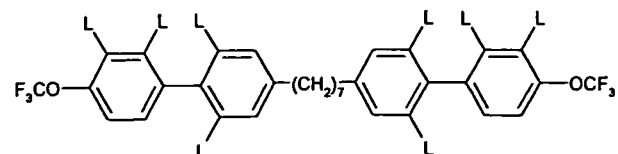
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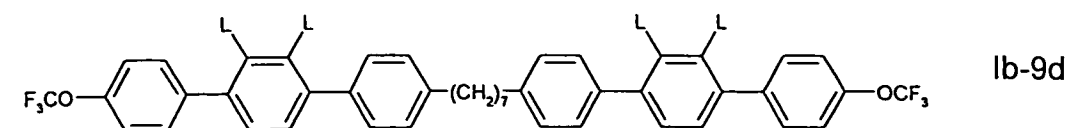
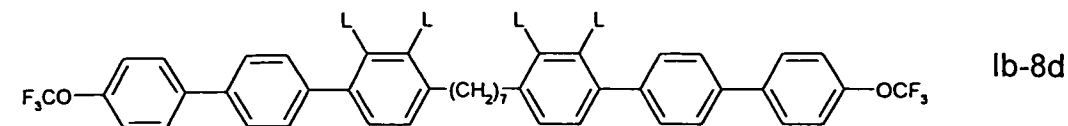
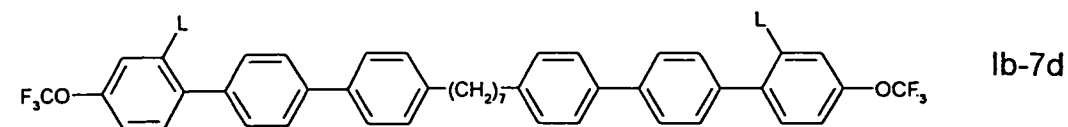
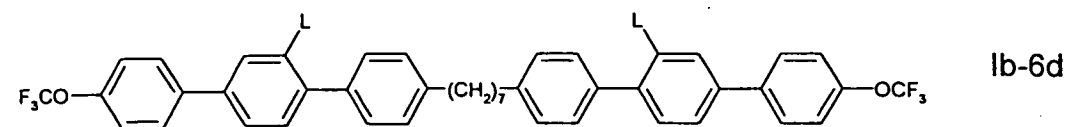
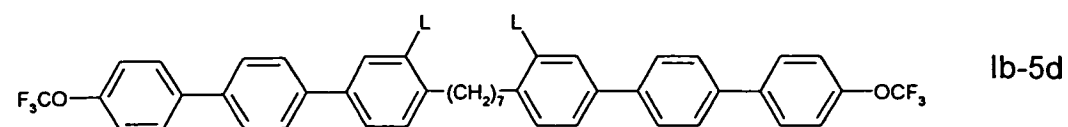
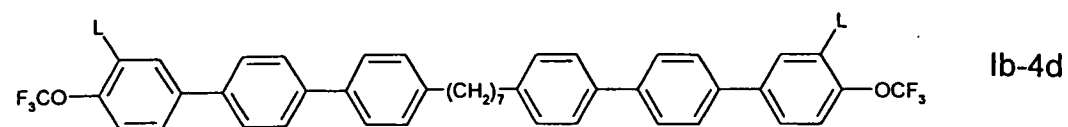
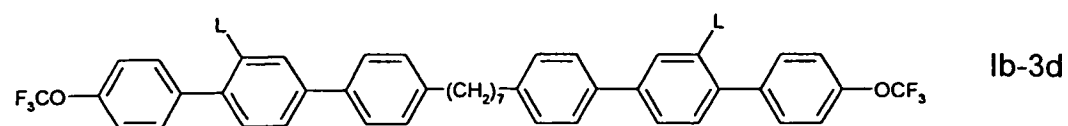
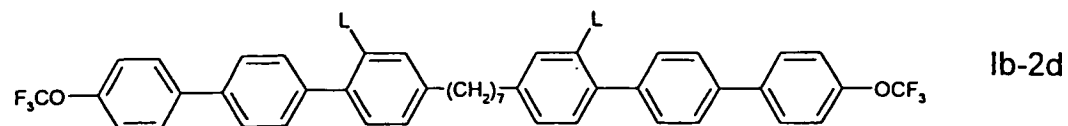
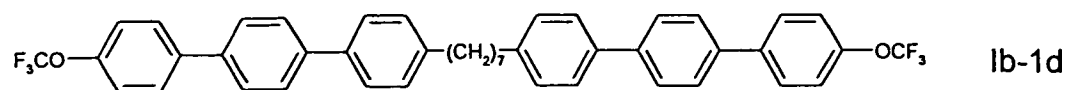
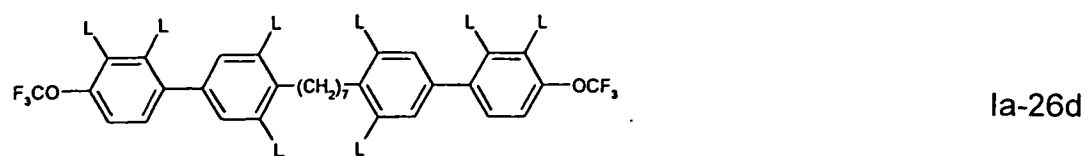
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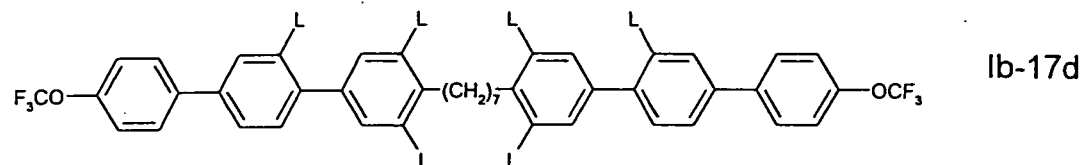
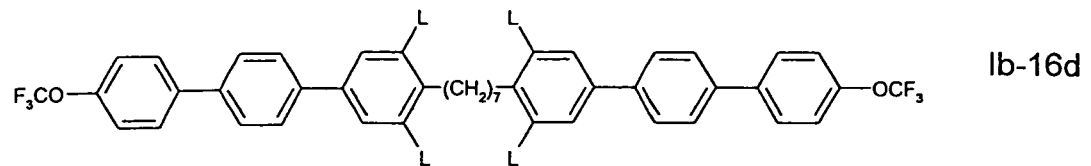
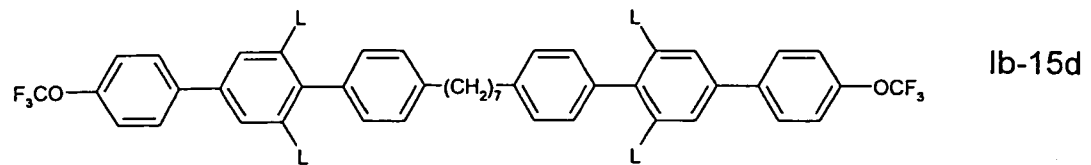
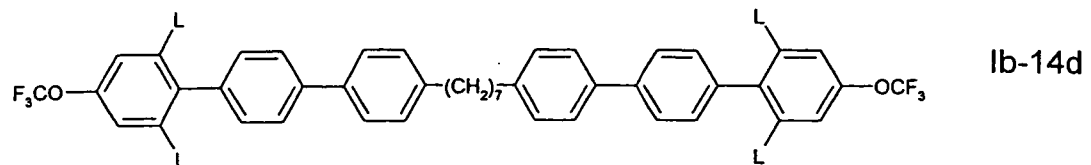
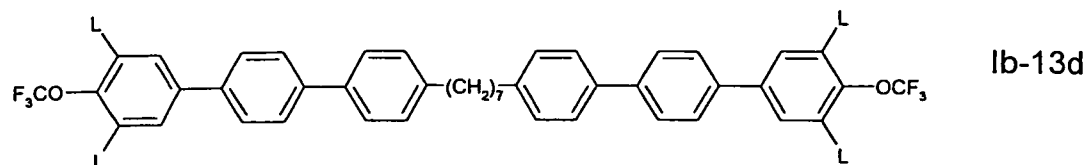
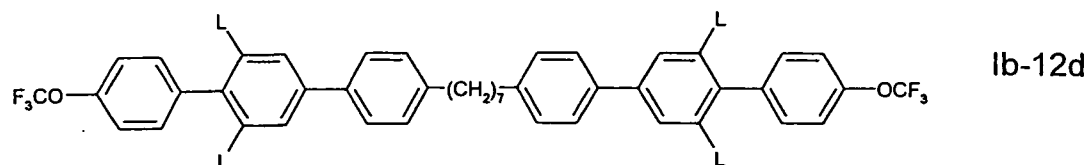
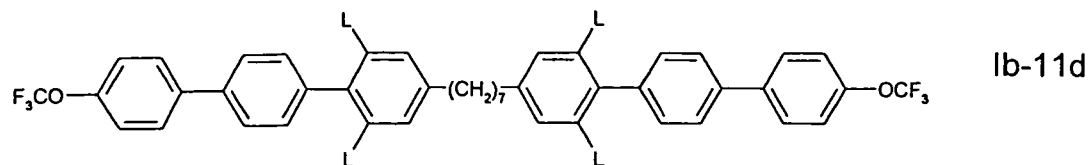
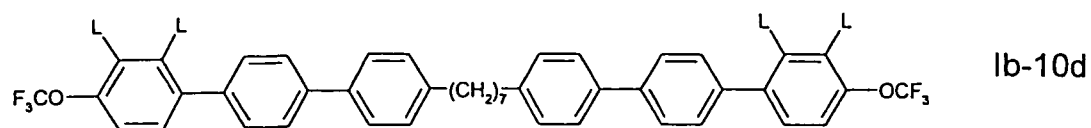


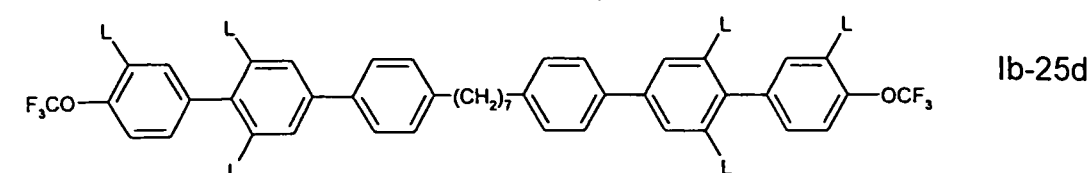
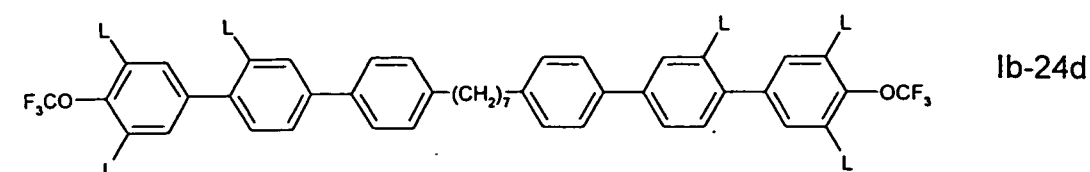
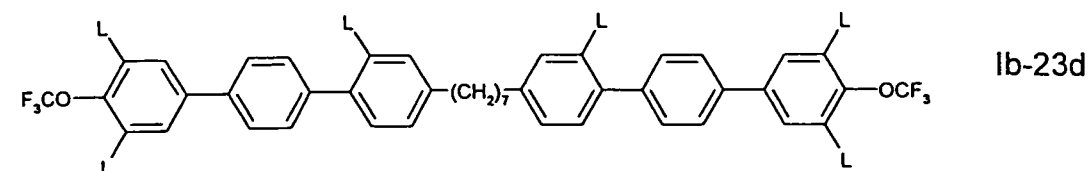
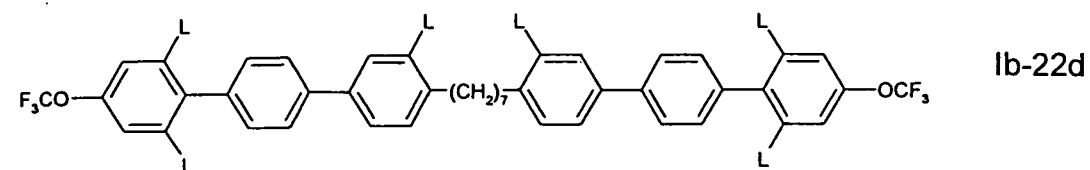
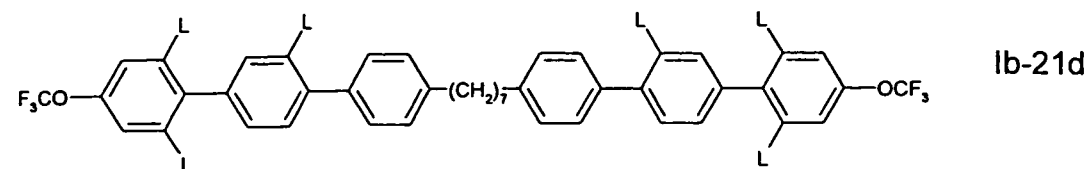
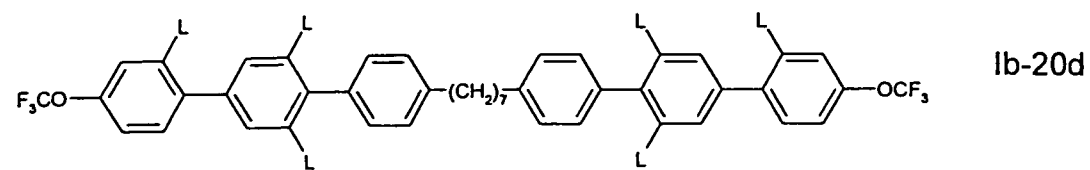
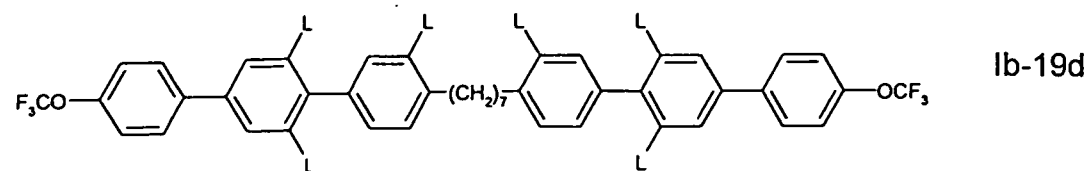
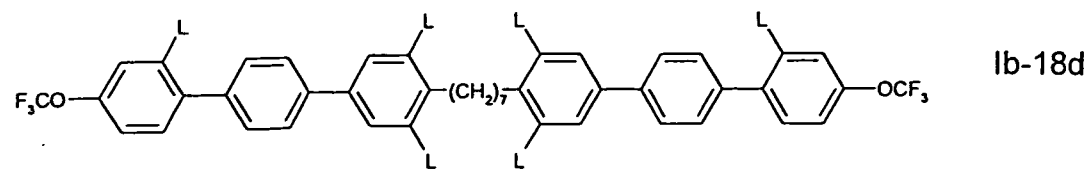
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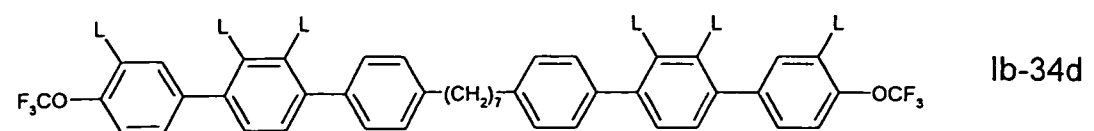
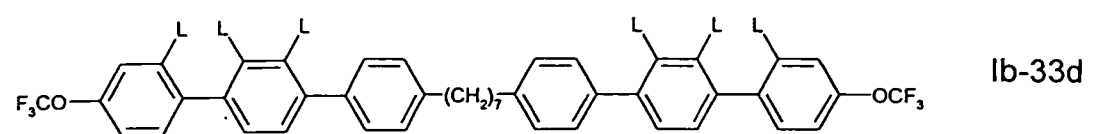
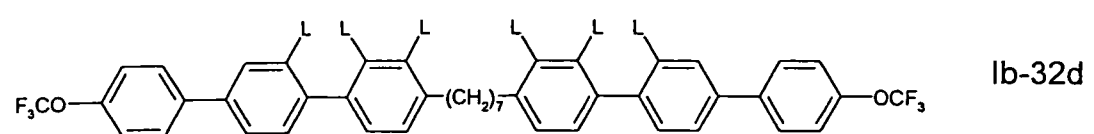
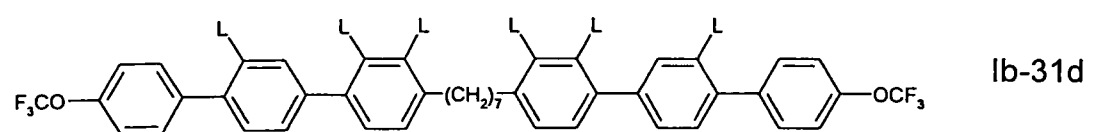
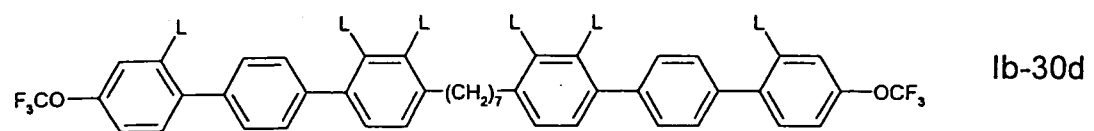
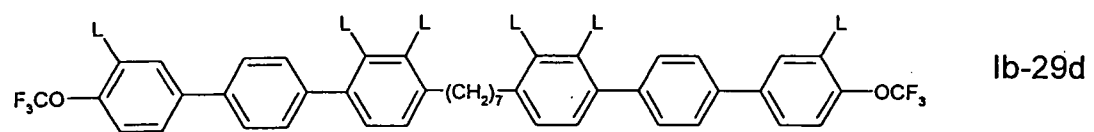
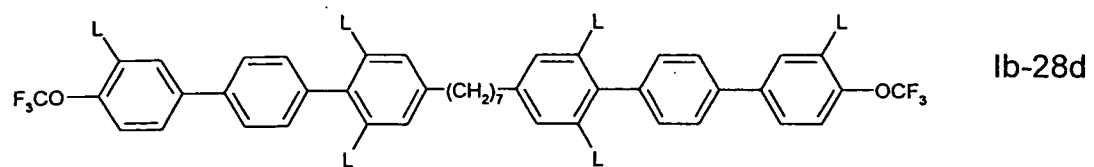
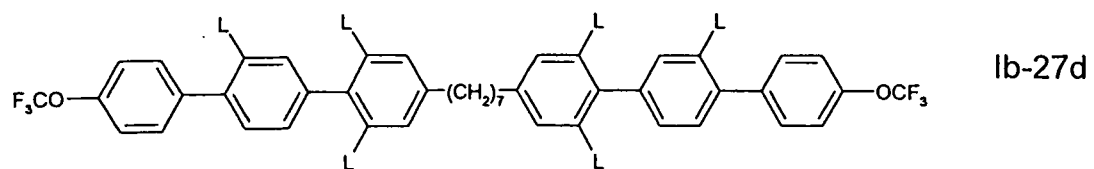
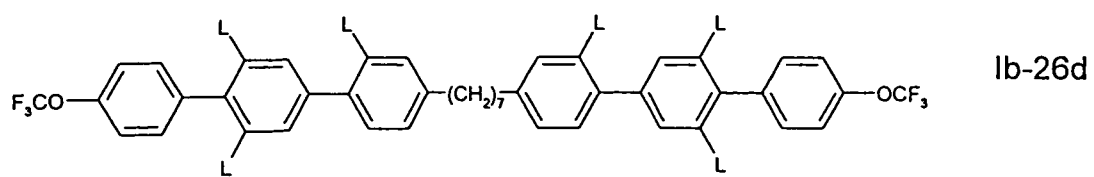


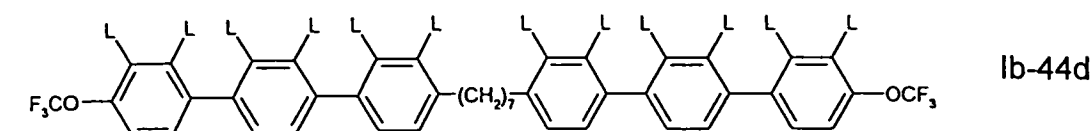
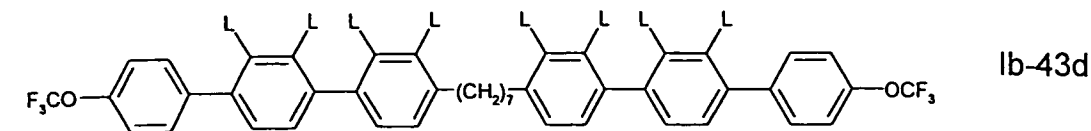
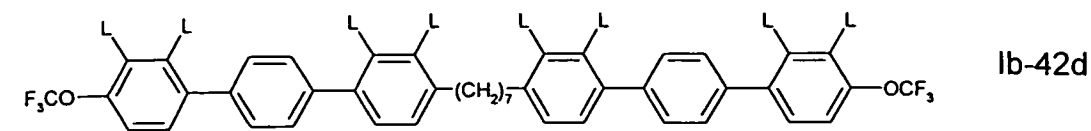
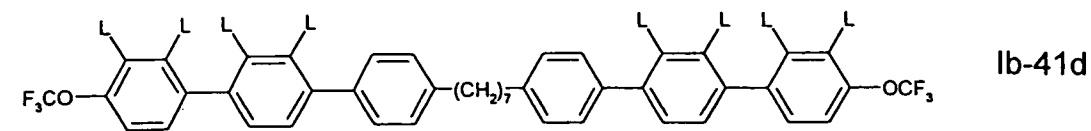
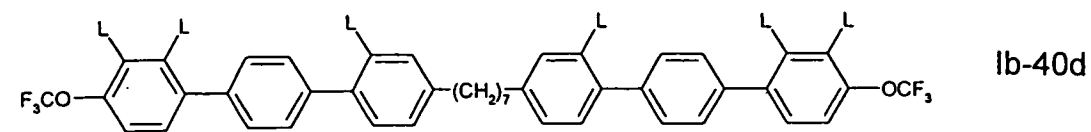
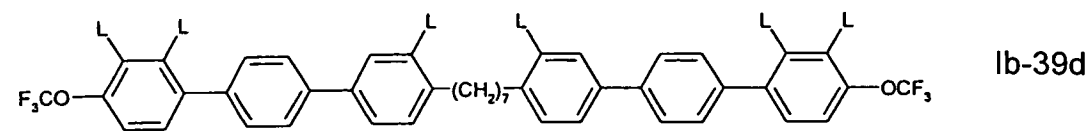
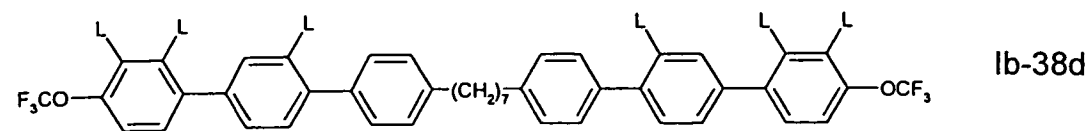
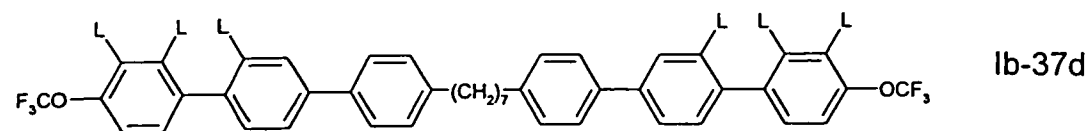
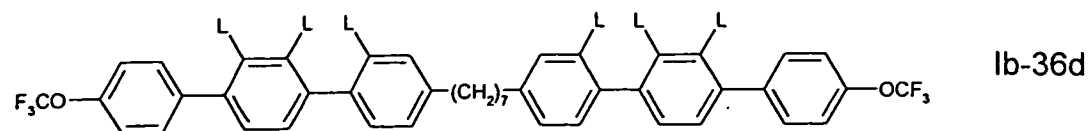
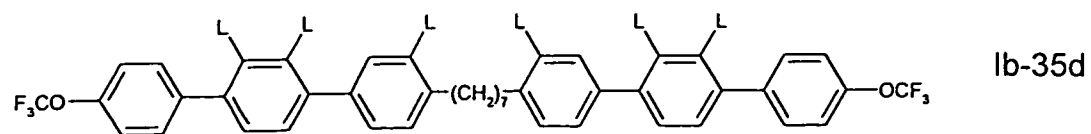
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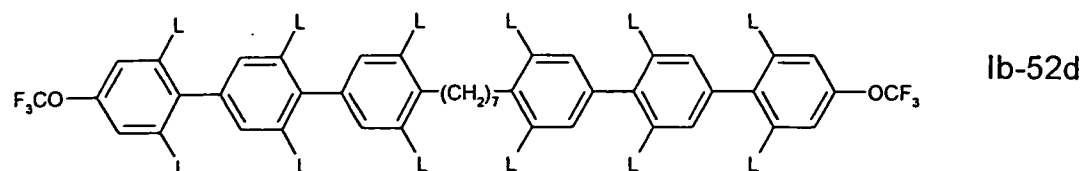
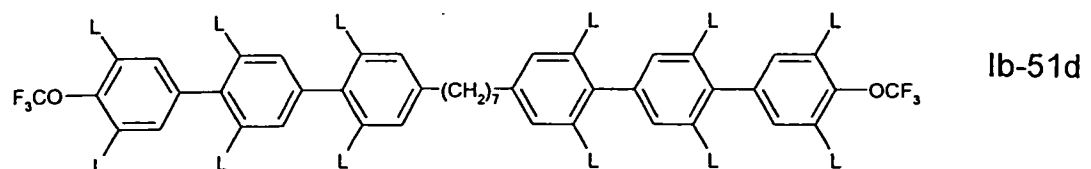
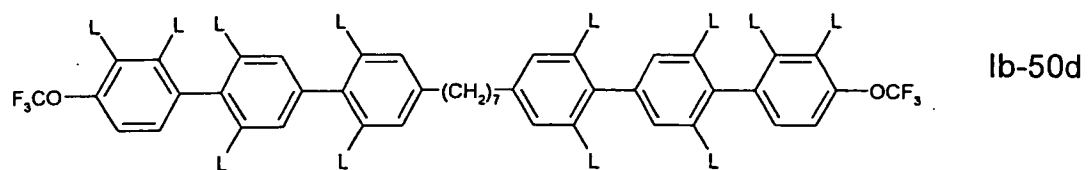
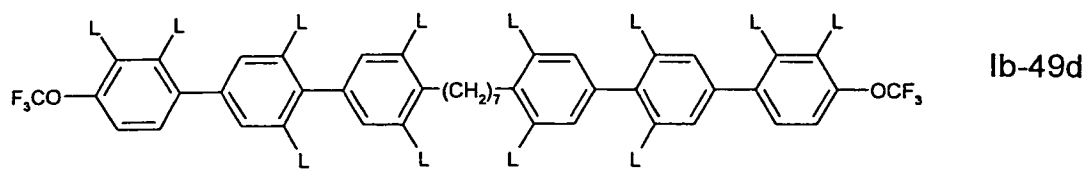
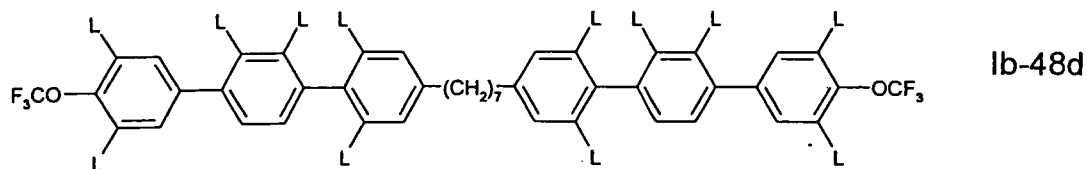
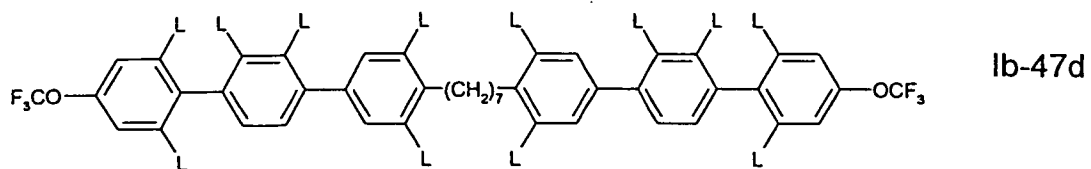
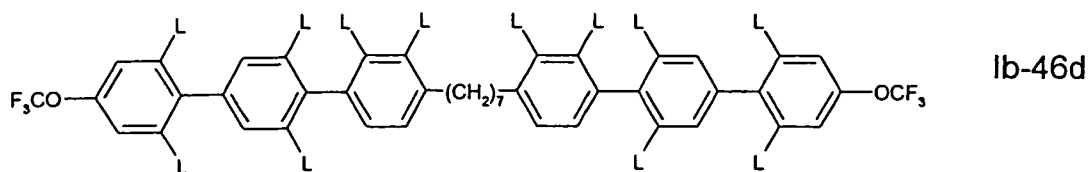
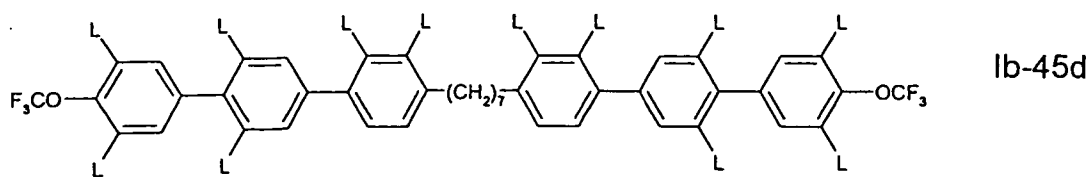


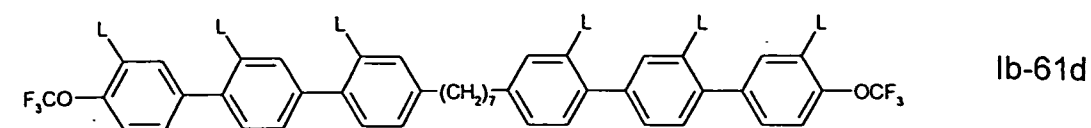
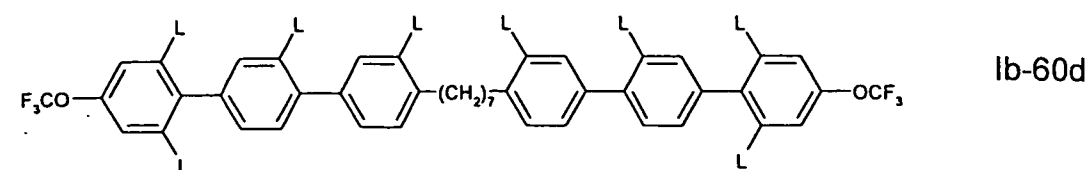
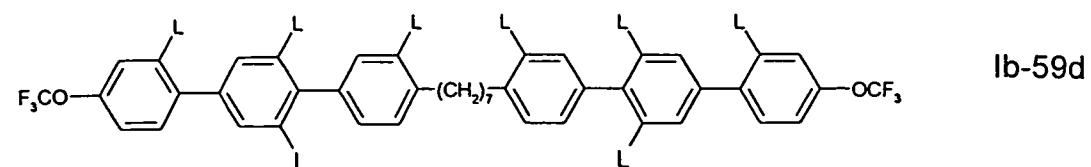
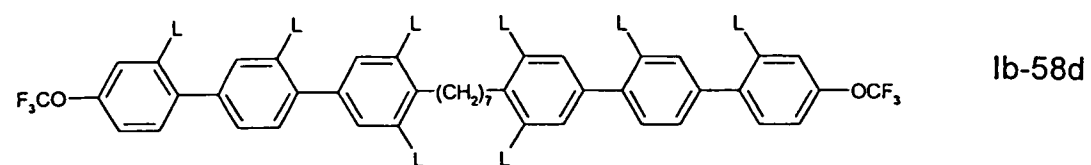
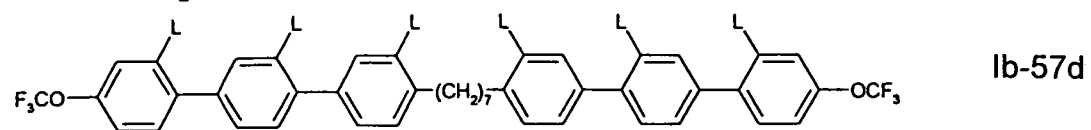
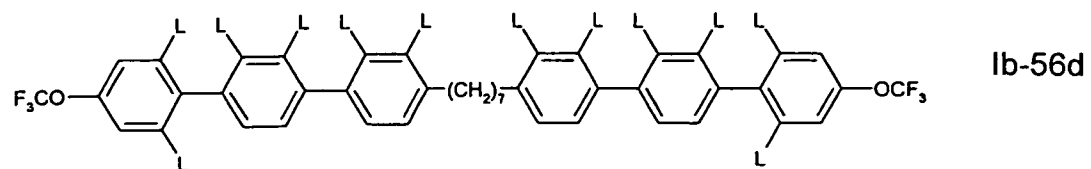
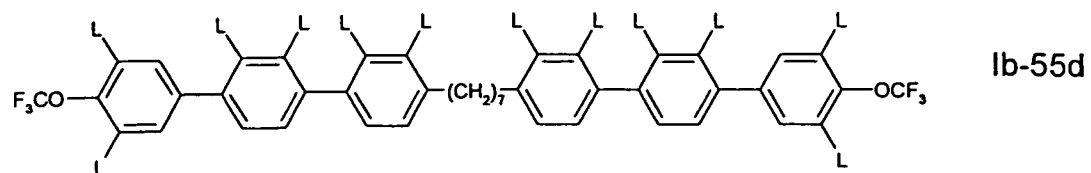
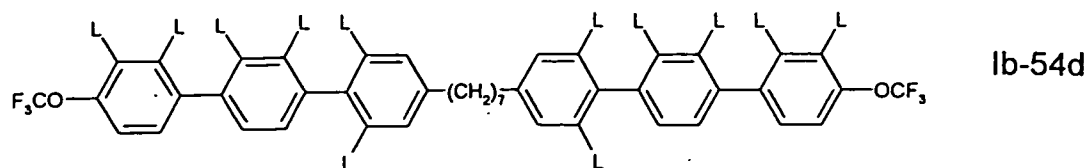
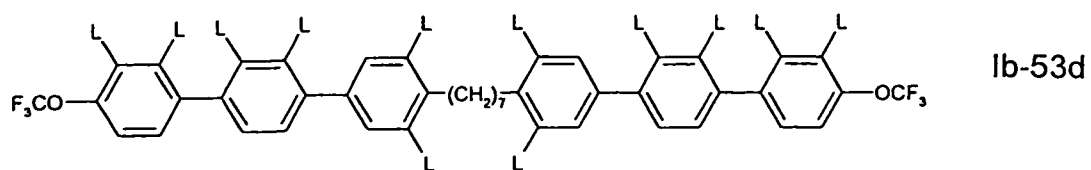


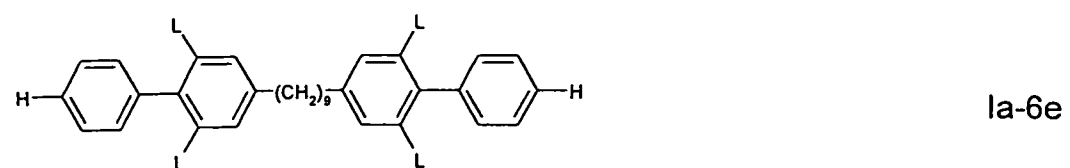
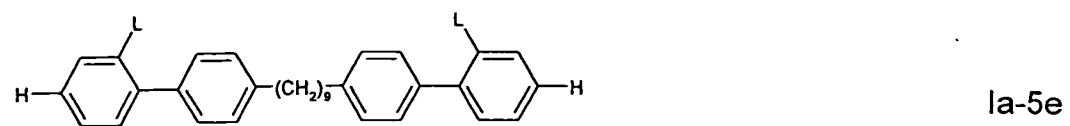
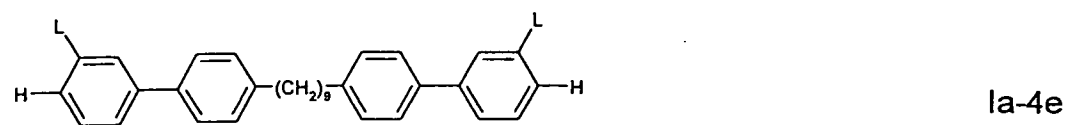
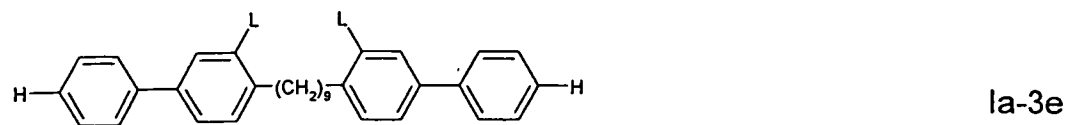
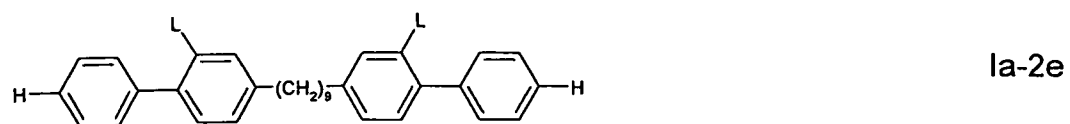
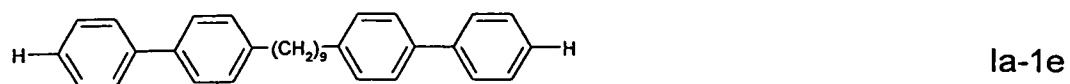
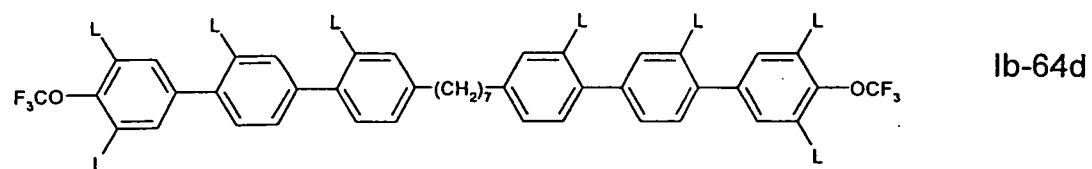
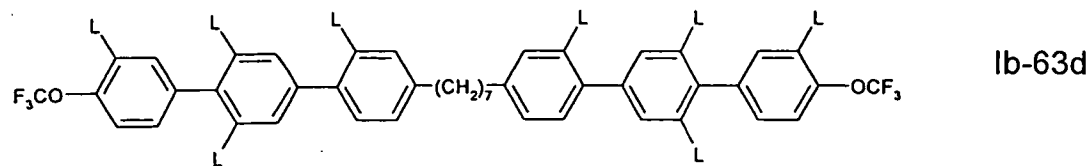
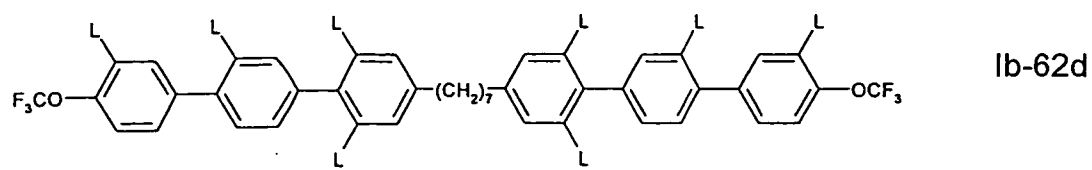


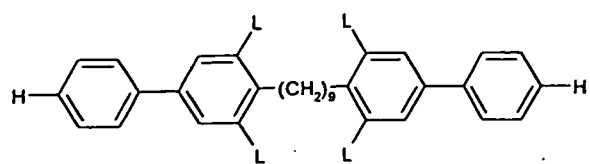




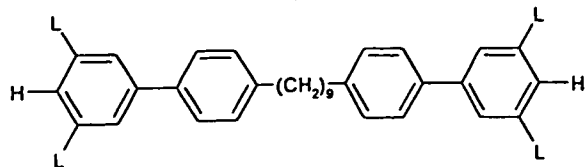




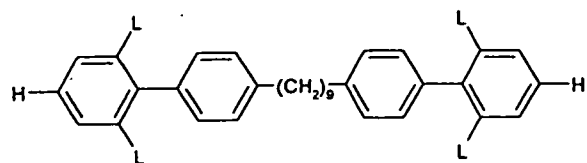




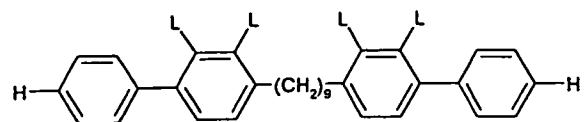
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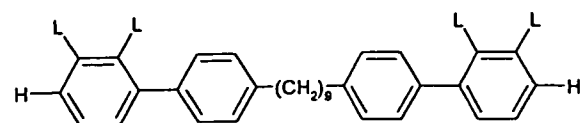
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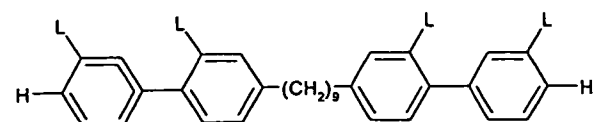
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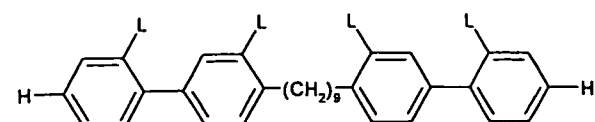
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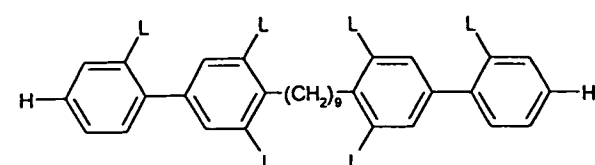
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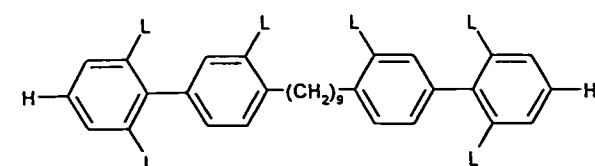
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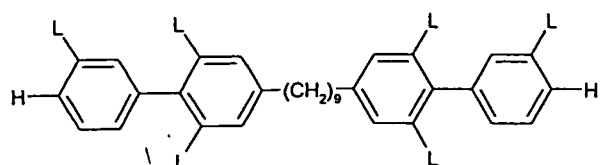
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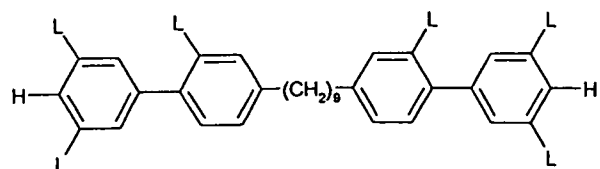
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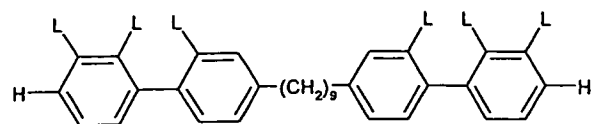
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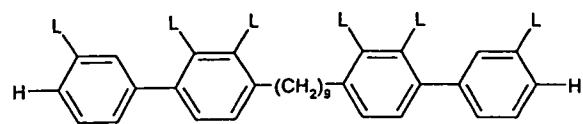
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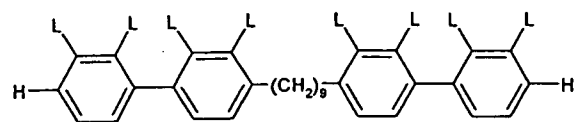
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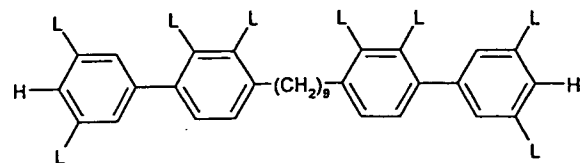
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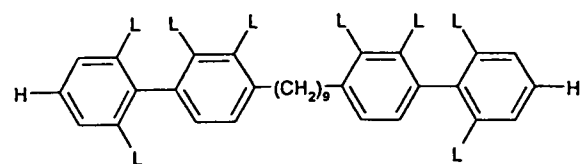
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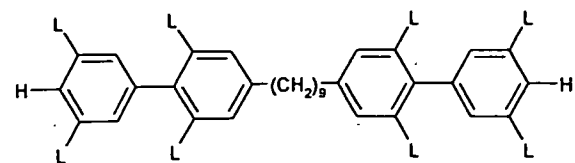
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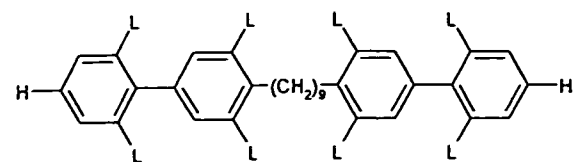
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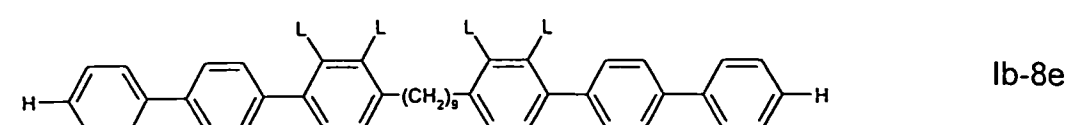
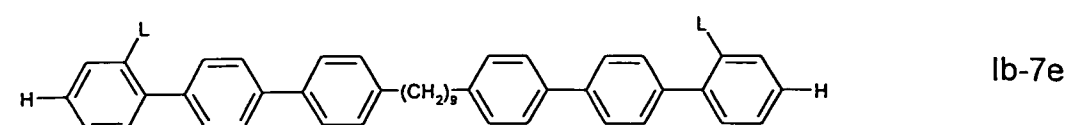
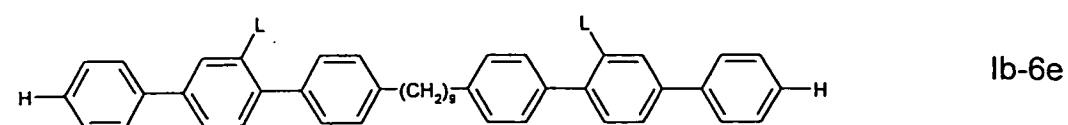
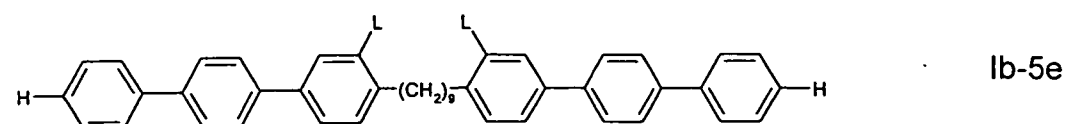
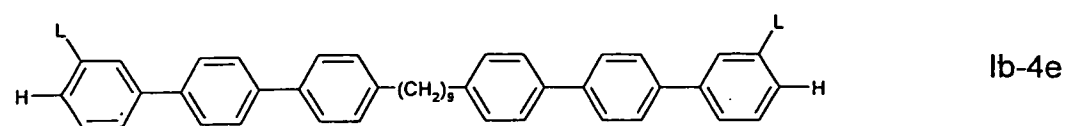
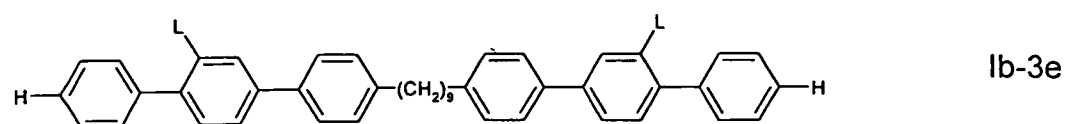
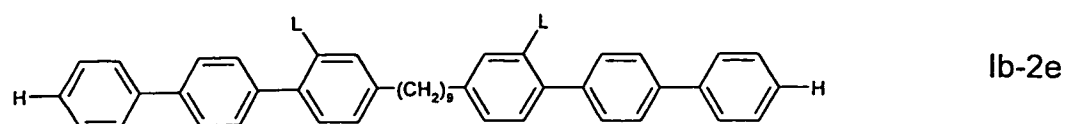
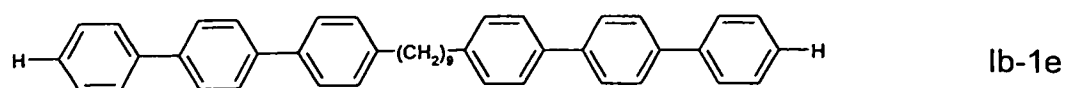
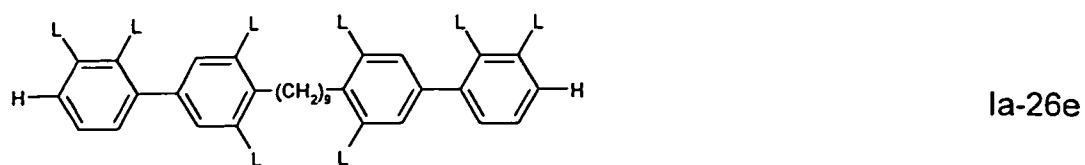
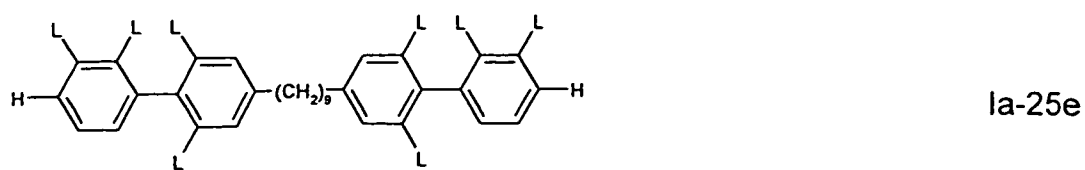
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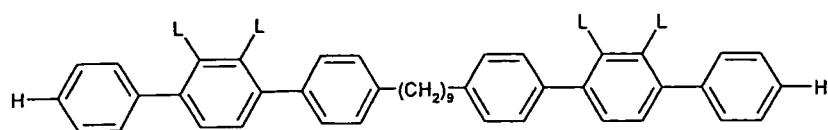


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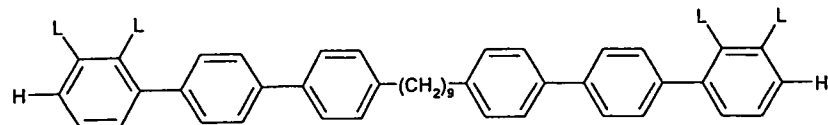


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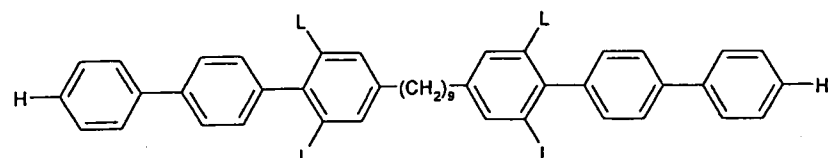




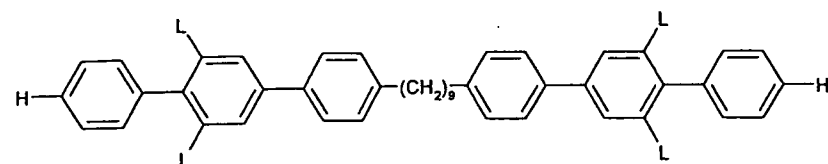
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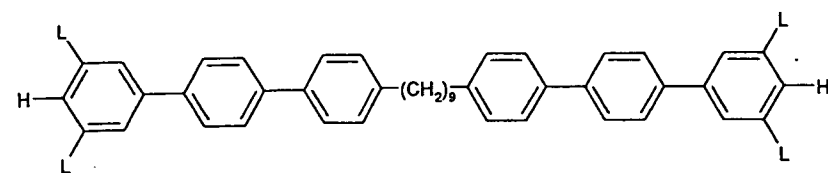
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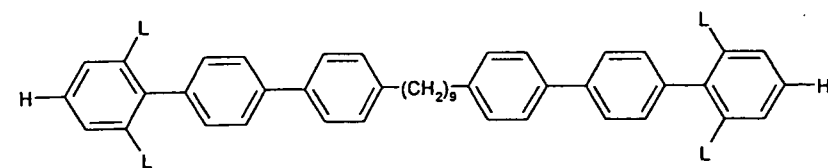
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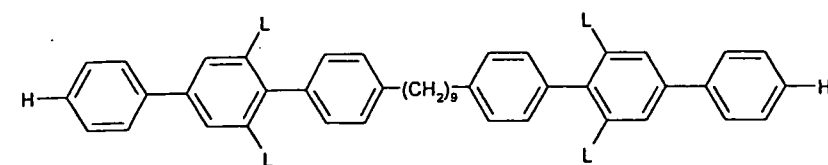
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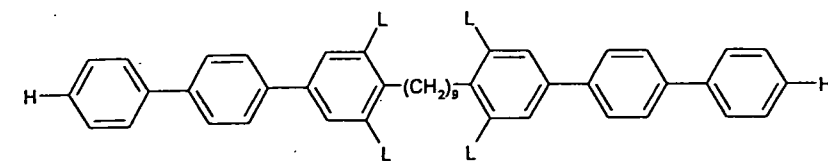
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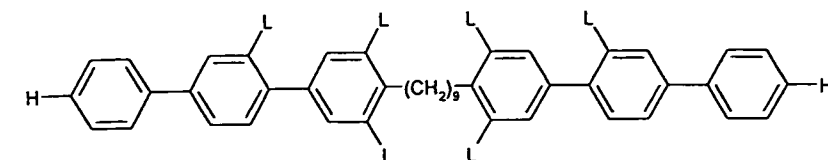
Ib-14e



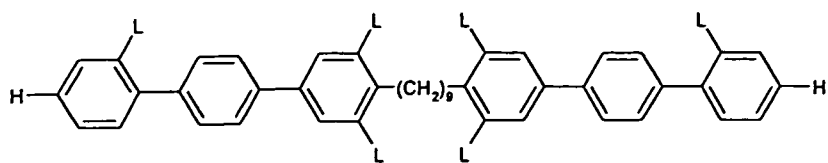
Ib-15e



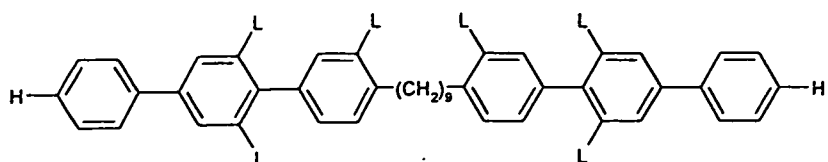
Ib-16e



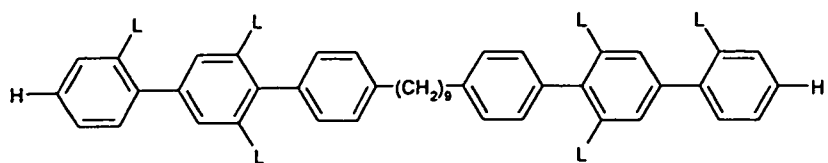
Ib-17e



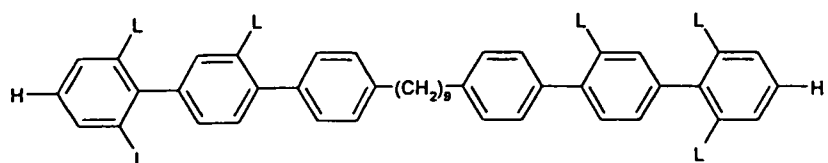
Ib-18e



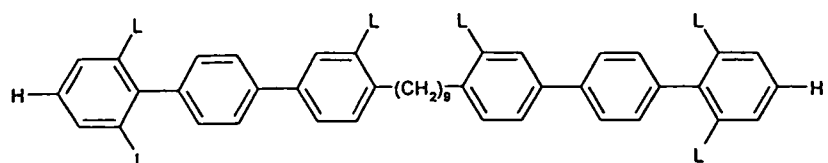
Ib-19e



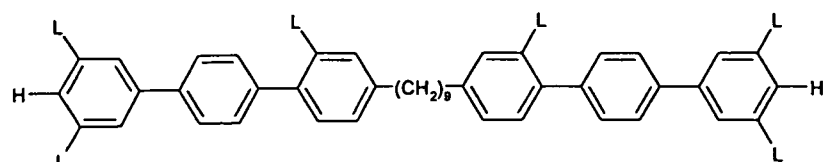
Ib-20e



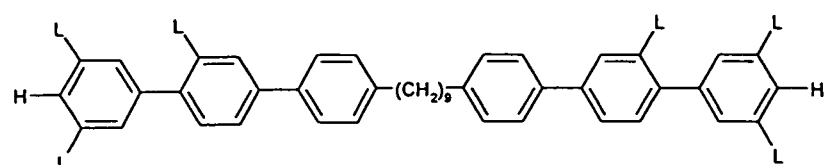
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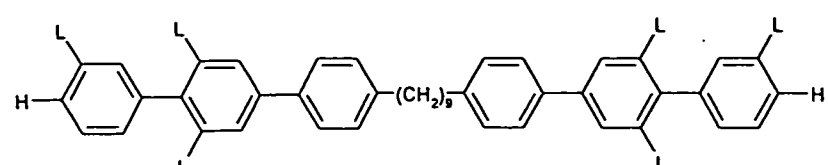
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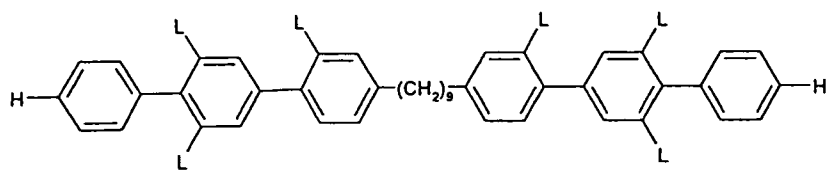
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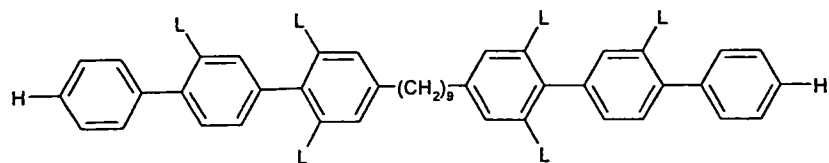
Ib-24e



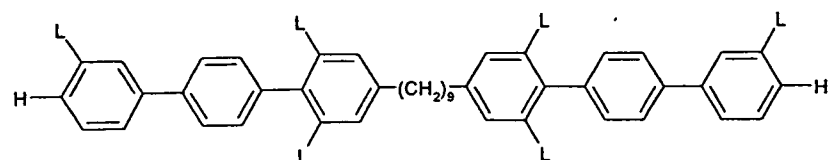
Ib-25e



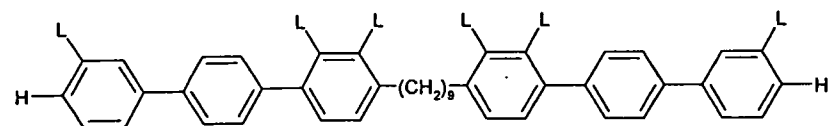
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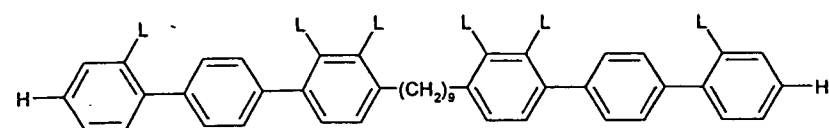
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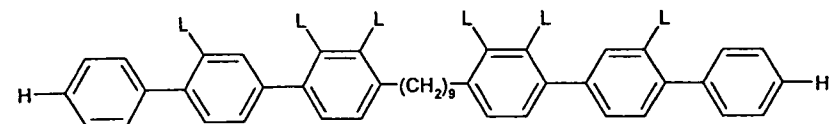
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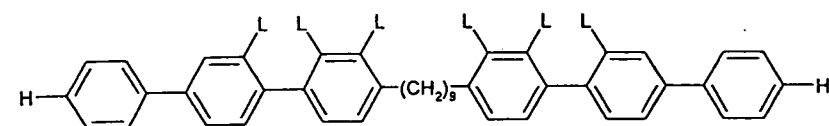
Ib-29e



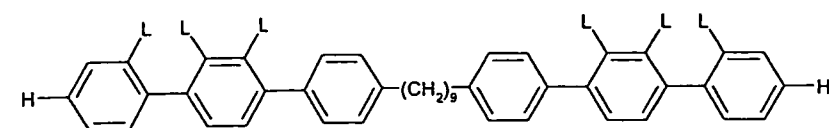
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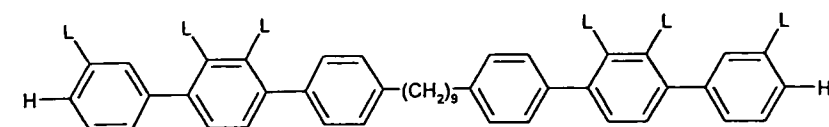
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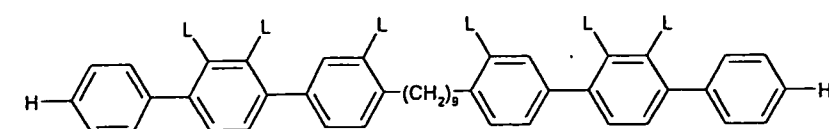
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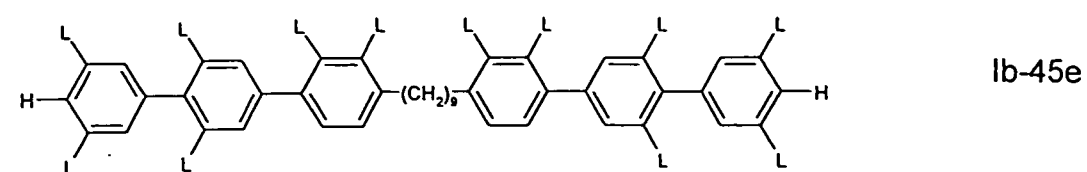
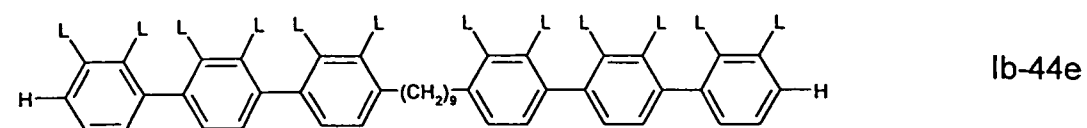
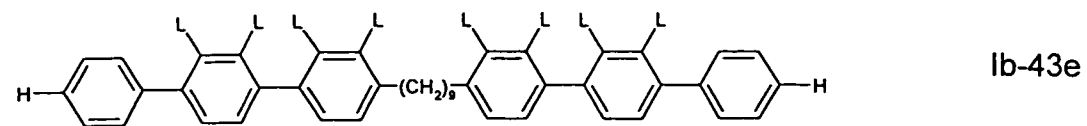
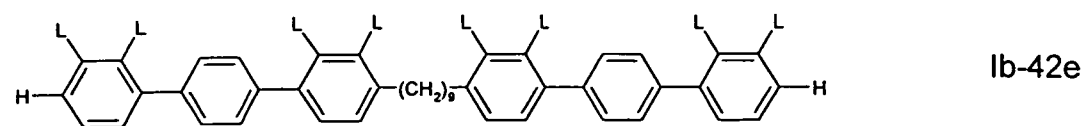
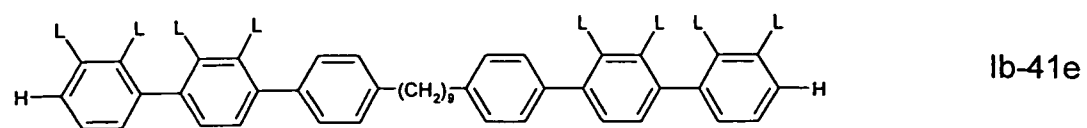
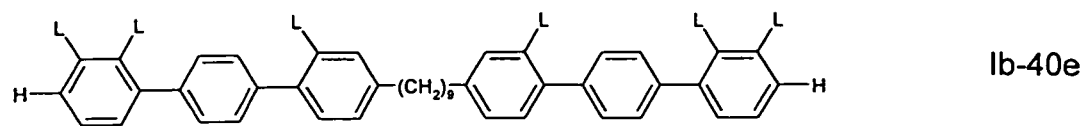
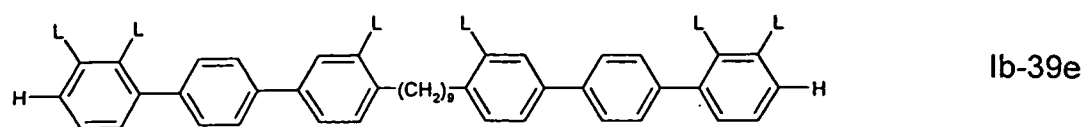
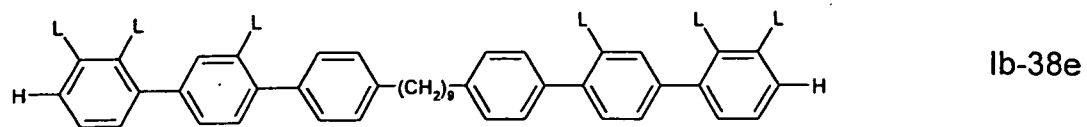
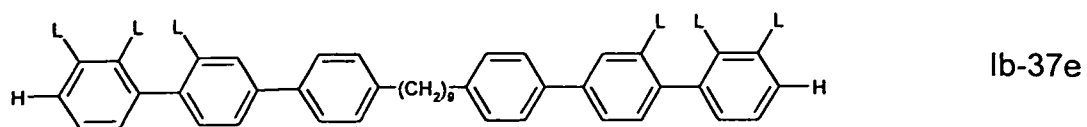
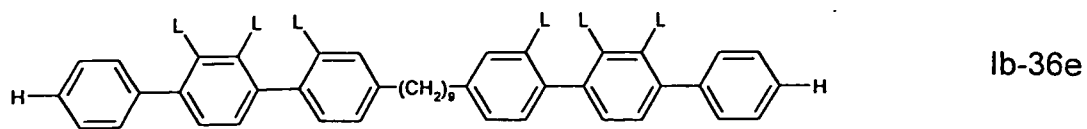
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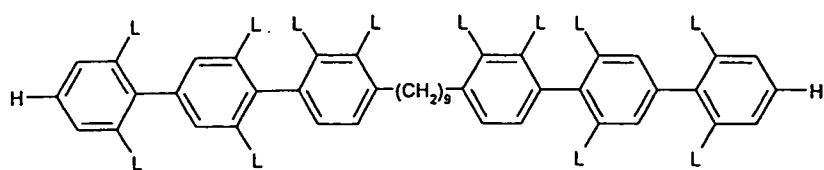


Ib-34e

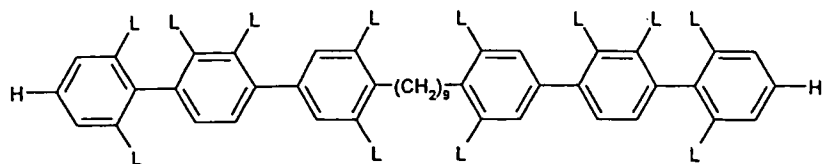


Ib-35e

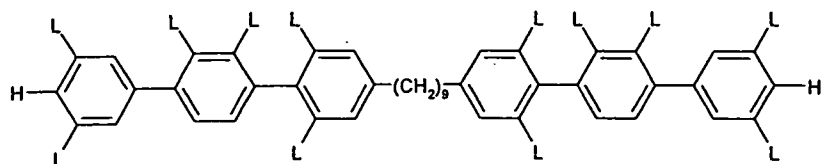




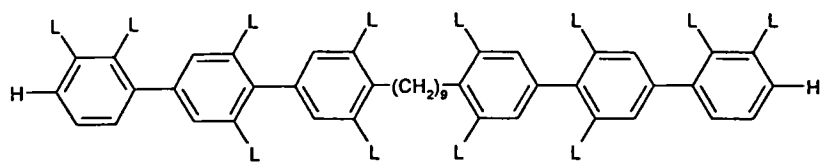
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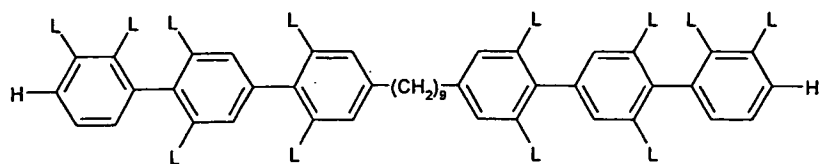
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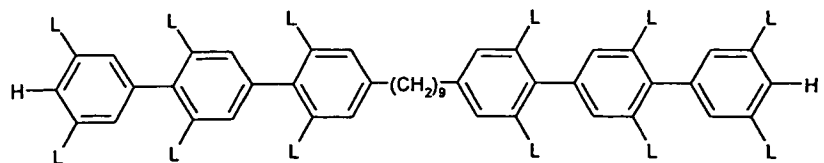
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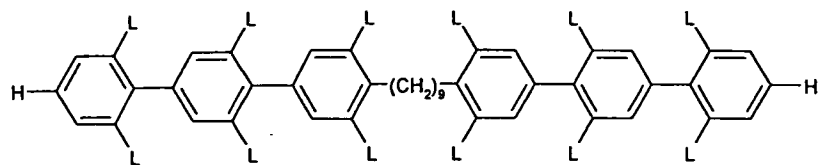
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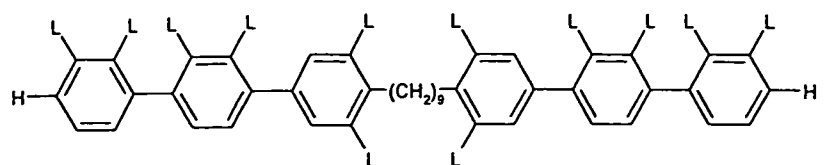
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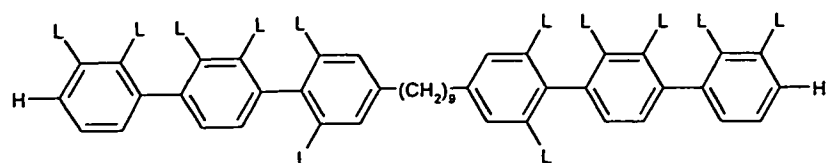
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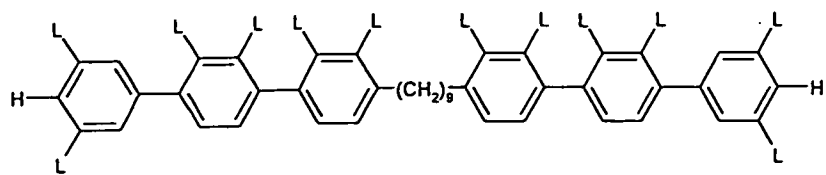
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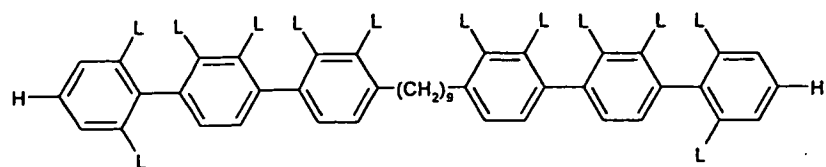
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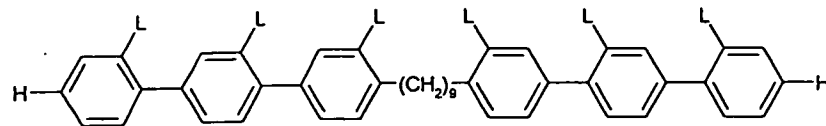
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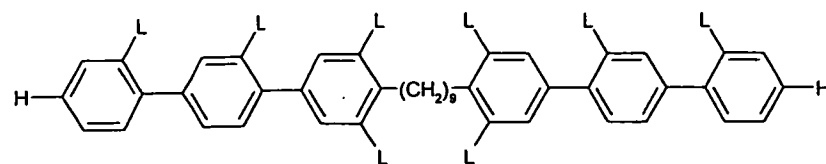
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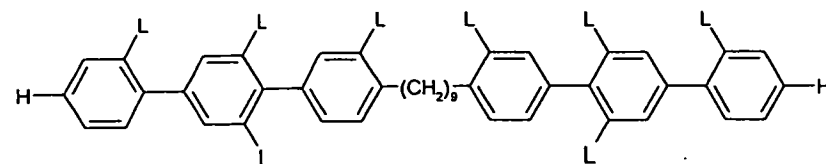
Ib-56e



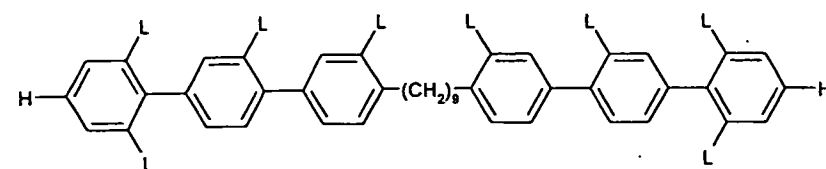
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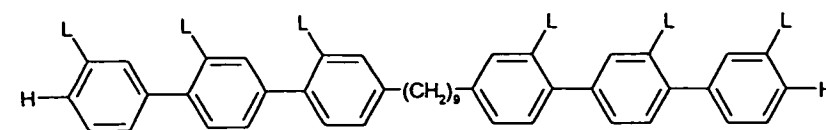
Ib-58e



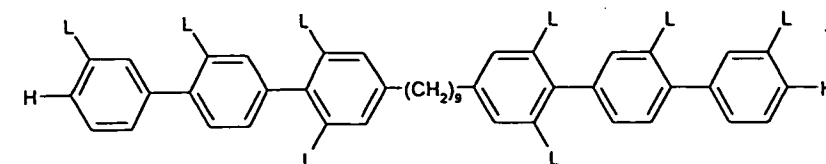
Ib-59e



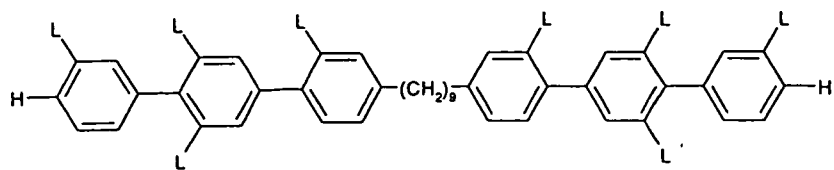
Ib-60e



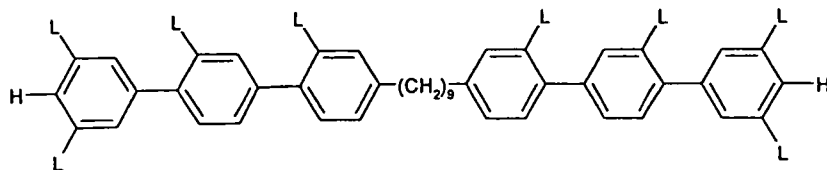
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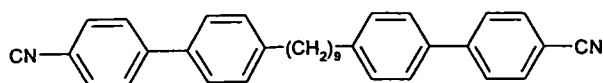
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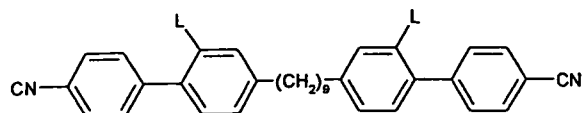
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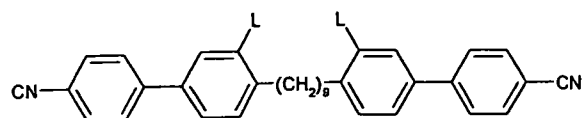
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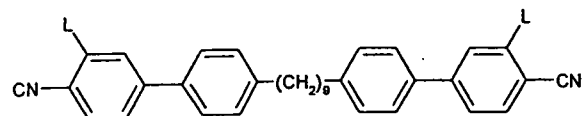
Ia-1f



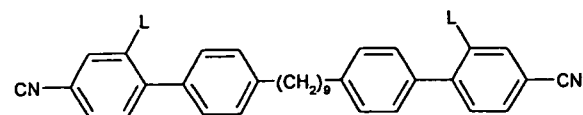
Ia-2f



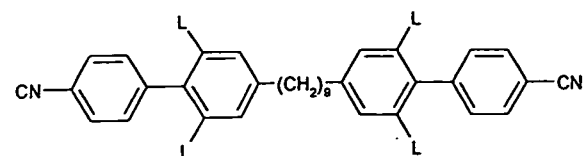
Ia-3f



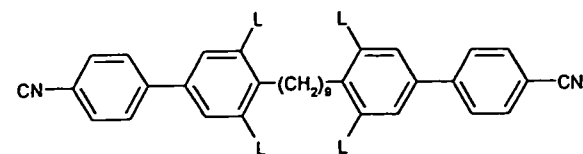
Ia-4f



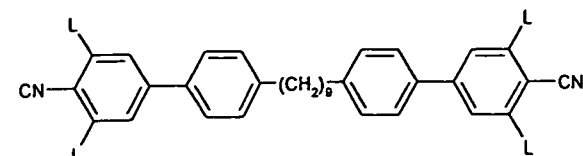
Ia-5f



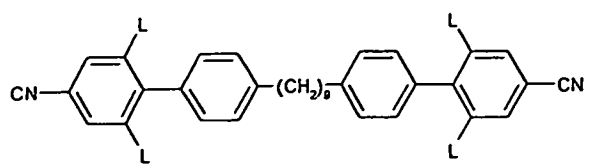
Ia-6f



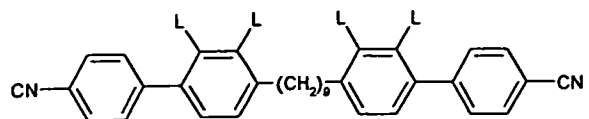
Ia-7f



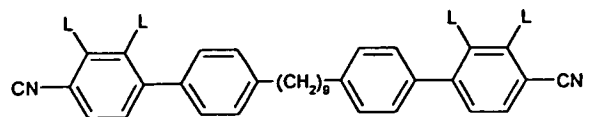
Ia-8f



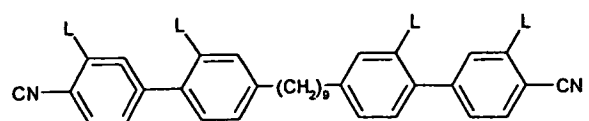
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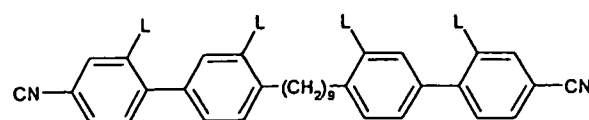
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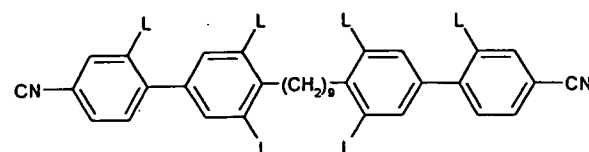
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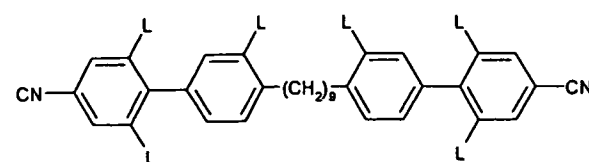
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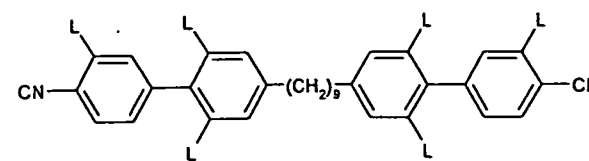
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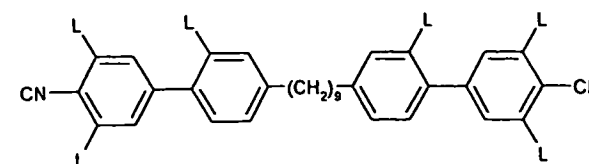
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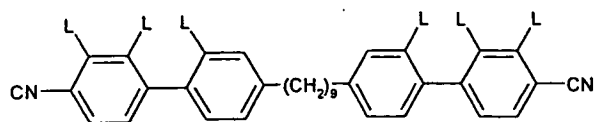
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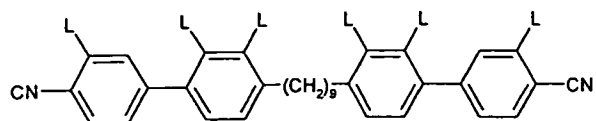
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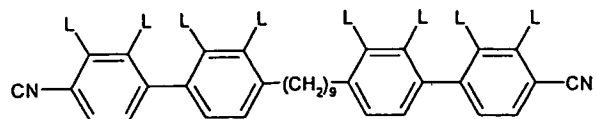
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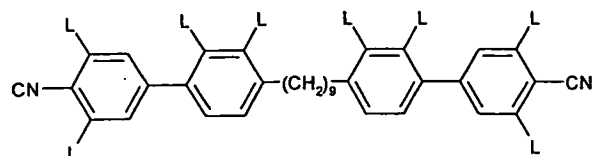
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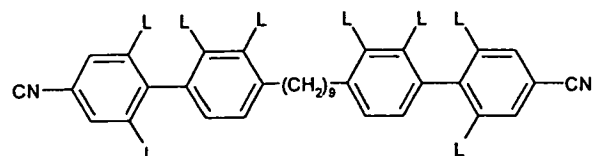
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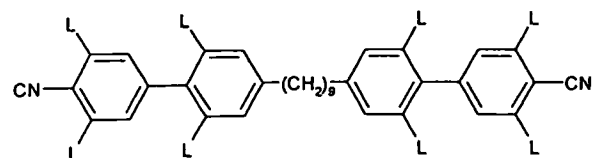
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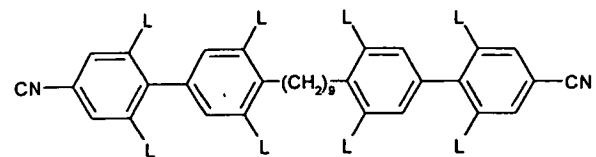
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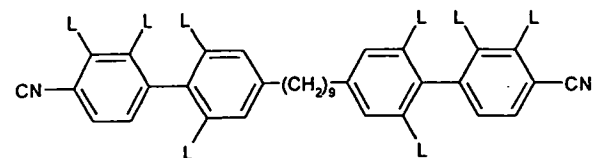
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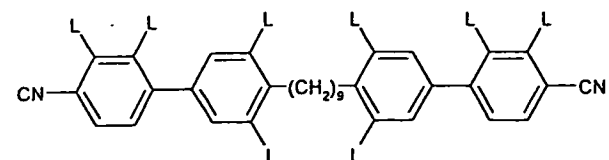
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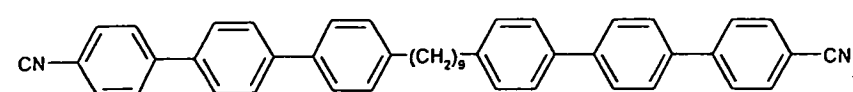
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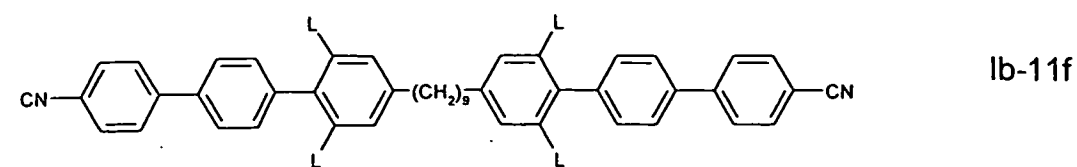
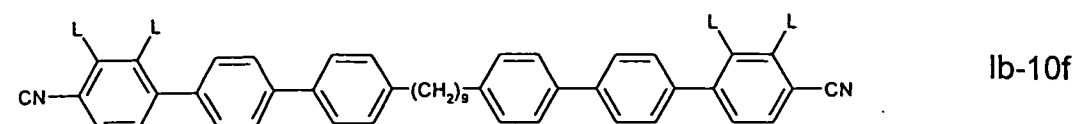
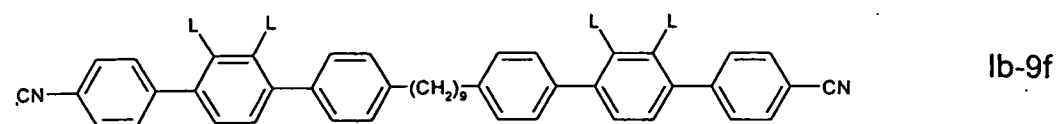
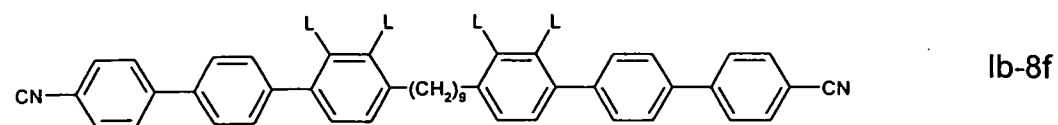
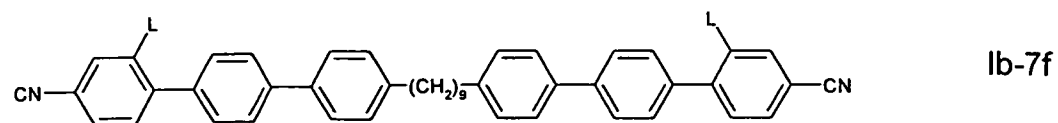
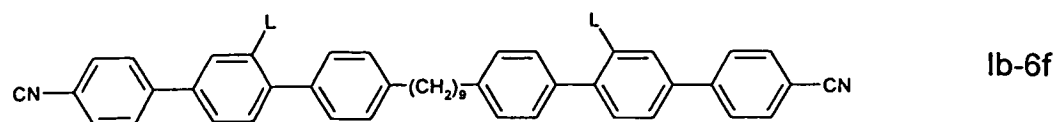
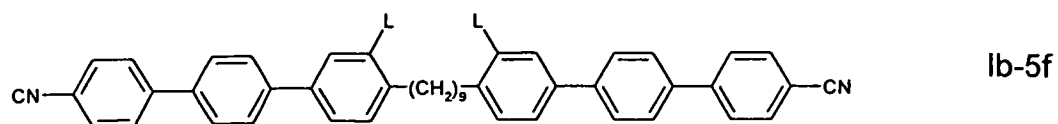
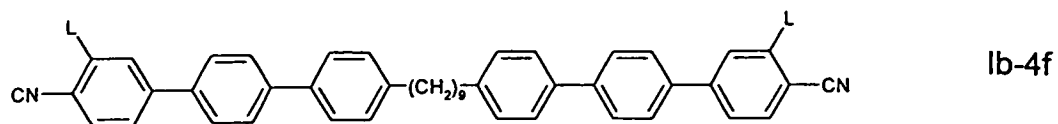
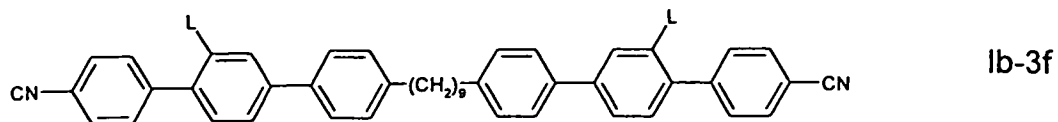
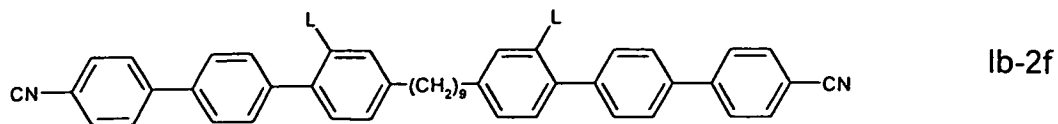
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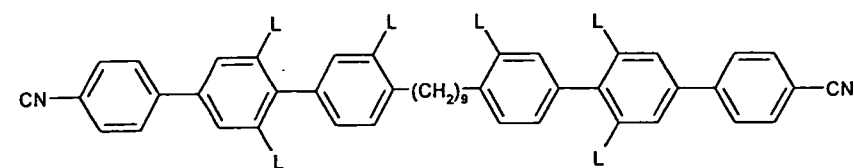
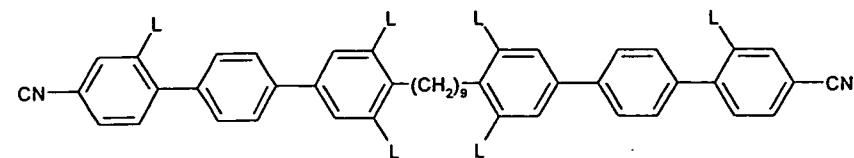
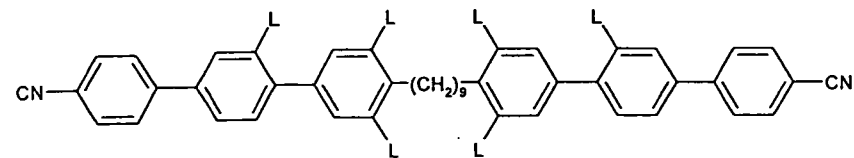
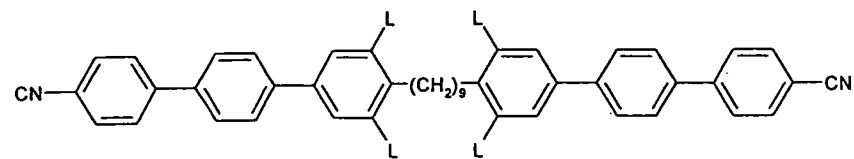
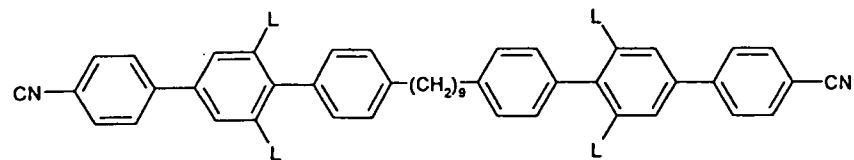
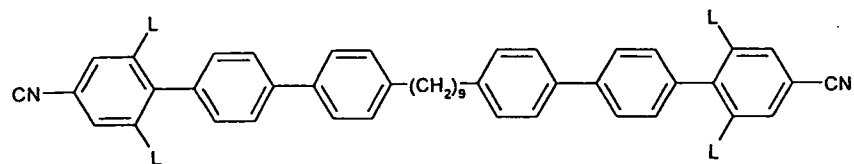
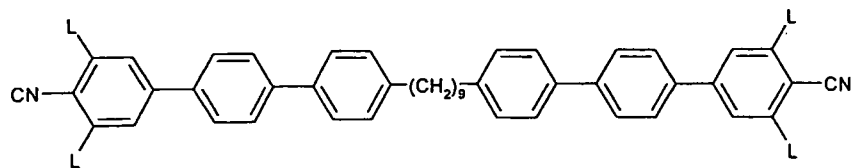
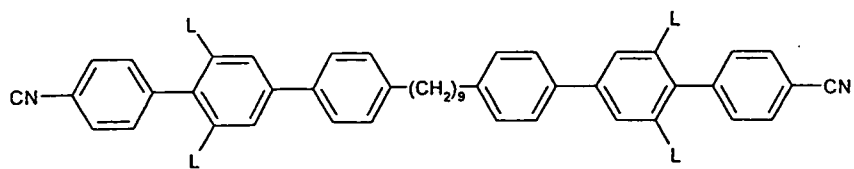


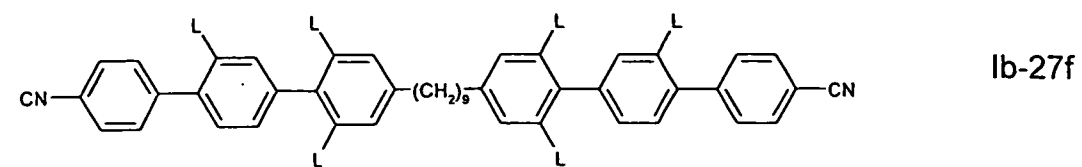
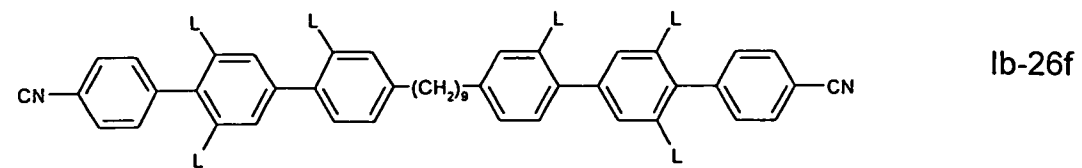
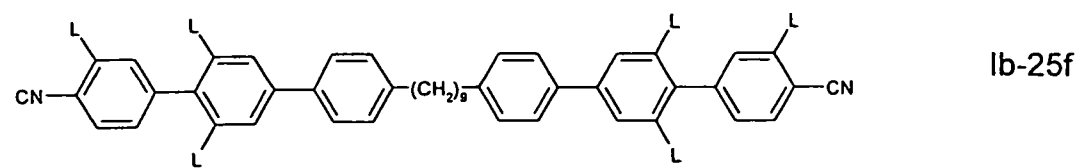
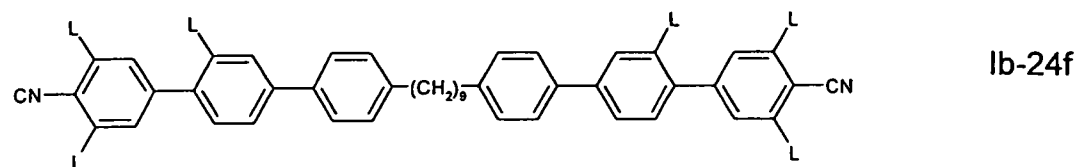
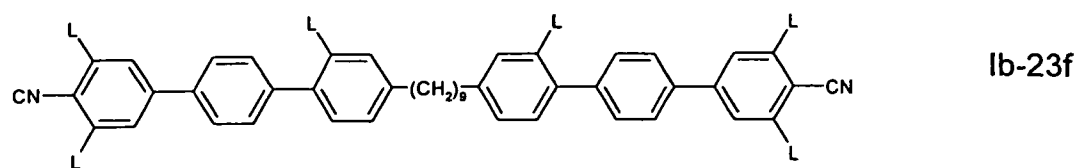
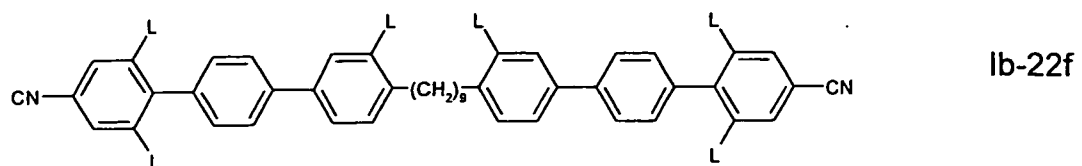
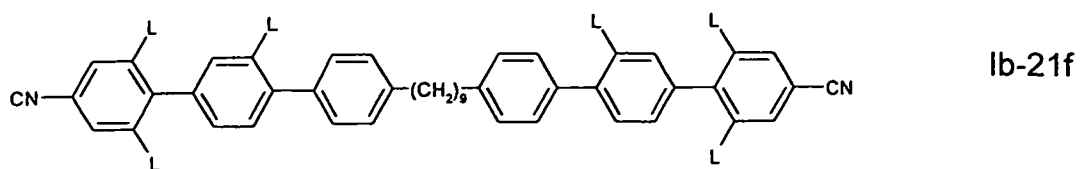
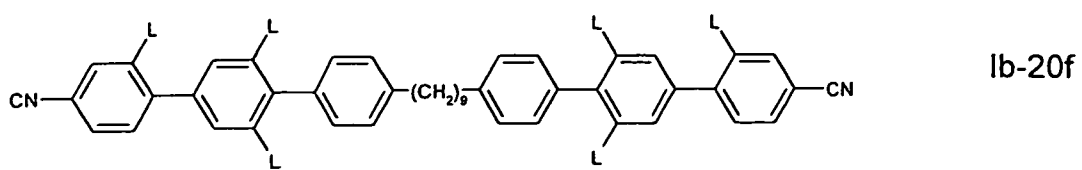
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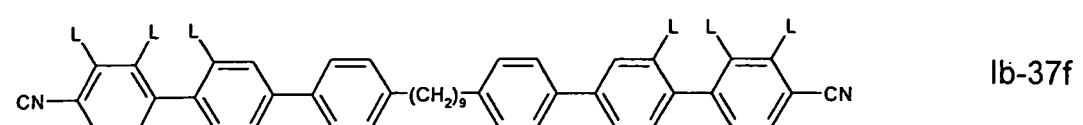
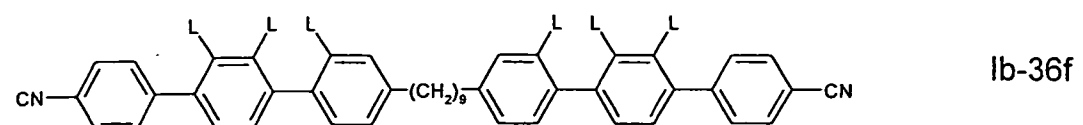
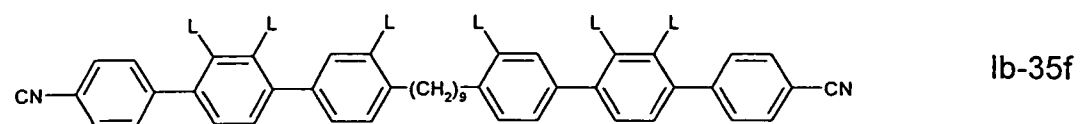
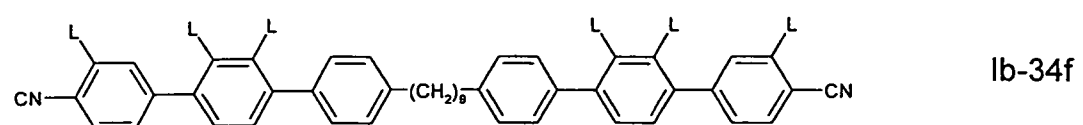
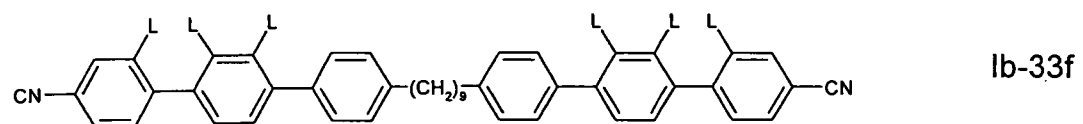
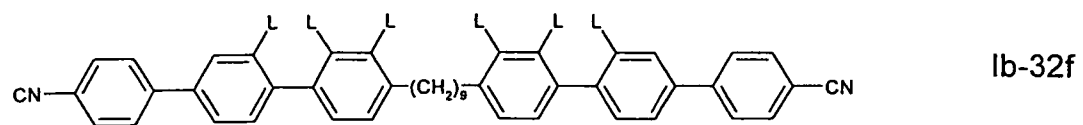
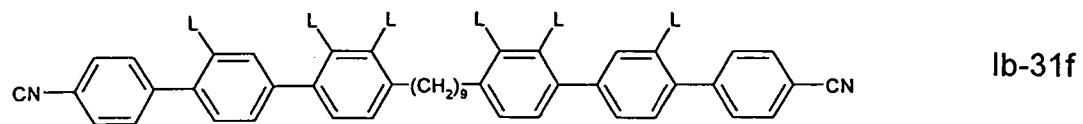
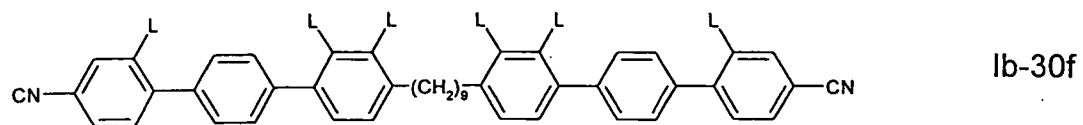
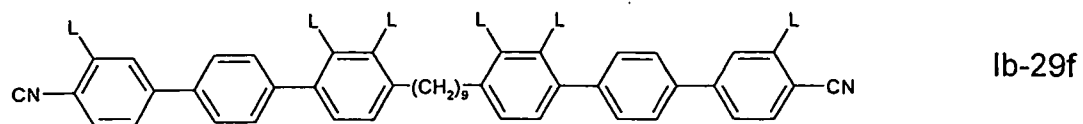
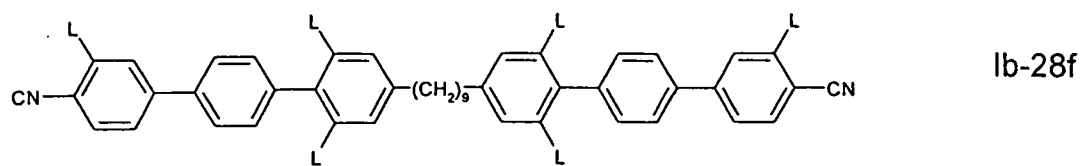


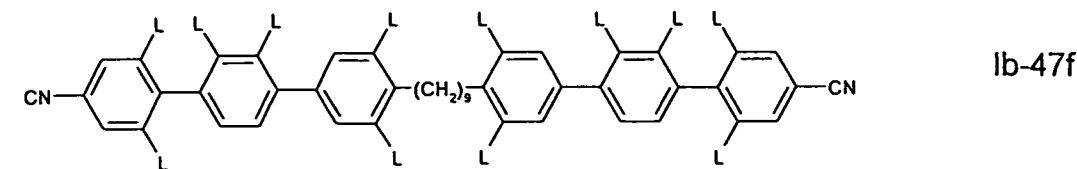
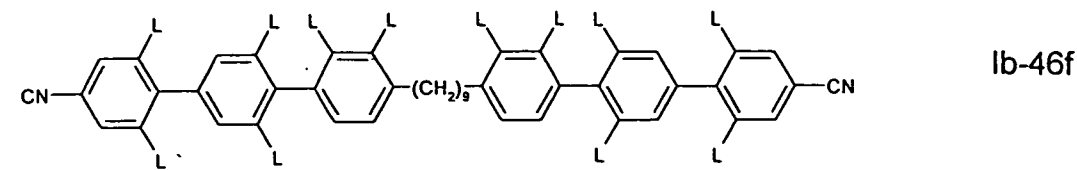
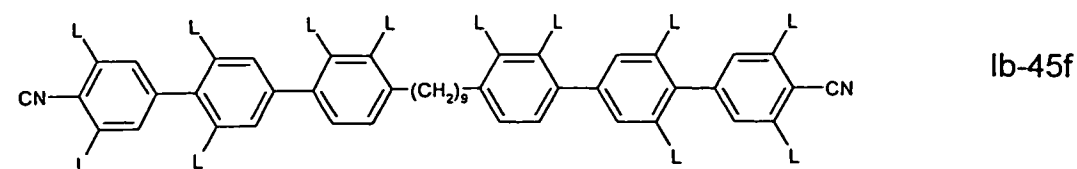
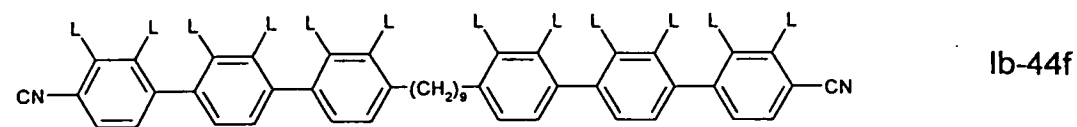
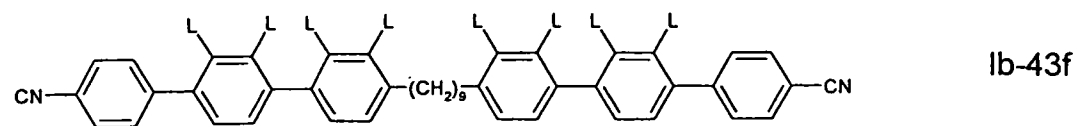
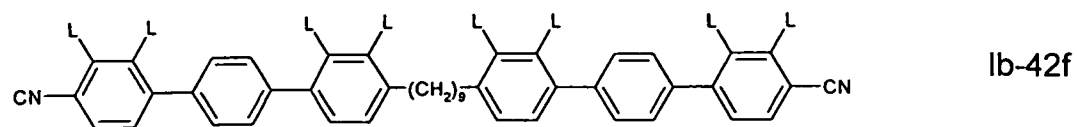
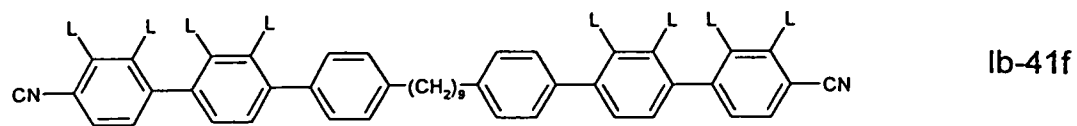
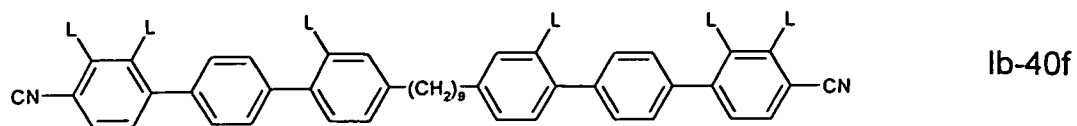
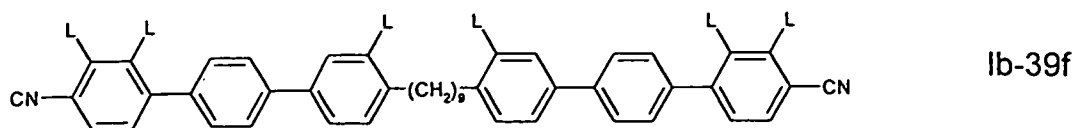
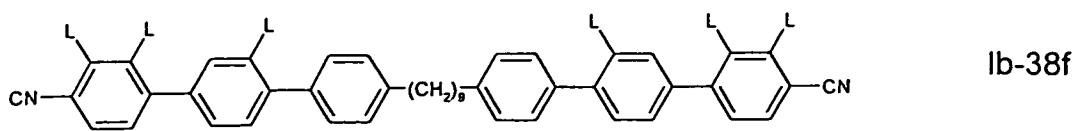
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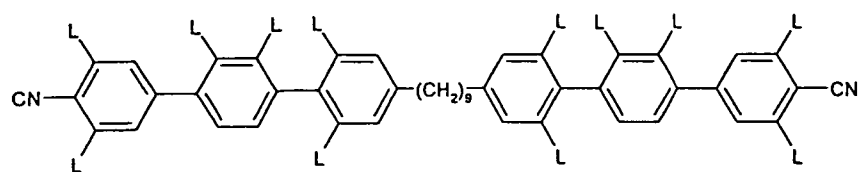




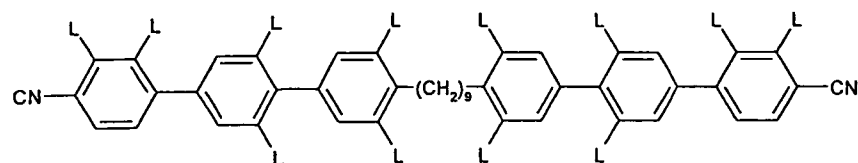




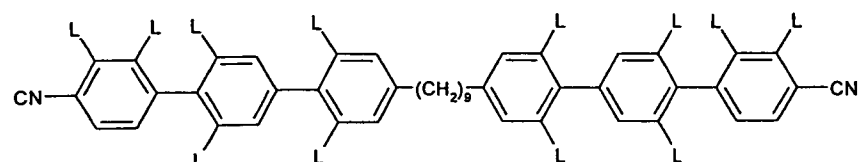




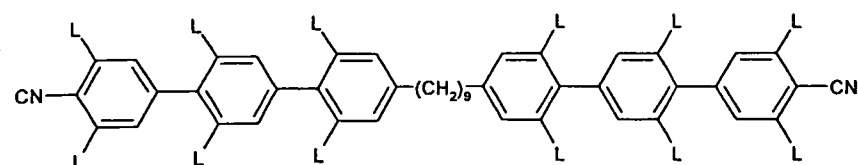
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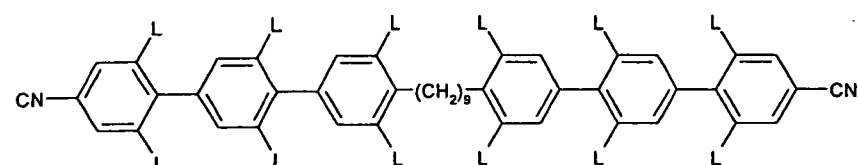
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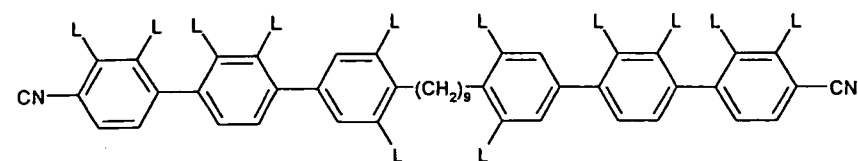
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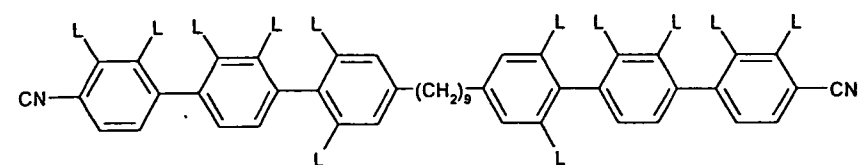
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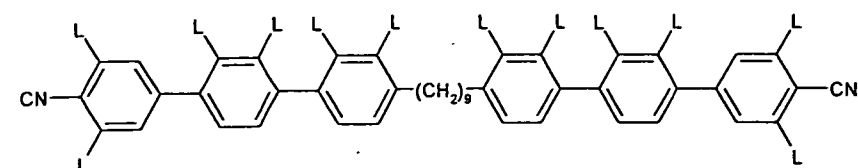
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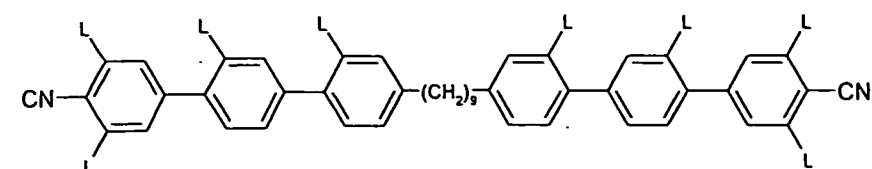
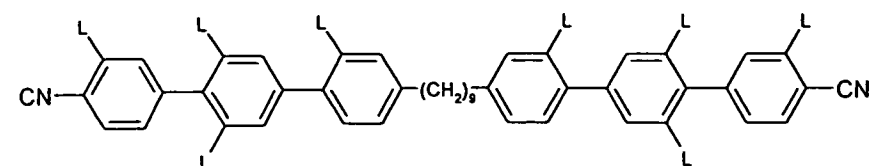
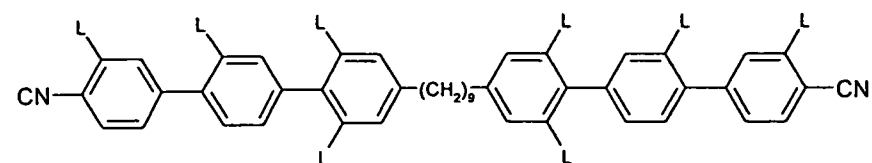
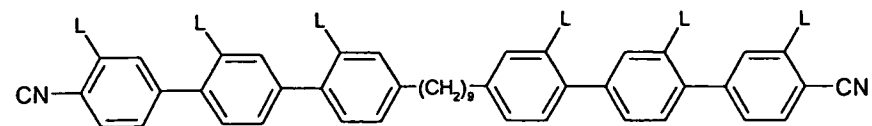
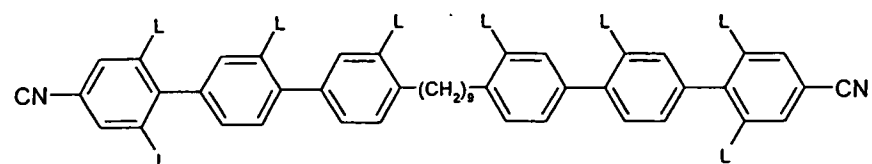
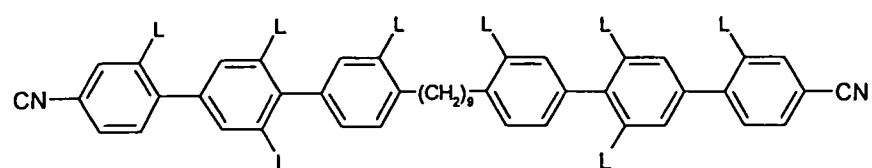
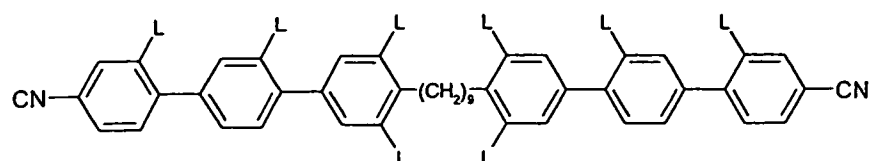
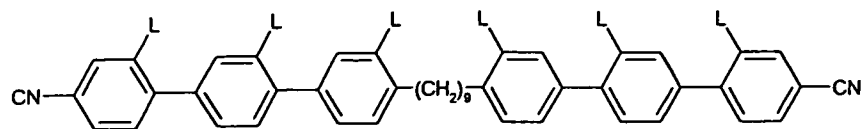
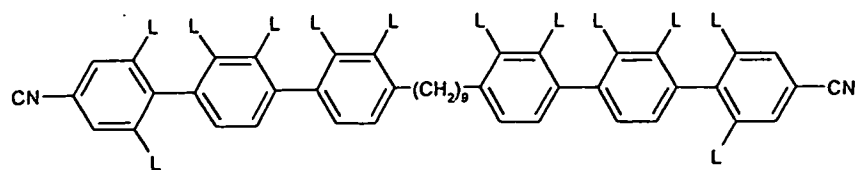
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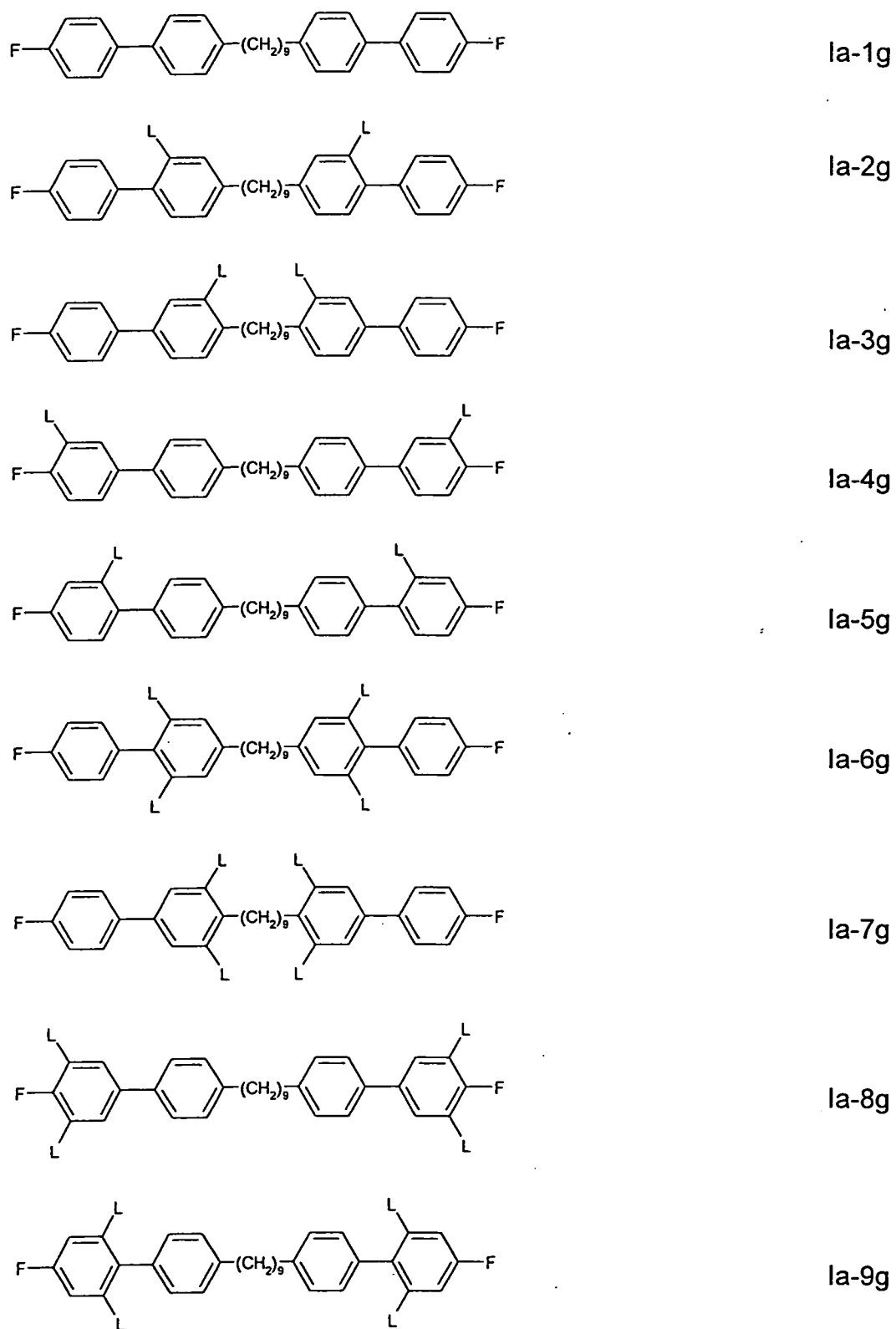


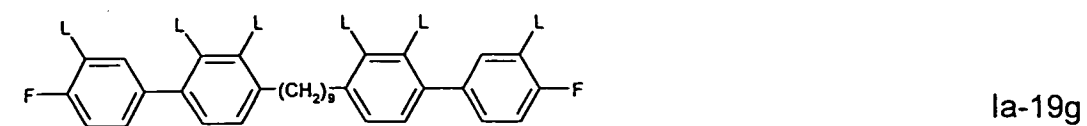
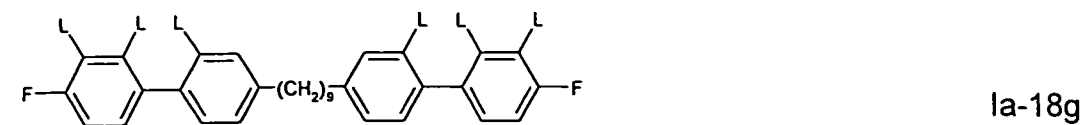
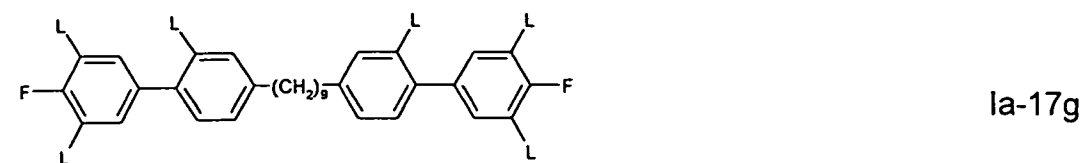
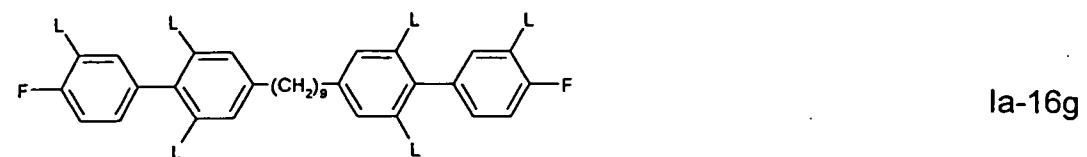
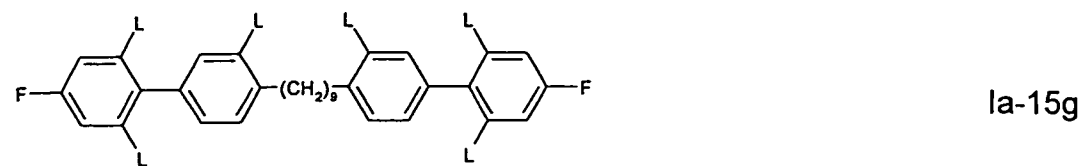
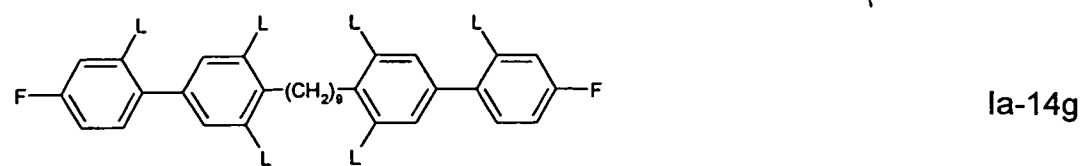
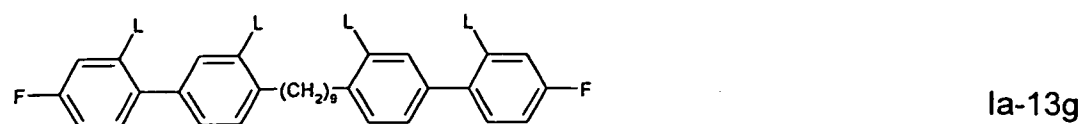
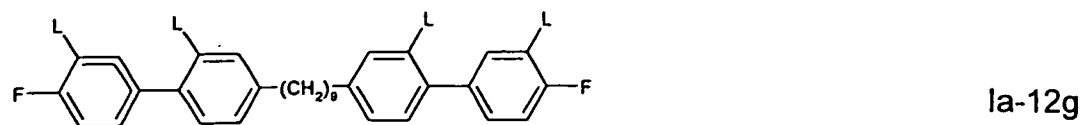
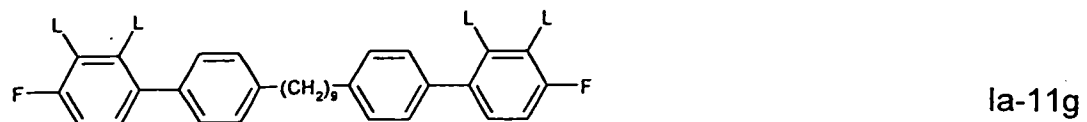
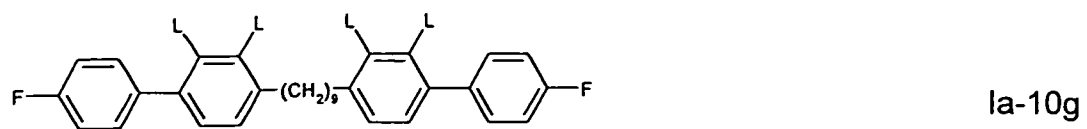
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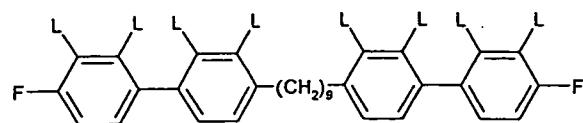


Ib-55f

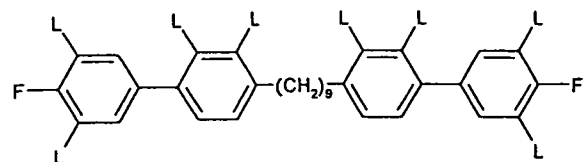




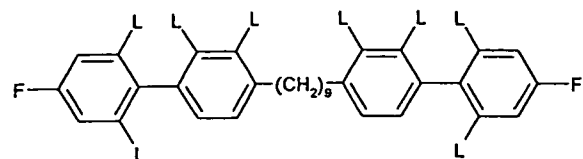




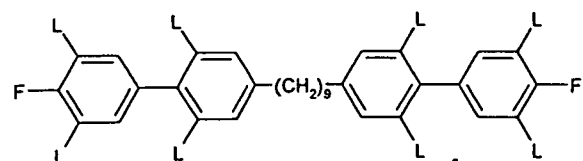
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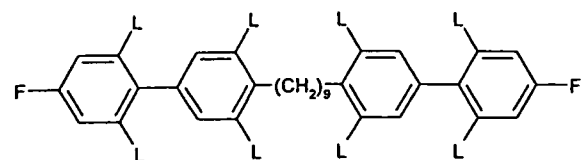
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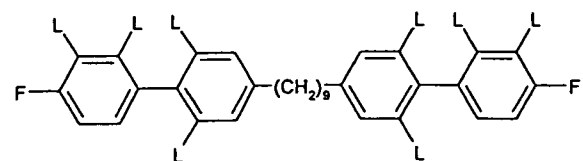
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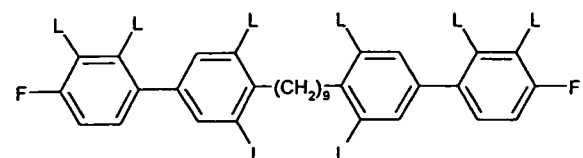
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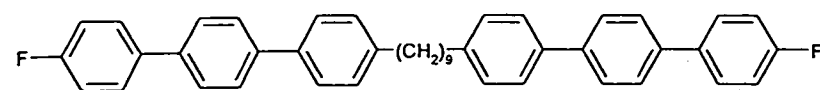
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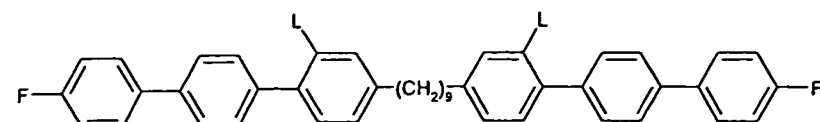
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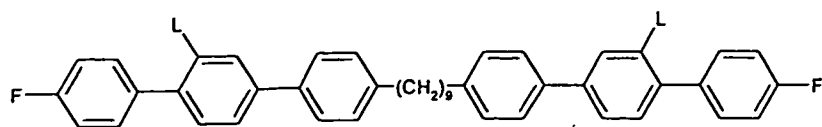
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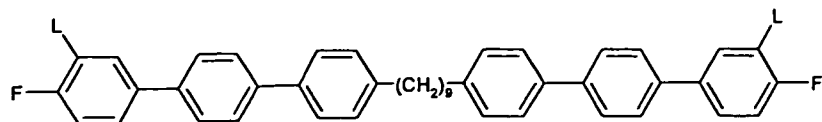
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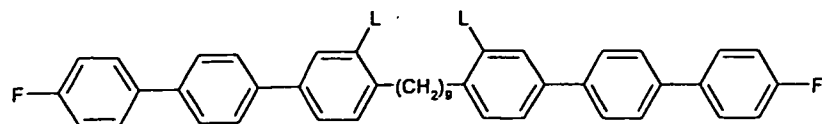
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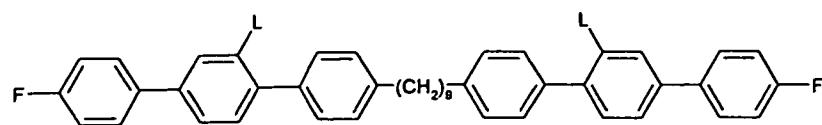
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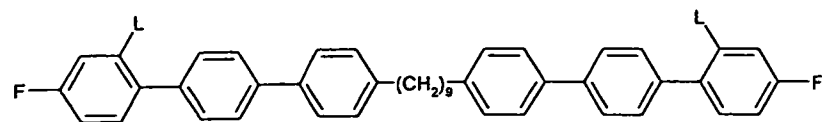
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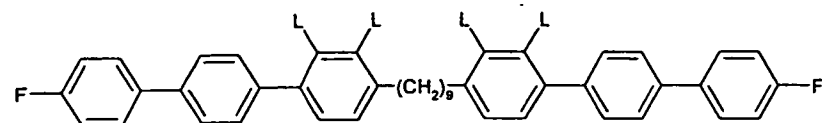
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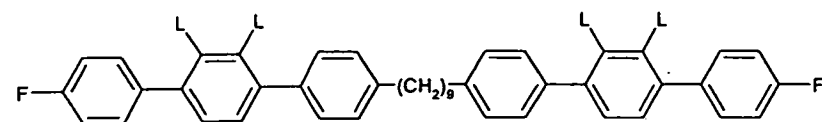
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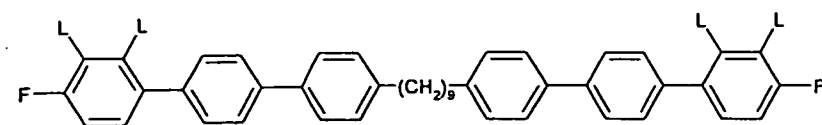
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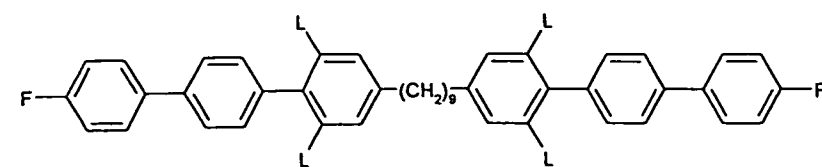
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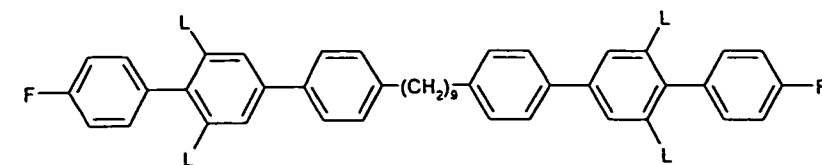
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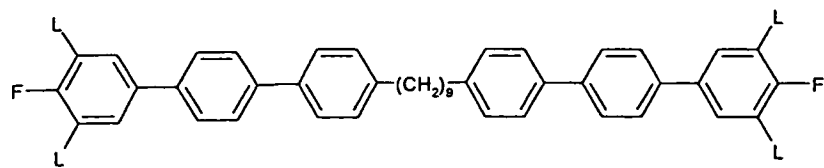
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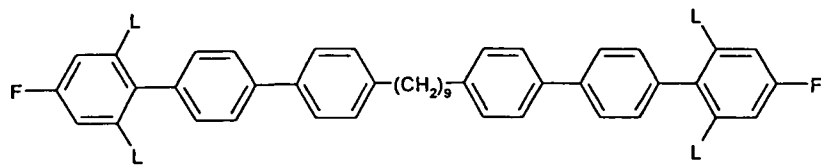
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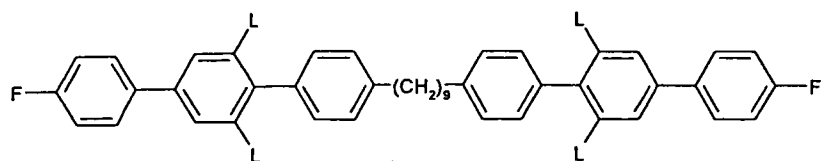
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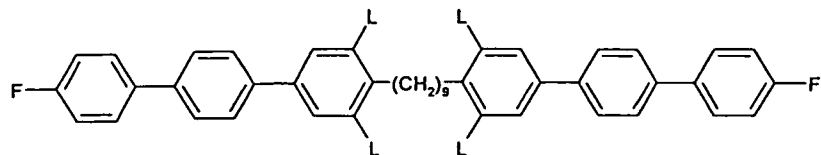
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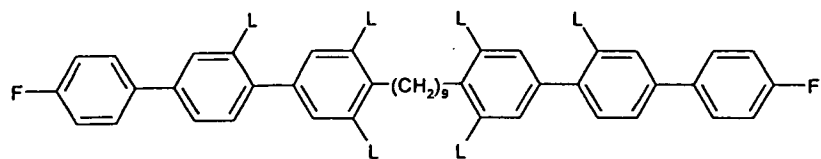
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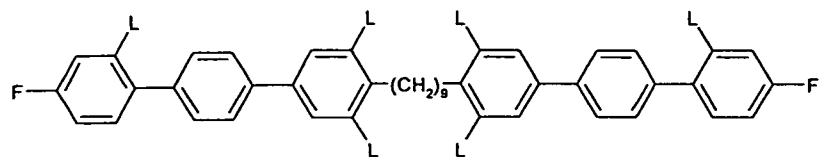
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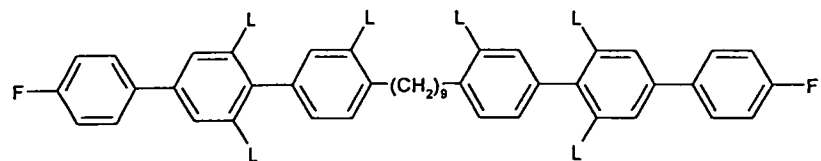
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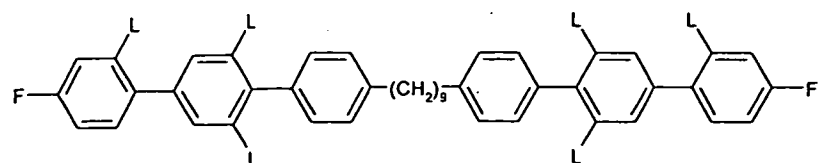
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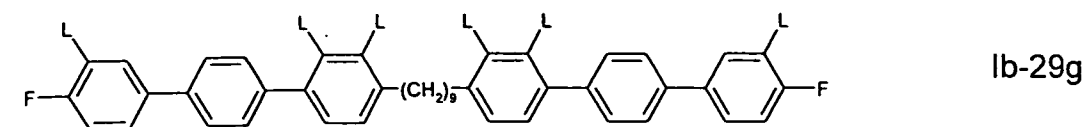
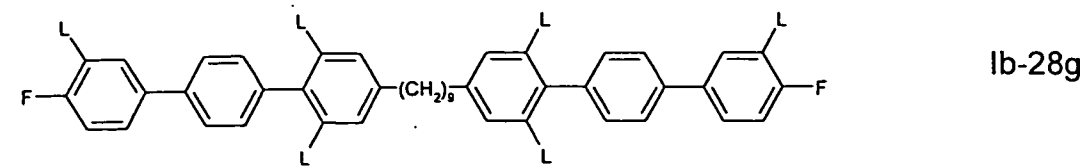
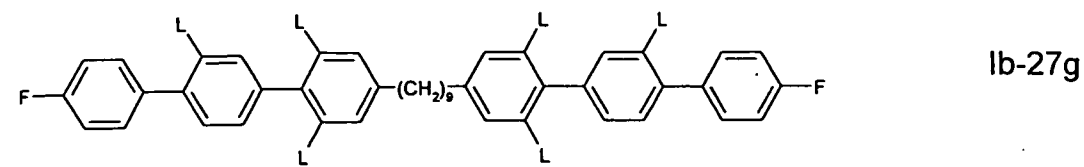
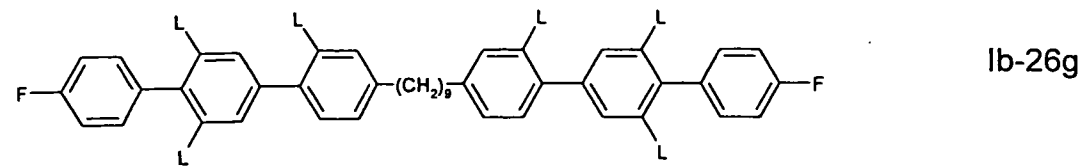
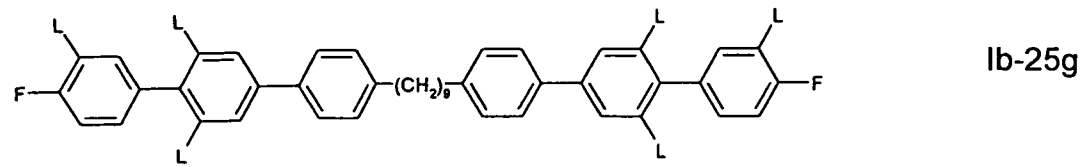
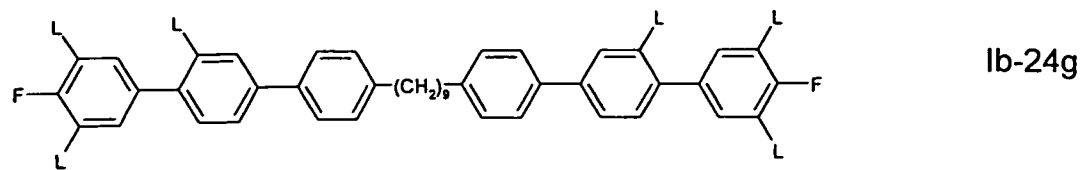
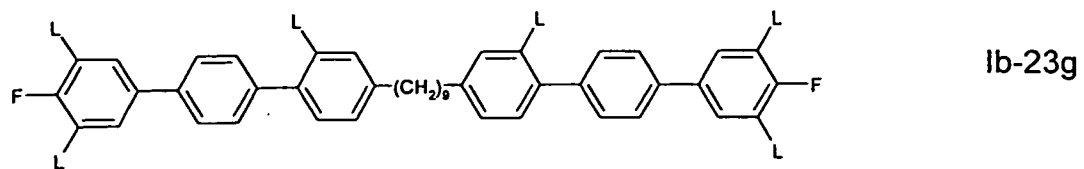
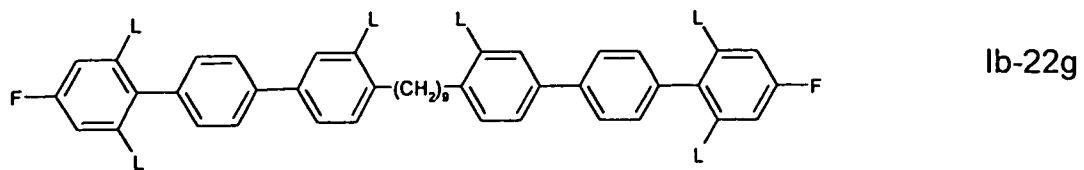
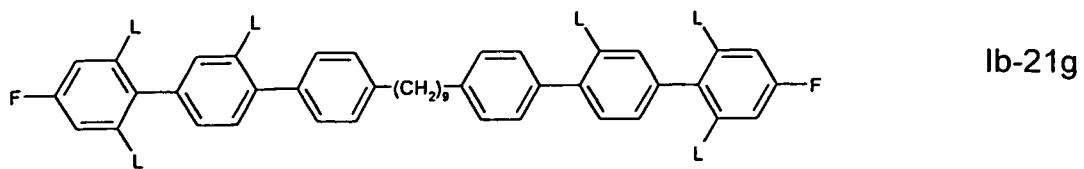
Ib-18g

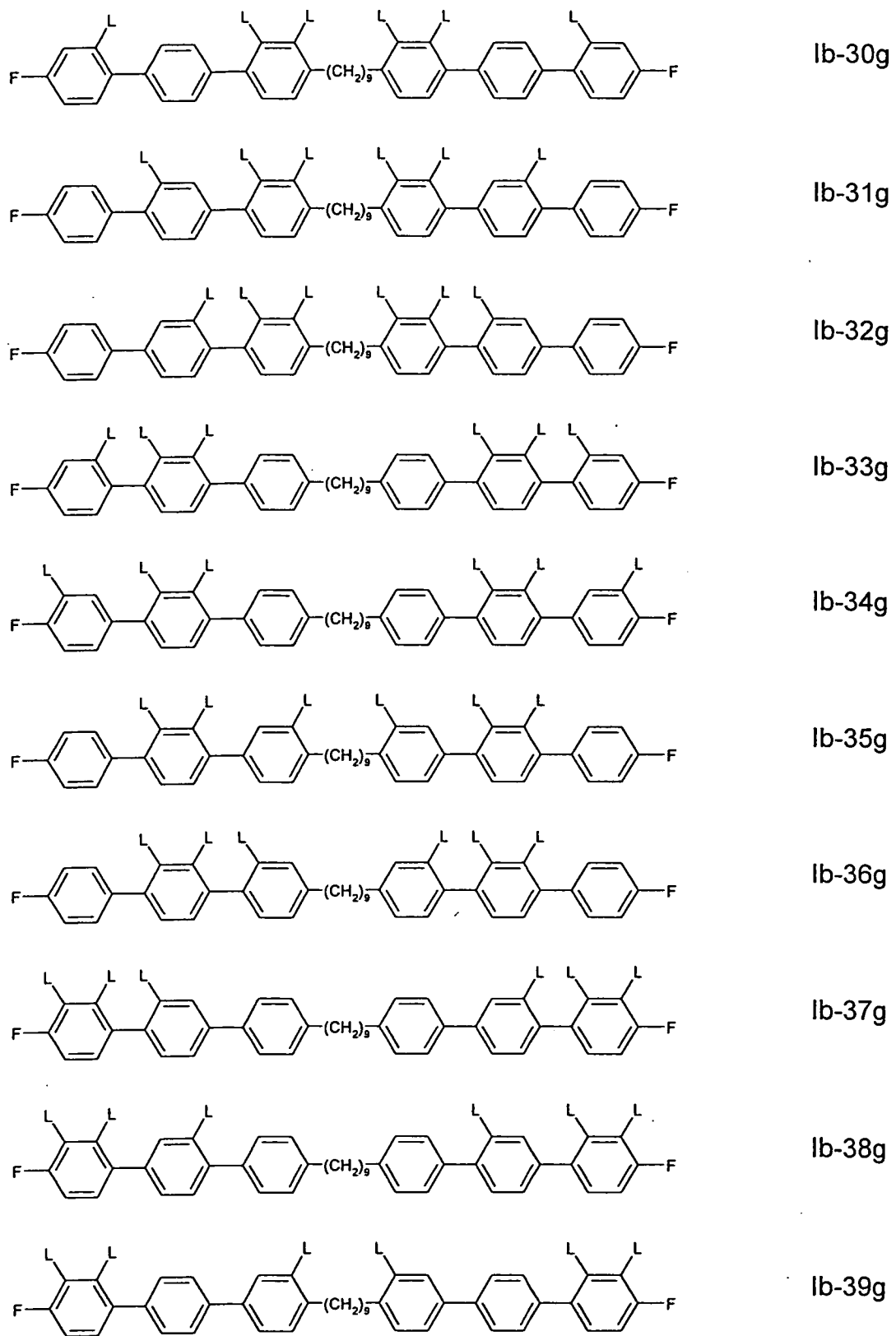


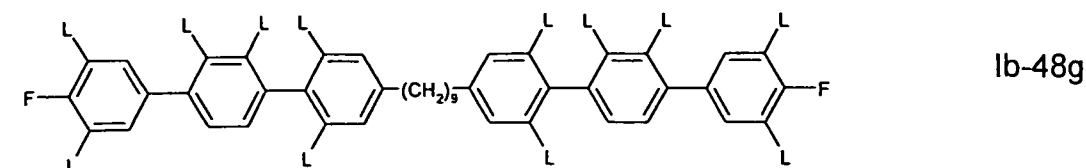
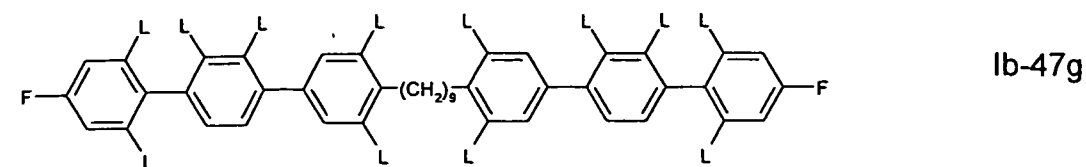
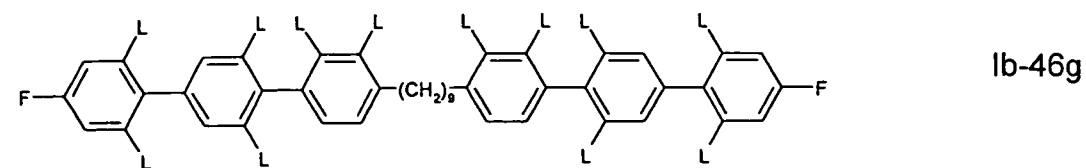
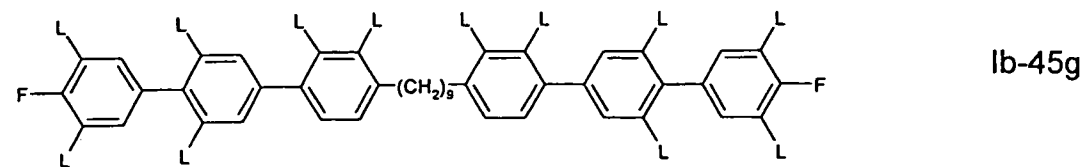
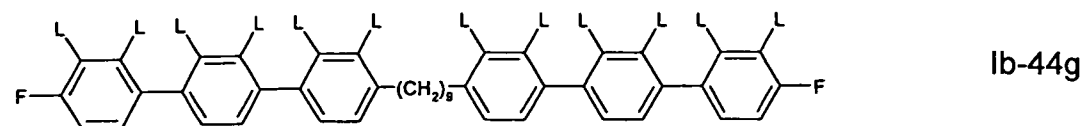
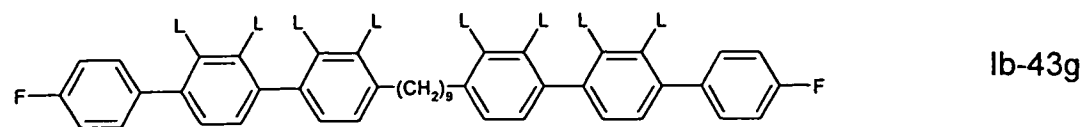
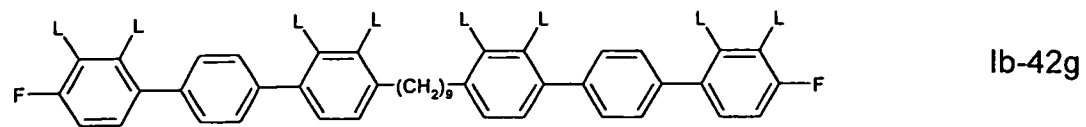
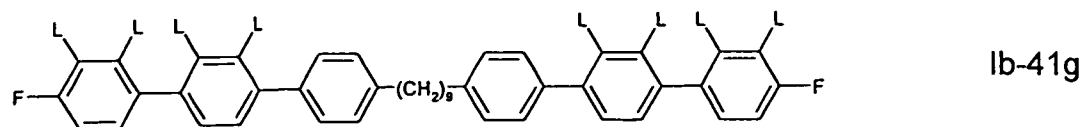
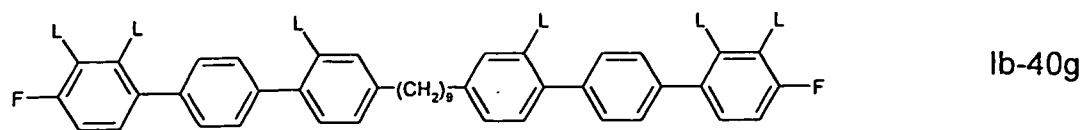
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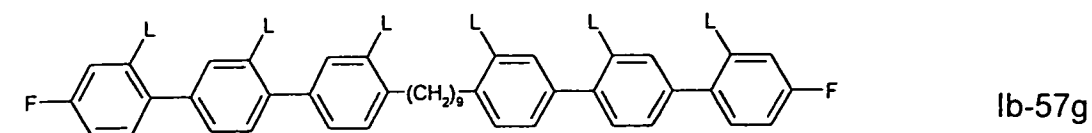
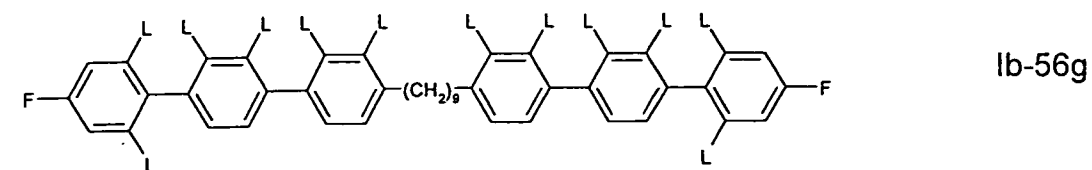
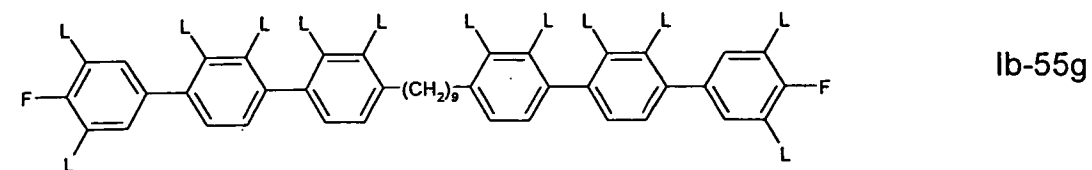
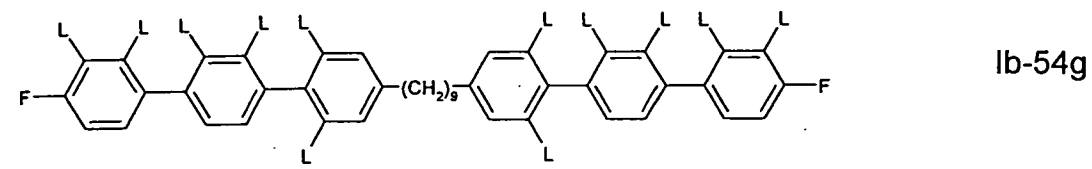
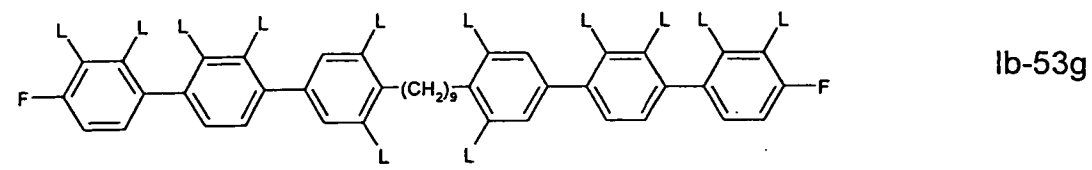
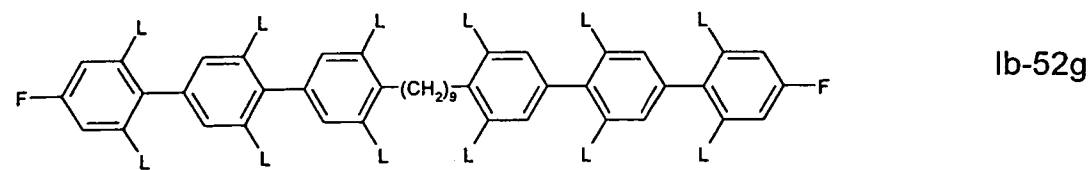
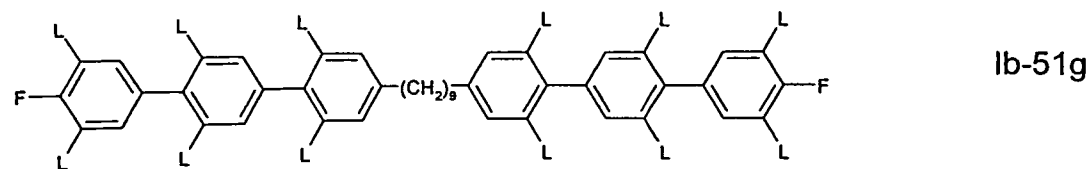
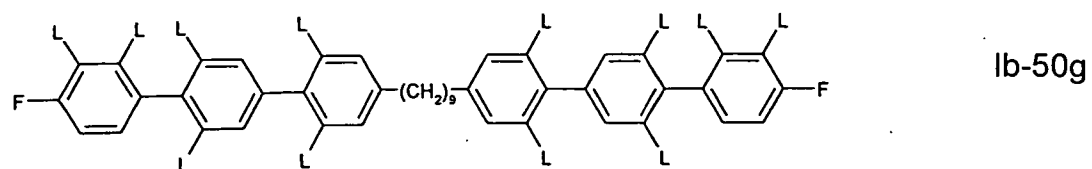
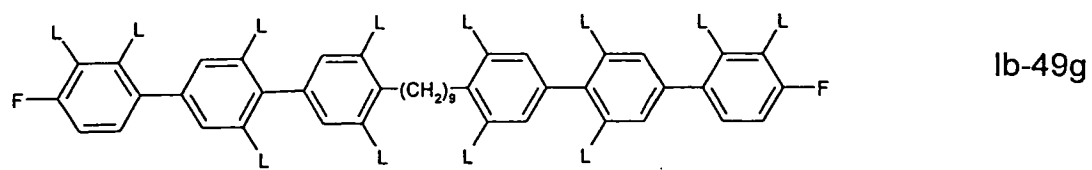


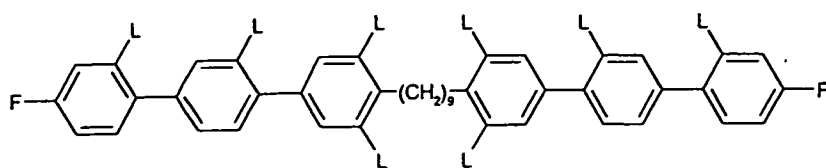
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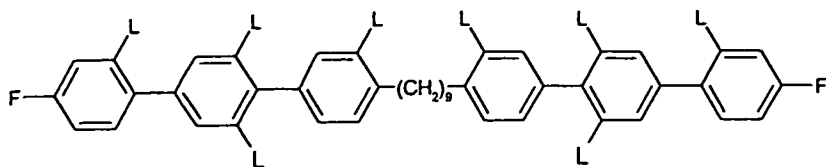




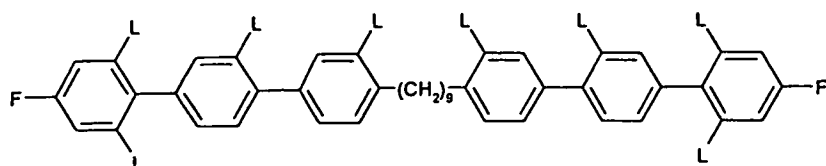




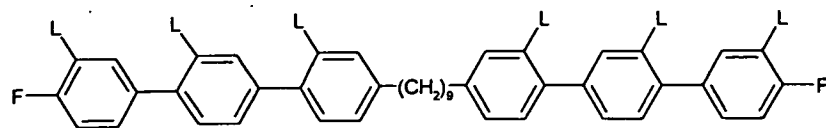
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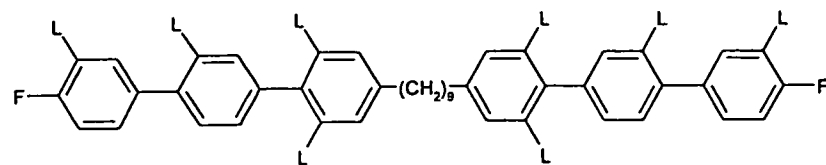
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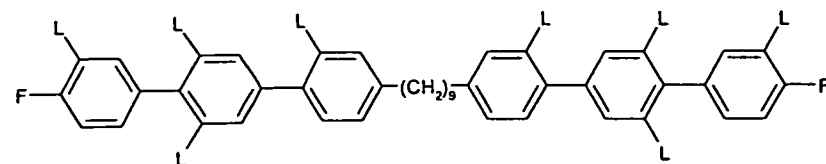
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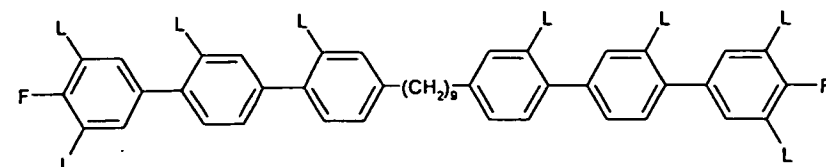
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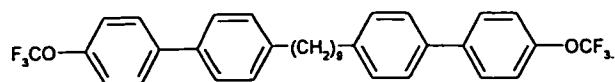
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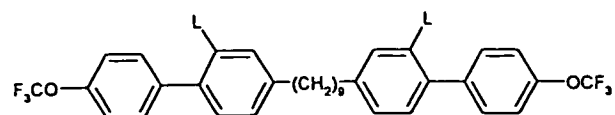
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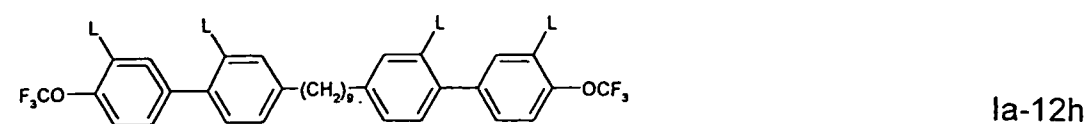
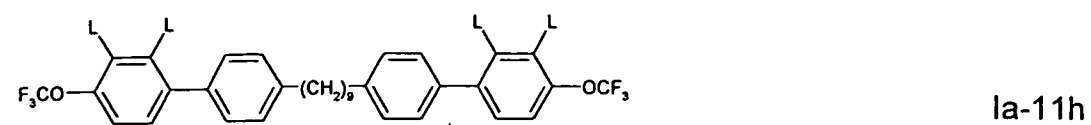
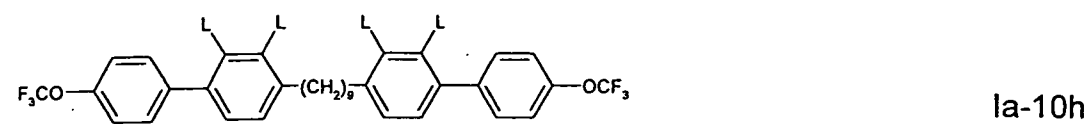
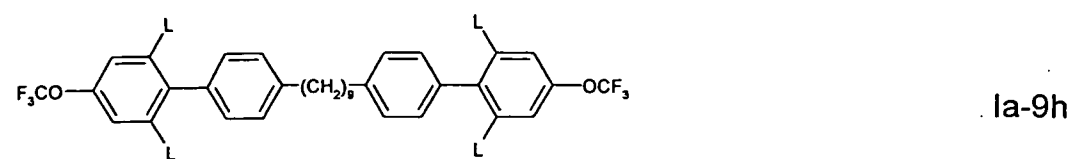
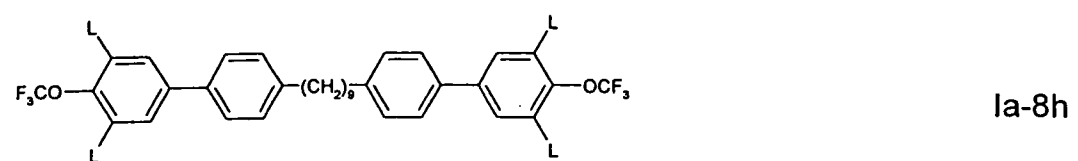
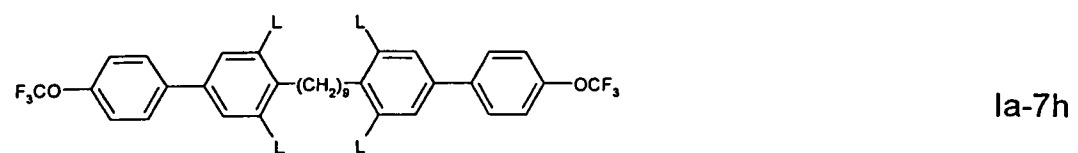
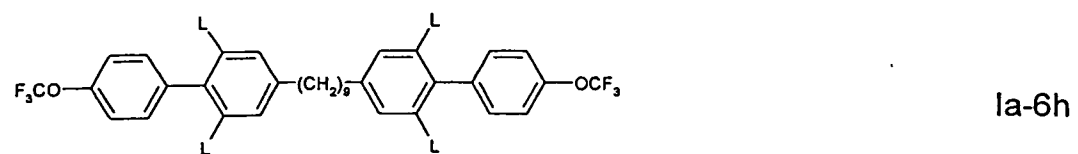
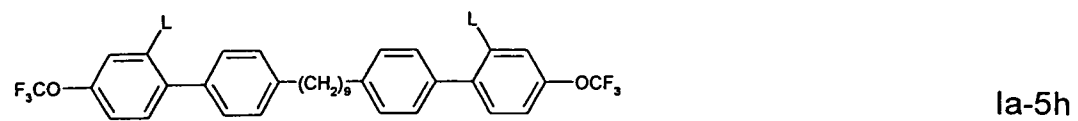
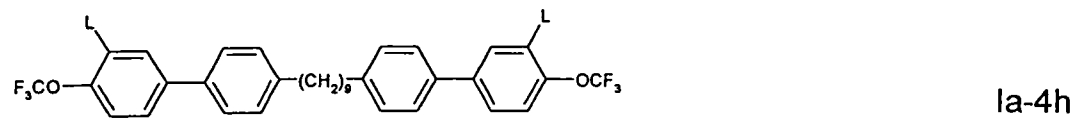
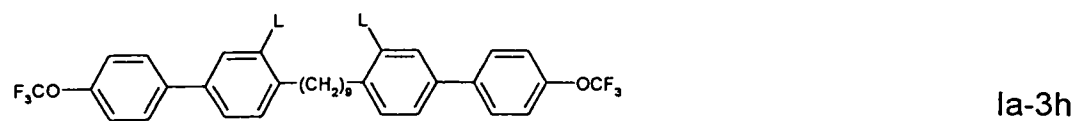
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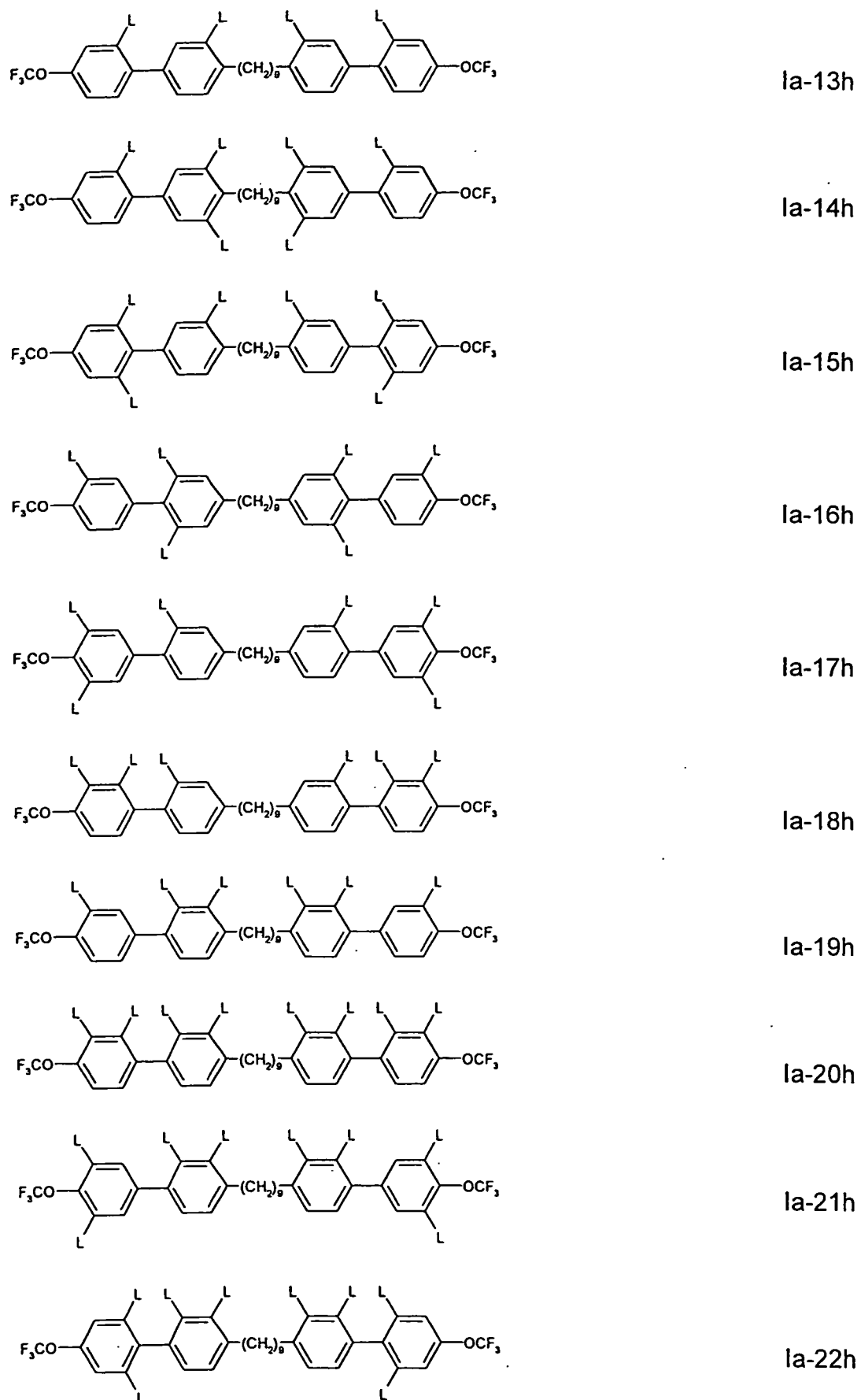


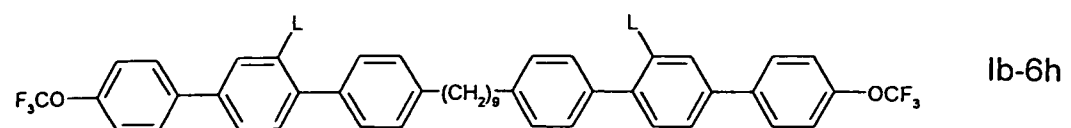
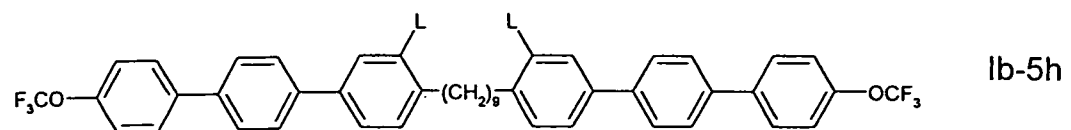
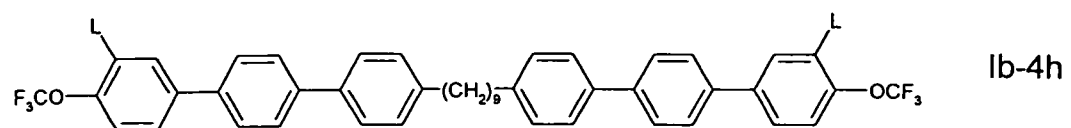
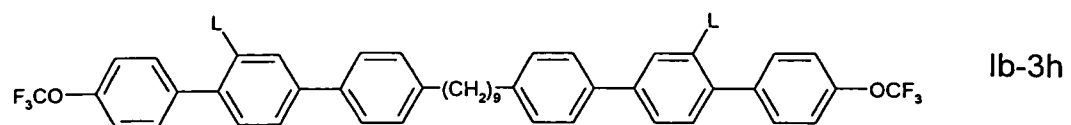
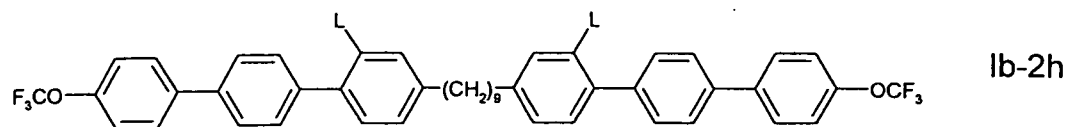
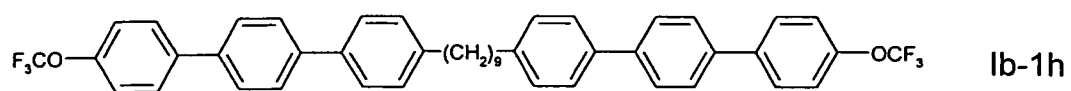
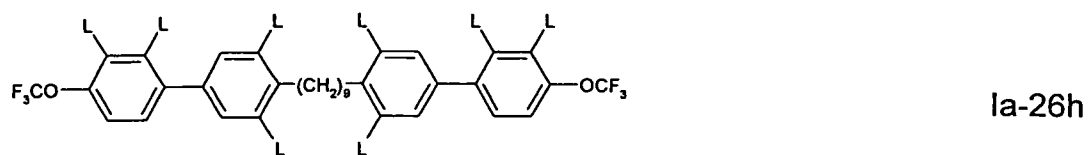
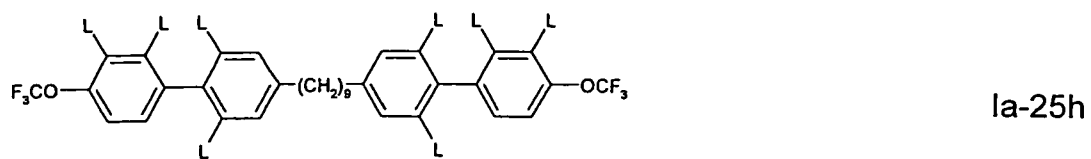
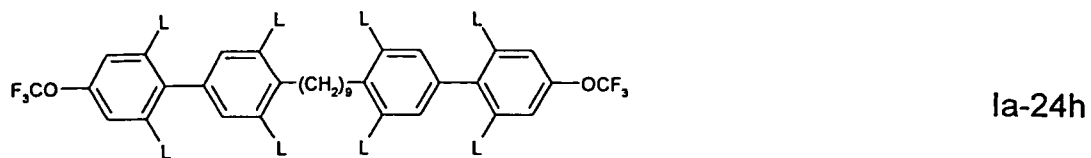
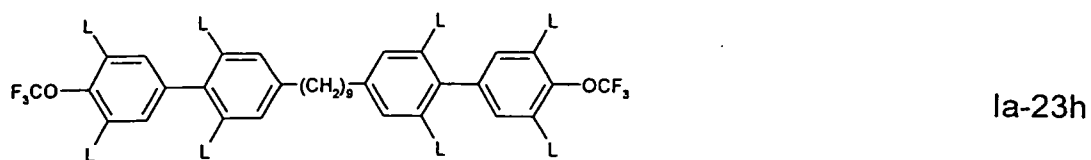
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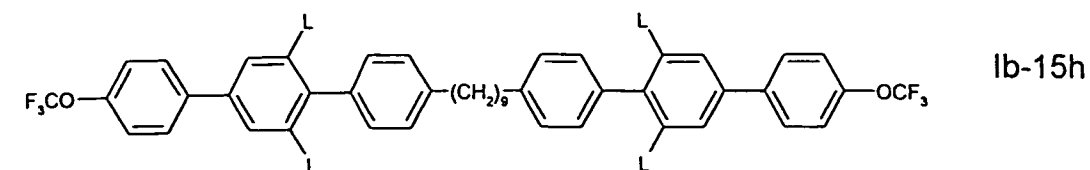
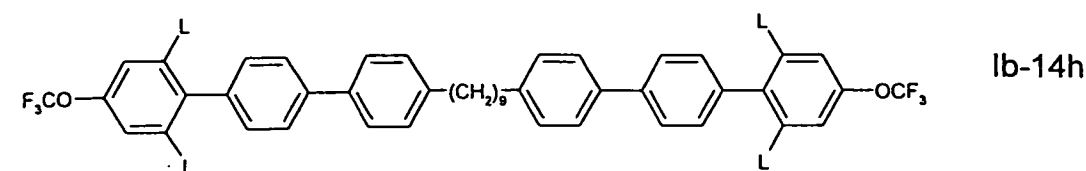
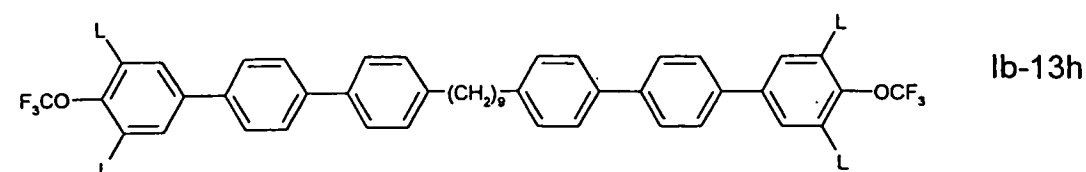
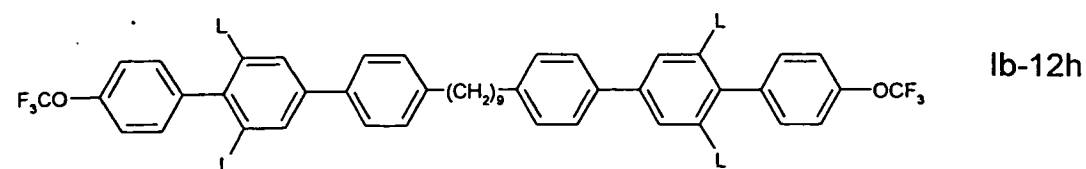
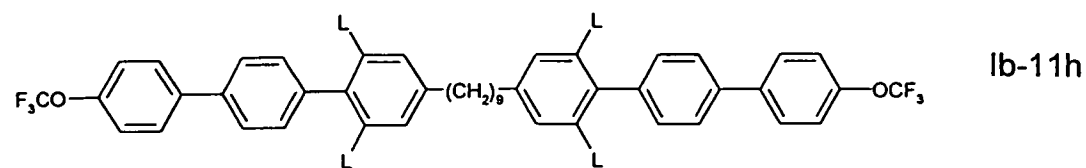
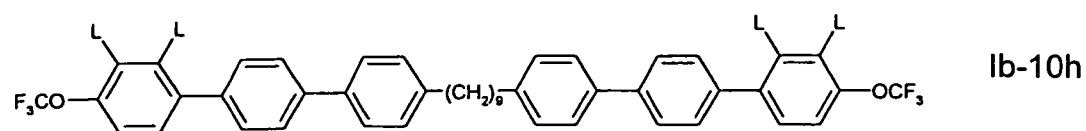
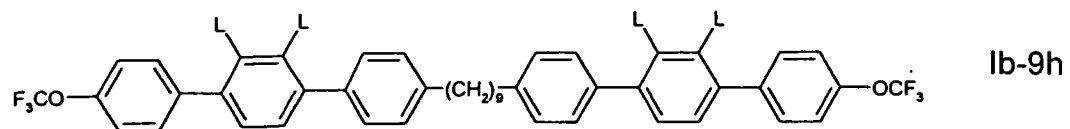
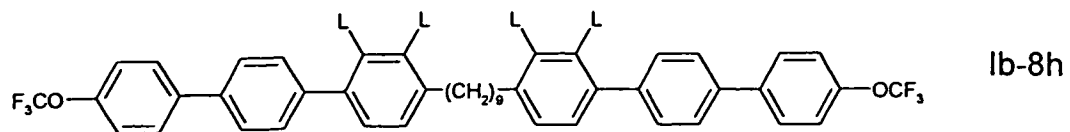
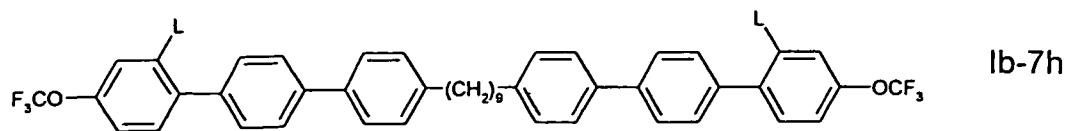


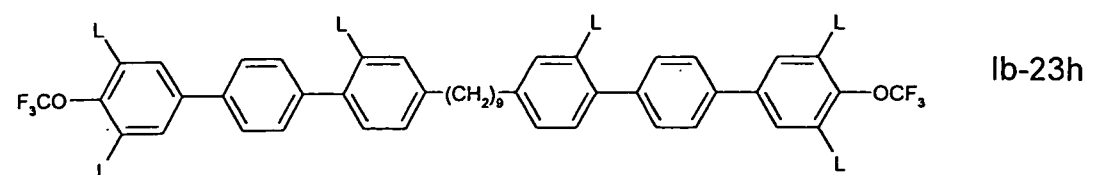
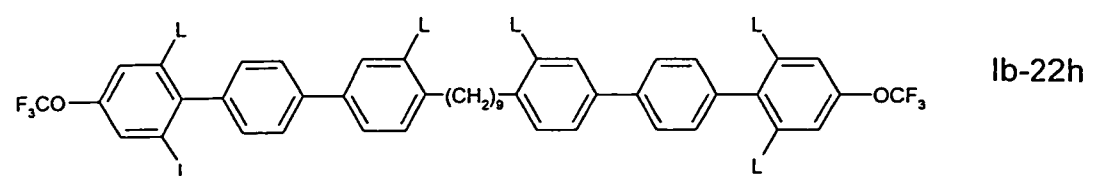
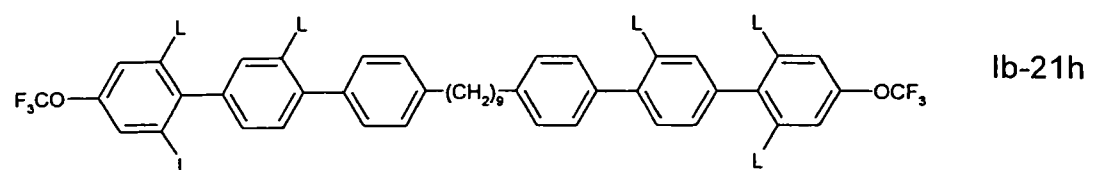
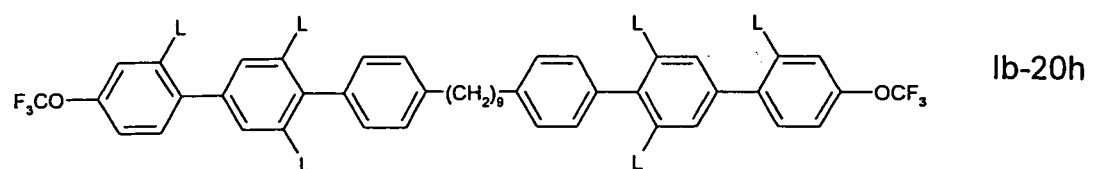
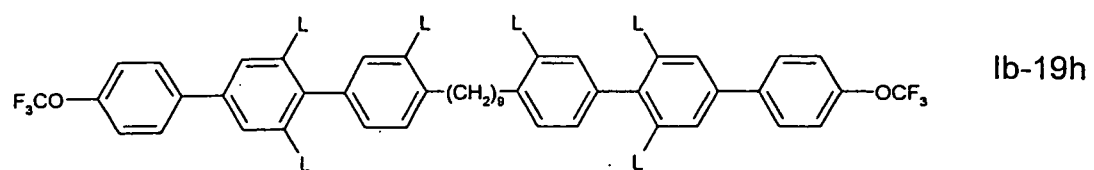
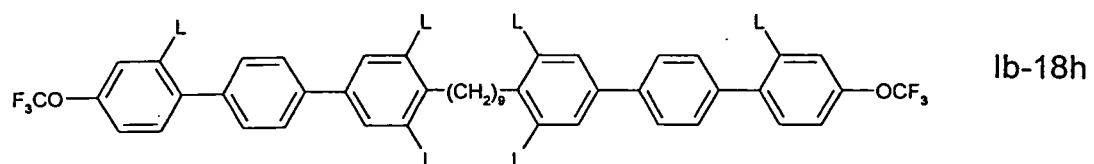
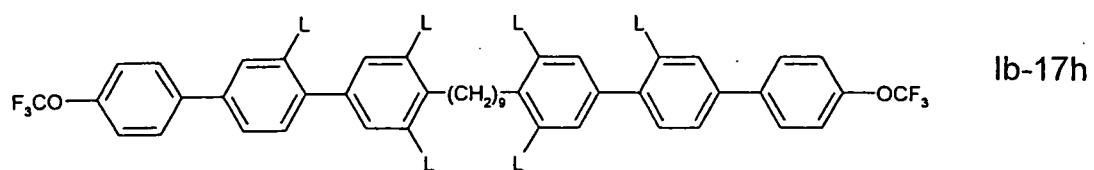
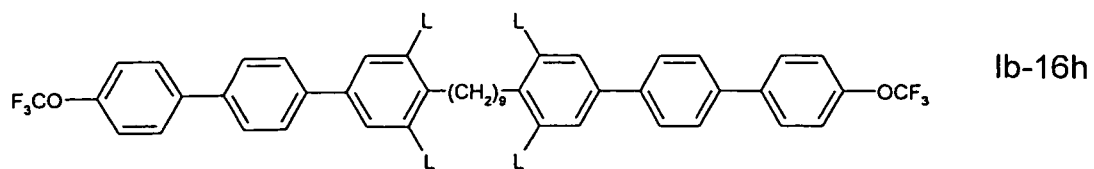
Ia-2h

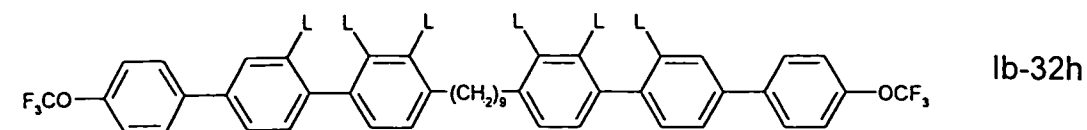
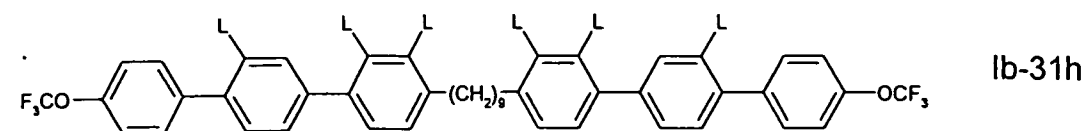
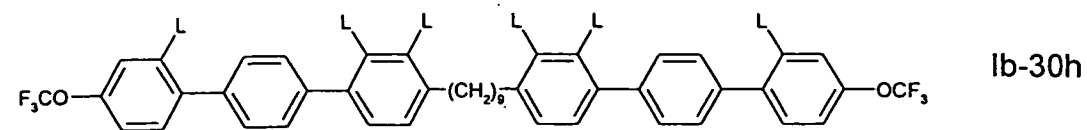
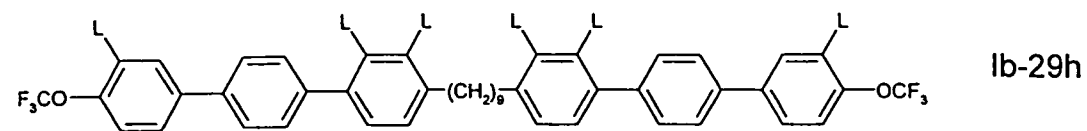
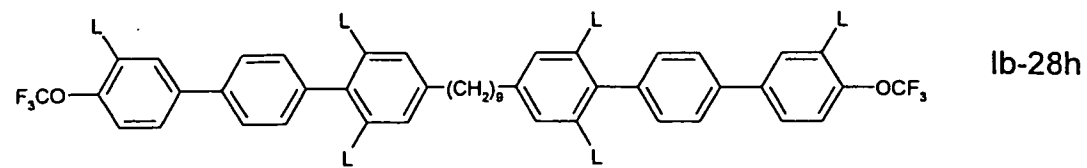
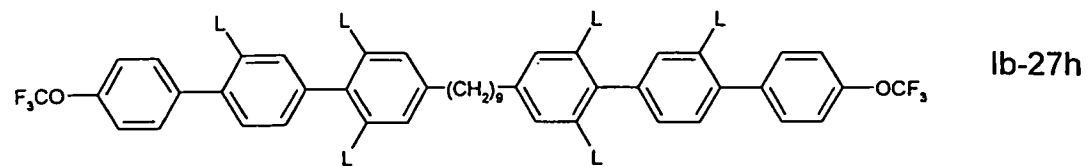
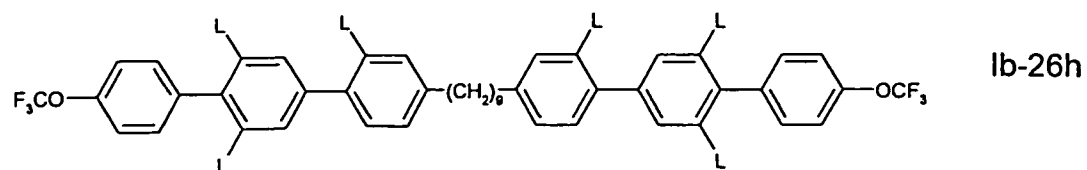
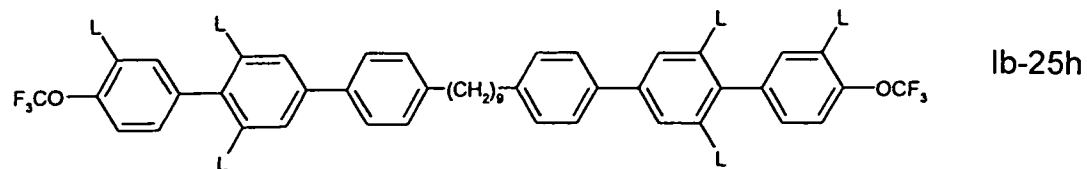
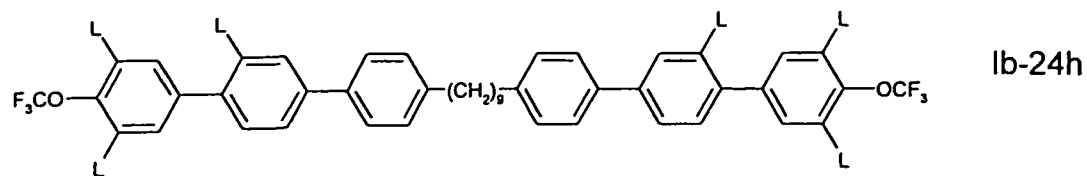


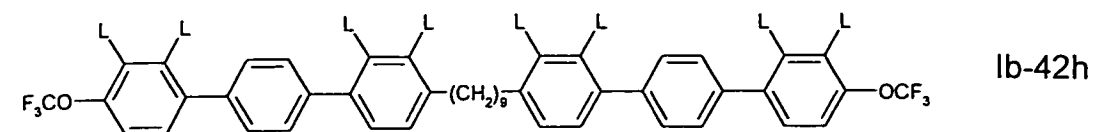
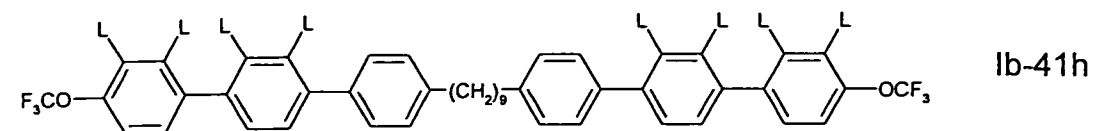
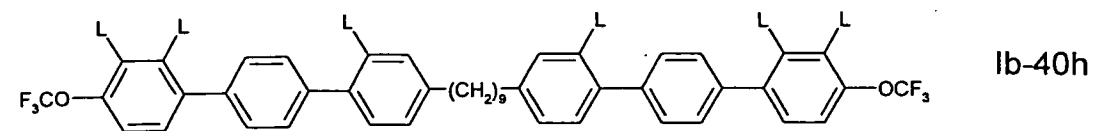
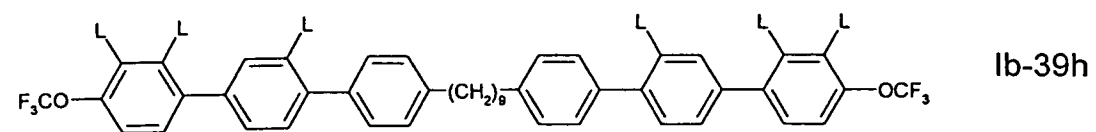
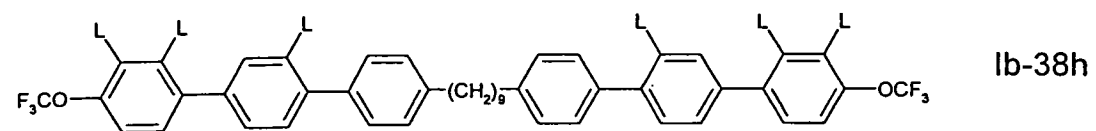
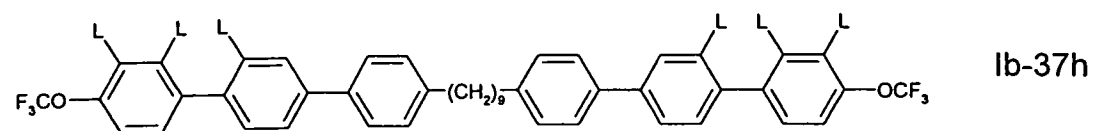
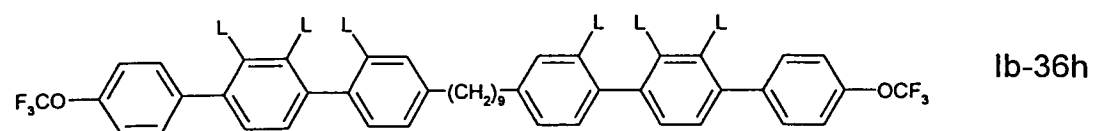
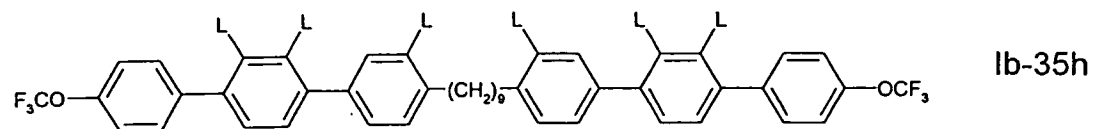
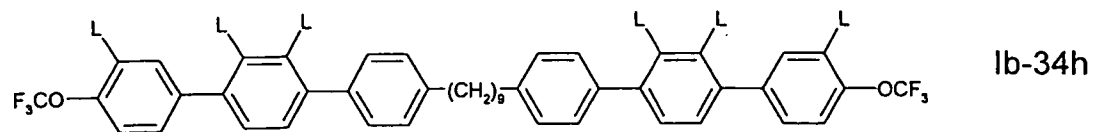
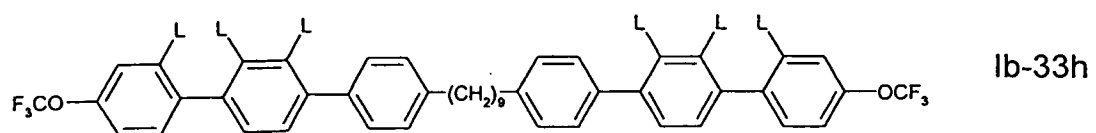


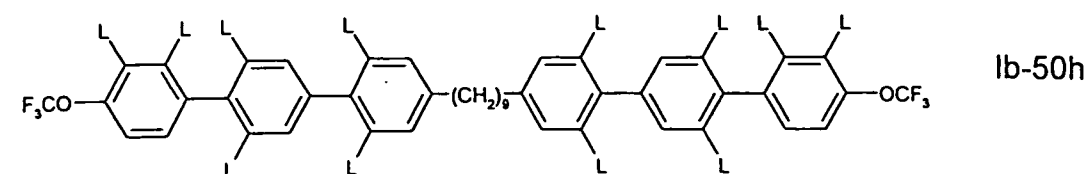
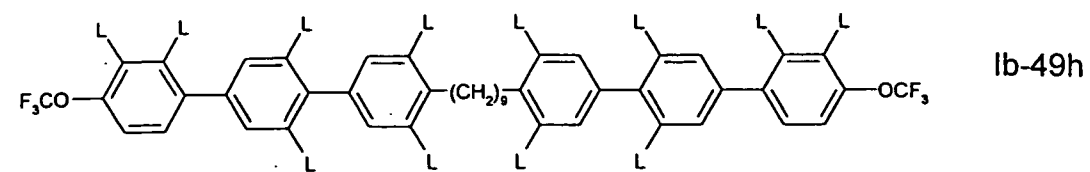
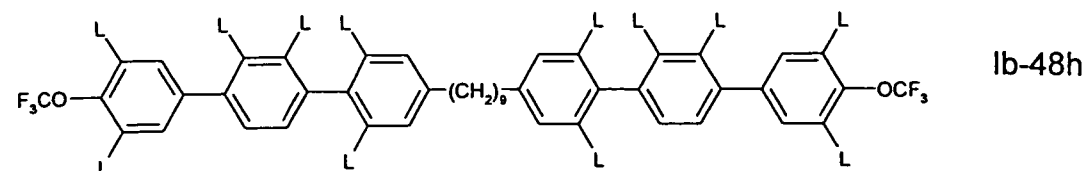
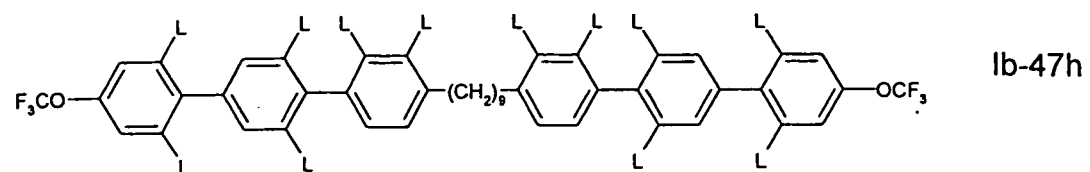
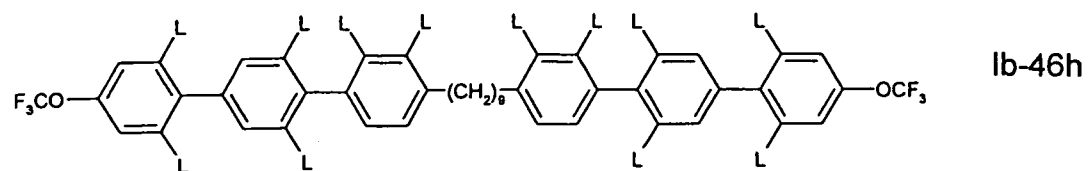
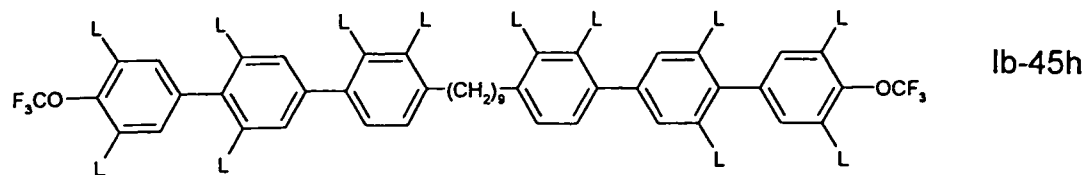
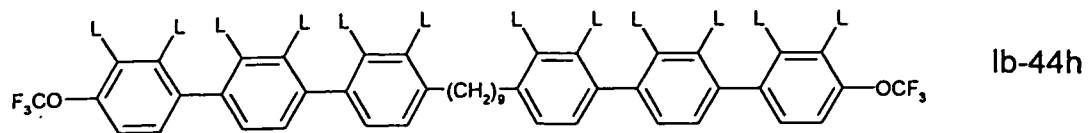
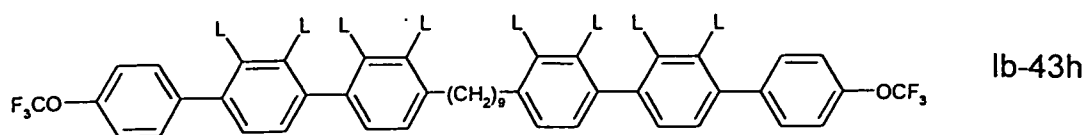


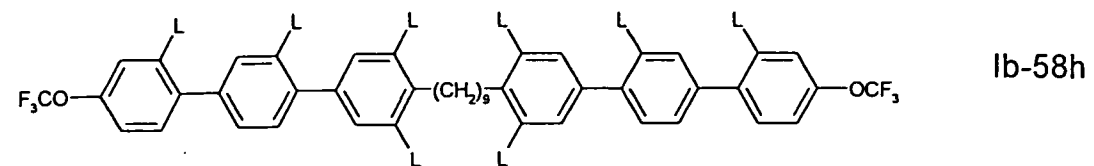
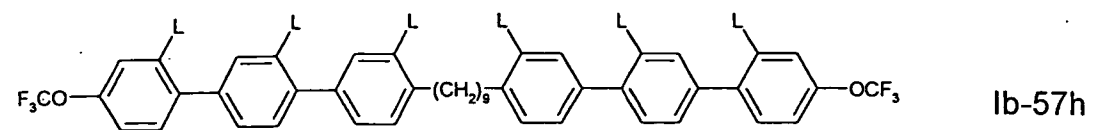
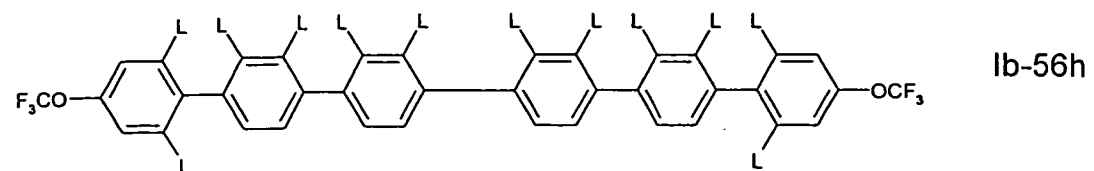
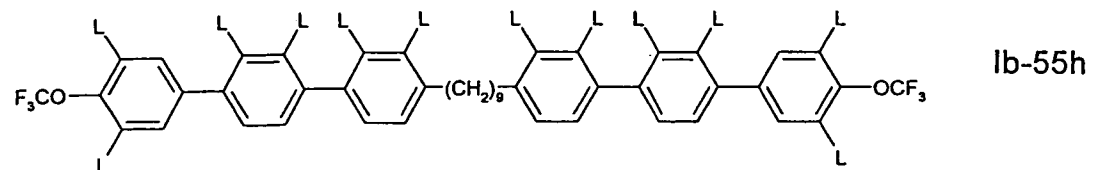
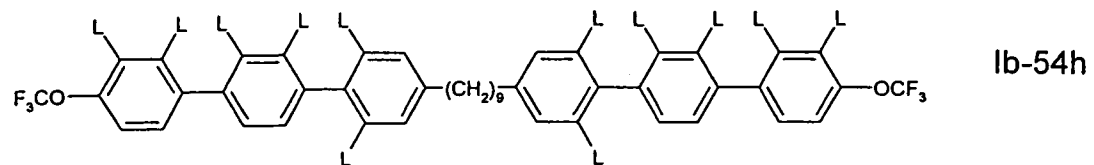
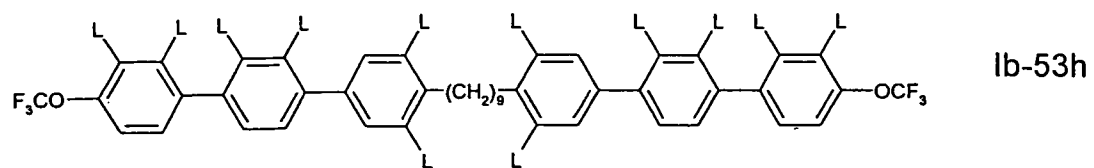
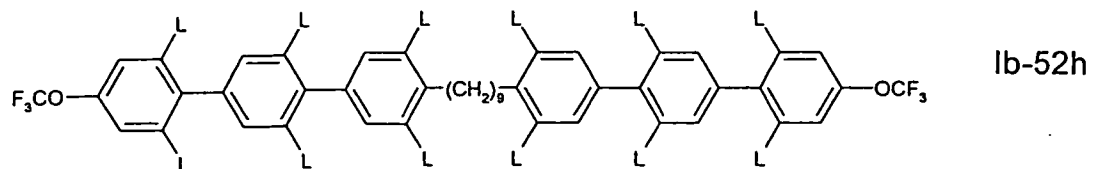
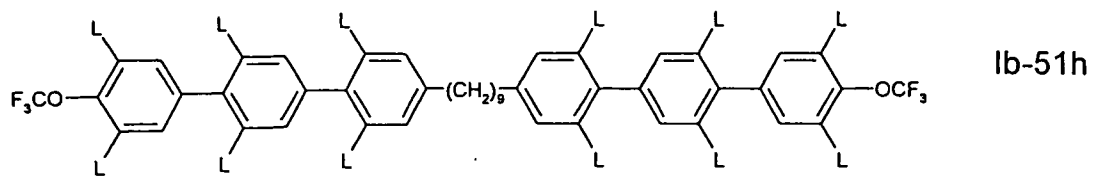


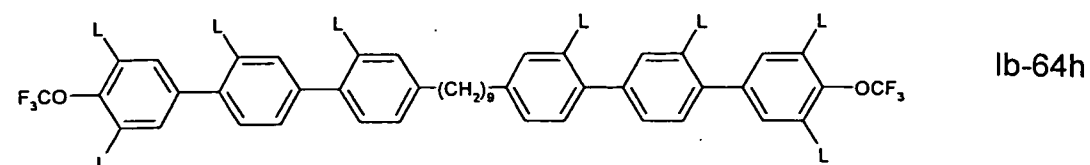
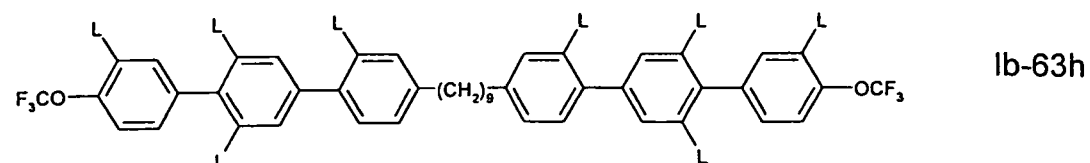
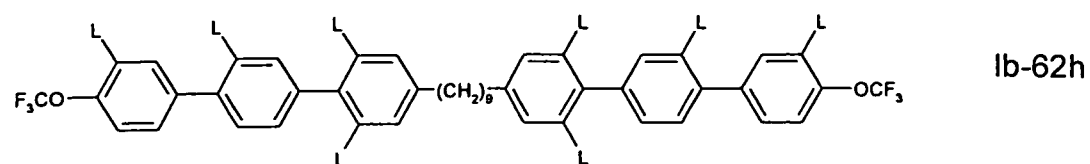
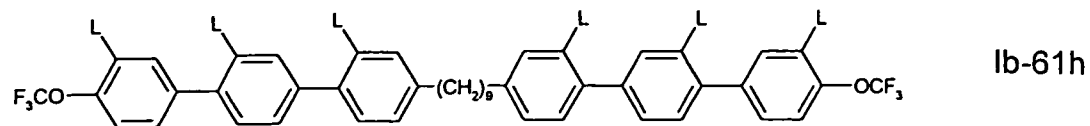
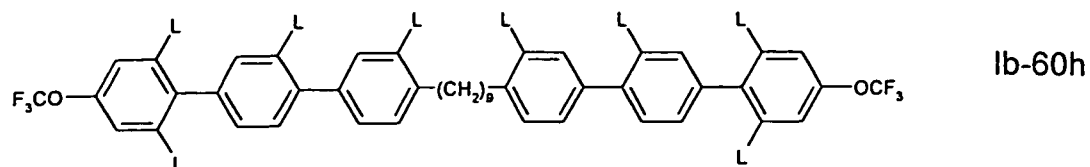
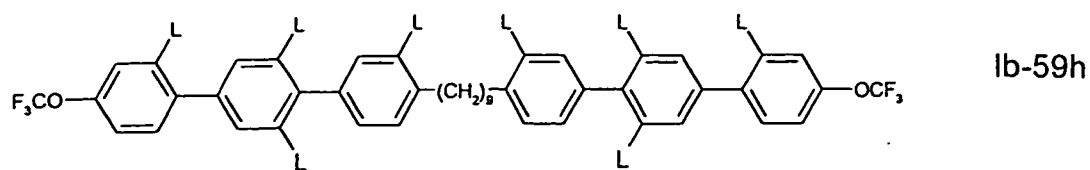










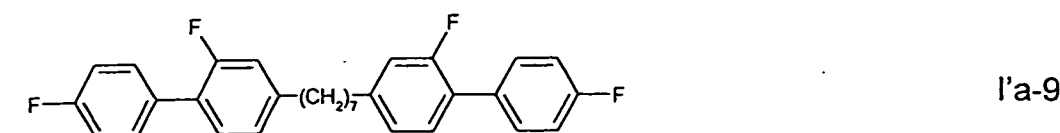
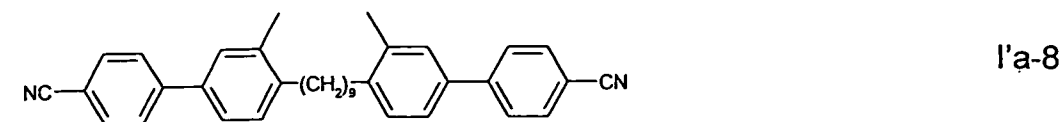
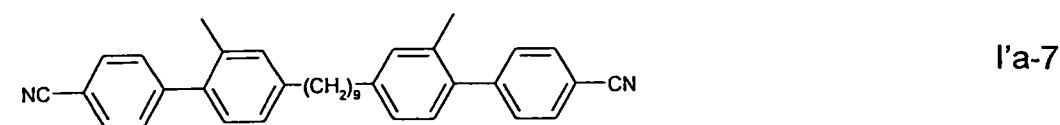
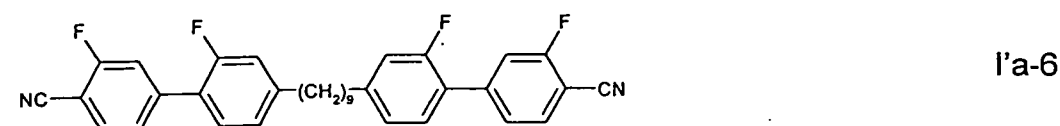
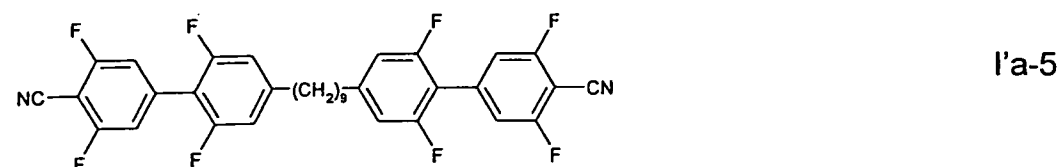
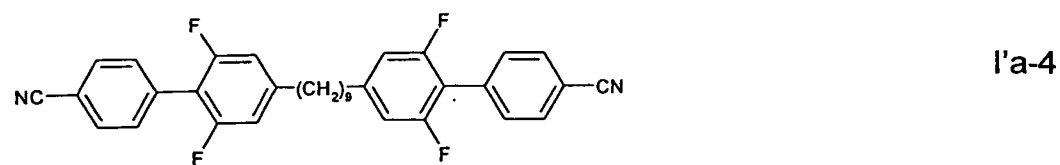
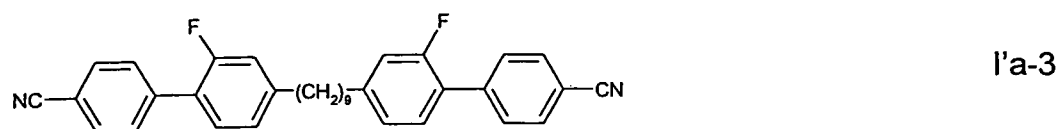
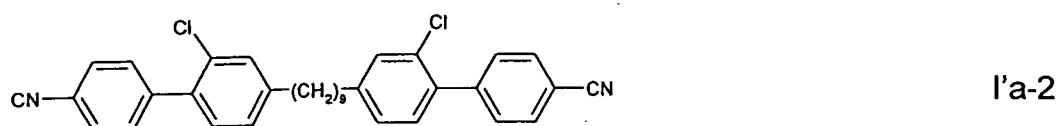
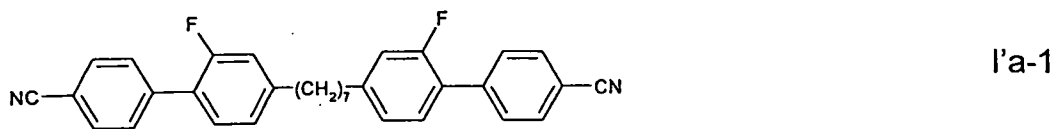


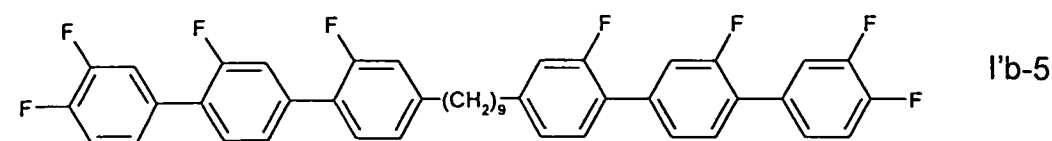
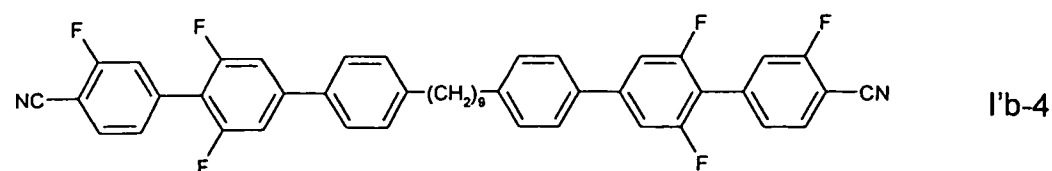
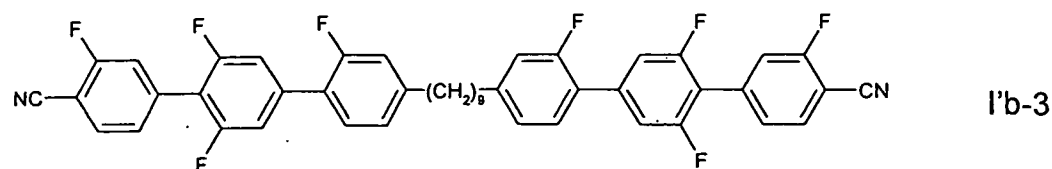
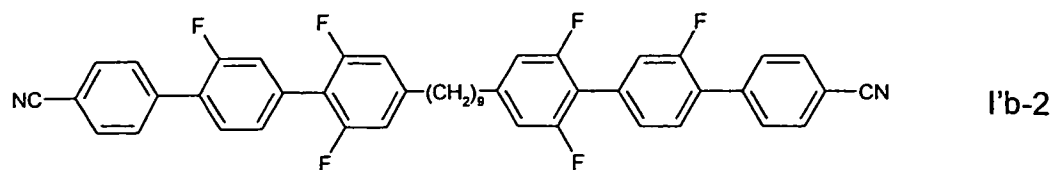
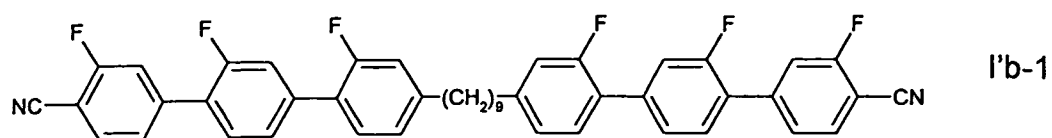
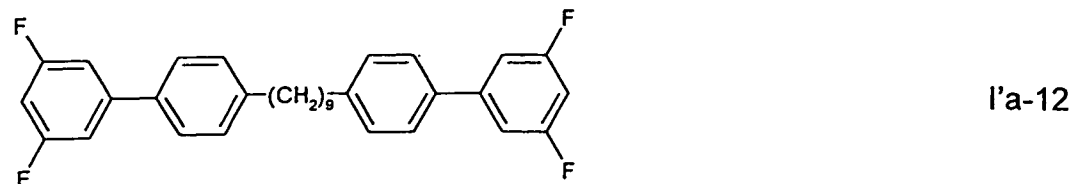
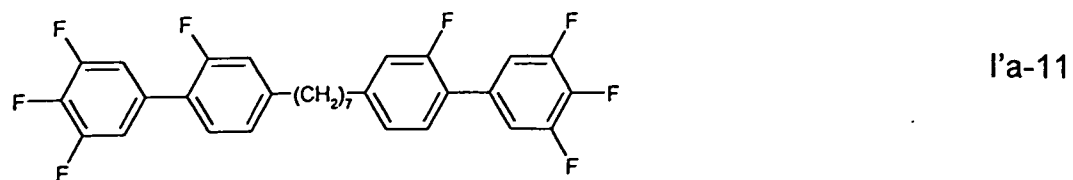
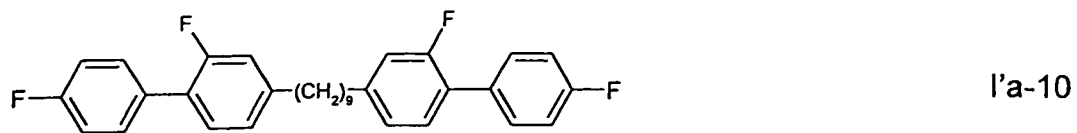
其中L在每次出現時彼此獨立地較佳地係F、Cl、CN、OH、NO₂或具有1至7個C原子之視情況氟化之烷基、烷氧基或烷醯基，極佳係F、Cl、CN、OH、NO₂、CH₃、C₂H₅、OCH₃、OC₂H₅、COCH₃、COC₂H₅、COOCH₃、COOC₂H₅、CF₃、OCF₃、OCHF₂、OC₂F₅，特定而言係F、Cl、CN、CH₃、C₂H₅、OCH₃、COCH₃及OCF₃，最佳係F、Cl、CH₃、OCH₃及COCH₃。

尤佳者係式Ia-1a、Ia-2a、Ia-2b、Ia-17c、Ia-8e、Ia-3f、Ia-5f、Ia-6f、Ia-12f、Ia-23f、Ib-27f、Ib-61f及Ib-63f

之化合物，其中L在每次出現時彼此獨立地較佳地係F、Cl、CH₃、OCH₃及COCH₃。

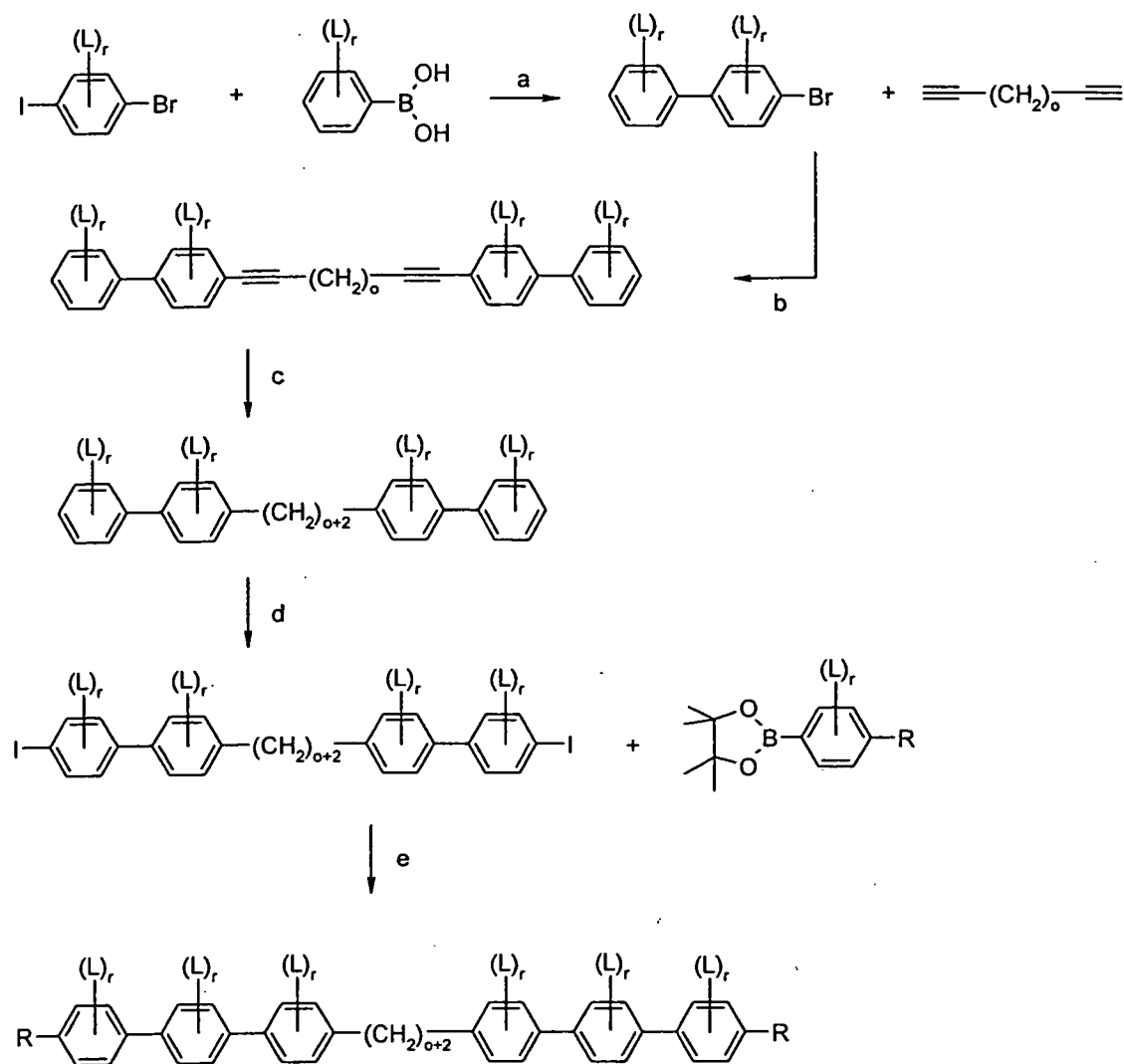
式 Ia-1a-h 至 Ia-26a-h 及 Ib-1a-h 至 Ib-56a-h 之極佳化合物如下文所指示：





式I化合物可根據原本已知且闡述於有機化學標準著作中之方法或以類似於該等方法之方式合成，例如，闡述於Houben-Weyl, Methoden der organischen Chemie, Thieme-

Verlag, Stuttgart中之方法。較佳製備方法可自下列合成反應圖獲得。



a) K₂CO₃, THF, H₂O, Pd觸媒, 80°C, 24小時

b) THF, Et₃N, CuI, Pd觸媒, 40°C, 24小時

c) THF, Pd/C, H₂, 60°C, 95巴

d) n-BuLi, THF, I₂, -70°C

e) Na₂CO₃, THF, H₂O, Pd觸媒, 80°C, 24小時

其中R具有R¹及R²之含義, o、L及r在每次出現時彼此獨立地如上文所定義, 包含該等基團之較佳含義。

本發明之另一目標係在液晶介質中使用式I之雙液晶原化合物。

在添加至向列液晶混合物中時，式I化合物產生位於向列相下方之相。在此上下文中，雙液晶原化合物對於向列液晶混合物之影響之第一指徵由Barnes, P.J., Douglas, A.G., Heeks, S.K., Luckhurst, G.R., *Liquid crystals*, 1993, 第13卷, 第4期, 603-613報導。此參考文獻例示高度極性之烷基間隔二聚體且發現位於向列相下方之相，從而總結出其係層列相類型。

在向列相下方之現有中間相之光學證據由Henderson, P.A., Niemeyer, O., Imrie, C.T.在*Liquid crystal*, 2001, 第28卷, 第3期, 463-472中公開，此並未進一步加以研究。

在*Liquid crystal*, 2005, 第32卷, 第11-12期, 1499-1513中，Henderson, P.A., Seddon, J.M.及Imrie, C.T.報導，在向列相下方之新相屬於層列C相之一些具體實例。在第一向列相下方之其他向列相由Panov, V.P., Ngaraj, M., Vij, J.K., Panarin, Y.P., Kohlmeier, A., Tamba, M.G., Lewis, R.A.及Mehl, G.H.報導於*Phys.Rev.Lett.* 2010, 105, 1678011-1678014中。

在此上下文中，包括式I之新發明性雙液晶原化合物之液晶混合物亦展現指定為第二向列相之新穎中間相。此中間相存在於低於原始向列液晶相之溫度下且已在本申請案所呈現之獨特混合物概念中觀察到。

因此，本發明之式I之雙液晶原化合物使得在通常並不具有第二向列相之向列混合物中誘導此相。另外，改變式I化合物之量可使得第二向列相之相行為適用於所需溫度。

本發明由此係關於包括至少一種式I化合物之液晶介質。

本發明混合物之一些較佳實施例如下文所指示。

較佳者係如下之式I化合物：其中液晶原基團 MG^1 及 MG^2 在每次出現時彼此獨立地包括一個、兩個或三個6員環、較佳地兩個或三個6員環。

尤佳者係子式II-1、II-4、II-6、II-7、II-13、II-14、II-15、II-16、II-17及II-18。

尤佳者係子式IIa、II d、II g、II h、II i、II k及II o，特定而言係子式IIa及IIg，其中L在每次出現時彼此獨立地較佳地係F、Cl、CN、OH、NO₂或具有1至7個C原子之視情況氟化之烷基、烷氧基或烷醯基，極佳係F、Cl、CN、OH、NO₂、CH₃、C₂H₅、OCH₃、OC₂H₅、COCH₃、COC₂H₅、COOCH₃、COOC₂H₅、CF₃、OCF₃、OCHF₂、OC₂F₅，特定而言係F、Cl、CN、CH₃、C₂H₅、OCH₃、COCH₃及OCF₃，最佳係F、Cl、CH₃、OCH₃及COCH₃。

較佳地，式I中之R¹及R²係選自H、F、Cl、CN、NO₂、OCH₃、COCH₃、COC₂H₅、COOCH₃、COOC₂H₅、CF₃、C₂F₅、OCF₃、OCHF₂及OC₂F₅，特定而言係H、F、Cl、CN、OCH₃及OCF₃，尤其係H、F、CN及OCF₃。

典型間隔基團 (Sp) 係 (例如) $-(CH_2)_o-$ 、 $-(CH_2CH_2O)_p-$ 、 CH_2CH_2- ，其中 o 為 5 至 40、特定而言 5 至 25、極佳地 5 至 15 之整數，且 p 為 1 至 8、特定而言 1、2、3 或 4 之整數。

較佳者係式 I 中之 R^1-MG^1- 及 R^2-MG^2- 相同之式 I 化合物。尤佳者係選自式 Ia 及 Ib 之化合物。尤佳者係選自子式 Ia-1 至 Ia-26 及 Ib-1 至 Ib-56、極佳地選自子式 Ia-1a-h 至 Ia-26a-h 及 / 或 Ib-1a-h 至 Ib-56a-h 之化合物。

本發明介質較佳地包括一種、兩種、三種、四種或更多種、較佳地一種、兩種或三種式 I 化合物。

液晶介質中之式 I 化合物之量較佳地為總混合物之 1 重量 % 至 50 重量 %、特定而言 5 重量 % 至 40 重量 %、極佳地 10 重量 % 至 30 重量 %。

在一較佳實施例中，本發明之液晶介質另外包括一或多種自 GB 2 356 629 已知之式 III 化合物。



其中

R^3 及 R^4 各自獨立地係 H、F、Cl、CN、NCS 或具有 1 至 25 個 C 原子之直鏈或具支鏈烷基，該烷基可未經取代、經鹵素或 CN 單-或多取代，其一或多個非毗鄰 CH_2 基團亦可在每一情形下彼此獨立地由 $-O-$ 、 $-S-$ 、 $-NH-$ 、 $-N(CH_3)-$ 、 $-CO-$ 、 $-COO-$ 、 $-OCO-$ 、 $-O-CO-O-$ 、 $-S-CO-$ 、 $-CO-S-$ 、 $-CH=CH-$ 、 $-CH=CF-$ 、 $-CF=CF-$ 或 $-C\equiv C-$ 以氧原子並不彼此直接連接之方式代替，

MG^3 及 MG^4 各自獨立地係液晶原基團，

Sp^1 係包括5至40個C原子之間隔基團，其中一或多個非毗鄰 CH_2 基團亦可由-O-、-S-、-NH-、-N(CH₃)-、-CO-、-O-CO-、-S-CO-、-O-COO-、-CO-S-、-CO-O-、-CH(鹵素)-、-CH(CN)-、-CH=CH-或-C≡C-代替，且

X^3 及 X^4 各自獨立地係-O-、-S-、-CO-、-COO-、-OCO-、-O-CO-O-、-CO-NH-、-NH-CO-、-CH₂CH₂-、-OCH₂-、-CH₂O-、-SCH₂-、-CH₂S-、-CH=CH-、-CH=CH-COO-、-OCO-CH=CH-、-C≡C-。

液晶原基團 MG^3 及 MG^4 較佳地選自式II。

尤佳者係 $R^3-MG^3-X^3$ -及 $R^4-MG^4-X^4$ -相同之式III化合物。

本發明之另一較佳實施例係關於 $R^3-MG^3-X^3$ -及 $R^4-MG^4-X^4$ -不同之式III化合物。

尤佳者係液晶原基團 MG^3 及 MG^4 包括一個、兩個或三個6員環之式III化合物，極佳地者係選自如下文所列示之式II之液晶原基團。

對於式III中之 MG^3 及 MG^4 而言，尤佳者係子式II-1、II-4、II-6、II-7、II-13、II-14、II-15、II-16、II-17及II-18。在該等較佳基團中，Z在每一情形下獨立地具有式II中所給出之Z¹含義中之一者。較佳地，Z係-COO-、-OCO-、-CH₂CH₂-、-C≡C-或單鍵。

極佳地，液晶原基團 MG^3 及 MG^4 係選自式 IIa 至 IIo 及其鏡像。

尤佳之 MG^3 及 MG^4 係子式 II d、II g、II h、II i、II k 及 II o，特定而言係子式 II d 及 II k。

在具有非極性極性基團之化合物之情形下， R^3 及 R^4 較佳係具有至多 15 個 C 原子之烷基或具有 2 至 15 個 C 原子之烷氧基。

若 R^3 或 R^4 係烷基或烷氧基(亦即，其中末端 CH_2 基團由 -O- 代替)，則其可係直鏈或具支鏈基團。其較佳為直鏈，具有 2、3、4、5、6、7 或 8 個碳原子，且因此較佳為乙基、丙基、丁基、戊基、己基、庚基、辛基、乙氧基、丙氧基、丁氧基、戊氧基、己氧基、庚氧基或辛氧基，其亦可為(例如)甲基、壬基、癸基、十一烷基、十二烷基、十三烷基、十四烷基、十五烷基、壬氧基、癸氧基、十一烷氧基、十二烷氧基、十三烷氧基或十四烷氧基。

氧雜烷基(亦即，其中一個 CH_2 基團由 -O- 代替)較佳係(例如)直鏈 2-氧雜丙基(=甲氧基甲基)、2-氧雜丁基(=乙氧基甲基)或 3-氧雜丁基(=2-甲氧基乙基)、2-、3-或 4-氧雜戊基、2-、3-、4-或 5-氧雜己基、2-、3-、4-、5-或 6-氧雜庚基、2-、3-、4-、5-、6-或 7-氧雜辛基、2-、3-、4-、5-、6-、7-或 8-氧雜壬基或 2-、3-、4-、5-、6-、7-、8-或 9-氧雜癸基。

在具有末端極性基團之化合物之情形下， R^3 及 R^4 係選自 CN、 NO_2 、鹵素、 OCH_3 、OCN、SCN、 COR^x 、 $COOR^x$ 或

具有1至4個C原子之單-、寡-或多氟化烷基或烷氧基。R^x係具有1至4個、較佳地1至3個C原子之視情況氟化之烷基。鹵素較佳地係F或Cl。

尤佳地，式III中之R³及R⁴係選自F、Cl、CN、NO₂、OCH₃、COCH₃、COC₂H₅、COOCH₃、COOC₂H₅、CF₃、C₂F₅、OCF₃、OCHF₂及OC₂F₅、特定而言F、Cl、CN、OCH₃及OCF₃。

對於式III中之間隔基團Sp¹而言，可使用熟習此項技術者已知用於此目的之所有基團。間隔基團Sp較佳係具有5至40個C原子、特定而言5至25個C原子、極佳地5至15個C原子之直鏈或具支鏈伸烷基，此外，其中一或多個非毗鄰CH₂基團可由-O-、-S-、-NH-、-N(CH₃)-、-CO-、-O-CO-、-S-CO-、-O-COO-、-CO-S-、-CO-O-、-CH(鹵素)-、-CH(CN)-、-CH=CH-或-C≡C-代替。

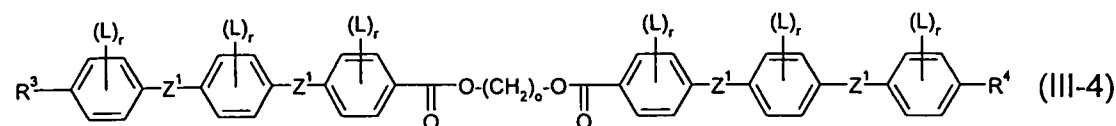
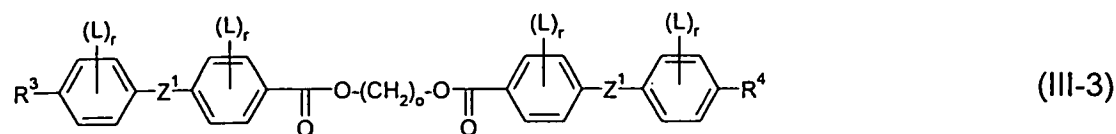
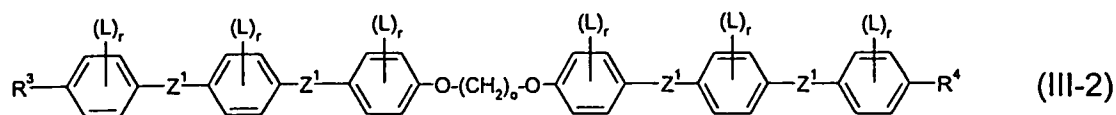
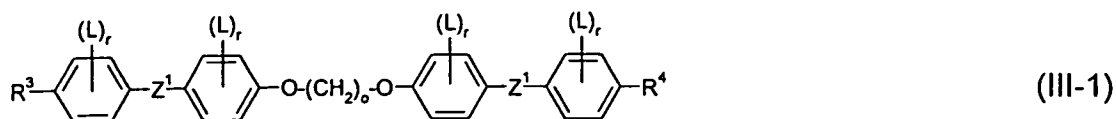
典型間隔基團係(例如)-(CH₂)_o-、-(CH₂CH₂O)_p-CH₂CH₂-、-CH₂CH₂-S-CH₂CH₂-或-CH₂CH₂-NH-CH₂CH₂-，其中o為5至40、特定而言5至25、極佳地5至15之整數，且p為1至8、特定而言1、2、3或4之整數。

較佳間隔基團係(例如)伸戊基、伸己基、伸庚基、伸辛基、伸壬基、伸癸基、伸十一烷基、伸十二烷基、伸十八烷基、二伸乙基氧基伸乙基、二亞甲基氧基伸丁基、伸戊烯基、伸庚烯基、伸壬烯基及伸十一烯基。

尤佳者係Sp¹表示具有5至15個C原子之伸烷基之式III之發明性化合物。尤佳者係直鏈伸烷基。

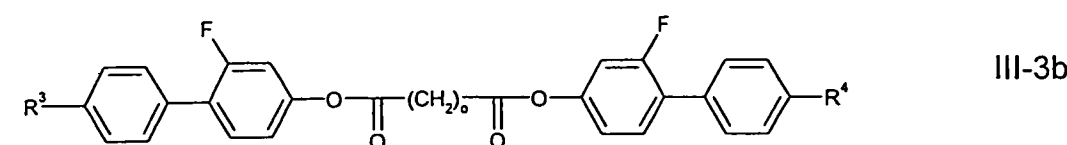
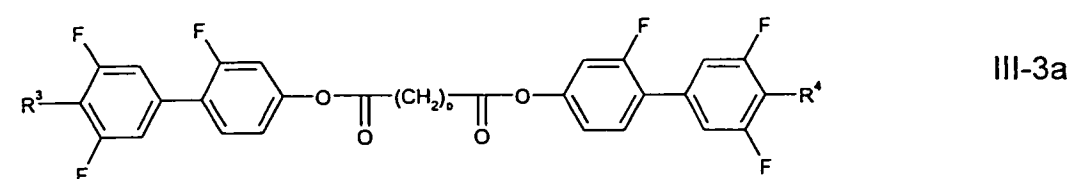
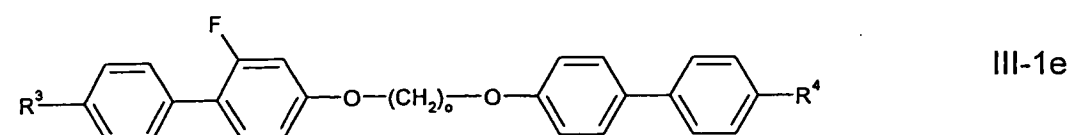
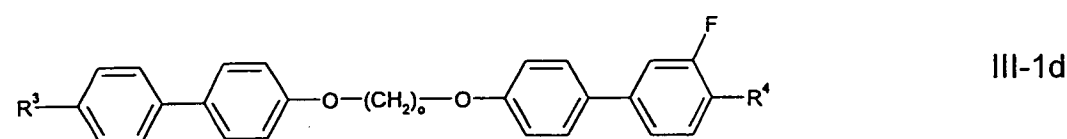
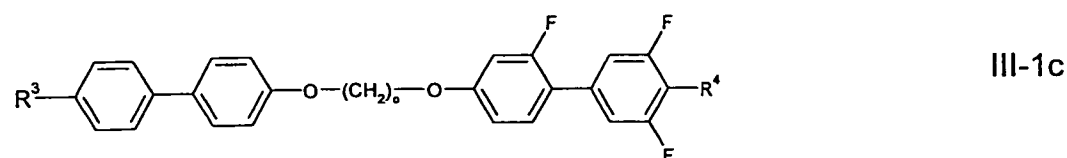
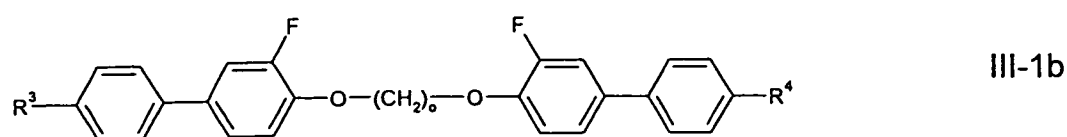
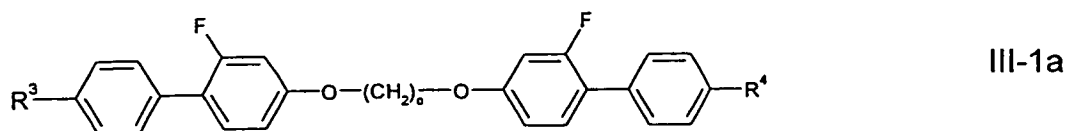
在本發明之另一較佳實施例中，式III之對掌性化合物包括至少一個係式IV之對掌性基團之間隔基團 Sp^1 。

式III中之 X^3 及 X^4 較佳地表示-O-、-CO-、-COO-、-OCO-、-O-CO-O-或單鍵。尤佳者係選自式III-1至III-4之下列化合物：



其中 R^3 及 R^4 定義於式III中， Z^1 定義於式II中且 o 及 r 在每次出現時獨立地如上文所定義，包含該等基團之較佳含義且其中 L 在每次出現時彼此獨立地較佳地係F、Cl、CN、OH、 NO_2 或具有1至7個C原子之視情況氟化之烷基、烷氧基或烷醯基，極佳係F、Cl、CN、OH、 NO_2 、 CH_3 、 C_2H_5 、 OCH_3 、 OC_2H_5 、 COCH_3 、 COC_2H_5 、 COOCH_3 、 COOC_2H_5 、 CF_3 、 OCF_3 、 OCHF_2 、 OC_2F_5 ，特定而言係F、Cl、CN、 CH_3 、 C_2H_5 、 OCH_3 、 COCH_3 及 OCF_3 ，最佳係F、Cl、 CH_3 、 OCH_3 及 COCH_3 。

本發明之尤佳混合物包括式 III-1a 至 III-1e 及 III-3a 至 III-3b 之一或多種化合物。



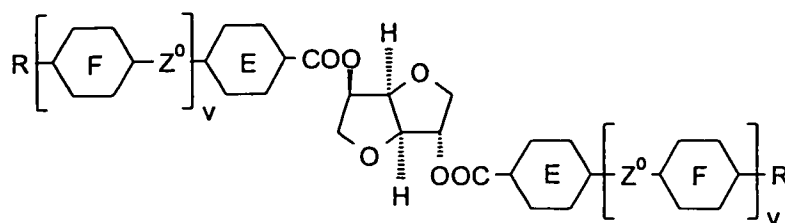
在本發明之一較佳實施例中，液晶介質係由 2 至 25、較佳地 3 至 15 種式 III 化合物組成。

液晶介質中之式 III 化合物之量較佳為總混合物之 10 重量% 至 95 重量%、特定而言 15 重量% 至 90 重量%、極佳地 20 重量% 至 85 重量%。

較佳地，介質中之式 III-1a 及 / 或 III-1b 及 / 或 III-1c 及 / 或 III-1e 及 / 或 III-3a 及 / 或 III-3b 之化合物之總體比例較佳地為至少 70 重量%。

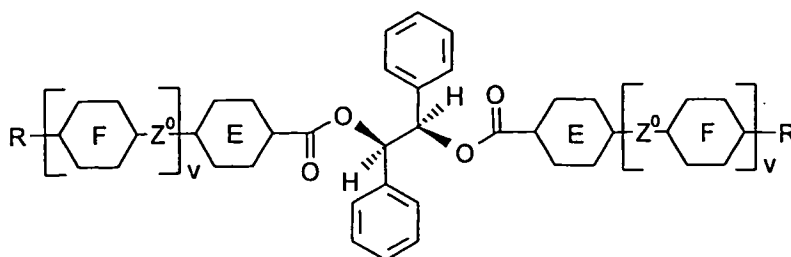
本發明之尤佳介質包括至少一或多種自身無需展現液晶相且自身得到良好均勻配向之對掌性摻雜劑。

尤佳者係選自以下之對掌性摻雜劑：式 IV



IV

及式 V



V

包含各別 (S,S) 對映異構體，

其中 E 及 F 各自獨立地係 1,4-伸苯基或反式-1,4-伸環己基， v 為 0 或 1， Z^0 係 $-COO-$ 、 $-OCO-$ 、 $-CH_2CH_2-$ 或單鍵，且 R 係具有 1 至 12 個 C 原子之烷基、烷氧基或烷醯基。

式 IV 化合物及其合成闡述於 WO 98/00428 中。尤佳者係如下表 D 中所展現之化合物 CD-1。式 V 化合物及其合成闡述於 GB 2,328,207 中。

尤佳者係具有高螺旋扭轉力 (HTP) 之對掌性摻雜劑，特定而言係彼等揭示於 WO 98/00428 中者。

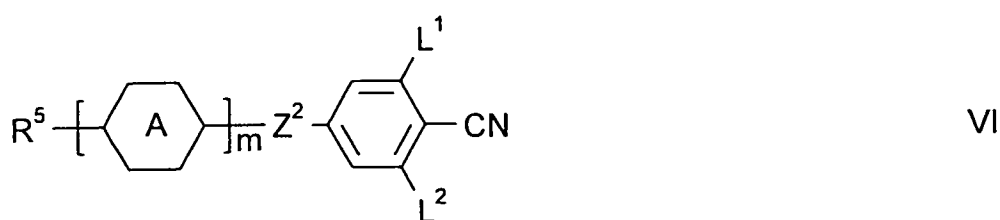
其他常用對掌性摻雜劑係(例如)市售R/S-5011、CD-1、R/S-811及CB-15(來自Merck KGaA, Darmstadt, 德國)。

上述對掌性化合物R/S-5011及CD-1及式IV及V之化合物展現極高螺旋扭轉力(HTP)，且由此尤其用於本發明目的。

液晶介質較佳地包括較佳地1至5種、特定而言1至3種、極佳地1或2種較佳地選自上式IV、特定而言CD-1及/或式V及/或R-5011或S-5011之對掌性摻雜劑，極佳地對掌性化合物係R-5011、S-5011或CD-1。

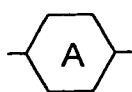
液晶介質中之對掌性化合物之量較佳為總混合物之1重量%至20重量%、特定而言1重量%至15重量%、極佳地1重量%至10重量%。

其他較佳者係包括一或多種選自下列式VI之添加劑之液晶介質

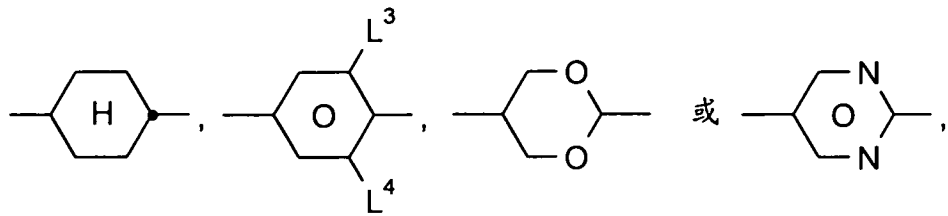


其中

R^5 係具有至多12個C原子之烷基、烷氧基、烯基或烯氧基，



係

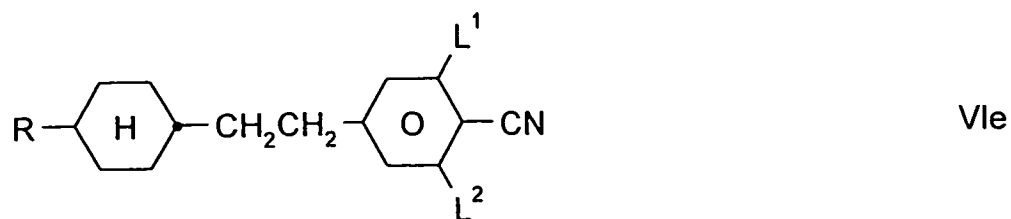
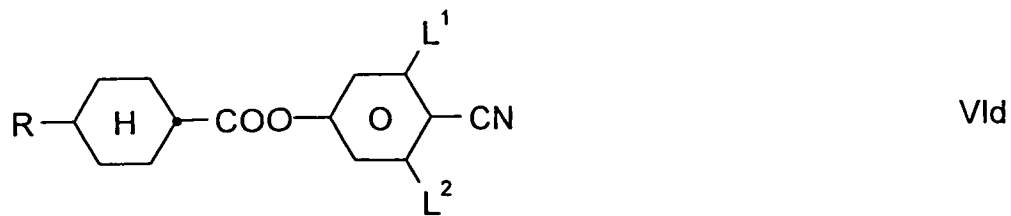
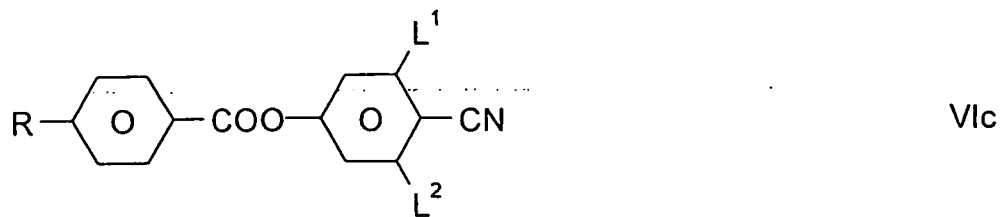
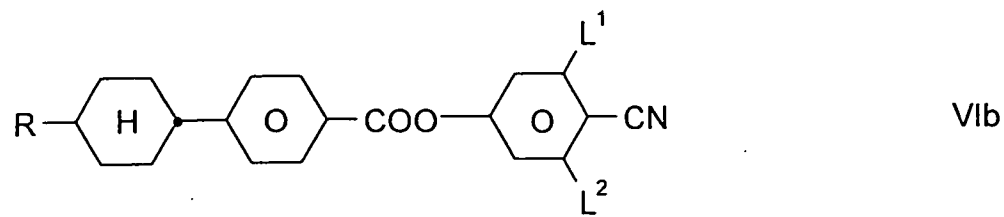


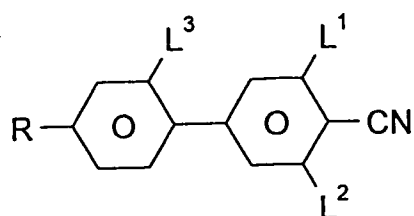
L^1 至 L^4 各自獨立地係 H 或 F，

Z^2 係 -COO-、-CH₂CH₂- 或單鍵，

m 為 1 或 2

式 VI 之尤佳化合物係選自下列式





VI f

其中R具有上述R⁵含義中之一者且L¹、L²及L³具有上述含義。

液晶介質較佳地包括較佳地1至5種、特定而言1至3種、極佳地1或2種較佳地選自上述式VIa至VI f、極佳地選自式VI f之添加劑。

液晶介質中之式VI之適宜添加劑之量較佳為總混合物之1重量%至20重量%、特定而言1重量%至15重量%、極佳地1重量%至10重量%。

本發明之液晶介質可以常規濃度含有其他添加劑。該等其他成份之總濃度以總混合物計介於0.1%至10%、較佳地0.1%至6%之間。所用個別化合物各自之濃度較佳地介於0.1%至3%之間。在本申請案中該等及類似添加劑之濃度並不計入液晶介質之液晶組份及化合物之濃度值及範圍內。此亦適用於混合物中所使用之二向色性染料之濃度，該等二向色性染料在分別指定主體介質之化合物或組份之濃度時並不計算在內。各別添加劑之濃度總是相對於最終摻雜混合物給出。

本發明之液晶介質係由若干種、較佳地3至30種、更佳地4至20種及最佳地4至16種化合物組成。以習用方式混合該等化合物。通常，將以較少量使用之所需量化合物溶於以較大量使用之化合物中。在溫度高於以較高濃度使用之

化合物之澄清點之情形下，尤其易於觀察到溶解過程之完成。然而，亦可藉由其他習用方法製備該等介質，例如使用可為(例如)化合物之均質或低共熔混合物之所謂的預混合物或使用所謂的多瓶系統，該等成份自身為即用混合物。

尤佳混合物概念如下文所指示(所用首字母縮寫詞闡釋於表A中)。

本發明混合物較佳地包括

- 一或多種式I化合物，其總濃度範圍為總混合物之1重量%至50重量%、特定而言5重量%至40重量%、極佳地10重量%至30重量%，較佳地該等化合物係選自式Ia-1a、Ia-2a、Ia-2b、Ia-17c、Ia-8e、Ia-3f、Ia-5f、Ia-6f、Ia-12f、Ia-23f、Ib-27f、Ib-61f及Ib-63f之群，尤佳地其包括

- N-GIGIGI-n-GGG-N、特定而言N-GIGIGI-9-GGG-N，基於總體混合物，其較佳濃度>5%、特定而言10-30%，

及/或

- N-PGI-n-GP-N、較佳地N-PGI-9-GP-N，基於總體混合物，其較佳濃度>5%、特定而言15-50%，

及/或

- 一或多種式III化合物，其總濃度範圍為總混合物之10重量%至95重量%、特定而言15重量%至90重量%、極佳地

20重量%至85重量%，較佳地該等化合物係選自式III-1a至III-1e及III-3a至III-3b，尤佳地其包括

- N-PGI-ZI-n-Z-GP-N、較佳地N-PGI-ZI-7-Z-GP-N及/或N-PGI-ZI-9-Z-GP-N，基於總體混合物，其較佳濃度>5%、特定而言10-30%，

及/或

- F-UIGI-ZI-n-Z-GU-F、較佳地F-UIGI-ZI-9-Z-GU-F，基於總體混合物，其較佳濃度>5%、特定而言10-30%，

及/或

- F-PGI-O-n-O-PP-N、較佳地F-PGI-O-9-O-PP-，基於總體混合物，其較佳濃度>1%、特定而言1-20%，

及/或

- N-PP-O-n-O-PG-OT、較佳地N-PP-O-7-O-PG-OT，基於總體混合物，其較佳濃度>5%、特定而言5-30%，

及/或

- N-PP-O-n-O-GU-F、較佳地N-PP-O-9-O-GU-F，基於總體混合物，其較佳濃度>1%、特定而言1-20%，

及/或

- F-PGI-O-n-O-GP-F、較佳地F-PGI-O-7-O-GP-F及/或F-PGI-O-9-O-GP-F，基於總體混合物，其較佳濃度>1%、特定而言1-20%，

及/或

- 一或多種式VI之適宜添加劑，其總濃度範圍為總混合物之1重量%至20重量%、特定而言1重量%至15重量%、極佳地1重量%至10重量%，較佳地該等化合物選自式VI-1至VI-f，尤佳地其包括
 - K15，基於總體混合物，其較佳濃度 $>1\%$ 、特定而言1-20%，

及/或

- 一或多種對掌性化合物，較佳地其總濃度範圍為總混合物之1重量%至20重量%、特定而言1重量%至15重量%、極佳地1重量%至10重量%，較佳地該等化合物係選自式IV、V及R-5011或S-5011，尤佳地其包括
 - R-5011、S-5011或Cd-1，基於總體混合物，其較佳濃度 $>1\%$ 、特定而言1-20%。

式I之雙液晶原化合物及包括其之液晶介質可用於液晶顯示器中，例如STN、TN、AMD-TN、溫度補償、賓-主、相變或表面穩定或聚合物穩定膽固醇結構(SSCT, PSCT)顯示器，特定而言用於以下中：撓變電子裝置、主動及被動光學元件(例如偏振器、補償器、反射器、配向層、濾色器或全像攝影元件)、黏著劑、具有各向異性機械性質之合成樹脂、化妝品、診斷學、液晶顏料、裝飾及安全應用、非線性光學、光學資訊儲存或對掌性摻雜劑。

式I化合物及可自其獲得之混合物尤其可用於撓變電子液晶顯示器。因此，本發明之另一目標係撓變電子顯示

器，其包括一或多種式I化合物或包括含有一或多種式I化合物之液晶介質。

式I之發明性雙液晶原化合物及其混合物可藉由專家已知之方法(例如表面處理或電場)以其膽固醇相配向成不同定向狀態。舉例而言，其可配向成平面(格蘭瓊(Grandjean))狀態、焦點圓錐狀態或垂直狀態。包括極性基團且具有強偶極矩之式I之發明性化合物可進一步經受撓變電子切換，且可由此用於光電切換或液晶顯示器中。

下文針對式I之發明性化合物試樣以實例方式詳細闡述本發明一較佳實施例之不同定向狀態間之切換。

根據此較佳實施例，將試樣置於包括兩個使用電極層(例如ITO層)塗覆之平面平行玻璃片之單元中，並以其膽固醇相配向成平面狀態，其中膽固醇螺旋之軸垂直於單元壁進行定向。此狀態亦稱為格蘭瓊狀態，且可在(例如)偏振顯微鏡中觀察到之試樣結構稱為格蘭瓊結構。可(例如)藉由對單元壁進行表面處理(例如藉由使用諸如聚醯亞胺等配向層進行擦拭及/或塗覆)來達成平面配向。

可進一步藉由以下方式來達成具有高配向品質及僅較少缺陷之格蘭瓊狀態：將試樣加熱至各向同性相，隨後在接近對掌性向列相-各向同性相轉變之溫度下冷卻至對掌性向列相，及擦拭單元。

在平面狀態中，試樣展現選擇性反射入射光，其中反射之中心波長取決於材料之螺旋節距及平均折射率。

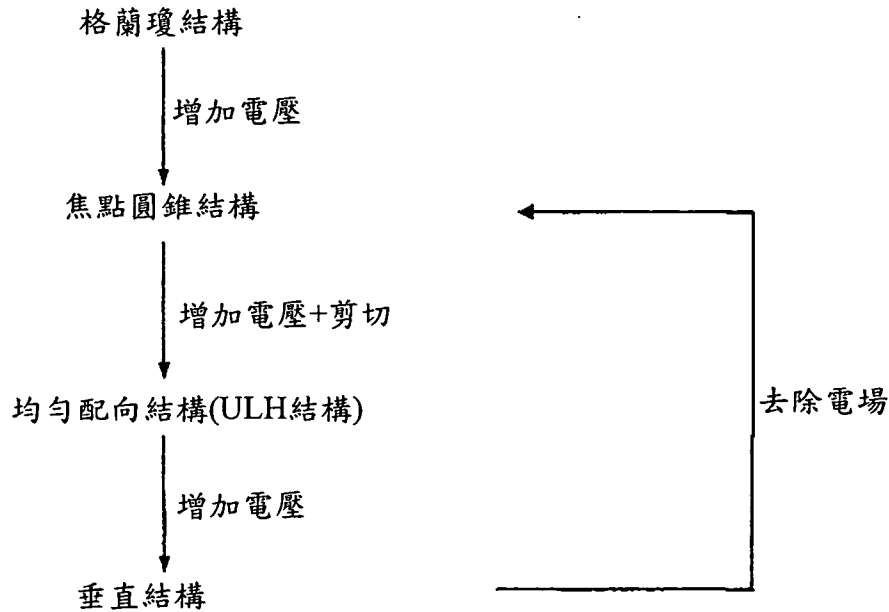
在向電極施加電場(例如以10 Hz至kHz之頻率及至多12 $V_{rms}/\square m$ 之幅值)時，試樣切換至垂直狀態，其中螺旋解開且分子平行於電場(亦即垂直於電極平面)進行定向。在垂直狀態中，在垂直日光中觀看時試樣可透光，且在置於交叉偏振器之間時表現為黑色。

在垂直狀態中減小或去除電場後，試樣採用焦點圓錐結構，其中分子展現螺旋扭轉結構且螺旋軸垂直於電場(亦即平行於電極平面)進行定向。亦可藉由僅向平面狀態之試樣施加弱電場來達成焦點圓錐狀態。在焦點圓錐狀態中，在垂直日光中觀看時試樣發生散射，且在交叉偏振器之間表現為明亮。

處於不同定向狀態中之發明性化合物之試樣展現不同光透射。因此，可藉由量測試樣端視所施加電場強度之光透射來控制各別定向狀態以及其配向品質。因此，亦可測定達成特定定向狀態及該等不同狀態間之轉變所需之電場強度。

在式I之發明性化合物之試樣中，上述焦點圓錐狀態係由許多無序雙折射小結構域組成。藉由施加大於用於使焦點圓錐結構成核(較佳地使用額外單元剪切)之電場的電場，達成均勻配向結構，其中在較大配向良好之區域中螺旋軸平行於電極平面。根據關於現有狀態對掌性向列材料之文獻(例如P. Rudquist等人，*Liq. Cryst.* 23 (4), 503 (1997))，此結構亦稱為均勻臥式螺旋(ULH)結構。需要此結構來描述發明性化合物之撓變電子性質。

在下文中給出在增加或降低電場後於經擦拭聚醯亞胺基板上之式I之發明性化合物試樣中通常所觀察到之結構順序：



自ULH結構開始，可藉由施加電場使發明性撓變電子化合物及混合物經受撓變電子切換。此使得材料之光軸在單元基板之平面中發生旋轉，從而在將材料置於交叉偏振器之間時引起透射變化。發明性材料之撓變電子切換進一步詳細闡述於上文引言及實例中。

亦可藉由以下方式獲得ULH結構：自焦點圓錐結構開始，向試樣施加具有高頻率(例如10 kHz)之電場同時自各向同性相緩慢冷卻至膽固醇相並剪切單元。不同化合物之場頻率可有所不同。

式I之雙液晶原化合物尤其用於撓變電子液晶顯示器中，此乃因其可容易地配向成宏觀均勻定向，且在液晶介質中得到彈性常數 k_{11} 之較高值及較高撓變電子係數 e 。

液晶介質較佳地展現

$k_{11} > 1 \times 10^{-10}$ N及撓變電子係數

$e > 1 \times 10^{-10}$ C/m。

除用於撓變電子裝置中外，發明性雙液晶原化合物以及其混合物亦適用於其他類型顯示器及其他光學及光電應用中，例如光學補償或偏振膜、濾色器、反射性膽固醇、旋光強度及光學資訊儲存。

本發明之另一態樣係關於顯示單元，其中單元壁展現混合配向條件。術語顯示單元中或兩個基板之間之液晶或液晶原材料之「混合配向」或定向意指，毗鄰第一單元壁或位於第一基板上之液晶原基團展現垂直定向且毗鄰第二單元壁或位於第二基板上之液晶原基團展現平面定向。

術語顯示單元中或基板上之液晶或液晶原材料之「垂直配向」或定向意指，液晶或液晶原材料中之液晶原基團實質上分別垂直於單元或基板平面進行定向。

術語顯示單元中或基板上之液晶或液晶原材料之「平面配向」或定向意指，液晶或液晶原材料中之液晶原基團實質上分別平行於單元或基板平面進行定向。

本發明之一較佳實施例之撓變電子顯示器包括兩個平面平行基板(較佳係在其內表面上使用諸如氧化銦錫(ITO)等透明導電層覆蓋之玻璃片)及提供於基板之間之撓變電子液晶介質，其特徵在於內基板表面中之一者對於液晶介質而言展現垂直配向條件且相對內基板表面展現平面配向條件。

可(例如)藉助施加於基板頂部中配向層(例如擦拭聚醯亞胺或濺鍍 SiO_x 之層)來達成平面配向。

另一選擇為，可直接擦拭基板，亦即並不施加其他配向層。舉例而言，可藉助擦拭布(例如絲絨布)或使用經擦拭布塗覆之平坦條來達成擦拭。在本發明之一較佳實施例中，藉助至少一個擦拭輥(例如刷塗基板之快速旋轉輥)或藉由將基板置於至少兩個輥之間來達成擦拭，其中在每一情形下至少一個輥視情況經擦拭布覆蓋。在本發明之另一較佳實施例中，藉由至少部分地以界定角度圍繞較佳地經擦拭布塗覆之輥捲繞基板來達成擦拭。

可(例如)藉助塗覆於基板頂部之配向層來達成垂直配向。用於玻璃基板上之適宜配向劑係(例如)烷基三氯矽烷或卵磷脂，而對於塑膠基板而言，可使用卵磷脂、二氧化矽或高傾斜聚醯亞胺定向膜之薄層作為配向劑。在本發明之一較佳實施例中，經二氧化矽塗覆之塑膠膜用作基板。

達成平面或垂直配向之其他適宜方法闡述於(例如)J. Cognard, Mol.Cryst.Liq.Cryst. 78, 增刊1, 1-77(1981)中。

藉由使用具有混合配向條件之顯示單元，可達成撓變電子切換之極高切換角度、快速反應時間及良好對比度。

本發明之撓變電子顯示器亦可包括塑膠基板來代替玻璃基板。塑膠膜基板尤其適於藉由如上文所闡述之擦拭輥進行擦拭處理。

本發明之另一目標在於，式I化合物在添加至向列液晶混合物中時會產生位於向列相下方之相。

因此，本發明中式I之雙液晶原化合物使得在通常並不展現第二向列相證據之向列混合物中誘導此相。另外，改變式I化合物之量可使得第二向列相之相行為適用於所需溫度。

給出關於此情形之實例且其可獲得混合物尤其可用於撓變電子液晶顯示器中。因此，本發明之另一目標係包括一或多種展現第二向列相之式I化合物之液晶介質。

據信，無需進一步詳細闡述，熟習此項技術者即可使用前文闡述應用本發明至最詳盡的程度。因此，下列實例僅應理解為闡釋之目的，且無論如何不應理解為以任何方式限制其餘揭示內容。

除非上下文另外明確指明，否則本文術語之本文所用複數形式應理解為包含單數形式且反之亦然。

在本說明書之闡述及技術方案中，詞語「包括(comprise)」及「含有(contain)」及該等詞語之變化形式(例如「包括(comprising及comprises)」)意指「包括但不限於」且並非意欲(且不)將其他組份排除在外。

應瞭解，可對本發明之前述實施例作出改變，而仍屬於本發明之範圍內。除非另有說明，否則本說明書中所揭示之每一特徵皆可由適合於相同、等效或類似目的之替代特徵所代替。因此，除非另有說明，否則每一所揭示特徵僅係一類等效或類似特徵之一個實例。

本說明書中所揭示之全部特徵可以任一組合進行組合，只是至少一些該等特徵及/或步驟相互排斥之組合除外。

特定而言，本發明之較佳特徵適用於本發明之全部態樣且可以任一組合使用。同樣，非必需組合中所闡述之特徵可單獨使用(不組合使用)。

在上文及下列實例中，除非另有說明，否則所有溫度皆未經校正以攝氏度給出，且所有份數及百分比皆按重量計。

使用下列縮寫來闡釋化合物之液晶相行為：K=結晶；N=向列；N2=第二向列；S=層列；Ch=膽固醇；I=各向同性；Tg=玻璃轉變。符號之間之數值指示相變溫度(以 $^{\circ}\text{C}$ 表示)。


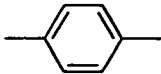
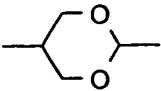
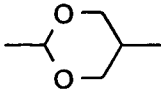
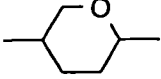
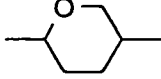
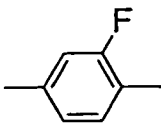
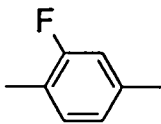
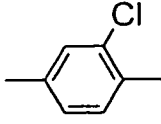
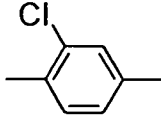
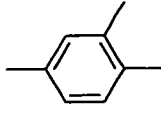
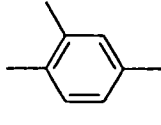
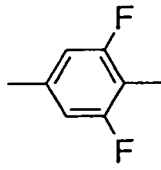
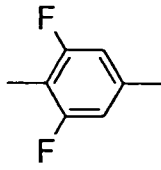
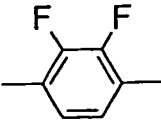
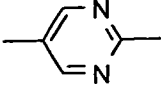
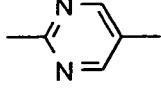
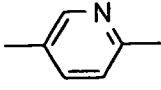
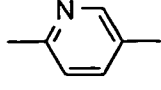
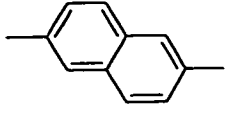
在本申請案且尤其下列實例中，液晶化合物之結構由縮寫(亦稱為「首字母縮寫詞」)表示。根據下列三個表A至C直接將縮寫轉變成相應結構。

所有基團 $\text{C}_n\text{H}_{2n+1}$ 、 $\text{C}_m\text{H}_{2m+1}$ 及 $\text{C}_l\text{H}_{2l+1}$ 較佳地係分別具有 n 、 m 及 l 個C原子之直鏈烷基，所有基團 C_nH_{2n} 、 C_mH_{2m} 及 C_lH_{2l} 較佳地分別係 $(\text{CH}_2)_n$ 、 $(\text{CH}_2)_m$ 及 $(\text{CH}_2)_l$ 且 $-\text{CH}=\text{CH}-$ 較佳地分別係反式-或E伸乙烯基。

表A列示用於環單元之符號，表B列示彼等用於連接基團之符號且表C列示彼等用於分子之左手端及右手端基團之符號。

表D列示實例性分子結構以及其各別代碼。

表 A：環單元

C		P	
D		DI	
A		AI	
G		GI	
G(Cl)		GI(Cl)	
G(Me)		GI(Me)	
U		UI	
Y			
M		MI	
N		NI	
np			

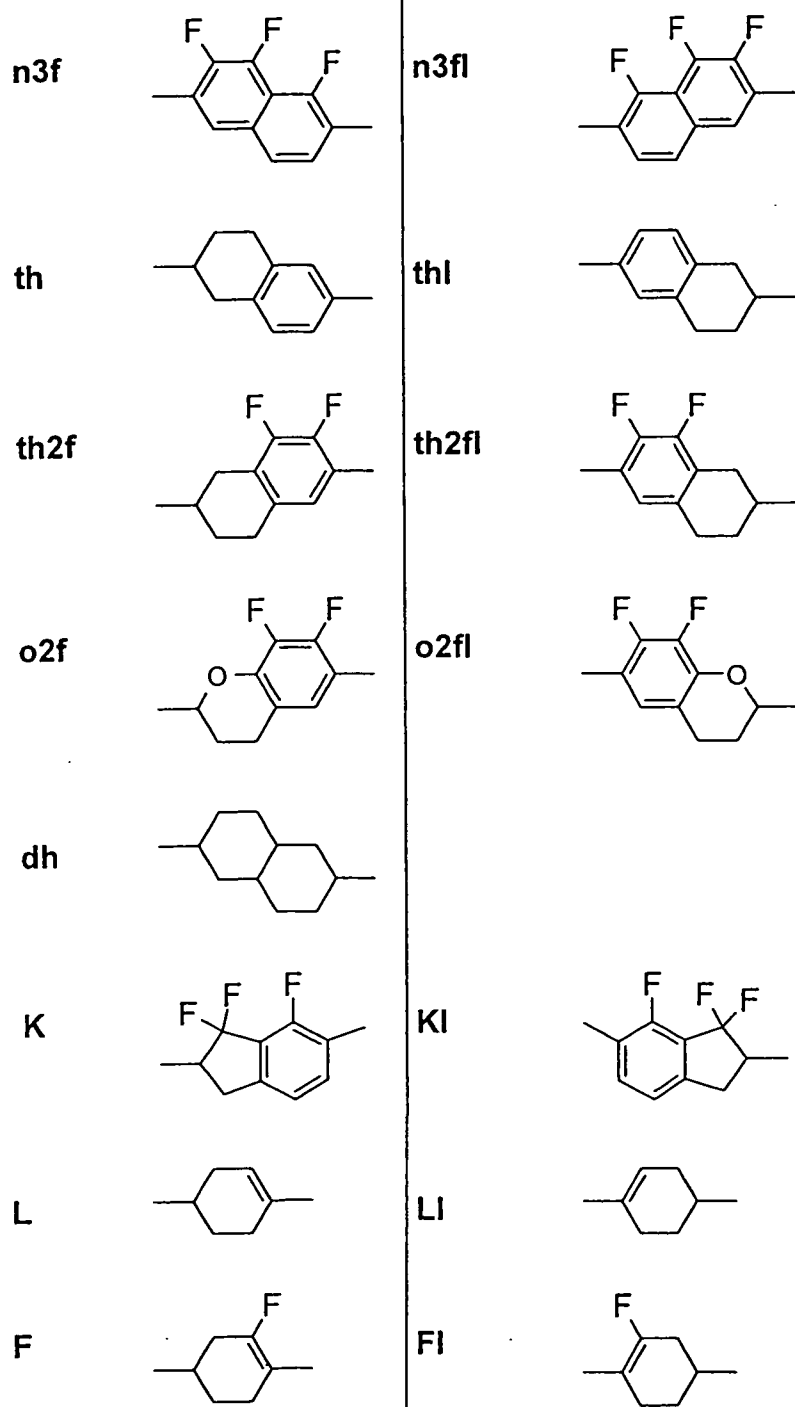


表 B：連接基團

E	-CH ₂ -CH ₂ -		
V	-CH=CH-		
T	-C≡C-		
W	-CF ₂ -CF ₂ -		
B	-CF=CF-		
Z	-CO-O-	ZI	-O-CO-
X	-CF=CH-	XI	-CH=CF-
O	-CH ₂ -O-	OI	-O-CH ₂ -
Q	-CF ₂ -O-	QI	-O-CF ₂ -

表 C：末端基團

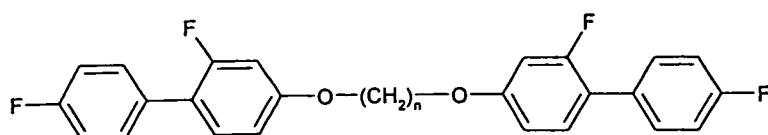
左手側，單獨或與其他基團組合使用		右手側，單獨或與其他基團組合使用	
-n-	C _n H _{2n+1} -	-n	-C _n H _{2n+1}
-nO-	C _n H _{2n+1} -O-	-nO	-O-C _n H _{2n+1}
-V-	CH ₂ =CH-	-V	-CH=CH ₂
-nV-	C _n H _{2n+1} -CH=CH-	-nV	-C _n H _{2n} -CH=CH ₂
-Vn-	CH ₂ =CH-C _n H _{2n} -	-Vn	-CH=CH-C _n H _{2n+1}
-nVm-	C _n H _{2n+1} -CH=CH-C _m H _{2m} -	-nVm	-C _n H _{2n} -CH=CH-C _m H _{2m+1}
-N-	N≡C-	-N	-C≡N
-S-	S=C=N-	-S	-N=C=S
-F-	F-	-F	-F
-CL-	Cl-	-CL	-Cl
-M-	CFH ₂ -	-M	-CFH ₂
-D-	CF ₂ H-	-D	-CF ₂ H
-T-	CF ₃ -	-T	-CF ₃
-MO-	CFH ₂ O-	-OM	-OCFH ₂
-DO-	CF ₂ HO-	-OD	-OCF ₂ H
-TO-	CF ₃ O-	-OT	-OCF ₃
-A-	H-C≡C-	-A	-C≡C-H
-nA-	C _n H _{2n+1} -C≡C-	-An	-C≡C-C _n H _{2n+1}
-NA-	N≡C-C≡C-	-AN	-C≡C-C≡N

左手側，僅與其他基團組合使用		右手側，僅與其他基團組合使用	
-...n...-	-C _n H _{2n} -	-...n...	-C _n H _{2n} -
-...M...-	-CFH-	-...M...	-CFH-
-...D...-	-CF ₂ -	-...D...	-CF ₂ -
-...V...-	-CH=CH-	-...V...	-CH=CH-
-...Z...-	-CO-O-	-...Z...	-CO-O-
-...ZI...-	-O-CO-	-...ZI...	-O-CO-
-...K...-	-CO-	-...K...	-CO-
-...W...-	-CF=CF-	-...W...	-CF=CF-

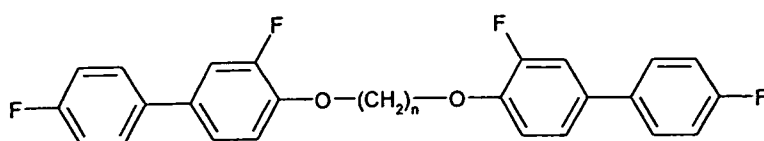
其中n及m各自係整數且三個點「...」指示用於此表之其他符號之空間。

較佳地，除式I化合物外，本發明之液晶介質包括一或多種選自下表中之式之化合物群的化合物。

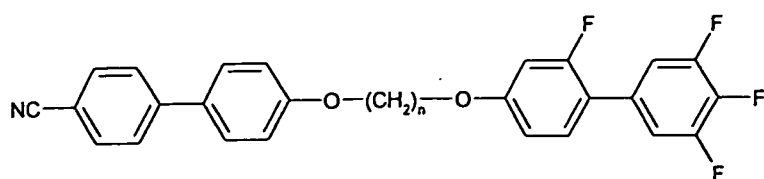
表D



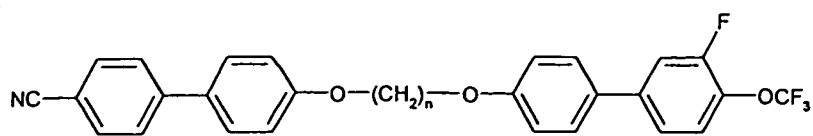
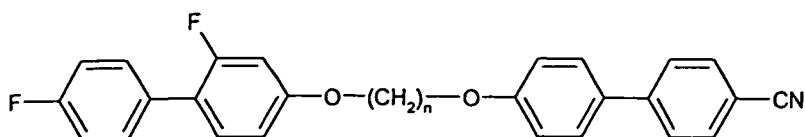
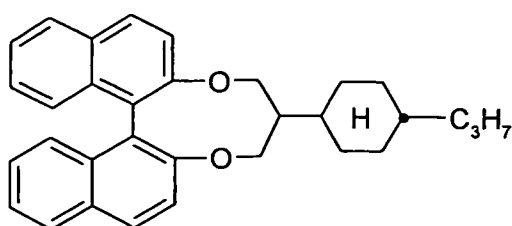
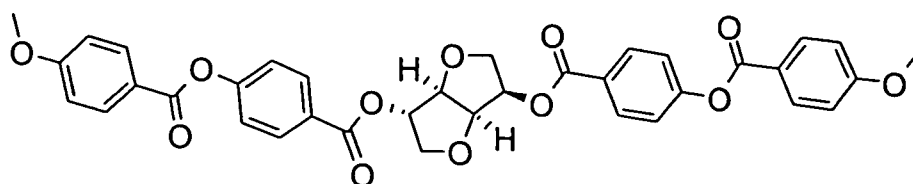
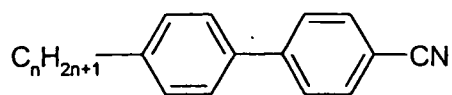
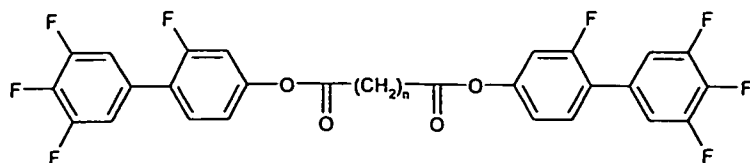
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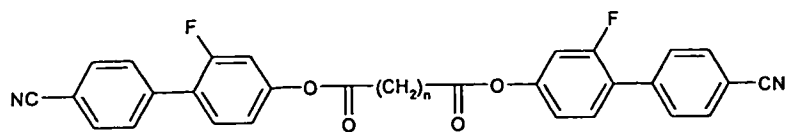


F-PG-O-n-O-GIP-F

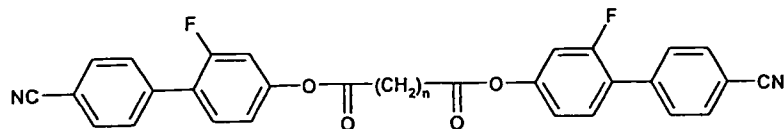


N-PP-O-n-O-GU-F

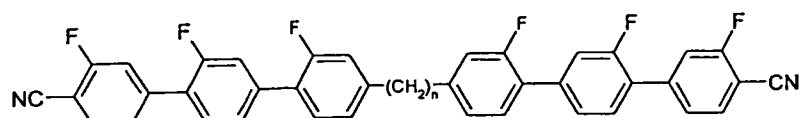
**N-PP-O-n-O-PG-OT****F-PGI-O-n-O-PP-N****R-5011 respectively S-5011****CD-1****K3n****F-UIGI-ZI-n-Z-GU-F**



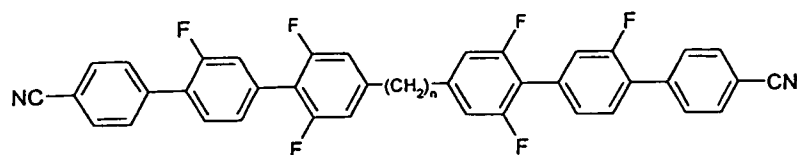
N-PGI-ZI-n-Z-GP-N



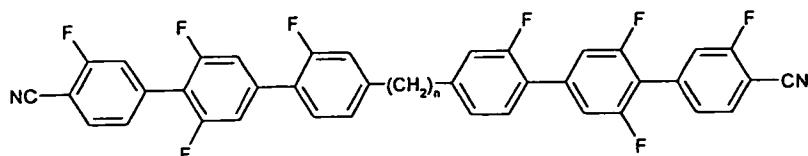
F-PGI-ZI-n-Z-GP-F



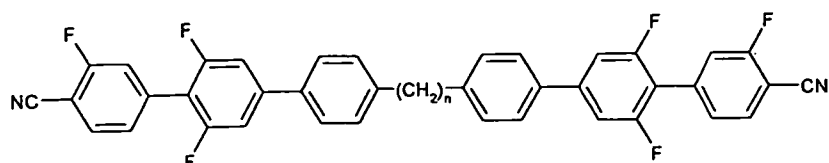
N-GIGIGI-n-GGG-N



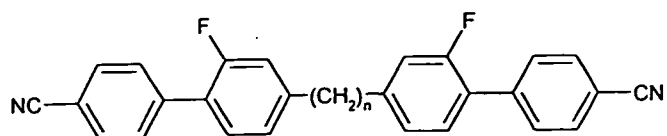
N-PGIUI-n-UGP-N



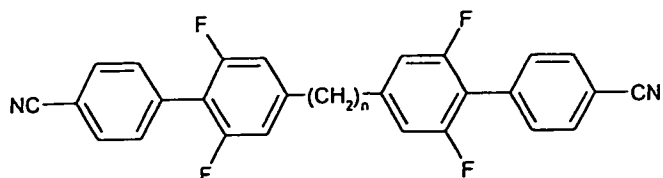
N-GIUIGI-n-GUG-N



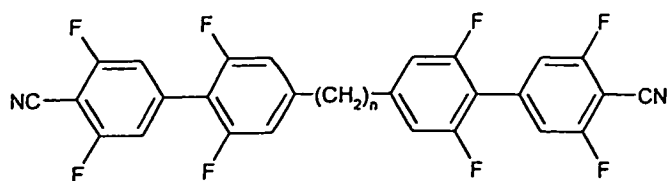
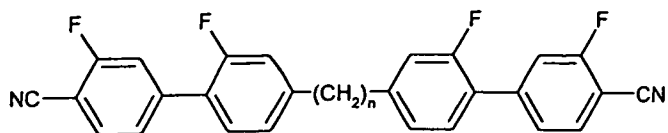
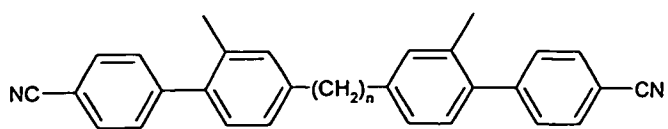
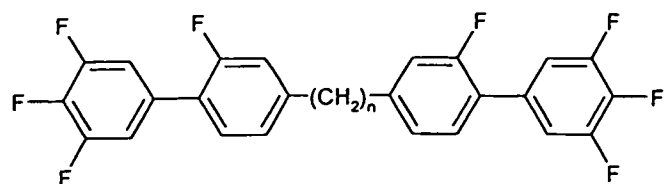
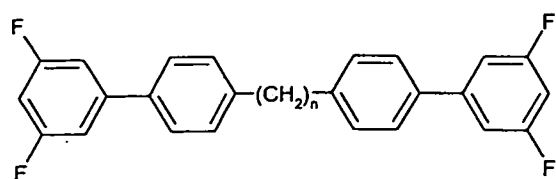
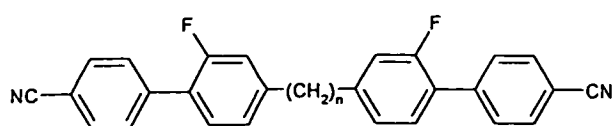
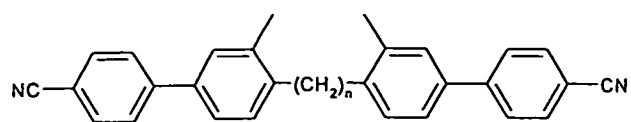
N-GIUIP-n-PUG-N



N-PGI-n-GP-N

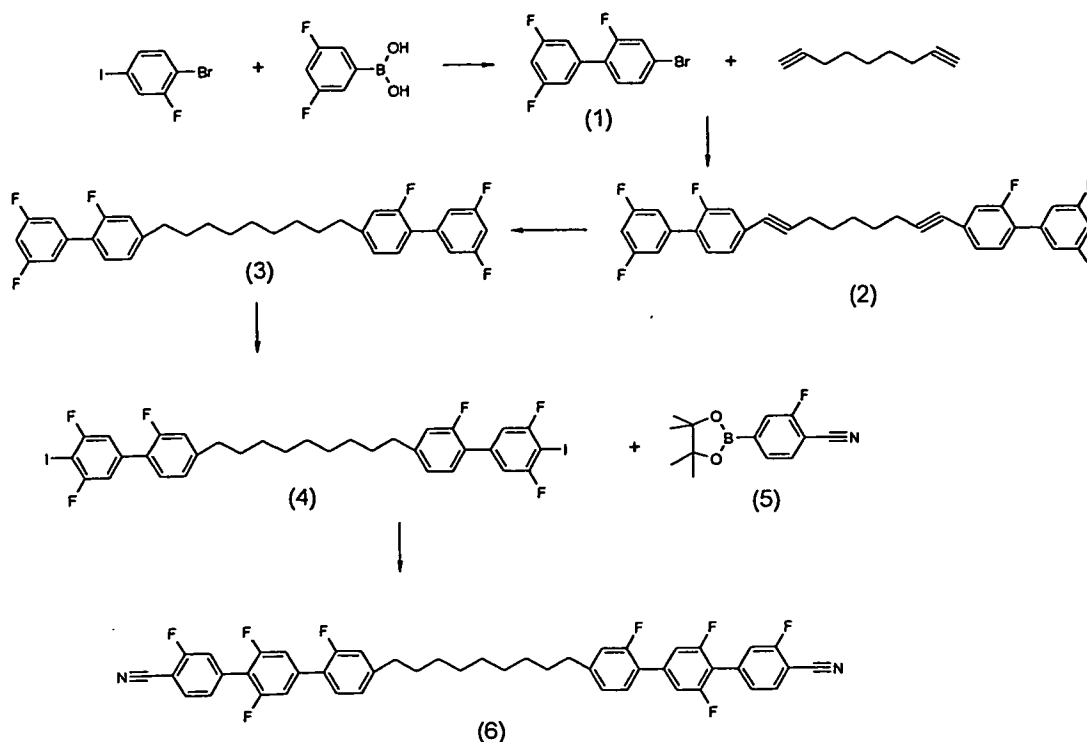


N-PUI-n-UP-N

**N-UIUI-n-UU-N****N-GIGI-n-GG-N****N-PGI(Me)-n-G(Me)P-N****F-UIGI-n-GU-F****UIP-n-PU****N-PGI-n-GP-N****N-PG(Me)-n-GI(Me)P-N****實例**

實例 1：式 I 化合物 (其中式 I 中之 R^1 -MG¹-及 R^2 -MG²-相同)

之一般合成



(1) 之合成

向圓底燒瓶中添加1-溴-3-氟碘苯(53.3 g, 0.177 mol)以及3,5-二氟苯硼酸(29.0 g, 0.184 mol)。添加四氫呋喃(500 ml)且在氮下攪拌混合物直至溶解為止。向反應液中添加碳酸鉀(36.7 g, 0.265 mol)之水溶液(100 ml)。添加觸媒雙(三苯基膦)-二氯化鈹(II)(1.98 g, 2.83 mmol)且將反應液加熱至回流保留18小時。冷卻反應液並使用水稀釋，然後使用稀鹽酸酸化。分離各層且使用水洗滌有機物，然後濃縮以獲得褐色固體產物。

將粗製固體溶於二氯甲烷中並藉由濃縮吸附於矽膠(100 g)上。藉由管柱層析(使用石油精(40-60°C)及二氯甲烷之混合物洗脫)來純化材料以獲得黃色固體形式之純化產物。

(2) 之合成

將2,-3'-5'-三氟-4-溴聯苯(26.1 g, 0.091 mol)添加至圓底燒瓶中。添加三乙胺(25.0 ml)及四氫呋喃(50.0 ml)且完全抽空並使用氮代替。添加碘化銅(I)(0.404 g, 2.12 mmol)及雙(三苯基膦)二氯化鈹(II)(0.71 g, 1.01 mmol)，且將反應液抽空並使用氮代替。將反應混合物加熱至40°C且經30分鐘緩慢添加1,8-壬二炔(5.25 g, 0.044 mol)。將混合物在40°C下再加熱24小時，隨後在80°C下加熱48小時。

冷卻反應液並在真空下過濾以去除沈澱物。使用稀鹽酸化濾液並使用二乙醚萃取。使用水洗滌有機材料，然後濃縮以提供黑色固體產物(26.0 g)。將粗製固體溶於二氯甲烷中並吸附於50.0 g矽膠上。藉由管柱層析(使用存於汽油中之二氯甲烷之混合物洗脫產物)純化材料。

(3) 之合成

將材料(2)(21.5 g, 0.040 mol)溶於四氫呋喃(600 ml)中並通過Thalesnano氫化器。材料需要70巴壓力及60°C之條件以產生淺白色固體產物。

(4) 之合成

向圓底燒瓶中添加材料(3)(21.5 g, 0.04 mol)以及四氫呋喃(150 ml)。在氮下攪拌反應液並冷卻至-70°C。經45分鐘緩慢添加正丁基鋰溶液(1.6 M，存於己烷中，55.0 ml，0.087 mol)，並將反應液在-70°C下進一步攪拌一小時。緩慢添加存於四氫呋喃(125 ml)中之碘(45.8 g, 0.179 mol)之溶液以將溫度保持於-60°C與-70°C之間。將反應液攪拌過夜並升溫至室溫。藉由緩慢添加濕潤THF來終止反應，然

後添加水且然後添加乙酸乙酯。分離各層並使用乙酸乙酯將水層萃取三次。使用硫代硫酸鈉溶液(100 ml, 2 M, 存於水中)將有機物洗滌兩次, 然後使用水洗滌。濃縮以提供褐色固體。藉由自工業甲基化乙醇、丙酮及乙腈/丙酮依序重結晶來純化材料。

合成(5)

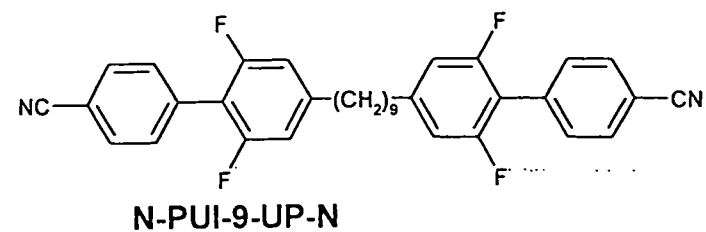
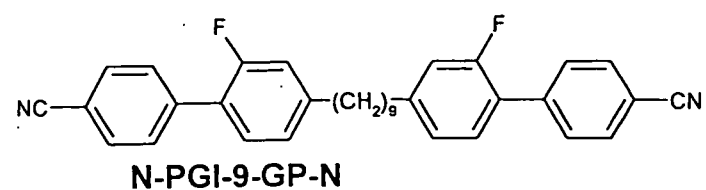
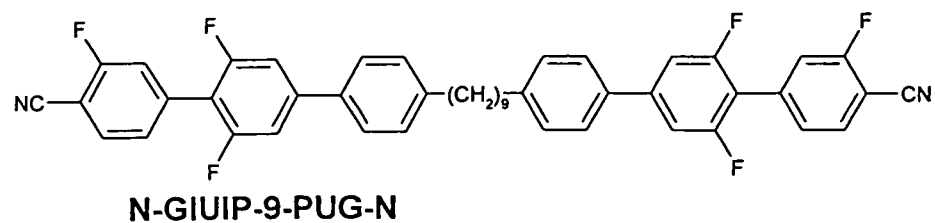
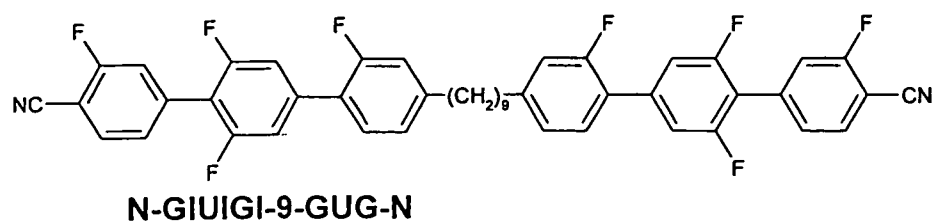
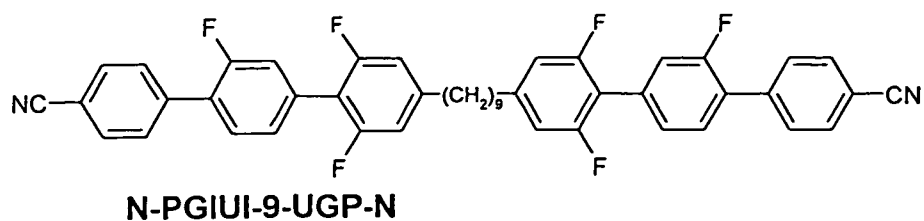
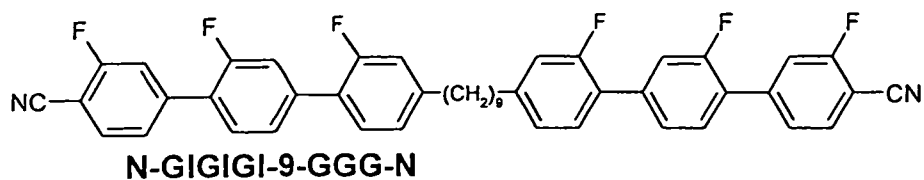
向圓底燒瓶中添加4-溴-2-氟苄腈(42.4 g, 212 mmol)以及雙(戊醯)二硼烷(59.8 g, 235 mmol)。將乙酸鉀(31.1 g, 317 mmol)、三氯己基膦(3.57 g, 12.7 mmol)、叁(二亞苄基丙酮)二鈹(0)(3.66 g, 6.36 mmol)及1,4-二噁烷(600 ml)一起添加至反應燒瓶中並將混合物在氮及80°C下攪拌72小時。冷卻反應混合物之後, 添加水及二乙醚並分離各層。使用鹽水及水洗滌有機材料, 然後濃縮成褐色固體。藉由自汽油/二氯甲烷重結晶來純化產物以獲得褐色結晶固體。

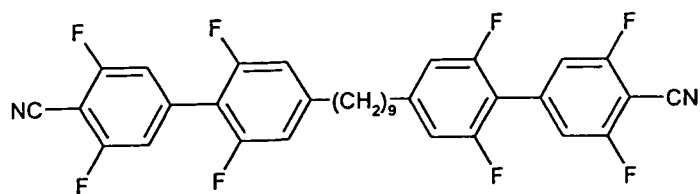
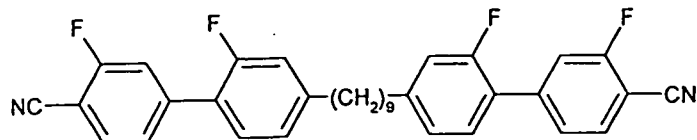
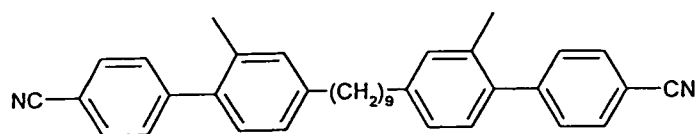
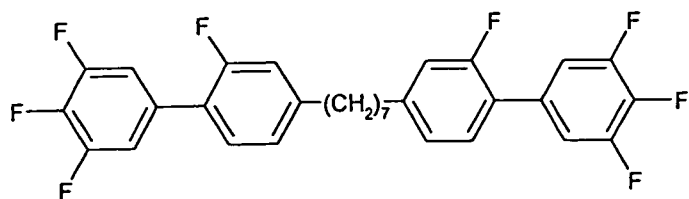
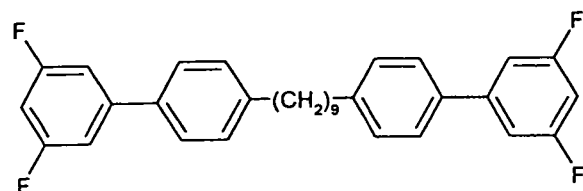
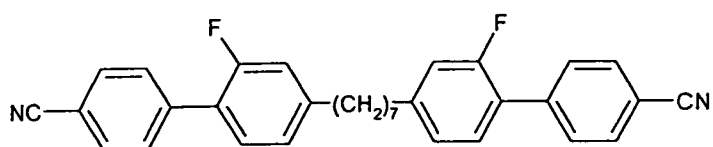
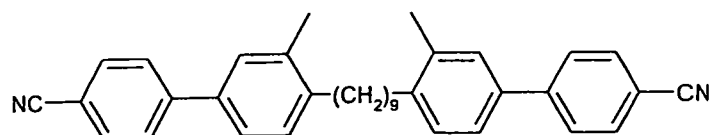
合成(6)

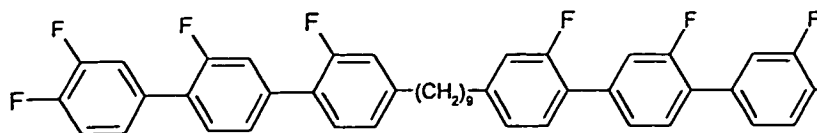
向圓底燒瓶中添加材料(4)(10.17 g, 12.8 mmol)及材料(5)(7.70 g, 31.2 mmol)並溶於四氫呋喃(250 ml)中。添加雙(三苯基膦)-二氯化鈹(II)(450.6 mg, 0.642 mmol)以及碳酸鈉(1 M, 存於水中, 77.0 ml, 77.0 mmol)之溶液。將反應液加熱至85°C保持24小時, 然後將其冷卻並使用水稀釋, 然後使用稀鹽酸酸化。分離各層且使用水洗滌有機層, 然後濃縮以得到褐色固產物體。藉由管柱層析(使用存於汽油中之40%乙酸乙酯洗脫產物)純化材料。藉由自首先丙

酮/甲醇、然後丙酮及最後IPA/汽油重結晶來進一步純化產物。

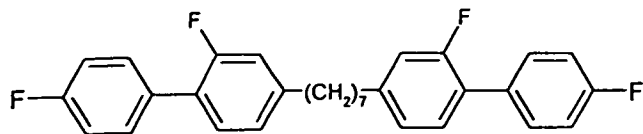
實例2：以類似方式製備式I之下列化合物



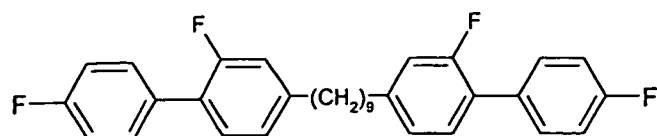
**N-UIUI-9-UU-N****N-GIGI-9-GG-N****N-PGI(Me)-9-G(Me)P-N****F-UIGI-7-GU-F****UIP-9-PU****N-PGI-7-GP-N****N-PG(Me)-9-GI(Me)P-N**



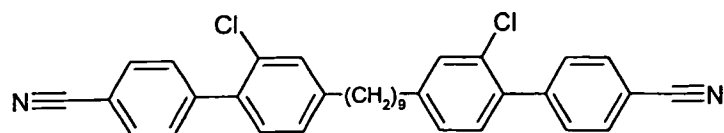
F-GIGIGI-9-GGG-F



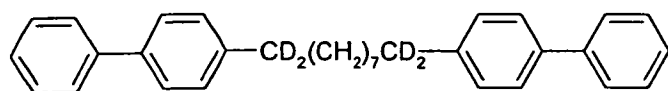
F-PGI-7-GP-F



F-PGI-9-GP-F

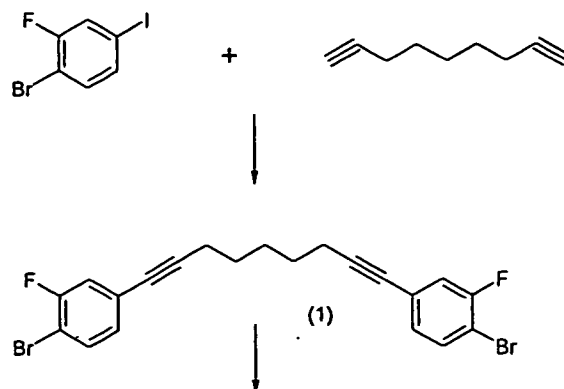


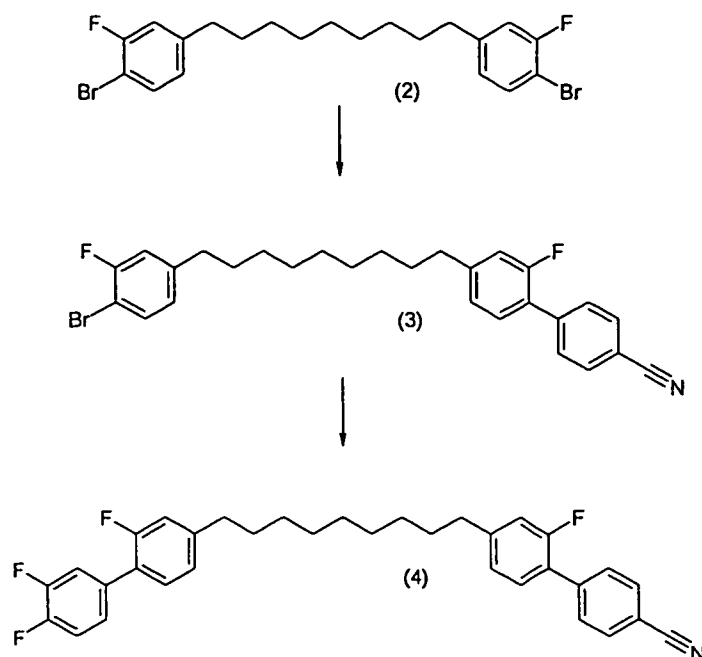
N-PGI(Cl)-9-G(Cl)P-N



PP-CD₂-7-CD₂-PP

實例 3：式 I 化合物 (其中式 I 中之 R¹-MG¹-及 R²-MG²-不同)
之一般合成





(1) 之合成

向圓底燒瓶中添加1-溴-3-氟碘苯(27.5 g, 92 mmol)以及四氫呋喃(30 ml)且在氮下攪拌混合物直至溶解為止。添加二異丙基胺(30 ml)並將反應液置於超音波浴中保持10分鐘。添加觸媒雙(三苯基-膦)二氯化鈣(II)(0.9 g, 1.28 mmol)及碘化銅(I)(0.2 g, 1.05 mmol)且將反應液在水浴中冷卻至20°C。向反應液中緩慢添加1,8-壬二炔(5.0 g, 41 mmol)並進一步攪拌20小時。冷卻反應液並在真空下過濾以去除沈澱物。使用稀鹽酸酸化濾液並使用二乙醚萃取。使用水洗滌有機材料，然後濃縮以提供黑色固體產物(19 g)。藉由管柱層析(使用存於汽油中之二氯甲烷之混合物洗脫產物)純化材料。此產生14 g (72%)期望產物。

(2) 之合成

將材料(1)(21.5 g, 40 mol)溶於四氫呋喃(600 ml)中並通過Thalesnano氫化器。材料需要70巴壓力及60°C之條件以產生淺白色固體產物(21.5 g, 99%)。

(3) 之合成

在氮氣氛下，將材料(2)(14.35 g, 30.3 mmol)、4-氟基苯基硼酸(4.45 g, 30.3 mmol)、磷酸鉀(25.4 g, 120 mmol)、二噁烷(57.4 ml)及水(28.7 ml)在超音波浴中超音波處理30分鐘。在室溫下攪拌混合物且添加Pd(DPPF)Cl₂-DCM複合物(215 mg)。將混合物在90°C下加熱2小時。冷卻混合物。分離兩個層並在真空中自有機層去除溶劑以得到黑色油狀物。將此油狀物溶於極少量DCM中並施加至使用1:1汽油：DCM洗脫之二氧化矽管柱上以得到期望產物(3.5 g, 23.3%)。

(4) 之合成

在氮氣氛下，將材料(3)(3.5 g, 7.05 mmol)、3,4-二氟苯基硼酸(1.7 g, 8 mmol)、磷酸鉀(1.7 g, 8 mmol)、二噁烷(10.6 ml)及水(5.3 ml)在超音波浴中超音波處理30分鐘。在室溫下攪拌混合物且添加Pd(DPPF)Cl₂-DCM複合物(59 mg)。將混合物在90°C下加熱5小時。分離兩個層並在真空中自有機層去除溶劑。將其溶於中極少量DCM中並施加至使用2:1汽油：DCM洗脫之二氧化矽管柱上。自DCM/乙腈將粗產物結晶兩次(使用乾冰/丙酮浴冷卻)且將產物溶於極少量DCM中並施加至使用2:1汽油：DCM洗脫之二氧化矽管柱

上。自乙腈將粗產物結晶(使用乾冰/丙酮浴冷卻)以得到期望產物(2.43 g, 65%)。

實例 4：混合物 A

組合物		
化合物		
編號	縮寫	濃度/%
1	R-5011	1.6
2	F-PGI-O-7-O-GP-F	4.0
3	F-PGI-O-9-O-GP-F	16.2
4	N-PP-O-9-O-GU-F	7.0
5	N-PP-O-7-O-PG-OT	18.5
6	F-PGI-O-9-O-PP-N	5.0
7	F-UIGI-ZI-9-Z-GU-F	25.0
8	N-PGI-ZI-9-Z-GP-N	7.7
9	N-PGI-9-GP-N	<u>15.0</u>
Σ		<u>100.0</u>

主體混合物(1至8項)展現自室溫直至68.5°C之向列相範圍。在添加15% N-PGI-9-GP-N之後，所得混合物A展現第二向列相之增加之相範圍。

實例 5：混合物 B

製備下列混合物(混合物 B)

組合物		
化合物		
編號	縮寫	濃度/%
1	F-PGI-O-7-O-GP-F	10.0
2	F-PGI-O-9-O-GP-F	40.0
3	N-PP-O-9-O-GU-F	10.0
4	N-PP-O-7-O-PGIOT	20.0
5	F-PGI-O-9-O-PP-N	20.0
Σ		100.0

此混合物具有下列性質：

澄清點：75.2

相序：K 44 N 75 I, Tg -17。

此混合物係主體混合物且並不顯示第二向列相。

實例 6：混合物 B-1

向混合物 B 中添加 10% N-PGI-9-GP-N 以得到具有下列熱性質之混合物 B-1：

相序：I 75-73 N 30 N2

隨著混合物中之 N-PGI-9-GP-N 之量增加至 10%，發生若干事件。首先，在原本並不顯示第二向列相之混合物中誘導此相，且其次，彈性彎曲常數 k_{33} 有所降低。

實例 7：混合物 B-2

向混合物 B 中添加 20% N-PGI-9-GP-N 以得到具有下列熱性質之混合物 B-2：

加熱之相序：K 37.9 N 73.6-74.2 I，

冷卻之相序：I 74 N 35.4-34.8 N2

隨著 N-PGI-9-GP-N 之濃度增加，在較高溫度下出現自向列相至第二彎曲扭轉向列相之轉變溫度。

混合物 B-2 在冷卻下自向列相顯示第二向列相（亦即在 35.4°C 以下）。自向列相至第二向列相之轉變似乎為二階性，且似乎並非急劇轉變。隨著添加量增加至 20%，與混合物 B-1 相比 k_{11} 保持基本不變，但 k_{33} 顯著減小。

另外，可假設在混合物中具有較高濃度 (>34%) N-PGI-9-GP-N 之組合物可具有負 k_{33} 。針對各組合物外推 k_{33} ，則關於 100% N-PGI-9-GP-N 之 k_{33} 值具有顯著負性 (-9.8 pN)。

表 2 匯總實例 5、6 及 7 之結果。

表 2 :

混合物	B	B-1	B-2	外推值
k_{11} (pN)	13.49	14.51	13.84	15.53
k_{33} (pN)	4.97	3.42	2.02	-9.79
$(k_{11}+k_{33})/2$ (pN)	9.23	8.97	7.93	2.87

實例 8 : 用於 USH 模式之撓變電子混合物 (混合物 C)

組合物		
化合物		
編號	縮寫	濃度/%
1	F-PGI-O-7-O-GP-F	3.2
2	F-PGI-O-9-O-GP-F	11.5
3	N-PP-O-9-O-GU-F	5.0
4	N-PP-O-7-O-PG-OT	13.1
5	F-PGI-O-9-O-PP-N	3.5
6	N-GIGIGI-9-GGG-N	20.0
7	K15	6.0
8	R-5011	4.0
9	F-UIGI-ZI-9-Z-GU-F	17.6
10	N-PGI-ZI-9-Z-GP-N	5.5
11	N-PGI-ZI-7-Z-GP-N	10.6
Σ		100.0

實例 9 : 用於 USH 模式之撓變電子混合物 (混合物 D)

組合物		
化合物		
編號	縮寫	濃度/%
1	F-PGI-O-7-O-GP-F	5.6
2	F-PGI-O-9-O-GP-F	11.5
3	N-PP-O-9-O-GU-F	5.0
4	N-PP-O-7-O-PG-OT	13.1
5	F-PGI-O-9-O-PP-N	3.5
6	N-GIGIGI-9-GGG-N	20.0
7	K15	6.0
8	R-5011	1.6
9	F-UIGI-ZI-9-Z-GU-F	17.6
10	N-PGI-ZI-9-Z-GP-N	5.5
11	N-PGI-ZI-7-Z-GP-N	10.6
Σ		100.0

實例 10：(混合物 E)

組合物		
化合物		
編號	縮寫	濃度/%
1	F-PGI-O-7-O-GP-F	8.0
2	F-PG-O-7-O-GIP-F	32.0
3	N-PP-O-9-O-GU-F	16.0
4	N-PP-O-7-O-PGIOT	8.0
5	F-PGI-O-9-O-PP-N	16.0
6	N-PGI-9-GP-N	20.0
Σ		100.0

此混合物適用於USH模式。

七、申請專利範圍：

1. 一種式I之雙液晶原化合物，



其中

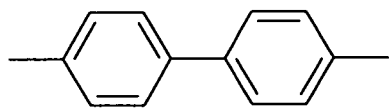
R^1 及 R^2 各自獨立地係H、F、Cl、CN、NCS或具有1至25個C原子之直鏈或具支鏈烷基，該烷基可未經取代、經鹵素或CN單-或多取代，其一或多個非毗鄰 CH_2 基團亦可在每一情形下彼此獨立地由-O-、-S-、-NH-、-N(CH₃)-、-CO-、-COO-、-OCO-、-O-CO-O-、-S-CO-、-CO-S-、-CH=CH-、-CH=CF-、-CF=CF-或-C≡C-以氧原子並不彼此直接連接之方式代替，

MG^1 及 MG^2 各自獨立地係液晶原基團，

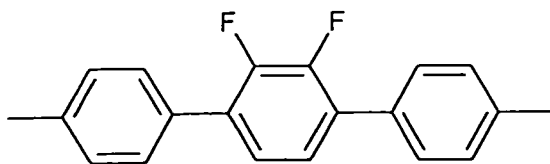
Sp 係Sp係-(CH₂)_o-且o為5至15之整數，

前提係若 R^1 及 R^2 皆係-CN，則

MG^1 及 MG^2 不會同時為



且若 MG^1 及 MG^2 皆係



，則 R^1 及 R^2 不會同時為直鏈烷基。

2. 如請求項1之雙液晶原化合物，其中 MG^1 及 MG^2 彼此獨立地選自式II



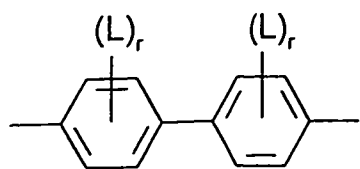
其中

Z^1 係 $-\text{COO}-$ 、 $-\text{OCO}-$ 、 $-\text{O}-\text{CO}-\text{O}-$ 、 $-\text{OCH}_2-$ 、 $-\text{CH}_2\text{O}-$ 、 $-\text{CH}_2\text{CH}_2-$ 、 $-(\text{CH}_2)_4-$ 、 $-\text{CF}_2\text{CF}_2-$ 、 $-\text{CH}=\text{CH}-$ 、 $-\text{CF}=\text{CF}-$ 、 $-\text{CH}=\text{CH}-\text{COO}-$ 、 $-\text{OCO}-\text{CH}=\text{CH}-$ 、 $-\text{C}\equiv\text{C}-$ 或單鍵，

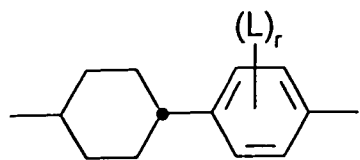
A^1 及 A^2 在每次出現時各自獨立地係1,4-伸苯基，另外其中一或多個CH基團可由N代替；反式-1,4-伸環己基，另外其中一或兩個非毗鄰 CH_2 基團可由O及/或S代替；1,4-伸環己烯基；1,4-雙環-(2,2,2)-伸辛基；六氫吡啶-1,4-二基；萘-2,6-二基；十氫-萘-2,6-二基；1,2,3,4-四氫-萘-2,6-二基；環丁烷-1,3-二基；螺[3.3]庚烷-2,6-二基；或二螺[3.1.3.1]癸烷-2,8-二基，所有該等基團皆可未經取代、經以下基團單-、二-、三-或四取代：F、Cl、CN或具有1至7個C原子之烷基、烷氧基、烷基羰基或烷氧基羰基，其中一或多個H原子可經F或Cl取代，

m 為0、1、2或3。

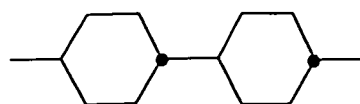
3. 如請求項1之雙液晶原化合物，其中 MG^1 及 MG^2 各自且獨立地選自下列式及其鏡像



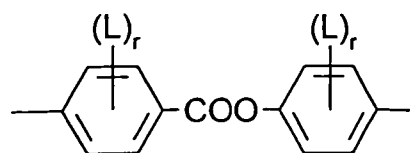
IIa



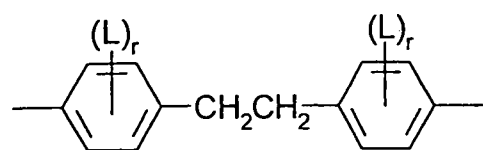
IIb



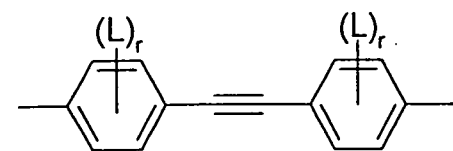
IIc



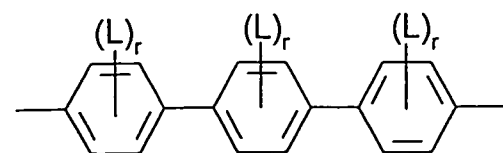
IIId



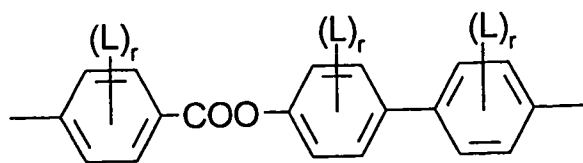
IIe



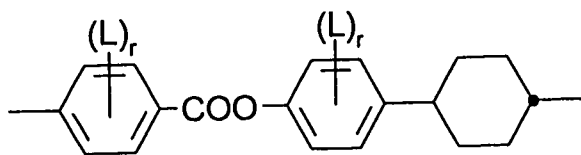
IIIf



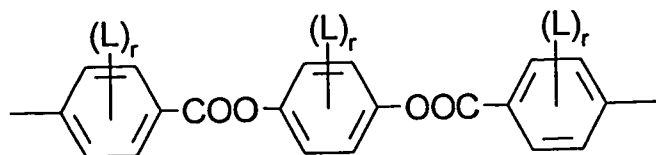
IIg



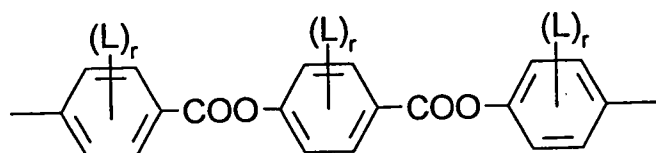
IIh



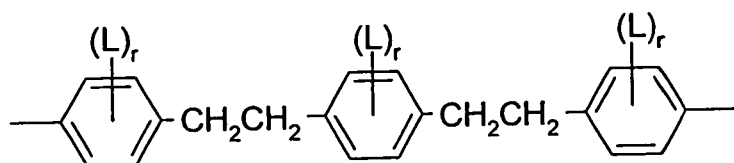
III



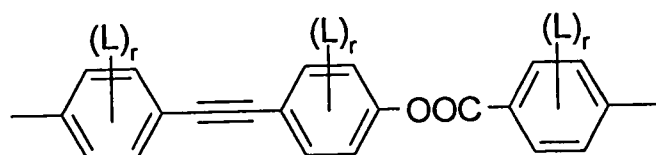
IIk



IIIm



IIIn



IIo

其中L在每次出現時彼此獨立地係F、Cl、CN、OH、NO₂或具有1至7個C原子之視情況氟化之烷基、烷氧基或烷醯基，且r在每次出現時彼此獨立地為0、1、2、3或4。

4. 如請求項1至3中任一項之雙液晶原化合物，其中R¹及R²係選自H、F、Cl、CN、NO₂、OCH₃、COCH₃、COC₂H₅、COOCH₃、COOC₂H₅、CF₃、C₂F₅、OCF₃、OCHF₂及OC₂F₅。

5. 一種如請求項1至4中任一項之雙液晶原化合物之用途，其係用於液晶介質中。
6. 一種液晶介質，其特徵在於其包括一或多種如請求項1至4中任一項之雙液晶原化合物。
7. 如請求項6之液晶介質，其中其另外包括一或多種選自式III化合物之群之化合物



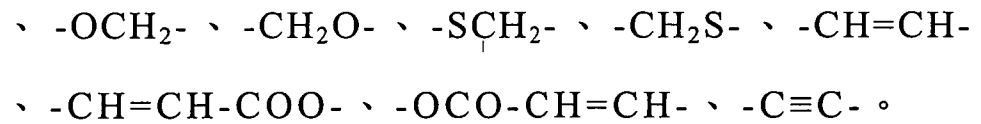
其中

R^3 及 R^4 各自獨立地係H、F、Cl、CN、NCS或具有1至25個C原子之直鏈或具支鏈烷基，該烷基可未經取代、經鹵素或CN單-或多取代，其一或多個非毗鄰 CH_2 基團亦可在每一情形下彼此獨立地由-O-、-S-、-NH-、-N(CH₃)-、-CO-、-COO-、-OCO-、-O-CO-O-、-S-CO-、-CO-S-、-CH=CH-、-CH=CF-、-CF=CF-或-C≡C-以氧原子並不彼此直接連接之方式代替，

MG^3 及 MG^4 各自獨立地係液晶原基團，

Sp^1 係包括5至40個C原子之間隔基團，其中一或多個非毗鄰 CH_2 基團亦可由-O-、-S-、-NH-、-N(CH₃)-、-CO-、-O-CO-、-S-CO-、-O-COO-、-CO-S-、-CO-O-、-CH(鹵素)-、-CH(CN)-、-CH=CH-或-C≡C-代替，且

X^3 及 X^4 各自獨立地係-O-、-S-、-CO-、-COO-、-OCO-、-O-CO-O-、-CO-NH-、-NH-CO-、-CH₂CH₂-



8. 如請求項6或7之液晶介質，其中其展現第二向列相。
9. 一種如請求項6至8中任一項之液晶介質之用途，其係用於液晶裝置中。
10. 一種液晶裝置，其包括含有兩種或更多種組份之液晶介質，該兩種或更多種組份中之一或多者係如請求項1至4中任一項之雙液晶原化合物。
11. 如請求項10之液晶裝置，其中其係撓變電子裝置。
12. 如請求項10或11之液晶裝置，其中其包括兩個平面平行電極，該兩個平面平行電極之內表面展現混合配向條件。