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Supporting Information

Phenothiazine/dimesitylborane Hybrid Materials as Bibipolar Transport Host of Red Phosphor

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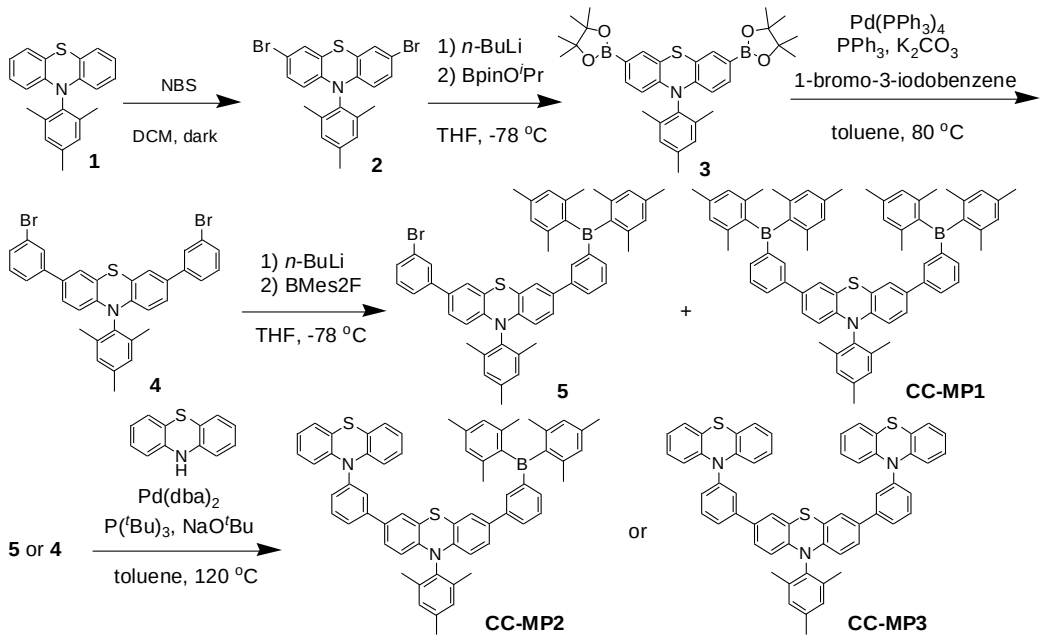
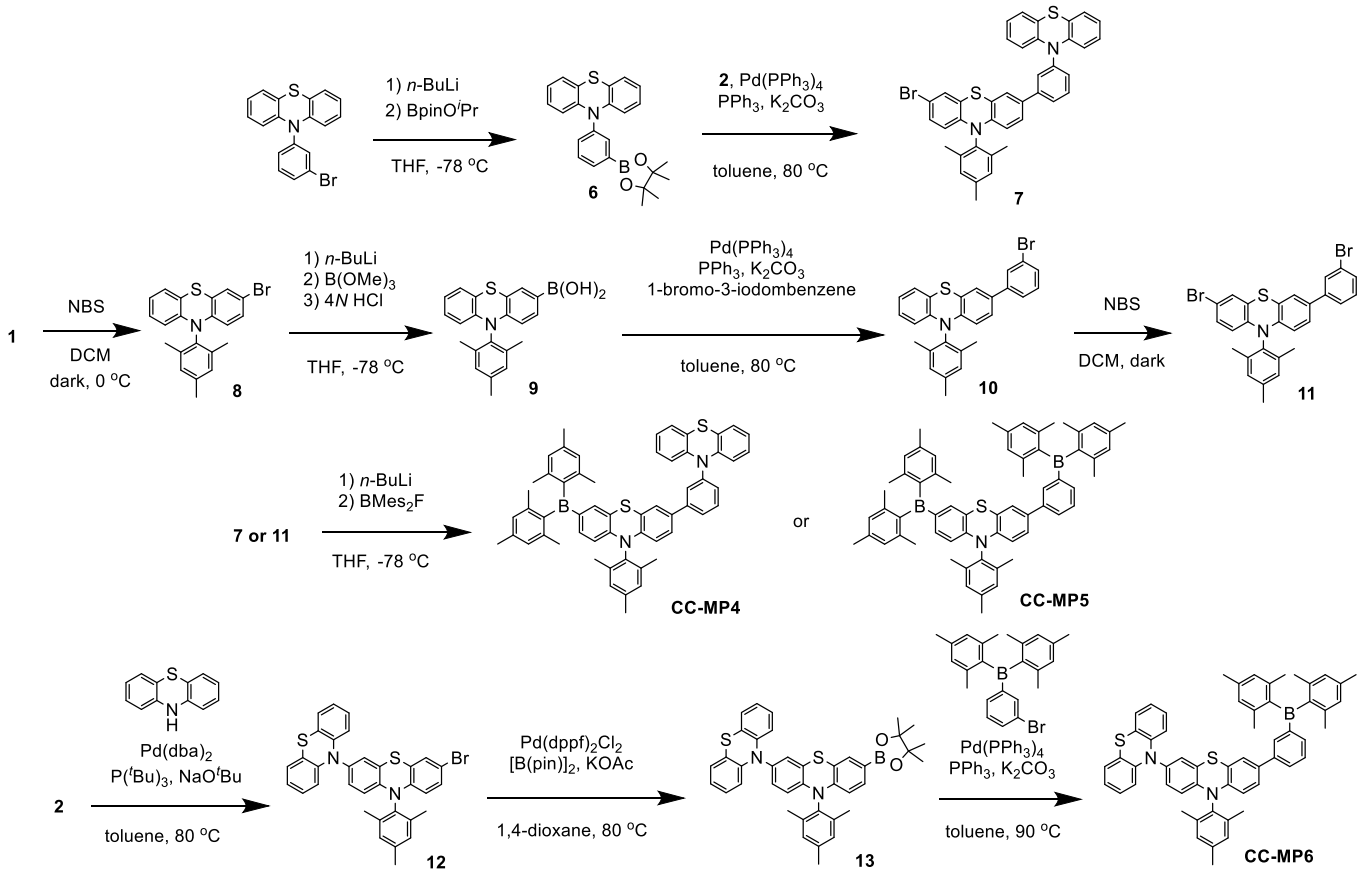
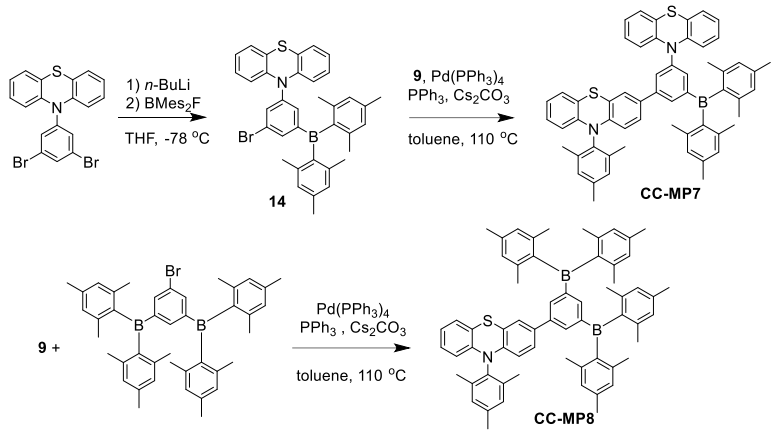


Scheme S1 Synthetic routes of **CC-MP1** to **CC-MP3**.



Scheme S2 Synthetic routes of **CC-MP4** to **CC-MP6**.



Scheme S3 Synthetic routes of **CC-MP7** and **CC-MP8**.

Synthesis of materials:

10-Mesityl-10H-phenothiazine (**1**). 10*H*-phenothiazine (5.00 g, 24.8 mmol), 2-bromo-1,3,5-trimethylbenzene (5.44 g, 1.1 eq), sodium *tert*-botoxide (3.58 g, 1.5 eq) and $Pd(dba)_2$ (0.29 g, 0.2 eq) were loaded in a 100 mL Schlenk flask with condenser. After addition of toluene (50 mL) and tri(*tert*-butyl)phosphine (0.49 M in toluene, 2.02 mL, 0.04 eq), the solution was heated at 110 °C for 8 h. After cooling, the mixture was filtered through Celite and the solvent was removed under vacuum. The residue was extracted with CH_2Cl_2/aqueous NH_4Cl for several times. Collected organic layer was dehydrated by anhydrous $MgSO_4$. After filtration, the filtrate was pumped dry. The crude product was purified by column chromatography using hexanes as the eluent. Further recrystallization of the crude product from CH_2Cl_2/MeOH provided the desired product as a white powder in 80% yield (6.28 g). ^{1}H NMR (acetone-d_6, 300 MHz): δ 7.16 (s, 2H), 6.92 (dd, 2H, J = 7.5; 1.5 Hz), 6.84 (td, 2H, J = 7.5; 1.5 Hz), 6.76 (td, 2H, J = 7.5; 1.2 Hz), 5.89 (dd, 2H, J = 7.5; 1.2 Hz), 2.37 (s, 3H), 2.14 (s, 6H). ^{13}C NMR (acetone-d_6, 75 MHz): δ 142.8, 139.9, 139.2, 136.3, 131.8, 128.9, 127.8, 123.7, 119.6, 115.4, 21.7, 18.5. HRMS (FAB, m/z): $[M]^+$ Calcd for $C_{21}H_{19}NS$, 317.1238; Found, 317.1234.

3,7-Dibromo-10-mesityl-10H-phenothiazine (**2**). Compound **1** (3.00 g, 9.45 mmol) was dissolved in CH_2Cl_2 (80 mL) in a 100 mL flask. NBS (3.87 g, 2.3 eq) was then added in dark and the solution was stirred for 3 h at room temperature. The mixture was quenched with aqueous $Na_2S_2O_3$ and extracted with CH_2Cl_2/aqueous NH_4Cl for several times. The collected organic layer was dehydrated by anhydrous $MgSO_4$. The soltion was filtered and the filtrate was pumped dry. The crude product obtained was recrystallized from CH_2Cl_2/MeOH to provide the desired product as a pale yellow powder in 92% yield (4.13 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.17 (s, 2H), 7.10 (d, 2H, J = 2.4 Hz), 7.00 (dd, 2H, J = 8.8; 2.4 Hz), 5.81 (d, 2H, J = 8.8Hz), 2.37 (s, 3H), 2.14 (s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.4, 139.0, 137.9, 134.2, 130.7, 130.2, 128.7, 120.2, 115.5, 114.4, 21.3, 17.9. HRMS (MALID, m/z): [M] Calcd for $C_{21}H_{17}Br_2NS$, 472.9443; Found, 472.9432.

10-Mesityl-3,7-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-10H-phenothiazine (**3**). Compound **2** (2.80 g, 5.87 mmol) was dissolved in THF (20 mL) in a 50 mL Schlenk flask under nitrogen and the solution was prechilled to -78 °C. *n*-BuLi (1.6 M in hexane, 7.70 mL, 2.1 eq) was added

dropwise into the solution and the mixture was stirred for 1 h at the same temperature. On completion, isopropyl pinacol borate (3.39 mL, 2.0 eq) was added and slowly warmed to room temperature at stirred for 8 h. The mixture was quenched with de-ionized water and THF was removed by a rotatory evaporator. The residue was extracted with CH_2Cl_2/aqueous NH_4Cl for several times. The collected organic layer was dehydrated by anhydrous $MgSO_4$. After filtration, the filtrate was pumped dry. The crude product was recrystallized from CH_2Cl_2/hexanes to provide the desired product as a brown powder in 87% yield (2.91 g).

3,7-Bis(3-bromophenyl)-10-mesityl-10H-phenothiazine (**4**). Compound **3** (2.60 g, 4.57 mmol), 1-bromo-3-iodobenzene (5.17 g, 4.0 eq), K_2CO_3 (3.79 g, 6.0 eq), PPh_3 (0.12 g, 0.1 eq) and $Pd(PPh_3)_4$ (0.53 g, 0.1 eq) were loaded in a 100 mL Schlenk flask with a condenser. Toluene (16 mL) and water/ethanol (5.5/2.5 mL) were added, and the solution was heated at 80 ^oC for 8 h. After removal of the solvent under high vacuum, the residue was extracted with CH_2Cl_2/aqueous NH_4Cl for several times. The collected organic layer was dehydrated by anhydrous $MgSO_4$. After filtration, the filtrate was pumped dry. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (1:9 by vol.) as the eluent. The desired product was isolated as a yellow powder in 87% yield (2.91 g). ^1H NMR (acetone-d_6, 400 MHz): δ 7.76 (t, 2H, J = 1.6 Hz), 7.58 (d, 2H, J = 8.0Hz), 7.47 (d, 2H, J = 8.0 Hz), 7.36 (t, 2H, J = 8.0 Hz), 7.31 (d, 2H, J = 2.4 Hz), 7.21 (s, 2H), 7.19 (dd, 2H, J = 8.4; 2.4 Hz), 5.99 (d, 2H, J = 8.4Hz), 2.40 (s, 3H), 2.21(s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz):δ 143.2, 142.2, 140.2, 138.9, 135.8, 134.9, 132.1, 131.9, 131.2, 130.2, 127.5, 126.3, 126.0, 124.0, 120.3, 115.8, 21.7, 18.5. HRMS (MALID, m/z): [M] Calcd for $C_{33}H_{25}Br_2NS$, 625.0069; Found, 625.0062.

3-(3-Bromophenyl)-7-(3-(dimesitylboranyl)phenyl)-10-mesityl-10H-phenothiazine (**5**) and *3,7-bis(3-(dimesityl-boranyl)phenyl)-10-mesityl-10H-phenothiazine* (**CC-MP1**). The compound **4** (8.89 g, 14.2 mmol) was dissolved in THF (50 mL) in a 100 mL Schlenk flask under nitrogen and the solution was prechilled to -78 ^oC , *n*-BuLi (1.6 M in hexane, 9.30 mL, 1.05 eq) was added dropwise into the solution and stirred for 1 h at the same temperature. On completion, a THF solution (20 mL) of dimesityl boronfluoride (3.80 g, 1.0 eq) was added and the solution was slowly warmed to room temperature and stirred for 8 h. The mixture was quenched with de-ionized water and THF was removed by a rotatory evaporator. The residue was extracted with CH_2Cl_2/aqueous NH_4Cl for several times. The collected organic layer was dehydrated by anhydrous $MgSO_4$. After filtration, the filtrate was pumped dry. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (1:20 by vol.) as the eluent. The compound **5** was isolated from the first band as a pale yellow powder in 38% yield (4.30 g). ^1H NMR (acetone-d_6, 500 MHz): δ 7.72-7.78 (m, 2H), 7.64 (s, 1H), 7.58 (d, 1H, J = 7.0 Hz), 7.44-7.49 (m, 2Hz), 7.39 (d, 1H, J = 8.0 Hz), 7.36 (t, 1H, J = 8.0 Hz), 7.28 (d, 1H, J = 2.0 Hz), 7.15-7.20 (m, 4H), 7.05 (dd, 1H, J = 8.5; 2.5 Hz), 6.84 (s, 4H), 5.98 (d, 1H, J = 8.5 Hz), 5.95 (d, 1H, J = 8.5 Hz), 2.34 (s, 3H), 2.28 (s, 6H), 2.18 (s, 6H), 2.01 (s, 12H). ^{13}C NMR (acetone-d_6, 125 MHz): δ 148.0, 143.2, 143.0, 142.3, 141.9, 141.7, 140.6, 140.2, 140.1, 138.9, 136.7, 136.0, 135.8, 134.8, 134.7, 132.1, 131.8, 131.3, 131.2, 130.1, 130.1, 129.6, 127.4, 127.3, 126.3, 126.0, 125.9, 123.9, 120.1, 120.0, 115.9, 115.7, 24.2, 21.8, 21.7, 18.4. HRMS (FAB, m/z): $[M]^+$ Calcd for $C_{51}H_{47}BBrNS$, 795.2706; Found, 795.2718. Using CH_2Cl_2/hexanes (1:10 by vol.) as the eluent, the compound **CC-MP1** was isolated from the second band and further

recrystallization from CH_2Cl_2/MeOH provided the desired product as a yellow powder in 25% yield (3.42 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.73 (d, 2H, J = 7.6 Hz), 7.65 (s, 2H), 7.46 (t, 2H, J = 7.6 Hz), 7.39 (d, 2H, J = 7.6 Hz), 7.17 (s, 2H), 7.14 (d, 2H, J = 2.0 Hz), 7.03 (dd, 2H, J = 8.8; 2.0 Hz), 6.84 (s, 8H), 5.93 (d, 2H, J = 8.8 Hz), 2.37 (s, 3H), 2.28 (s, 12H), 2.16 (s, 6H), 2.01 (s, 24H). ^{13}C NMR (acetone-d_6, 100 MHz): δ 148.2, 143.1, 142.0, 141.9, 140.7, 140.2, 140.1, 139.1, 136.6, 136.1, 136.0, 134.9, 131.9, 131.3, 130.2, 129.7, 127.4, 125.9, 120.1, 115.9, 24.3, 21.9, 21.7, 18.5. HRMS (MALID, m/z): [M] Calcd for $C_{69}H_{69}B_2NS$, 965.5352; Found, 965.5377. Anal. Calcd for $C_{69}H_{69}B_2NS$: C, 85.79; H, 7.20; N, 1.45; Found: C, 85.23; H, 7.17; N, 1.40.

3-(3-(10H-Phenothiazin-10-yl)phenyl)-7-(3-(dimesitylboranyl)-phenyl)-10-mesityl-10H-pheno-thiazine (**CC-MP2**). A procedure similar to that used for **1** was followed except that compound **5** (4.00 g, 5.02 mmol) was usedand the solution was heated at 120 ^{o}C for 8 h. The crude product was purified by aluminum gel column chromatography using CH_2Cl_2/hexanes (1:9 by vol.) as the eluent. Further recrystallization of the crude product from CH_2Cl_2/MeOH provided the desired product as a yellow powder in 57% yield (2.62 g). ^{1}H NMR (acetone-d_6, 500 MHz): δ 7.50-7.70 (m, 5H), 7.34 (t, 1H, J = 7.5 Hz), 7.20-7.30 (m, 2H), 7.22 (d, 1H, J = 7.5 Hz), 7.12 (d, 1H, J = 8.5 Hz), 7.00-7.10 (m, 3H), 6.90-6.95 (m, 3H), 6.78 (t, 2H), 6.70-6.75 (m, 6H), 6.17 (d, 2H, J = 8.0 Hz), 5.85 (d, 1H, J = 8.5 Hz), 5.81 (d, 1H, J = 8.5 Hz), 2.26 (s, 3H), 2.15 (s, 6H), 2.04 (s, 6H), 1.88 (s, 12H). ^{13}C NMR (acetone-d_6, 125 MHz): δ 147.8, 145.4, 143.4, 142.8, 142.0, 141.7, 141.5, 140.4, 140.0, 139.9, 138.7, 136.4, 135.9, 135.7, 134.9, 134.7, 132.7, 131.7, 131.1, 130.2, 130.0, 129.5, 129.1, 128.4, 127.8, 127.2, 127.1, 126.9, 125.8, 125.7, 123.9, 121.3, 112.0, 117.5, 115.7, 115.6, 24.1, 21.7, 21.6, 18.3. HRMS (MALID, m/z): [M] Calcd for $C_{63}H_{55}BN_2S_2$, 914.3904; Found, 914.3910. Anal. Calcd for $C_{63}H_{55}BN_2S_2$: C, 82.69; H, 6.06; N, 3.06; Found: C, 82.45; H, 6.09; N, 3.09.

10,10'-((10-Mesityl-10H-phenothiazine-3,7-diyl)bis(3,1-phenylene))bis-(10H-phenothiazine) (**CC-MP3**). A procedure similar to that used for **1** was followed except that compound **4** (5.00 g, 7.97 mmol) was used and the solution was heated at 120 ^{o}C for 8 h. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (2:8 by vol.) as the eluent. The crude product was recrystallized from CH_2Cl_2/MeOH to provide the desired product as a yellow powder in 91% yield (6.30 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.78 (dm, 2H, J = 7.6 Hz), 7.71 (t, 2H, J = 7.6 Hz), 7.66 (sm, 2H), 7.40 (d, 2H, J = 2.0 Hz), 7.34 (dm, 2H, J = 7.6 Hz), 7.28 (dd, 2H, J = 8.8; 2.0 Hz), 7.20 (s, 2H), 7.04 (dd, 4H, J = 7.6; 2.0 Hz), 6.91 (td, 4H, J = 7.6; 2.0 Hz), 6.85 (td, 4H, J = 7.6; 1.2 Hz), 6.31 (dd, 2H, J = 8.6; 1.2 Hz), 6.00 (d, 1H, J = 8.8 Hz), 2.39 (s, 3H), 2.20 (s, 6H). ^{13}C NMR (acetone-d_6, 100 MHz): δ 145.7, 143.7, 143.2, 142.2, 140.3, 139.0, 136.0, 135.3, 132.9, 132.0, 130.4, 129.4, 128.6, 128.1, 127.4, 127.2, 126.0, 124.2, 121.8, 120.4, 118.0, 116.0, 21.8, 18.5. HRMS (MALID, m/z): [M] Calcd for $C_{57}H_{41}N_3S_3$, 863.2457; Found, 863.2460. Anal. Calcd for $C_{57}H_{41}N_3S_3$: C, 79.22; H,4.78; N, 4.86; Found: C, 79.18; H,4.71; N, 4.90.

10-(3-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-10H-pheno-thiazine (**6**). A procedure similar to that used for **3** was followed except that 10-(3-bromophenyl)-10*H*-pheno-thiazine (1.00 g, 2.82 mmol) was used and the solution was stirred for 8 h. The crude product obtained was

recrystallized from CH_2Cl_2/hexanes to provide the desired product as a white powder in 76% yield (0.86 g).

3-(3-(10H-Phenothiazin-10-yl)phenyl)-7-bromo-10-mesityl-10H-pheno-thiazine (**7**). A procedure similar to that used for **4** was followed. A mixture of ompound **6** (1.63 g, 4.06 mmol), the compound **2** (2.5 eq), K_2CO_3 (3.0 eq), PPh_3 (0.05 eq) and $Pd(PPh_3)_4$ (0.05 eq), toluene (14 mL) and water/ethanol (2.5/1.0 mL) was heated at 80 ^oC for 8 h. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (1:9 by vol.) as the eluent. Further recrystallizationof the crude product from CH_2Cl_2/MeOH provided the desired product as a yellow powder in 64% yield (1.73 g). ^1H NMR (acetone-d_6, 400 MHz): δ 7.77 (dm, 1H, J = 7.6 Hz), 7.71 (t, 1H, J = 7.6 Hz), 7.66 (t, 1H, J = 1.6 Hz), 7.39 (sd, 1H, J = 2.0 Hz), 7.35 (dm, 1H, J = 7.6 Hz), 7.29 (dd, 1H, J = 8.8; 2.0 Hz), 7.18 (s, 2H), 7.01 (d, 1H, J = 2.4 Hz),7.04 (dd, 2H, J = 8.0; 1.6), 6.99 (dd, 1H, J = 8.8; 2.4 Hz), 6.91 (td, 2H, J = 8.0; 1.6 Hz), 6.85 (td, 2H, J = 8.0; 1.2 Hz), 6.31 (dm, 2H, J = 8.0 Hz), 6.00 (d, 1H, J = 8.8 Hz), 5.81 (d, 1H, J = 8.8 Hz), 2.38 (s, 3H), 2.17 (s, 6H). ^{13}C NMR (acetone-d_6, 100 MHz): δ 145.7, 143.6, 143.3, 142.1, 142.0, 140.4, 139.0, 135.8, 135.5, 132.9, 132.0, 131.6, 130.5, 129.8, 129.4, 128.6, 128.1, 127.7, 127.2, 126.1, 124.2, 122.2, 121.8, 119.8, 118.0, 117.1, 116.1, 115.2, 21.8, 18.5. HRMS (MALID, m/z): [M] Calcd for $C_{39}H_{29}BrN_2S_2$, 668.0950; Found, 668.0957.

3-(3-(10H-Phenothiazin-10-yl)phenyl)-7-(dimesitylboranyl)-10-mesityl-10H-phenothiazine (**CC-MP4**). A procedure similar to that used for **CC-MP1** was followed. A mixture of compound **7** (1.25 g, 1.86 mmol), *n*-BuLi (1.05 eq) in THF (6 mL) and dimesityl boronfluoride (1.0 eq) in THF (6 mL) was stirred for 8 h. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (1:9 by vol.) as the eluent. Further recrystallization of the crude product from EA/hexanes (30/20 mL each gram compound) provided the desired product as a yellow crystallization in 32% yield (0.75 g). ^1H NMR (DMSO-d_6, 400 MHz): δ 7.75 (d, 1H, J = 7.6 Hz), 7.67 (t, 1H, J = 7.6 Hz), 7.63 (s, 1H), 7.38 (s, 1H), 7.34 (d, 1H, J = 7.6 Hz), 7.28 (dm, 1H, J = 8.8;1.6 Hz), 7.18 (s, 2H), 7.07 (dm, 2H, J = 7.6 Hz), 6.93 (t, 2H, J = 7.6 Hz), 6.80-6.90 (m, 4H), 6.79 (s, 4H), 6.21 (d, 2H, J = 7.6 Hz), 5.89 (d, 1H, J = 8.8 Hz), 5.85 (d, 1H, J = 8.4 Hz), 2.34 (s, 3H), 2.23 (s, 6H), 2.10 (s, 6H), 1.95 (s, 12H). ^{13}C NMR (THF-d_8, 125 MHz): δ 145.4, 145.3, 143.4, 142.7, 142.3, 141.3, 141.1, 140.5, 139.7, 139.0, 138.5, 138.4, 135.7, 135.6, 135.5, 132.0, 131.3, 130.0, 129.2, 129.0, 127.7, 127.4, 126.5, 125.6, 123.3, 121.3, 120.8, 118.4, 117.1, 115.7, 114.3, 23.8, 21.3, 21.2, 17.9. HRMS (MALID, m/z): [M] Calcd for $C_{57}H_{51}BN_2S_2$, 838.3581; Found, 838.3592. Anal. Calcd for $C_{57}H_{51}BN_2S_2$: C, 81.60; H, 6.13; N, 3.34; Found: C, 81.83; H, 6.28; N, 3.15.

3-Bromo-10-mesityl-10H-phenothiazine (**8**). Compound **1** (3.00 g, 9.45 mmol) was dissolved with CH_2Cl_2 (80 mL) in a 100 mL flask and prechilled to 0 ^oC. To the solution was added a DMF solution (20 mL) of NBS (1.68 g, 9.45 mmol) in the dark. The solution was slowly warmed to room temperature and stirred for 3 h. The mixture was quenched with aqueous $Na_2S_2O_3$ and extracted with CH_2Cl_2/aqueous NH_4Cl for several times. The collected organic layer was dehydrated by anhydrous $MgSO_4$. After filtration, the filtrate was pumped dry. The crude product was purified by column chromatography using hexanes as the eluent. Further recrystallization of the crude product from CH_2Cl_2/MeOH provided the desired product as a white powder in 89% yield (3.32 g). ^1H NMR

(acetone-d_6, 400 MHz): δ 7.17 (s, 2H), 7.07 (d, 1H, J = 1.6 Hz), 6.97 (dd, 1H, J = 8.8; 1.6 Hz), 6.94 (d, 1H, J = 7.6 Hz), 6.86 (t, 1H, J = 7.6 Hz), 6.79 (t, 1H, J = 7.6 Hz), 5.89 (d, 1H, J = 7.6 Hz), 5.79 (d, 1H, J = 8.8 Hz), 2.37 (s, 3H), 2.14 (s, 6H). ^{13}C NMR (acetone-d_6, 100 MHz): δ 142.4, 142.3, 140.2, 139.1, 135.9, 132.0, 131.5, 129.7, 129.2, 127.9, 124.2, 122.3, 118.9, 116.9, 115.7, 115.0, 21.8, 18.5. HRMS (MALID, m/z): [M] Calcd for $C_{21}H_{18}BrNS$, 395.0338; Found, 395.0329.

10-Mesityl-10H-phenothiazin-3-ylboronic acid (**9**). A procedure similar to that used for **3** was followed except that compound **8** (2.89 g, 7.29 mmol) was used and the solution was stirred for 8 h. The extracted filtrate was pumped dry and without further purification to provide the desired product as a yellow powder in 100% yield (2.63 g).

3-(3-Bromophenyl)-10-mesityl-10H-phenothiazine (**10**). A procedure similar to that used for **4** was followed except that compound **9** (2.63 g, 7.29 mmol) was used and the solution was heated at 80 ^{o}C for 8 h. The crude product was purified by column chromatography using hexanes as the eluent. The desired product was isolated as a yellow powder in 74% yield (2.56 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.74 (t, 1H, J = 2.0 Hz), 7.57 (d, 1H, J = 8.0 Hz), 7.47 (d, 1H, J = 8.0 Hz), 7.35 (t, 1H, J = 8.0 Hz), 7.27 (d, 1H, J = 2.0 Hz), 7.14-7.20 (m, 3H), 6.96 (dd, 1H, J = 7.6; 1.2 Hz), 6.83 (td, 1H, J = 7.6; 1.2 Hz), 6.76 (td, 1H, J = 7.6; 1.2 Hz), 5.97 (d, 1H, J = 8.4 Hz), 5.92 (dd, 1H, J = 7.6; 1.2 Hz), 2.39 (s, 3H), 2.18 (s, 6H). ^{13}C NMR (acetone-d_6, 125 MHz): δ 142.8, 142.2, 141.9, 139.6, 138.6, 135.5, 134.2, 131.7, 131.4, 130.7, 129.7, 128.5, 127.3, 126.9, 125.8, 125.5, 123.6, 123.5, 120.0, 118.9, 115.2, 115.1, 21.3, 18.0. HRMS (MALID, m/z): [M] Calcd for $C_{27}H_{22}BrNS$, 471.0651; Found, 471.0629.

3-Bromo-7-(3-bromophenyl)-10-mesityl-10H-phenothiazine (**11**). A procedure similar to that used for **2** was followed except that compound **10** (2.00 g, 4.23 mmol) was used and the solution was stirred for 3 h. The crude product obtained was recrystallized from CH_2Cl_2/MeOH to provide the desired product as a pale yellow powder in 87% yield (2.03 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.75 (s, 1H), 7.58 (d, 1H, J = 8.0 Hz), 7.47 (d, 1H, J = 8.0 Hz), 7.36 (t, 1H, J = 8.0 Hz), 7.29 (d, 1H, J = 2.0 Hz), 7.15-7.25 (m, 3H), 7.12 (d, 1H, J = 2.0 Hz), 7.00 (dd, 1H, J = 8.8; 2.0 Hz), 5.98 (d, 1H, J = 8.8 Hz), 5.82 (d, 1H, J = 8.8 Hz), 2.38 (s, 3H), 2.18 (s, 6H). ^{13}C NMR (acetone-d_6, 125 MHz): δ 142.9, 142.0, 141.7, 140.2, 138.7, 135.4, 134.9, 132.0, 131.8, 131.4, 131.2, 130.1, 129.6, 127.5, 126.2, 126.0, 123.8, 121.8, 119.6, 116.8, 115.8, 115.1, 21.6, 18.3. HRMS (MALID, m/z): [M] Calcd for $C_{27}H_{21}Br_2NS$, 548.9756; Found, 548.9746.

3-(Dimesitylboryl)-7-(3-(dimesitylboryl)phenyl)-10-mesityl-10H-pheno-thiazine (**CC-MP5**). A procedure similar to that used for **CC-MP1** was followed ecept that compound **11** (1.03 g, 1.86 mmol) was used and the solution was stirred for 8 h. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (1:9 by vol.) as the eluent. The desired product was obtained as a yellow powder in 39% yield (0.64 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.72 (dm, 1H, J = 7.6 Hz), 7.63 (s, 1H), 7.46 (t, 1H, J = 7.6 Hz), 7.39 (d, 1H, J = 7.6 Hz), 7.16 (s, 2H), 7.11 (d, 1H, J = 2.0 Hz), 7.04 (dd, 1H, J = 8.4; 2.0 Hz), 7.00 (d, 1H, J = 1.2 Hz),6.96 (dd, 1H, J = 8.4; 1.2 Hz), 6.83 (s, 4H), 6.81 (s, 4H), 5.96 (d, 1H, J = 8.4 Hz), 5.93 (d, 1H, J = 8.4 Hz), 2.36 (s, 3H), 2.27 (s, 6H), 2.26

(s, 6H) , 2.16 (s, 6H), 2.02 (s, 12H), 1.99 (s, 12H). ^{13}C NMR (THF-d_8, 125 MHz): δ *1*47.4, 145.6, 142.5, 142.3, 141.4, 141.3, 140.6, 140.3, 139.6, 139.5, 139.0, 138.6, 138.4, 137.0, 135.8, 135.7, 135.4, 134.5, 131.2, 130.8, 129.4, 129.1, 129.0, 126.6, 125.5, 120.5, 118.3, 115.7, 114.2, 23.8, 21.4, 21.3, 21.2, 17.9 . HRMS (MALID, m/z): [M] Calcd for $C_{63}H_{65}B_2NS$, 888.5060; Found, 888.5039. Anal. Calcd for $C_{63}H_{65}B_2NS$: C, 85.03; H, 7.36; N, 1.57; Found: C, 85.10; H, 7.38; N, 1.70.

7-Bromo-10-mesityl-10H-3,10'-biphenothiazine (**12**). A procedure similar to that used for **1** was followedexcept that compound **2** (2.0 eq) was used and the solution was heated at 80 ^{o}C for 8 h. The crude product was purified by aluminum column chromatography using hexanes as the eluent. Further recrystallization of the crude product from CH_2Cl_2/MeOH provided the desired product as a yellow-white powder in 60% yield (4.10 g). ^{1}H NMR (acetone-d_6, 300 MHz): δ 7.21 (s, 2H), 7.14 (d, 1H, J = 2.4 Hz), 6.97-7.10 (m, 4H), 6.90-6.96 (m, 3H), 6.84 (t, 2H, J = 8.0 Hz), 6.36 (d, 2H, J = 8.0 Hz), 6.15 (d, 1H, J = 8.8 Hz), 5.88 (d, 1H, J = 8.8 Hz), 2.38 (s, 3H), 2.24 (s, 6H). ^{13}C NMR (acetone-d_6, 75 MHz): δ 145.6, 142.3, 142.0, 140.5, 139.0, 136.9, 135.7, 132.1, 131.8, 131.6, 130.0, 129.9, 128.6, 128.0, 124.1, 121.8, 121.6, 121.5, 117.6, 117.4, 117.3, 115.6, 21.9, 18.7. HRMS (FAB, m/z): $[M]^+$ Calcd for $C_{33}H_{25}BrN_2S_2$, 592.0643; Found, 592.0638.

10-Mesityl-7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-10H-3,10'-biphenothiazine (**13**). Compound **12** (2.88 g, 4.85 mmol), bis(pinacolato)diboron (2.46 g, 9.70 mmol), potassium acetate (2.86 g, 29.1 mmol) and $Pd(dppf)_2Cl_2$ (0.12 g, 0.146 mmol) were loaded into a 50 mL Schlenk flask with condenser. The solution was added 1,4-dioxane (10 mL) and heated at 80 ^{o}C for 8 h. After removal of the solvent under high vacuum, the residue was extracted with CH_2Cl_2/aqueous NH_4Cl for several times. The collected organic layer was dehydrated by anhydrous $MgSO_4$. After filtration, the filtrate was pumped dry. The crude product obtained was recrystallized from CH_2Cl_2/MeOH to provide the desired product as a pale brown powder in 94% yield (2.93 g).

7-(3-(Dimesitylboranyl)phenyl)-10-mesityl-10H-3,10'-bi-phenothiazine (**CC-MP6**). A procedure similar to that used for **4** was followed except that compound **13** (2.80 g, 4.37 mmol)was used and the solution was heated at 90 ^{o}C for 8 h. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (1:9 by vol.) as the eluent. Further recrystallization of the crude product from CH_2Cl_2/MeOH provided the desired product as a yellow-white powder in 70% yield (2.57 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.76 (d, 1H, J = 7.6 Hz), 7.67 (s, 1H), 7.48 (t, 1H, J = 7.6 Hz), 7.40 (d, 1H, J = 7.6 Hz), 7.21 (s, 2H), 7.19 (d, 1H, J = 2.0 Hz), 7.09 (dd, 1H, J = 8.4; 2.0 Hz), 7.03 (d, 1H, J = 2.4 Hz), 7.00 (dm, 2H, J = 8.4 Hz), 6.89-6.97 (m, 3H), 6.80-6.87 (m, 6H), 6.36 (d, 2H, J = 8.4 Hz), 6.15 (d, 1H, J = 8.8 Hz), 6.10 (d, 1H, J = 8.4 Hz), 2.39 (s, 3H), 2.27 (s, 6H), 2.24 (s, 6H), 2.01 (s, 12H). ^{13}C NMR (THF-d_8, 125 MHz): δ 147.5, 145.3, 142.6, 142.0, 141.5, 141.3, 140.3, 139.6, 139.5, 138.7, 136.6, 136.0, 135.8, 135.6, 134.5, 131.4, 130.8, 130.7, 129.6, 129.4, 129.1, 127.8, 127.3, 126.9, 125.6, 123.2, 121.9, 120.9, 119.5, 116.7, 116.3, 115.4, 23.8, 21.4, 21.3, 18.1. HRMS (EI, m/z): $[M]^+$ Calcd for $C_{57}H_{51}BN_2S_2$, 838.3587; Found, 838.3584. Anal. Calcd for $C_{57}H_{51}BN_2S_2$: C, 81.60; H, 6.13; N, 3.34; Found: C, 81.47; H, 6.09; N, 3.39.

10-(3-Bromo-5-(dimesitylboranyl)phenyl)-10H-phenothiazine (**14**). A procedure similar to that used for **CC-MP1** was followed except that 10-(3,5-dibromophenyl)-10*H*-phenothiazine (1.00 g, 2.31 mmol) was used and the solution was stirred for 8 h. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (1:9 by vol.) as the eluent. The desired product was isolated as a yellow powder in 45% yield (0.63 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.80 (s, 1H), 7.66 (s, 1H), 7.36 (s, 1H), 7.09 (d, 2H, J = 7.6 Hz), 6.99 (t, 2H, J = 7.6 Hz), 6.91 (t, 2H, J = 7.6 Hz), 6.85 (s, 4H), 6.36 (d, 2H, J = 7.6 Hz), 2.26 (s, 3H), 2.04 (s, 12H). ^{13}C NMR (acetone-d_6, 100 MHz): δ 144.8, 144.4, 142.0, 141.0, 138.3, 136.8, 136.2, 129.8, 129.7, 128.6, 128.3, 128.0, 125.1, 124.7, 122.9, 118.6, 24.2, 21.7. HRMS (FAB, m/z): $[M+H]^+$ Calcd for $C_{36}H_{33}BBrNS$, 601.1610; Found, 601.1613.

3-(3-(Dimesitylboranyl)-5-(10H-phenothiazin-10-yl)phenyl)-10-mesityl-10H-phenothiazine (CC-MP7). A procedure similar to that used for **4** was followed except that compound **9** (1.98 g, 5.48 mmol) and compound **14** (1.0 eq) were used and the solution was heated at 110 ºC for 8 h. The crude product was purified by column chromatography using CH_2Cl_2/hexanes (1:9 by vol.) as the eluent. Further recrystallization of the crude product from CH_2Cl_2/MeOH provided the desired product as a yellow powder in 56% yield (2.57 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.82 (d, 1H, J = 1.6 Hz), 7.81 (s, 1H), 7.31 (s, 1H), 7.26 (d, 1H, J = 1.6 Hz), 7.10-7.15 (m, 3H), 6.98 (dm, 2H, J = 8.0 Hz), 6.77-6.90 (m, 10H), 6.74 (t, 1H, J = 8.0 Hz), 6.25 (d, 2H, J = 8.0 Hz), 5.91 (d, 1H, J = 8.8 Hz), 5.86 (d, 1H, J = 8.0 Hz), 2.34 (s, 3H), 2.22 (s, 6H), 2.11 (s, 6H), 2.04 (s, 12H). ^{13}C NMR (acetone-d_6, 100 MHz): δ 151.9, 145.6, 143.7, 142.9, 142.8, 142.7, 142.4, 142.0, 140.7, 140.1, 139.1, 137.3, 136.1, 135.0, 134.2, 133.5, 131.9, 129.9, 129.0, 128.5, 128.1, 127.8, 127.5, 126.0, 124.1, 124.0, 121.2, 120.6, 119.3, 117.5, 115.8, 115.6, 24.4, 21.9, 21.8, 18.5. HRMS (EI, m/z): $[M]^+$ Calcd for $C_{57}H_{51}BN_2S_2$, 838.3587; Found, 838.3577. Anal. Calcd for $C_{57}H_{51}BN_2S_2$: C, 81.60; H, 6.13; N, 3.34; Found: C, 81.66; H, 6.09; N, 3.35.

3-(3,5-Bis(dimesitylboranyl)phenyl)-10-mesityl-10H-phenothiazine (**CC-MP8**). A procedure similar to that used for **4** was followed except that compound **9** (2.38 g, 6.58 mmol) was used and the solution was heated at 110 ºC for 8 h. The crude product was purified by column chromatography using CH2Cl2/hexanes (1:9 by vol.) as the eluent. Further recrystallization of the crude produt from CH_2Cl_2/MeOH provided the desired product as a yellow powder in 45% yield (2.65 g). ^{1}H NMR (acetone-d_6, 400 MHz): δ 7.74 (sd, 2H, J = 1.2 Hz), 7.55 (d, 1H, J = 1.2 Hz), 7.14 (s, 2H), 7.00 (sd, 1H, J = 2.0 Hz), 6.88-6.93 (m, 2H), 6.83 (tm, 1H, J = 7.6 ;1.6 Hz), 6.72-6.79 (m, 9H), 5.86-5.89 (m, 2H), 2.36 (s, 3H), 2.24 (s, 12H), 2.12 (s, 6H), 1.98 (s, 24H). ^{13}C NMR (acetone-d_6, 100 MHz): δ 148.7, 143.2, 142.6, 142.5, 142.3, 142.0, 140.6, 140.4, 140.0, 139.1, 138.1, 136.5, 136.1, 131.8, 129.7, 129.0, 127.8, 127.5, 125.9, 123.9, 120.4, 119.2, 115.9, 115.5, 24.3, 21.9, 21.7, 18.5. HRMS (FAB, m/z): $[M]^+$ Calcd for $C_{63}H_{65}B_2NS$, 889.5024; Found, 889.5005. Anal. Calcd for $C_{63}H_{65}B_2NS$: C, 85.03; H, 7.36; N, 1.57; Found: C, 85.07; H, 7.45; N, 1.67.

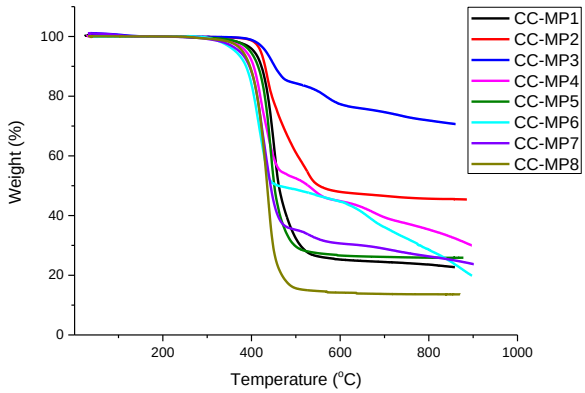


Fig. S1 TGA curves for **CC-MP** compounds.

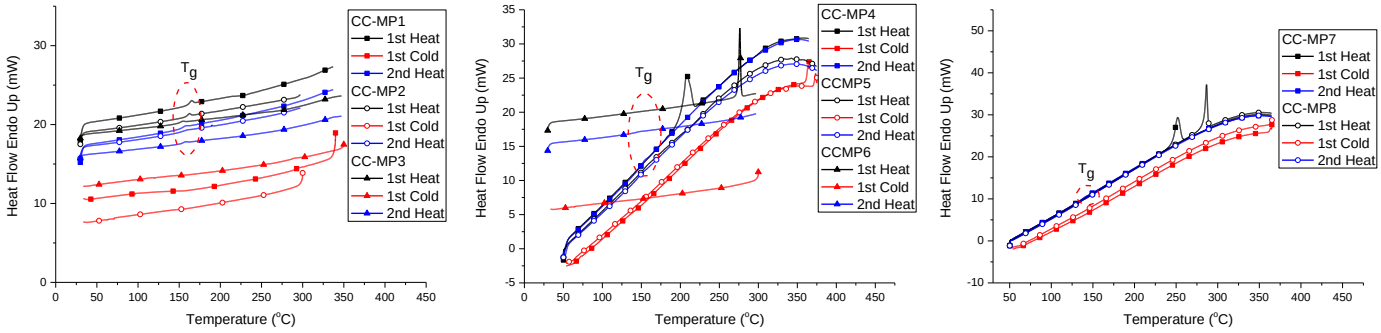


Fig. S2 DSC curves for **CC-MP** compounds (after heated at 110 °C for 1h) at a scan rate of 10 °C/min.

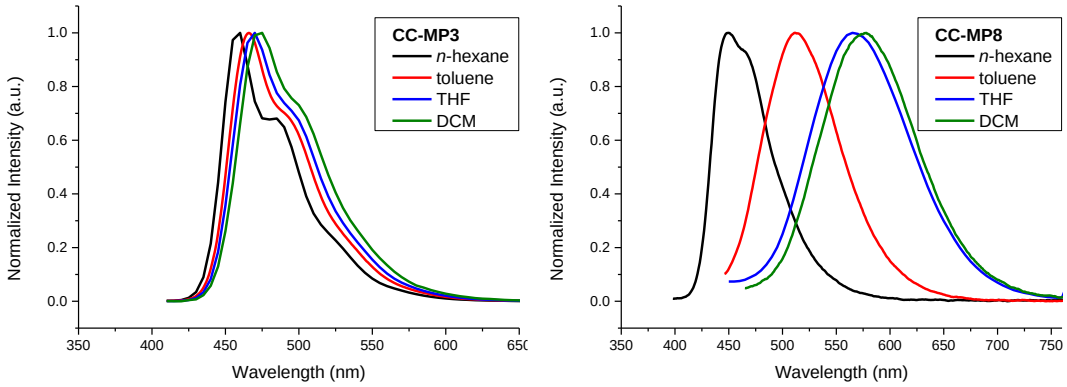


Fig. S3 PL spectra of **CC-MP3** and **CC-MP8** in different solvents.

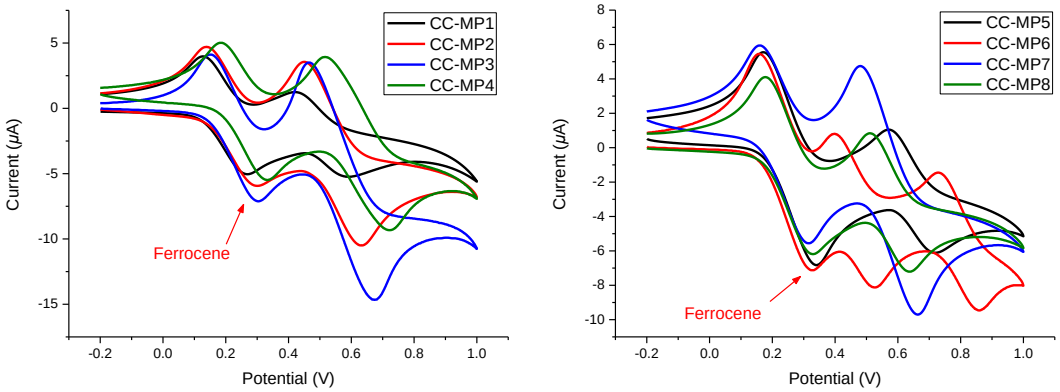


Fig. S4 Cyclic voltammograms measurements in THF.

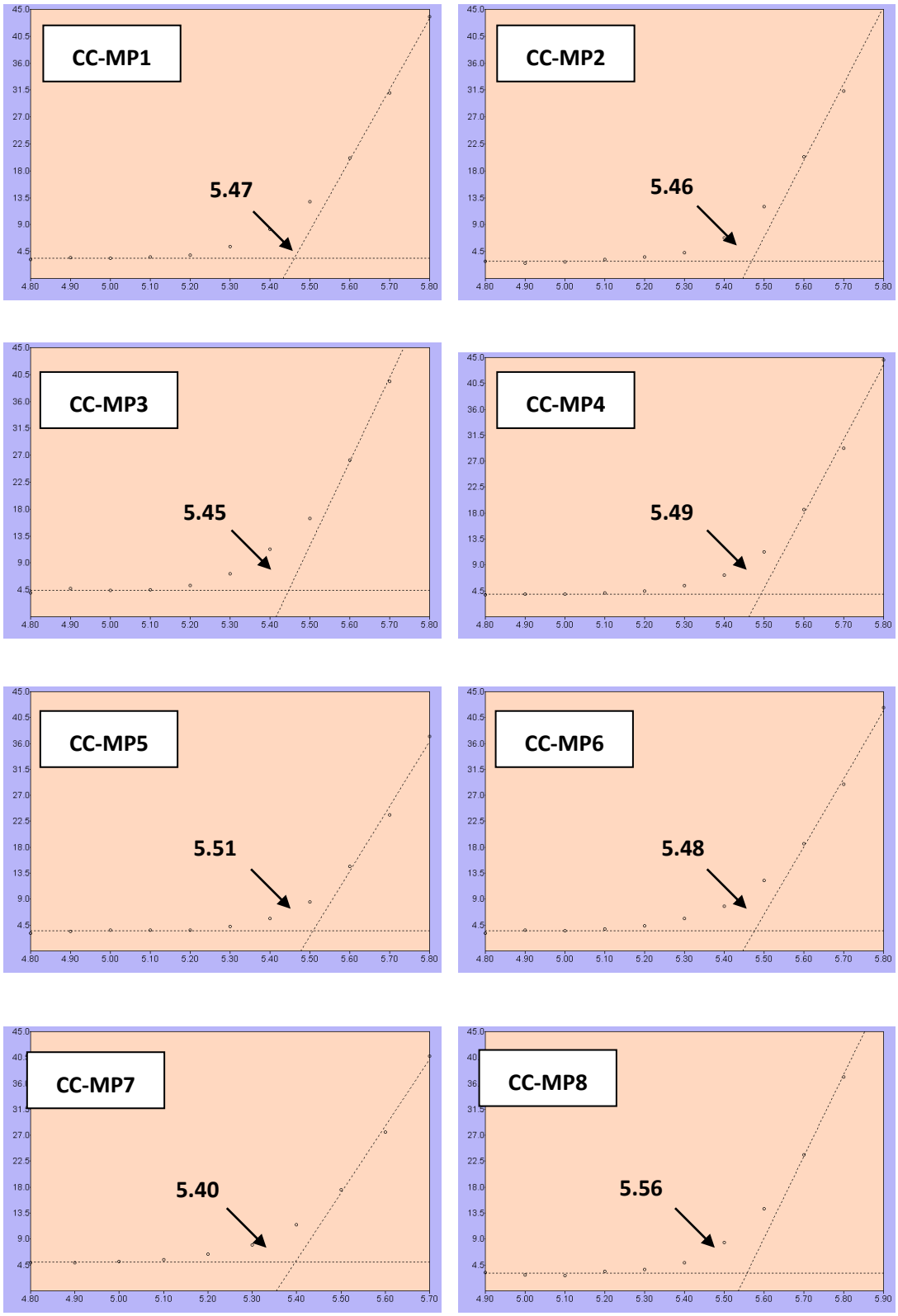
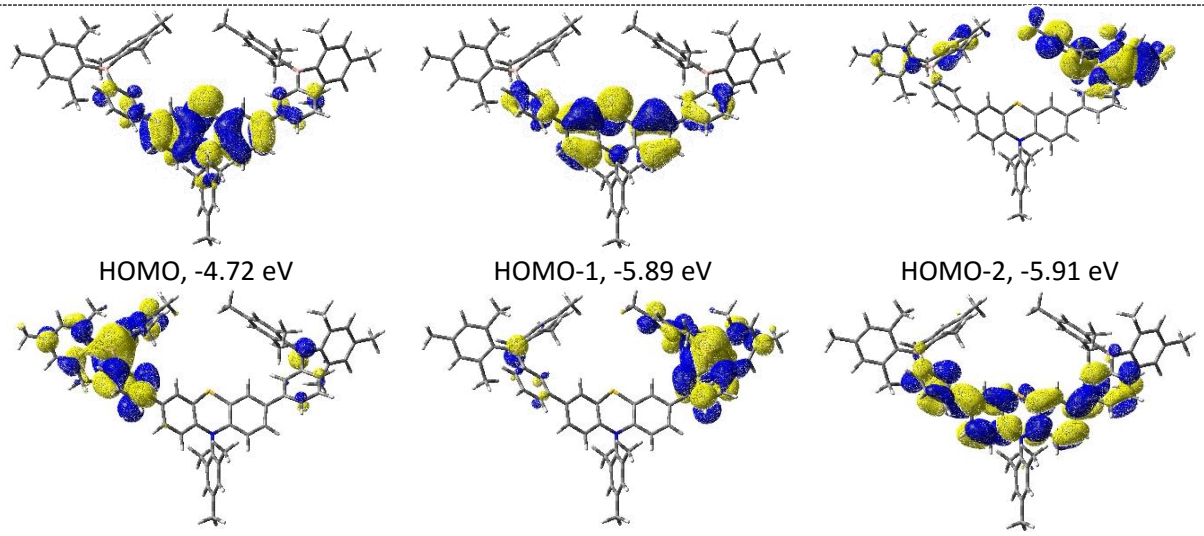


Fig. S5 Low-energy photoelectron spectra of all compounds.

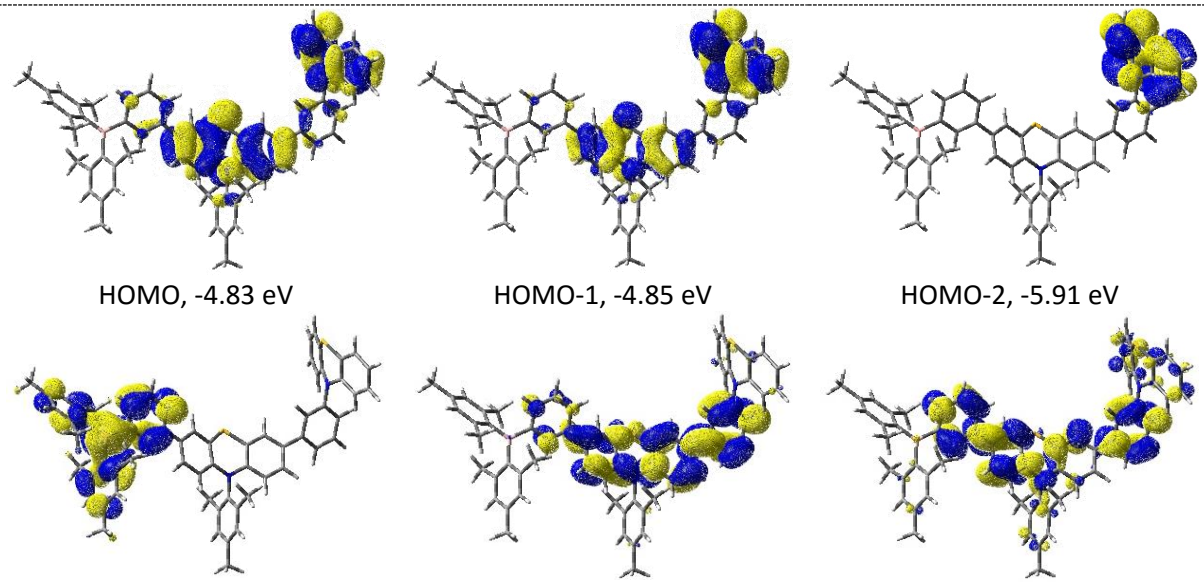
CC-MP1, ΔE = 3.12 eV (397.91 nm)



HOMO, -4.72 eV | HOMO-1, -5.89 eV | HOMO-2, -5.91 eV

LUMO, -1.60 eV | LUMO+1,-1.57 eV | LUMO+2, -0.89 eV

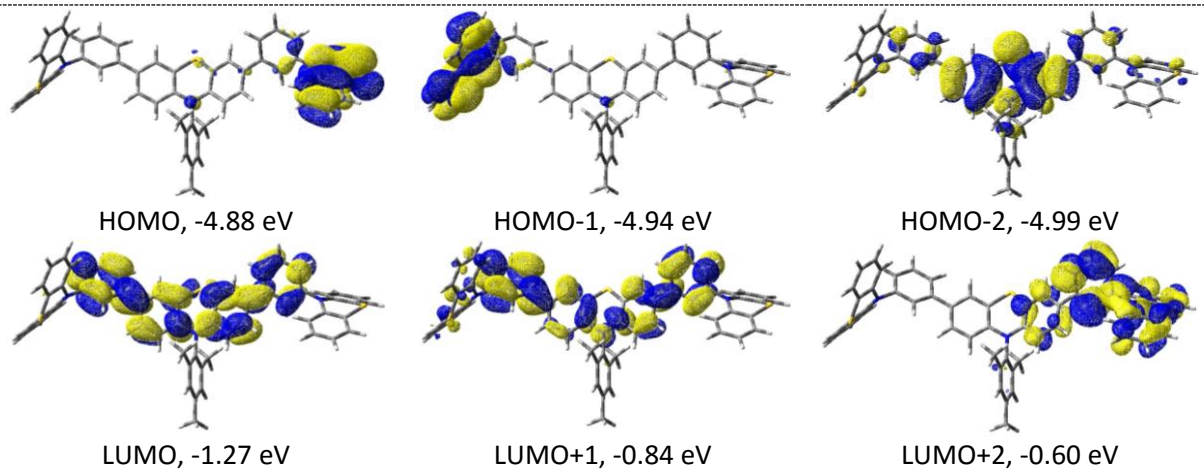
CC-MP2, ΔE = 3.20 eV (387.79 nm)



HOMO, -4.83 eV | HOMO-1, -4.85 eV | HOMO-2, -5.91 eV

LUMO, -1.63 eV | LUMO+1, -1.14 eV | LUMO+2, -0.60 eV

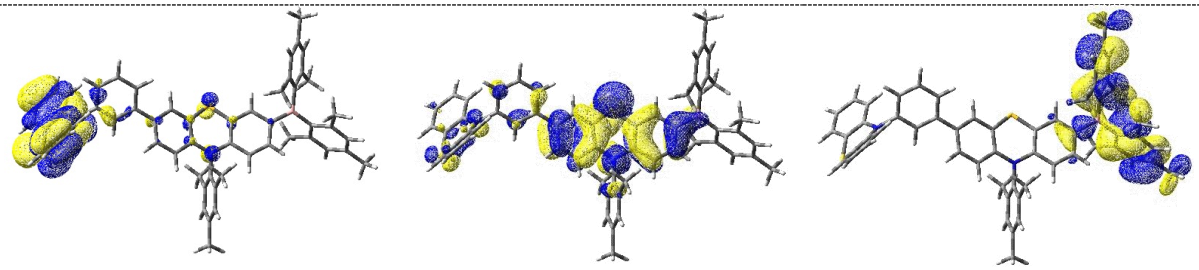
CC-MP3, ΔE = 3.61 eV (344.06 nm)



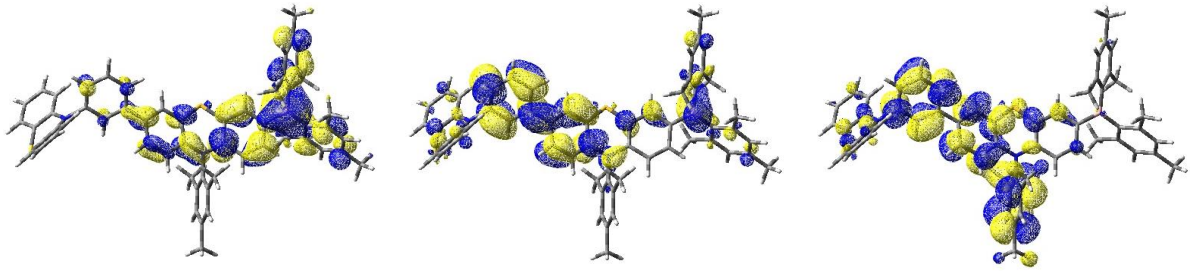
HOMO, -4.88 eV | HOMO-1, -4.94 eV | HOMO-2, -4.99 eV

LUMO, -1.27 eV | LUMO+1, -0.84 eV | LUMO+2, -0.60 eV

CC-MP4, ΔE = 3.25 eV (381.33 nm)

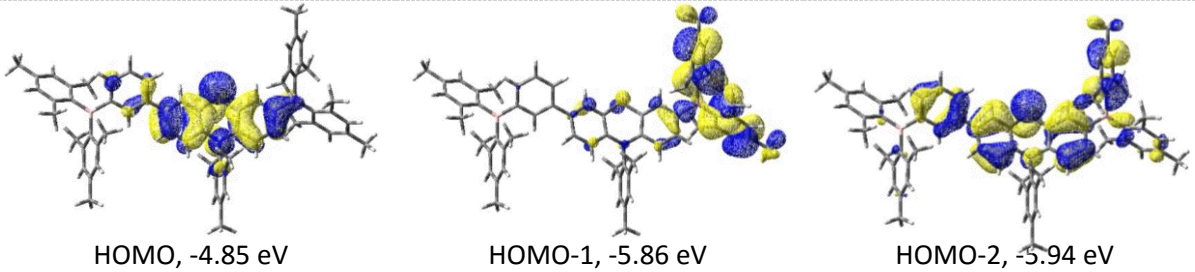


HOMO, -4.88 eV | HOMO-1, -4.96 eV | HOMO-2, -5.91 eV

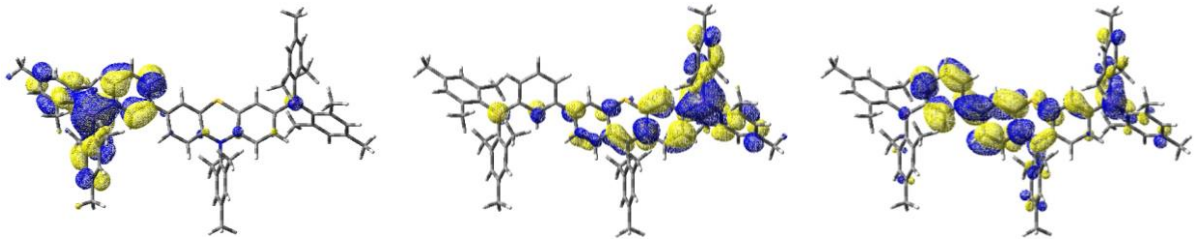


LUMO, -1.63 eV | LUMO + 1, -0.98 eV | LUMO + 2, -0.49 eV

CC-MP5, ΔE = 3.20 eV (387.79 nm)

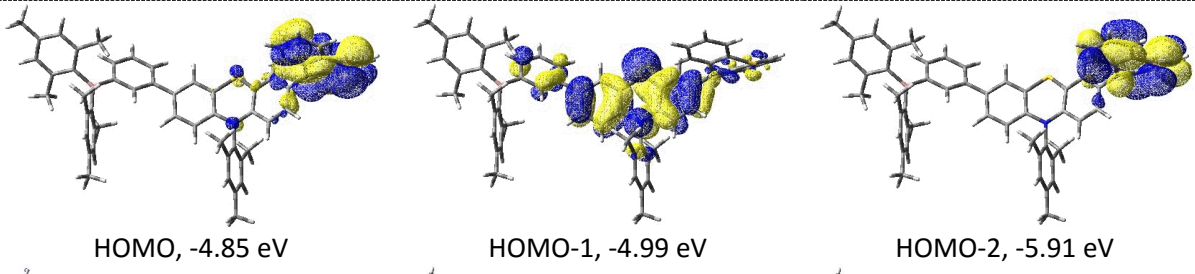


HOMO, -4.85 eV | HOMO-1, -5.86 eV | HOMO-2, -5.94 eV

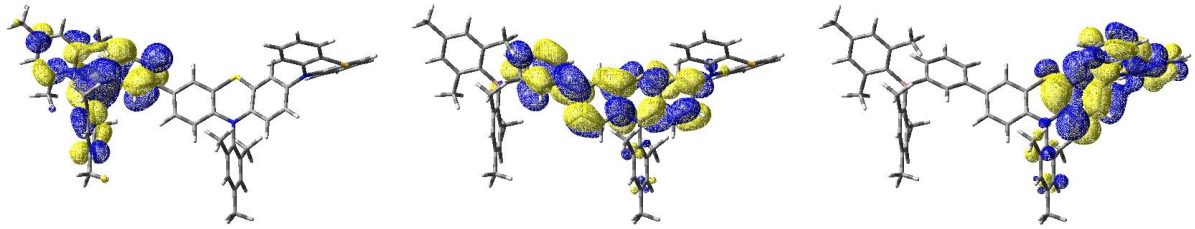


LUMO, -1.65 eV | LUMO+1, -1.55 eV | LUMO+2, -0.71 eV

CC-MP6, ΔE = 3.17 eV (391.11 nm)



HOMO, -4.85 eV | HOMO-1, -4.99 eV | HOMO-2, -5.91 eV



LUMO, -1.68 eV | LUMO+1, -0.95 eV | LUMO+2, -0.57 eV

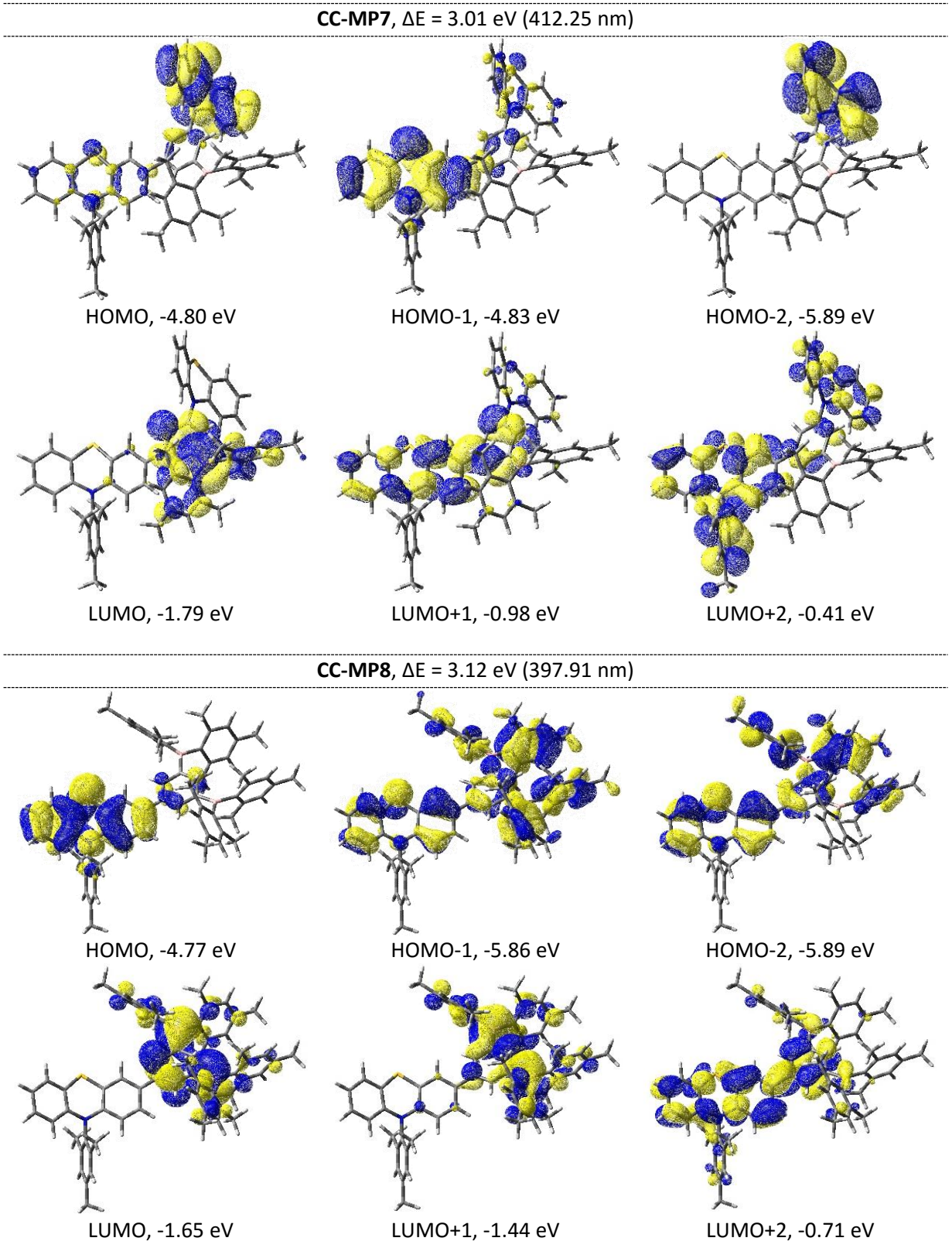


Fig. S6 Frontier orbitals of the compounds.

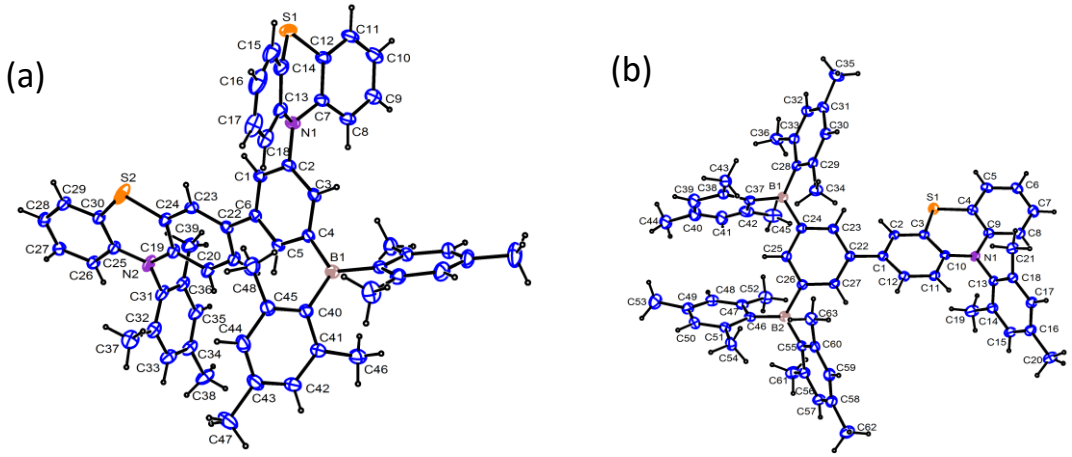


Fig. S7 ORTEP plots of **CC-MP7** (a) and **CC-MP8** (b).

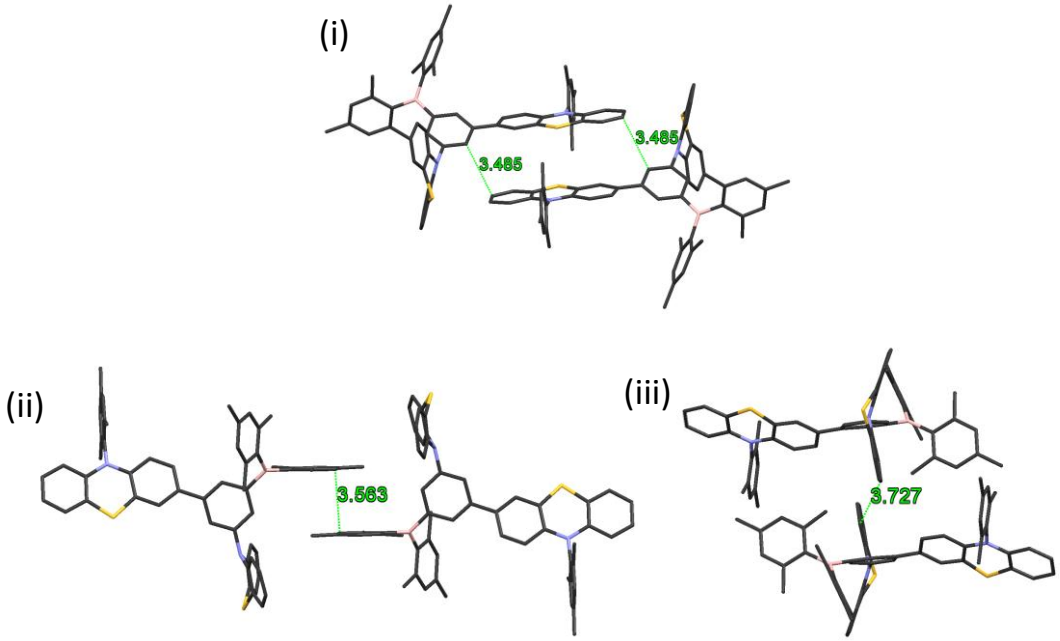


Fig. S8 Packing of **CC-MP7** molecules in the crystal.

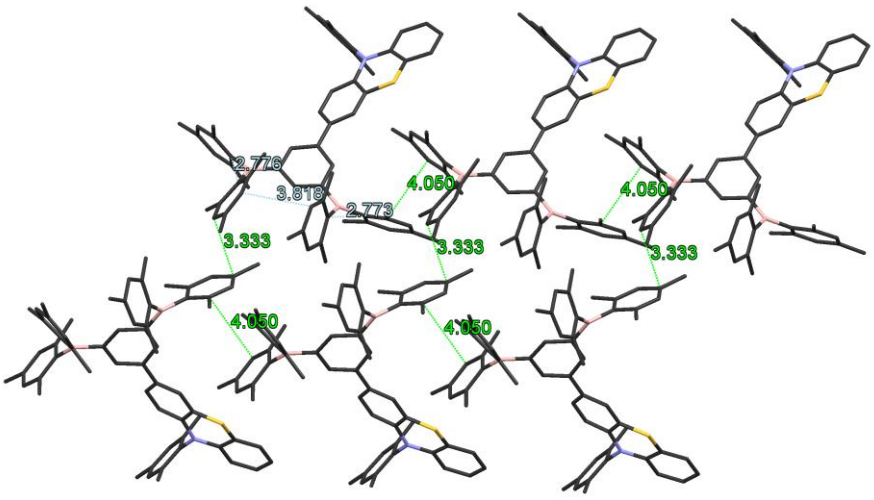
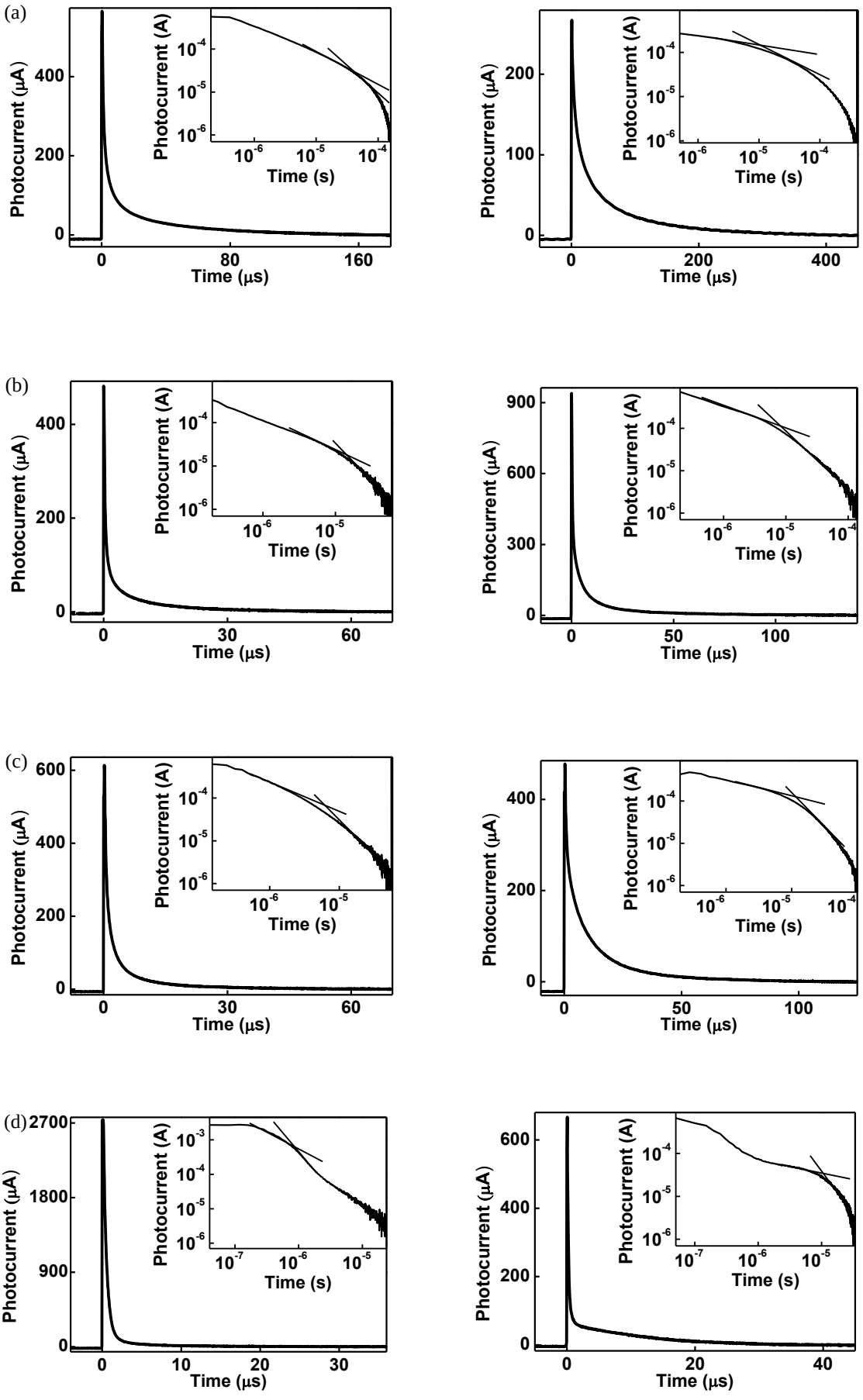


Fig. S9 Packing of **CC-MP8** molecules in the crystal.


(a)
Photocurrent (μA)
Time (μs)
Photocurrent (A)
Time (s)
(b)
(c)
(d)

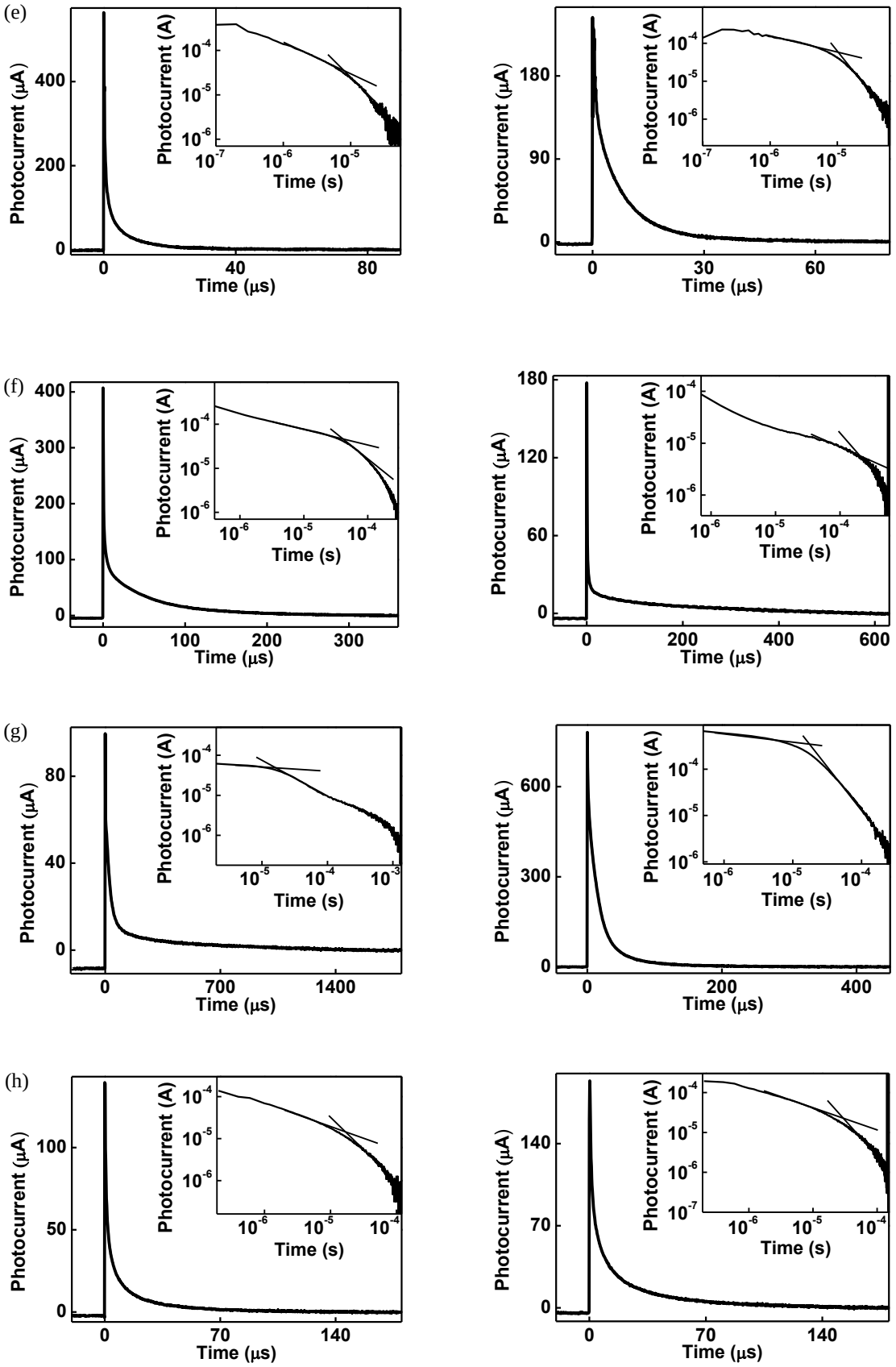


Fig. S10 The representative TOF transients for electrons (left) and holes (right) of **CC-MP1** (a)**, CC-MP2** (b), **CC-MP3** (c), **CC-MP4** (d)**, CC-MP5** (e)**, CC-MP6** (f) **, CC-MP7** (g) **,** and **CC-MP8** (h).

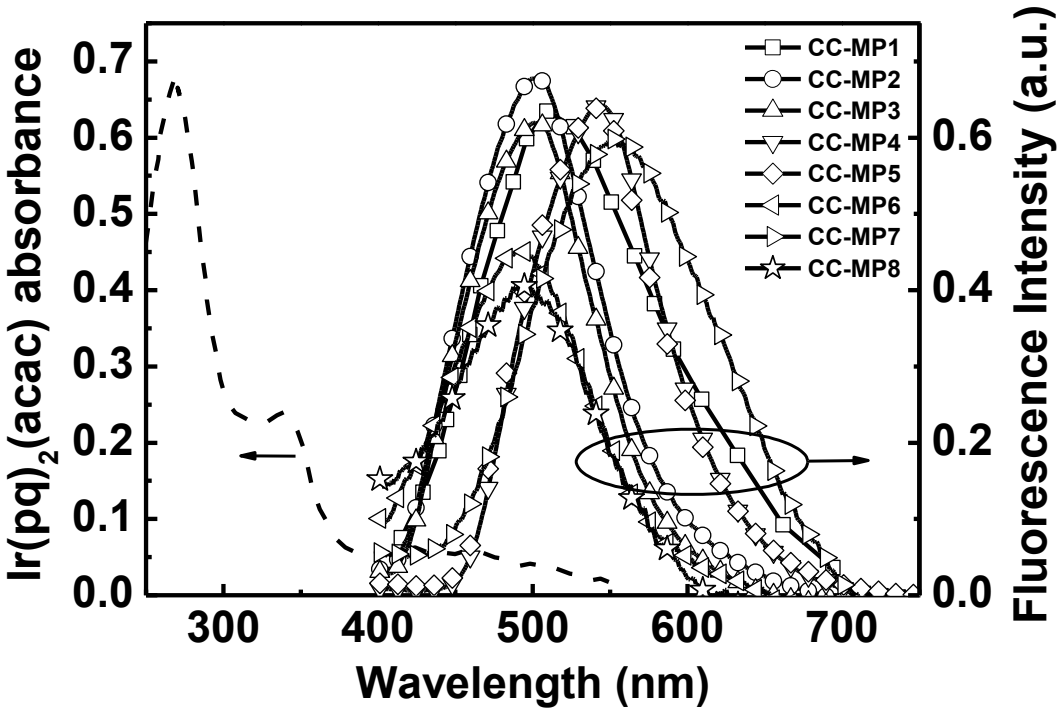
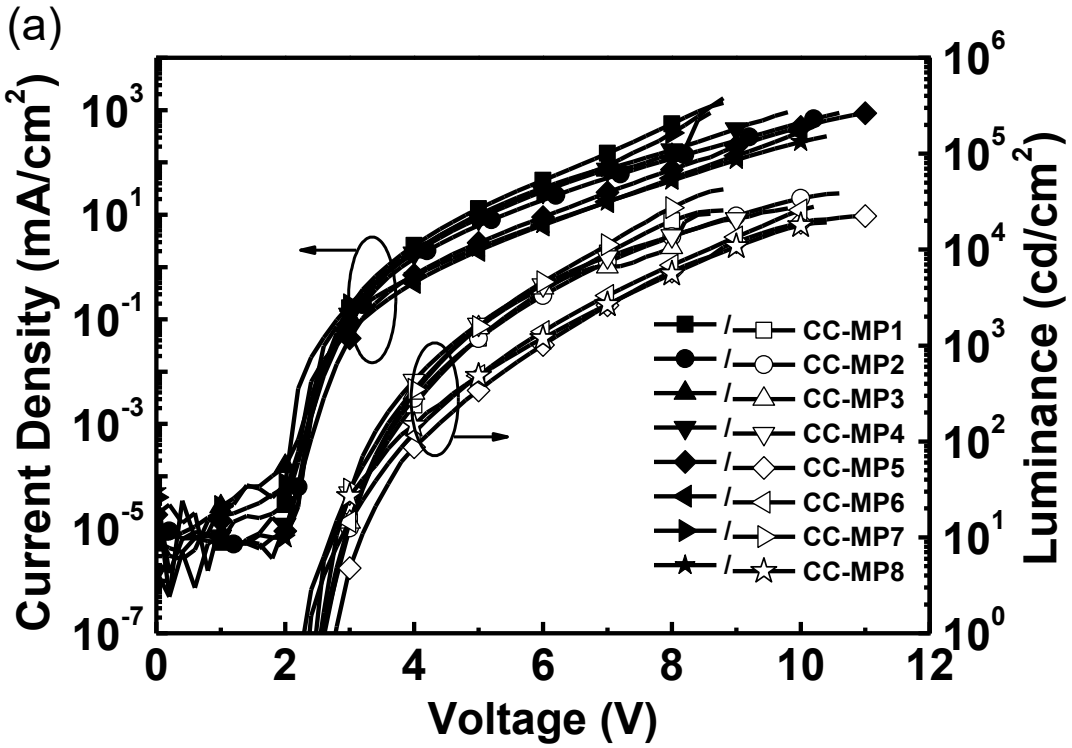


Fig. S11 Film PL spectra of selected **CC-MP** dyes and absorption spectrum of $Ir(pq)_2(acac)$.



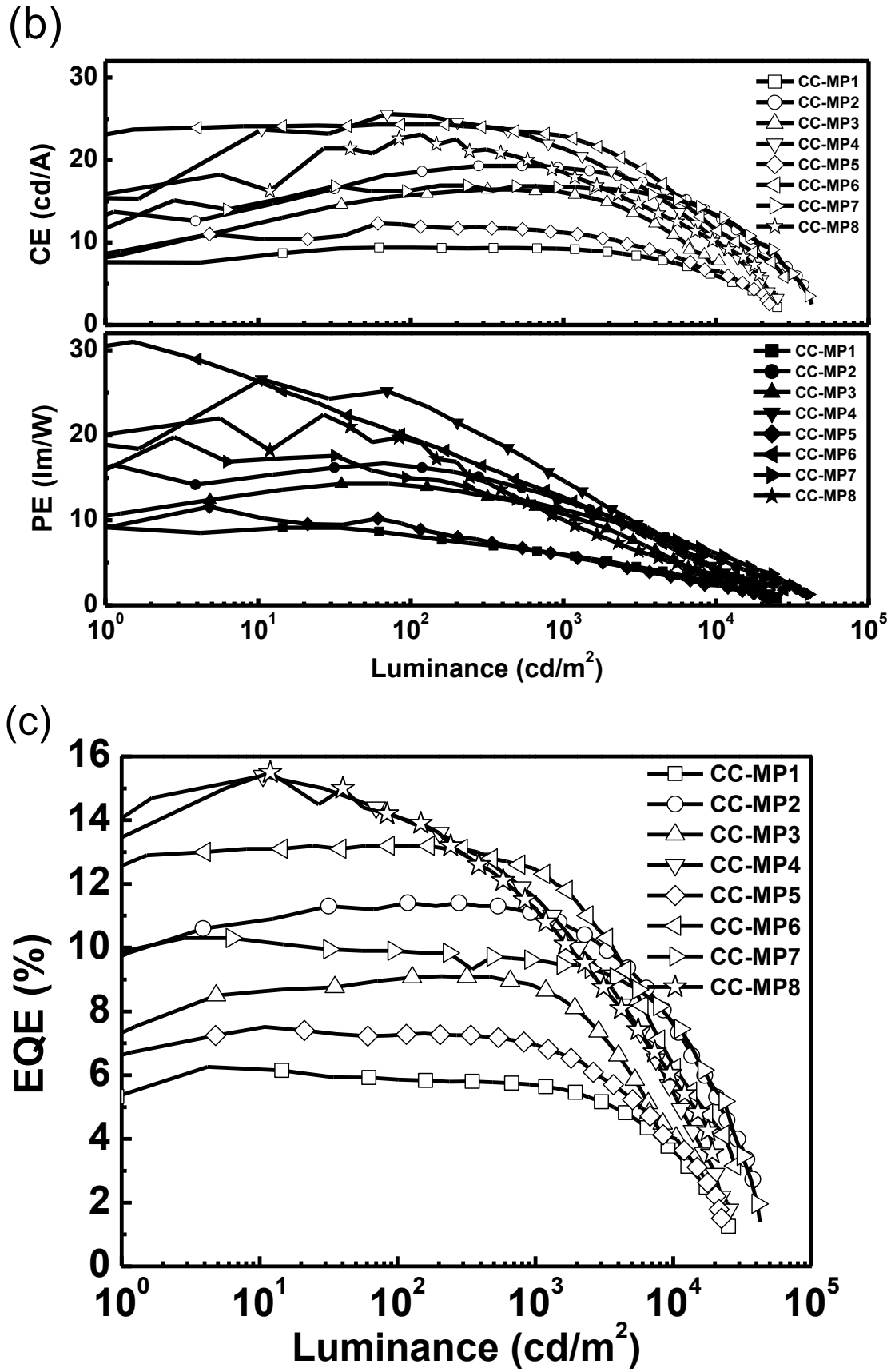


Fig. S12 J–V–L (a), CE–L–PE (b), EQE-L (c) plots of the OLED device.

Table S1 Calculated lower-lying transitions of the dyes.[a]

dye	State	excitation[b]	eV	*f*	dye	State	excitation[b]	eV	*f*
CC-MP1	S_1	H → L (93%) H → L1 (6%)	2.74	0.017	**CC-MP2**	S_1	H1 → L (30%) H → L (69%)	2.86	0.014
	S_2	H → L (6%) H → L1 (93%)	2.76	0.003		S_2	H1 → L (69%) H → L (30%)	3.06	0.000
	S_3	H → L2 (94%)	3.19	0.253		S_3	H1 → L1 (26%) H → L1 (68%)	3.12	0.290
CC-MP3	S_1	H2 → L (80%) H1 → L (5%) H → L (10%)	3.12	0.324	**CC-MP4**	S_1	H1 → L (87%) H → L (9%)	2.79	0.299
	S_2	H2 → L (5%) H1 → L (80%) H1 → L1 (13%)	3.22	0.001		S_2	H1 → L (9%) H → L (85%) H → L1 (5%)	3.01	0.001
	S_3	H2 → L (9%) H → L (77%) H → L1 (10%)	3.24	0.003		S_3	H → L (6%) H → L1 (84%)	3.40	0.002
CC-MP5	S_1	H → L1 (31%) H → L (66%)	2.79	0.278	**CC-MP6**	S_1	H1 → L (60%) H → L (40%)	2.92	0.010
	S_2	H → L (68%) H → L1 (31%)	2.87	0.036		S_2	H1 → L (39%) H → L (60%)	2.99	0.003
	S_3	H3 → L (93%)	3.56	0.077		S_3	H1 → L1 (76%) H → L1 (17%)	3.32	0.135
CC-MP7	S_1	H1 → L (5%) H → L (94%)	2.49	0.000	**CC-MP8**	S_1	H → L (99%)	2.70	0.008
	S_2	H1 → L (95%) H → L (5%)	2.67	0.035		S_2	H → L1 (99%)	2.96	0.037
	S_3	H1 → L1 (61%) H1 → L2 (5%) H → L1 (29%)	3.25	0.155		S_3	H → L2 (89%)	3.38	0.098

[a]Results are based on gas-phase TD-DFT calculation.

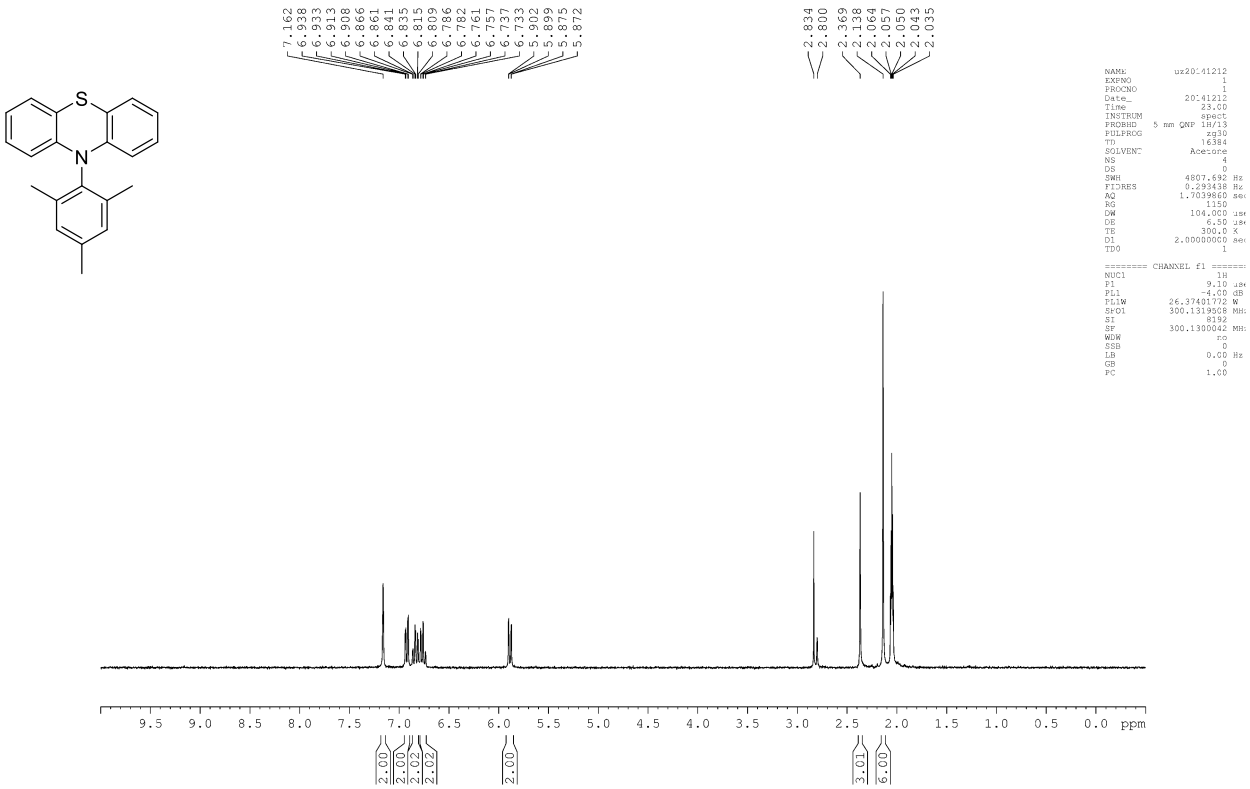
[b]H = HOMO, L = LUMO, H1 = The next highest occupied molecular orbital, or HOMO – 1, Hn = HOMO – n, Ln = LUMO + n. In parentheses is the population of a pair of MO excitations.

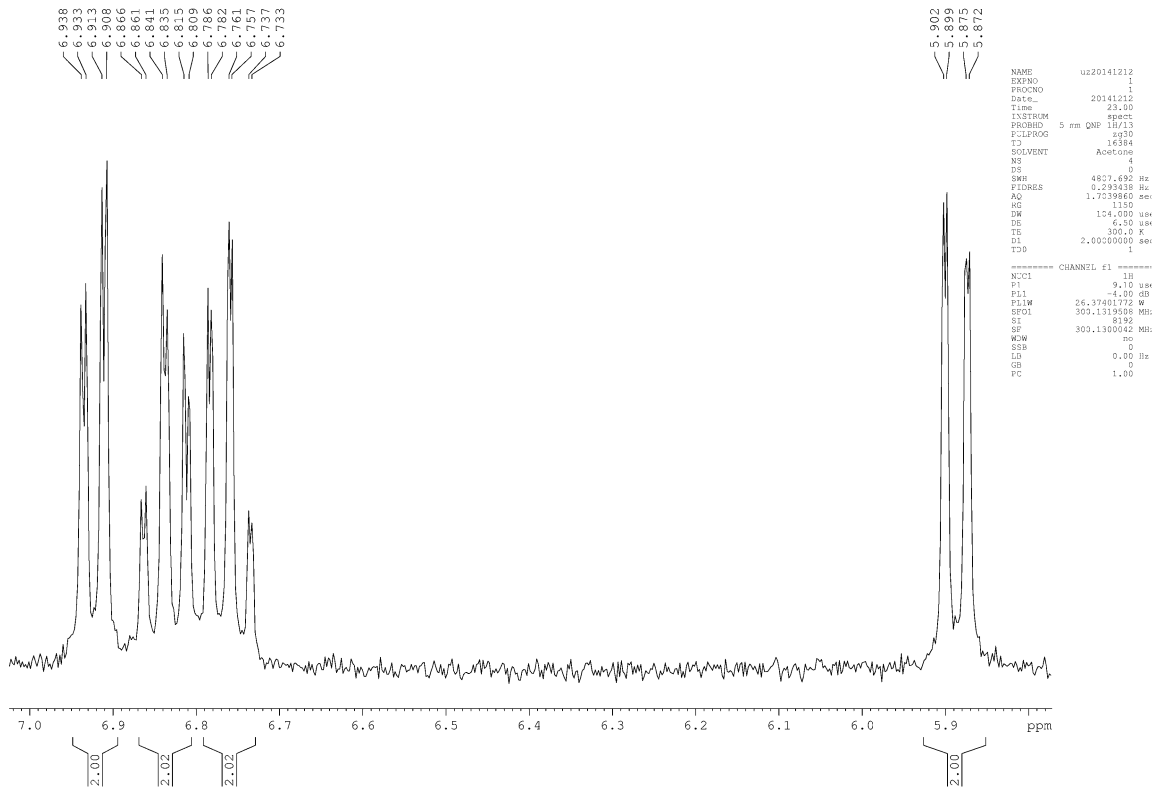
Table S2 Selected bond distances (Å) and angles (°) of the compounds.

CC-MP4					
S(1)-C(6)	1.762(2)	S(2)-C(25)	1.745(7)	S(1)-C(7)	1.762(2)
S(2)-C(26)	1.759(6)	N(1)-C(1)	1.398(3)	N(2)-C(15)	1.426(5)
N(1)-C(12)	1.411(3)	N(2)-C(20)	1.349(8)	N(1)-C(32)	1.445(3)
N(2)-C(31)	1.449(8)	B(1)-C(4)	1.557(3)	B(1)-C(41)	1.582(4)
B(1)-C(50)	1.578(4)	C(9)-C(13)	1.485(3)		
C(1)-N(1)-C(12)	123.3(2)	C(15)-N(2)-C(20)	115.7(5)	C(1)-N(1)-C(32)	119.7(2)
C(15)-N(2)-C(31)	116.0(4)	C(12)-N(1)-C(32)	117.0(2)	C(20)-N(2)-C(31)	123.6(5)
N(1)-C(1)-C(2)	120.5(2)	N(2)-C(15)-C(14)	120.9(3)	N(1)-C(1)-C(6)	121.8(2)
N(2)-C(15)-C(16)	118.0(3)	N(1)-C(12)-C(7)	122.0(2)	N(2)-C(20)-C(21)	123.0(5)
N(1)-C(12)-C(11)	120.7(2)	N(2)-C(20)-C(25)	119.4(6)	N(1)-C(32)-C(33)	116.8(2)
N(2)-C(31)-C(26)	119.0(5)	N(1)-C(32)-C(37)	121.9(2)	N(2)-C(31)-C(30)	123.0(5)
S(1)-C(6)-C(1)	121.8(2)	S(2)-C(25)-C(20)	121.2(5)	S(1)-C(7)-C(8)	117.2(2)
S(2)-C(25)-C(24)	119.0(4)	S(1)-C(6)-C(5)	117.4(2)	S(2)-C(26)-C(27)	117.6(4)

S(1)-C(7)-C(12)	121.4(2)	S(2)-C(26)-C(31)	120.5(5)	C(4)-B(1)-C(41)	117.5(2)
C(4)-B(1)-C(50)	118.9(2)	C(41)-B(1)-C(50)	123.6(2)	B(1)-C(4)-C(3)	123.6(2)
B(1)-C(4)-C(5)	119.9(2)	B(1)-C(41)-C(42)	121.7(2)	B(1)-C(41)-C(46)	119.9(2)
B(1)-C(50)-C(51)	119.3(2)	B(1)-C(50)-C(55)	122.8(2)	C(13)-C(9)-C(8)	120.3(2)
C(13)-C(9)-C(10)	122.2(2)	C(9)-C(13)-C(14)	120.5(3)	C(9)-C(13)-C(18)	121.5(2)
CC-MP7					
S(1)-C(12)	1.753 (2)	S(2)-C(24)	1.759(2)	S(1)-C(14)	1.754(2)
S(2)-C(30)	1.755(2)	N(1)-C(2)	1.444(2)	N(2)-C(19)	1.402(2)
N(1)-C(7)	1.416(2)	N(2)-C(25)	1.404(2)	N(1)-C(13)	1.418(2)
N(2)-C(31)	1.442(2)	B(1)-C(4)	1.570(2)	B(1)-C(40)	1.571(2)
B(1)-C(49)	1.567(2)	C(6)-C(22)	1.482(2)		
C(6)-N(1)-C(7)	121.9(2)	C(30)-N(2)-C(19)	123.83(19)	C(6)-N(1)-C(13)	116.7(2)
C(30)-N(2)-C(17)	117.4(2)	C(7)-N(1)-C(13)	116.2(2)	C(19)-N(2)-C(17)	118.13(19)
N(1)-C(2)-C(1)	118.3(1)	N(2)-C(31)-C(32)	118.8(2)	N(1)-C(2)-C(3)	120.9(1)
N(2)-C(31)-C(36)	118.7(2)	N(1)-C(7)-C(8)	121.8(1)	N(2)-C(19)-C(20)	119.6(1)
N(1)-C(7)-C(12)	120.2(2)	N(2)-C(19)-C(24)	123.0(1)	N(1)-C(13)-C(14)	119.7(2)
N(2)-C(25)-C(26)	119.2(1)	N(1)-C(13)-C(18)	122.4(1)	N(2)-C(25)-C(30)	122.8(1)
C(12)-S(1)-C(14)	98.88(8)	C(30)-S(2)-C(24)	101.36(7)	S(1)-C(12)-C(7)	120.4(1)
S(2)-C(24)-C(23)	160.1(1)	S(1)-C(12)-C(11)	119.0(1)	S(2)-C(24)-C(29)	123.3(1)
S(1)-C(14)-C(13)	120.3(1)	S(2)-C(30)-C(25)	123.9(1)	S(1)-C(14)-C(15)	118.9(1)
S(2)-C(30)-C(29)	106.1(1)	C(2)-N(1)-C(7)	116.7(1)	C(19)-N(2)-C(25)	124.6(1)
C(7)-N(1)-C(13)	120.7(1)	C(25)-N(2)-C(31)	118.4(1)	C(2)-N(1)-C(13)	117.6(1)
C(19)-N(2)-C(31)	117.0(1)	C(4)-B(1)-C(40)	115.5(1)	C(4)-B(1)-C(49)	120.1(1)
C(40)-B(1)-C(49)	124.3(1)	B(1)-C(4)-C(3)	121.8(1)	B(1)-C(4)-C(5)	120.2(1)
B(1)-C(40)-C(41)	120.8(1)	B(1)-C(40)-C(45)	121.1(1)	B(1)-C(49)-C(50)	120.8(1)
B(1)-C(49)-C(54)	121.2(1)	C(22)-C(6)-C(1)	122.1(1)	C(22)-C(6)-C(5)	120.0(1)
C(6)-C(22)-C(21)	120.7(1)	C(6)-C(22)-C(23)	122.1(1)		
CC-MP8					
S(1)-C(3)	1.756(2)	S(1)-C(4)	1.758(2)	N(1)-C(9)	1.412(2)
N(1)-C(10)	1.404(2)	N(1)-C(13)	1.443(2)	C(1)-C(22)	1.481(2)
B(1)-C(24)	1.567(3)	B(2)-C(26)	1.575(3)	B(1)-C(28)	1.574(3)
B(2)-C(46)	1.578(3)	B(1)-C(37)	1.572(3)	B(2)-C(55)	1.576(3)
C(9)-N(1)-C(10)	124.1(1)	C(9)-N(1)-C(13)	118.1(1)	C(10)-N(1)-C(13)	117.3(1)
N(1)-C(9)-C(4)	121.9(2)	N(1)-C(9)-C(8)	120.2(2)	N(1)-C(10)-C(3)	122.6(2)
N(1)-C(10)-C(11)	120.1(2)	N(1)-C(13)-C(14)	118.4(2)	N(1)-C(13)-C(18)	120.0(2)
C(24)-B(1)-C(28)	120.9(2)	C(24)-B(1)-C(37)	115.5(2)	C(28)-B(1)-C(37)	123.6(2)
C(26)-B(2)-C(46)	117.0(2)	C(26)-B(2)-C(55)	119.7(2)	C(46)-B(2)-C(55)	123.3(2)
B(1)-C(24)-C(23)	121.8(2)	B(1)-C(24)-C(25)	120.8(2)	B(1)-C(28)-C(29)	121.8(2)
B(1)-C(28)-C(33)	120.7(2)	B(1)-C(37)-C(38)	120.0(2)	B(1)-C(37)-C(42)	121.0(2)
B(2)-C(26)-C(25)	121.3(2)	B(2)-C(26)-C(27)	121.3(2)	B(2)-C(46)-C(47)	120.9(2)
B(2)-C(46)-C(51)	121.5(2)	B(2)-C(55)-C(56)	120.1(2)	B(2)-C(55)-C(60)	121.7(2)
C(1)-C(22)-C(23)	120.5(2)	C(1)-C(22)-C(27)	121.8(2)	C(22)-C(1)-C(2)	121.0(2)
C(22)-C(1)-C(12)	122.4(2)				

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **1**:





MesPh

[Elemental Composition]

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Date : 24-Mar-2014 17:02
Sample: MesPh
Note : NBA
Inlet : Direct
Ion Mode : FAB+
RT : 0.19 min
Scan#: 4
Elements : C 400/0, H 1000/0, N 1/1, S 1/1
Mass Tolerance : 10mmu
Unsaturation (U.S.) : -0.5 - 1000.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
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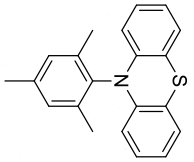

[Mass Spectrum]
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Spectrum Type : Normal Ion (EF-Linear)
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Int. : 15.02
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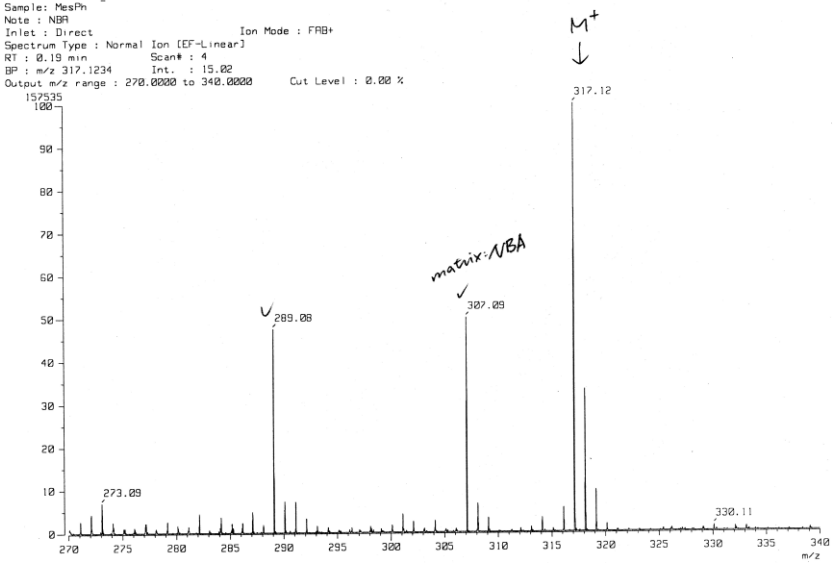
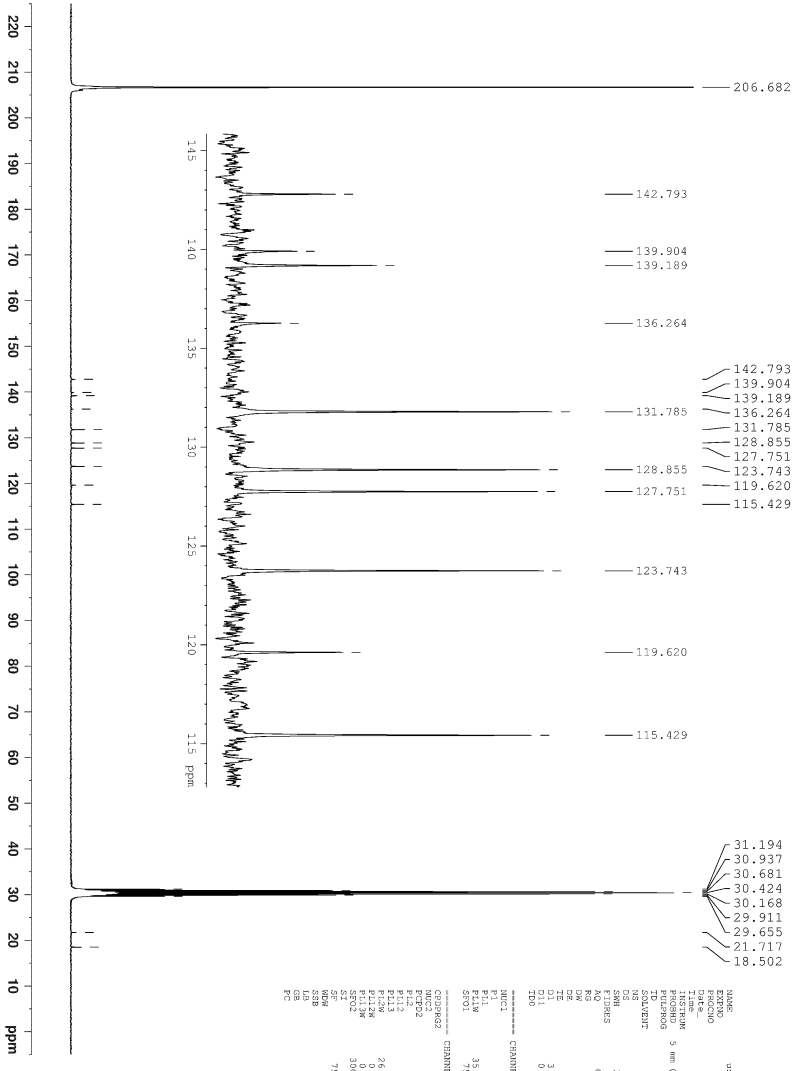
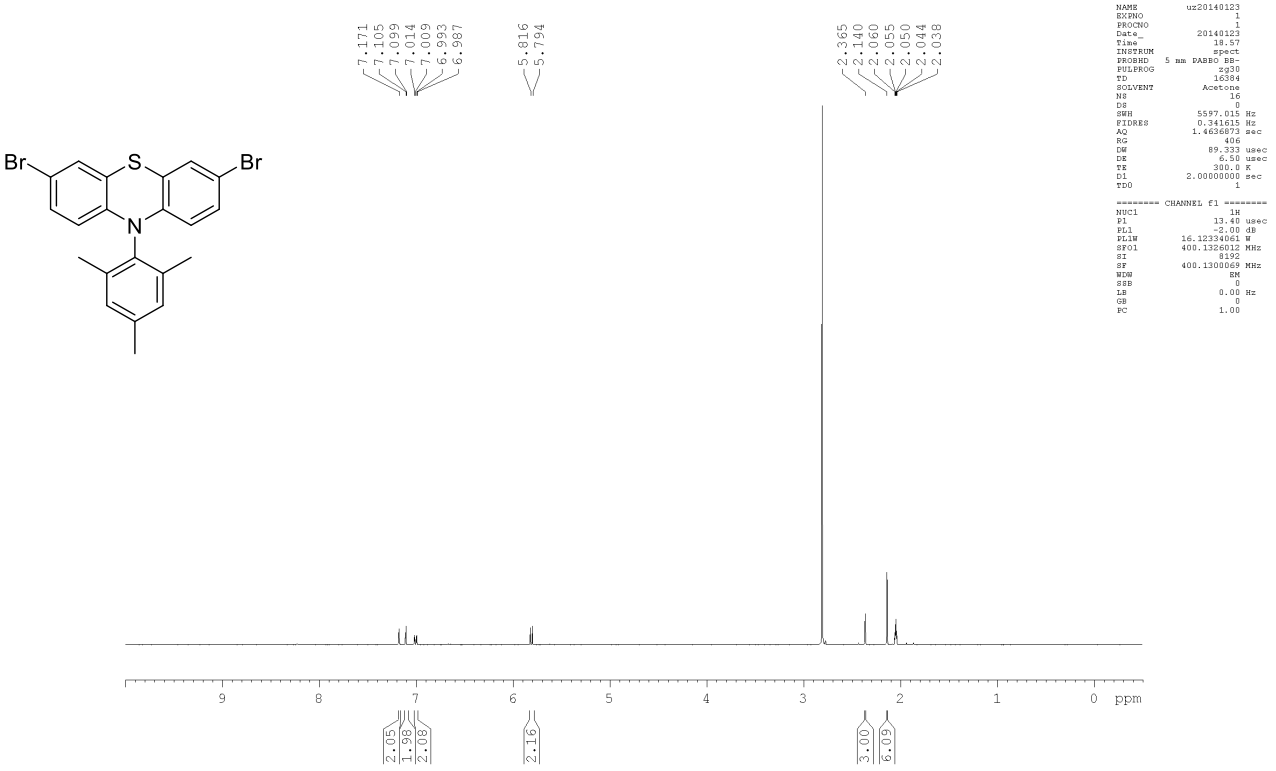
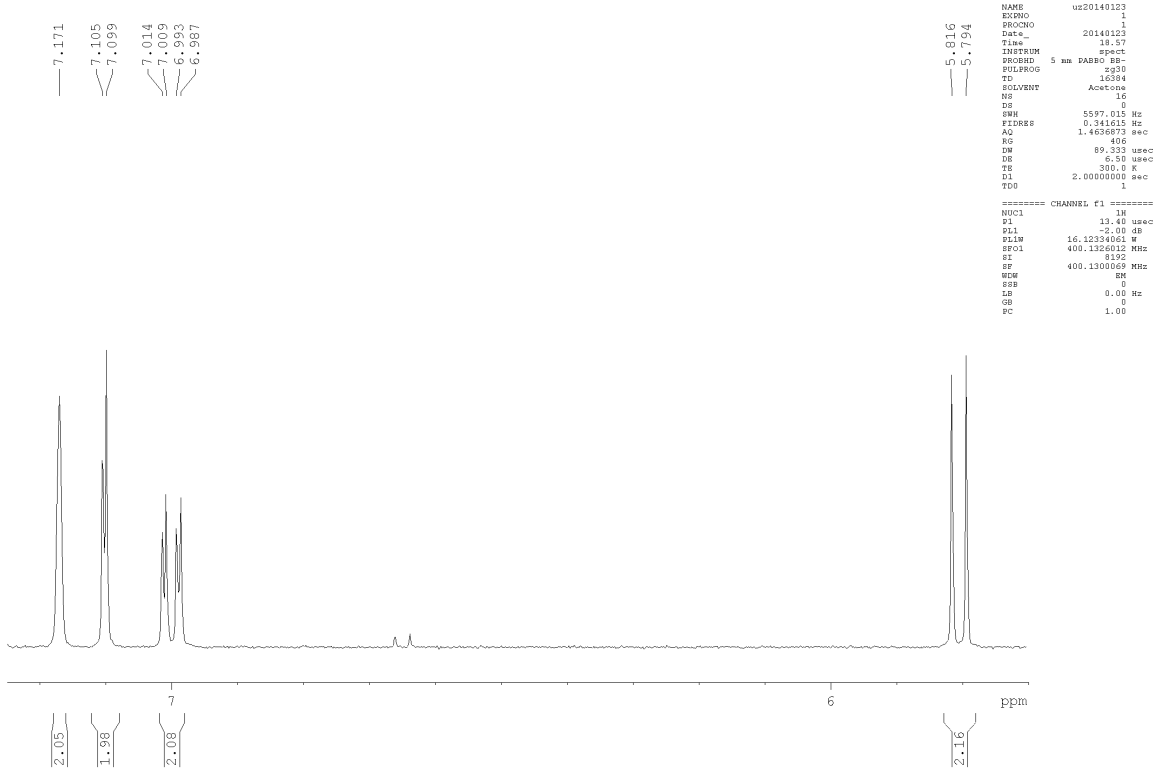
Cut Level : 0.00 %

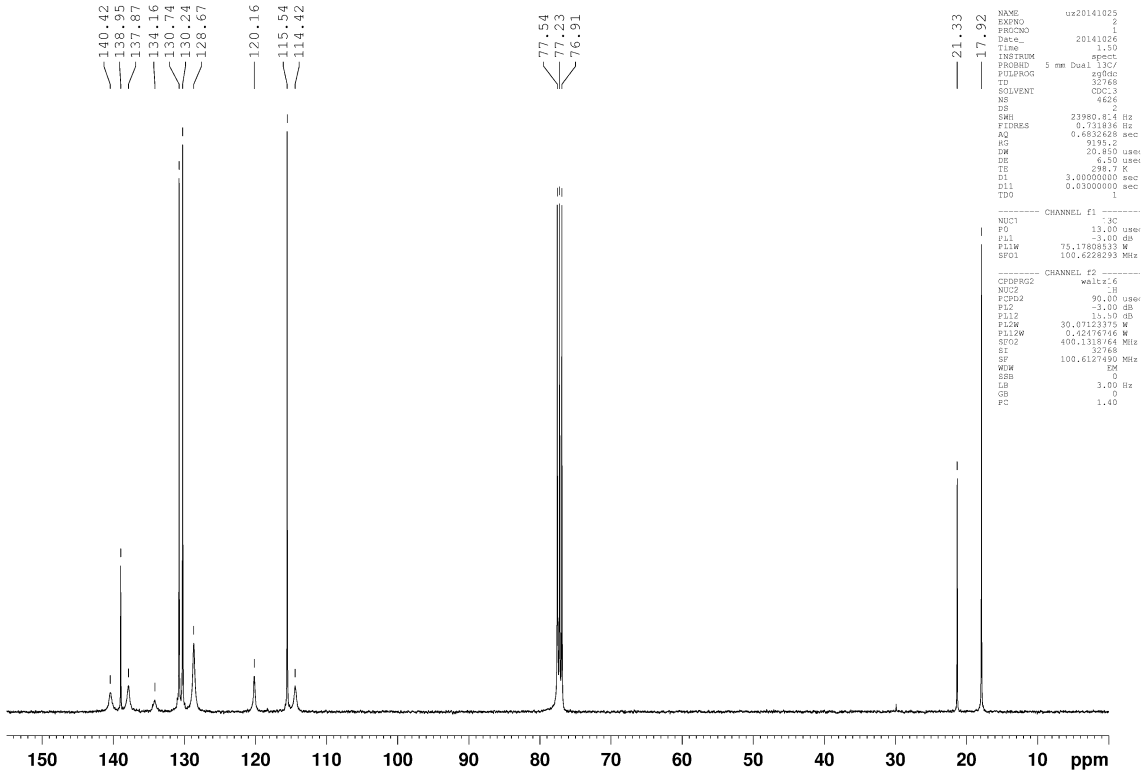




^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **2**:



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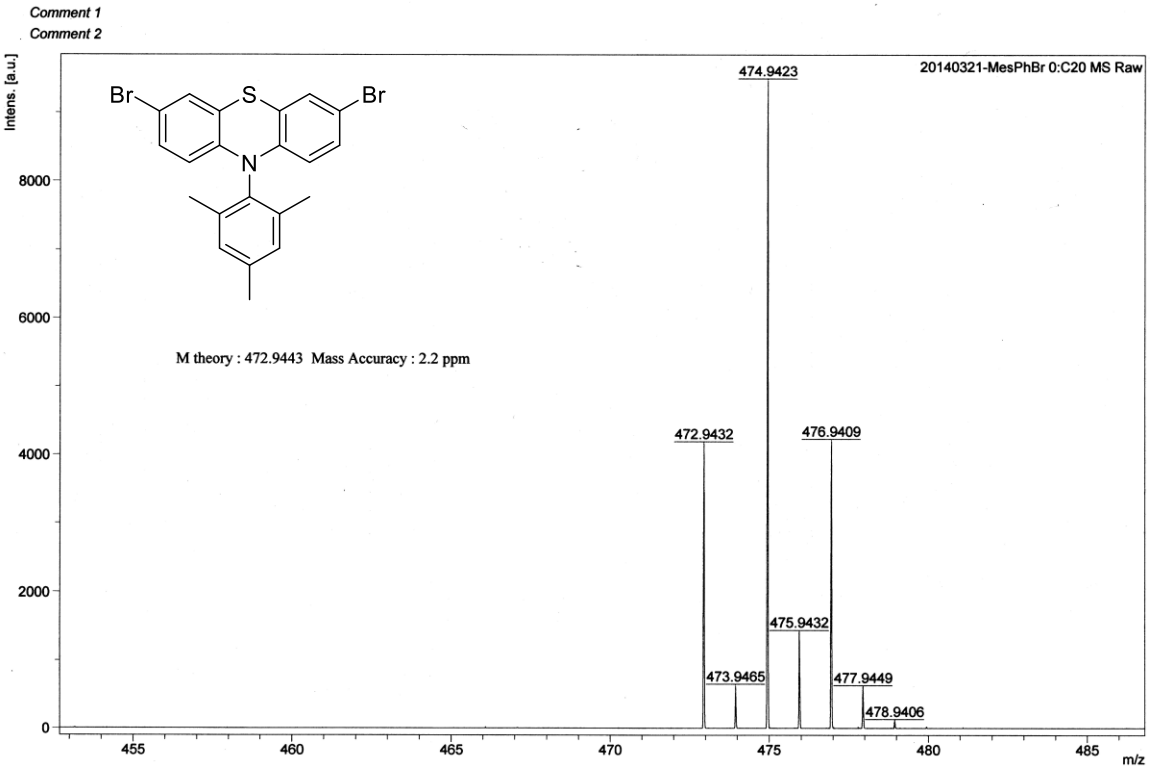
10
ppm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Comment 2
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S
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N
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472.9432
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475
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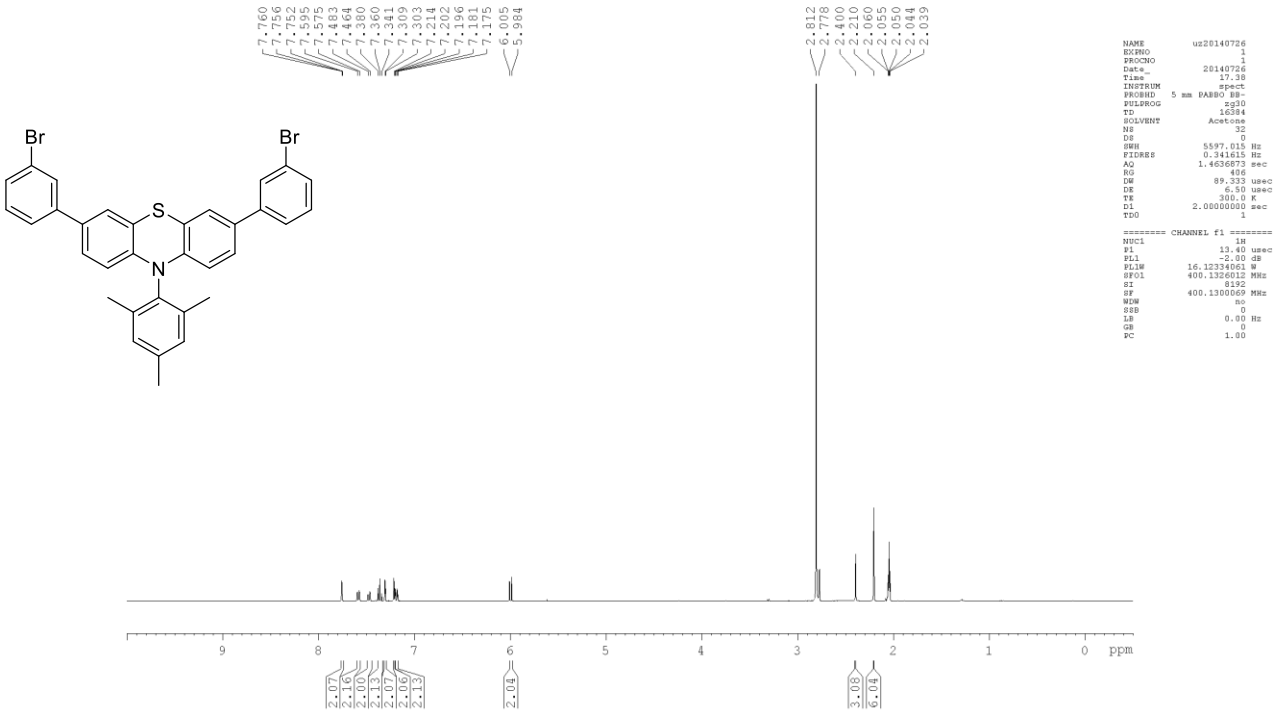
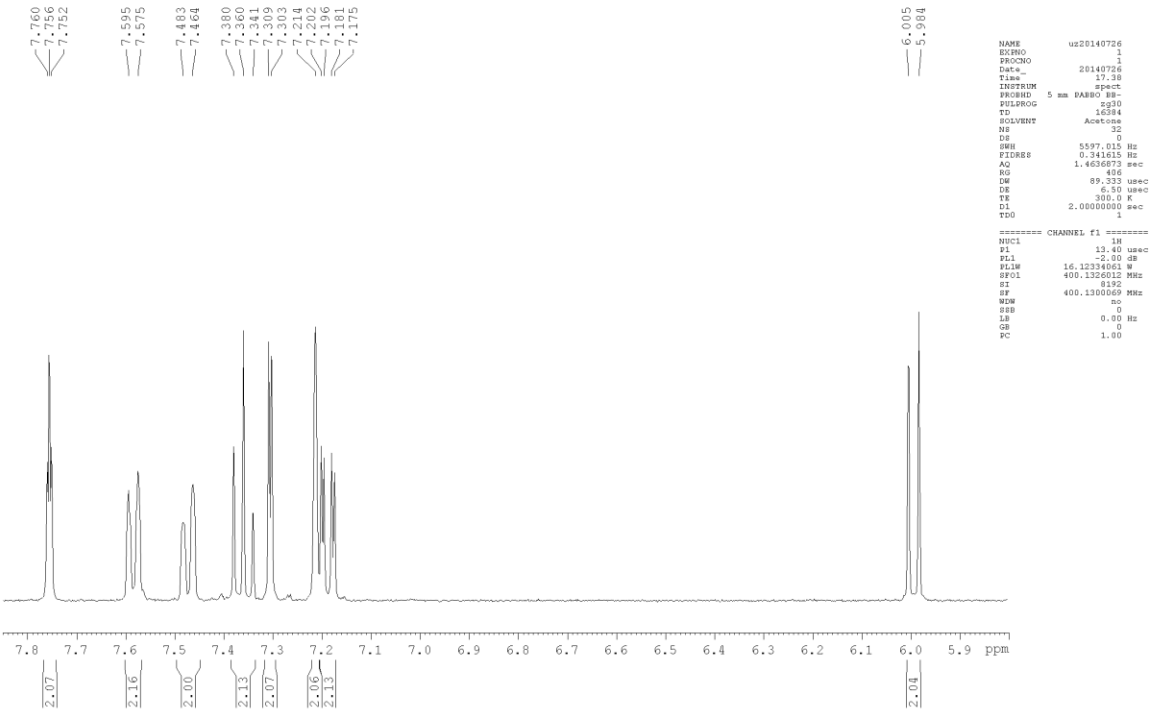
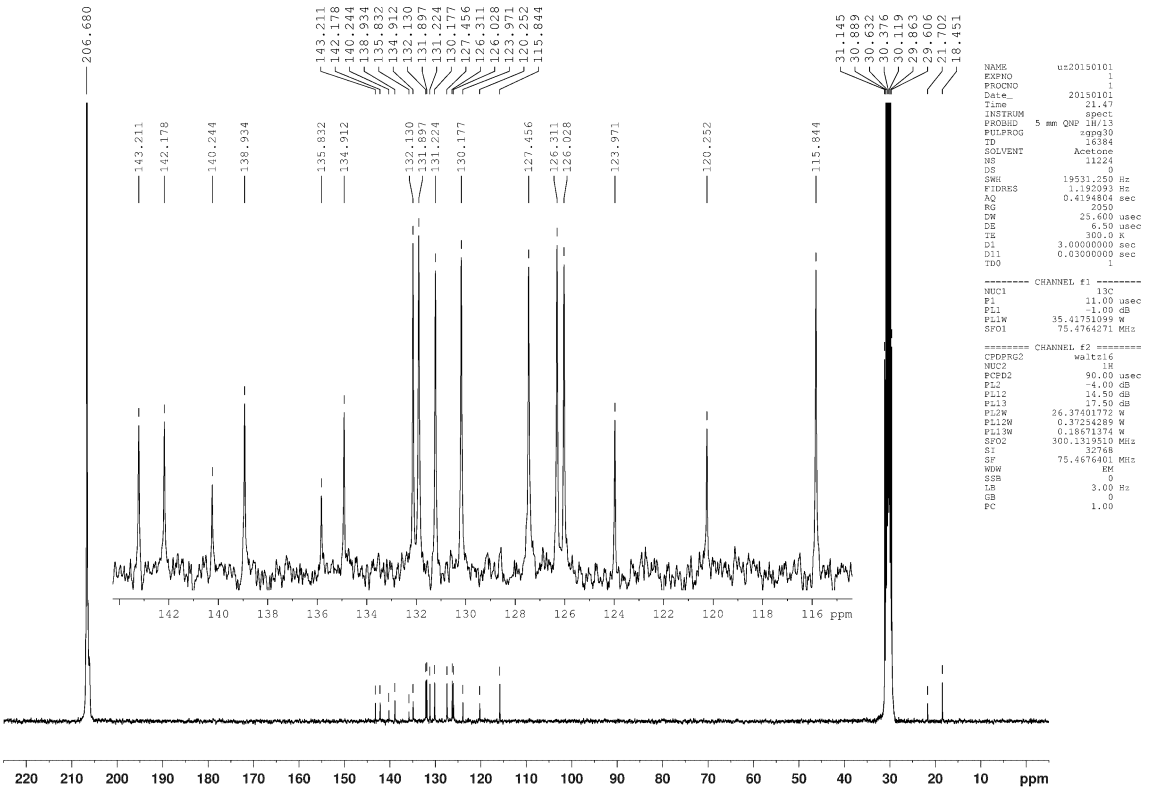
485
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **4**:



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31.145
30.889
30.632
30.376
30.119
29.863
29.606
21.702
18.451
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EXPNO 1
PROCNO 1
Date_ 20150101
Time 21.47
INSTRUM spect
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PULPROG zgpg30
TD 16384
SOLVENT Acetone
NS 11224
DS 0
SWH 19531.250 Hz
FIDRES 1.192093 Hz
AQ 0.4194804 sec
RG 2050
DW 25.600 usec
DE 6.50 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
PL1W 35.41751099 W
SFO1 75.4764271 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 14.50 dB
PL13 17.50 dB
PL2W 26.37401772 W
PL12W 0.37254289 W
PL13W 0.18671374 W
SFO2 300.1319510 MHz
SI 32768
SF 75.4676401 MHz
WDW EM
SSB 0
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GB 0
PC 1.00
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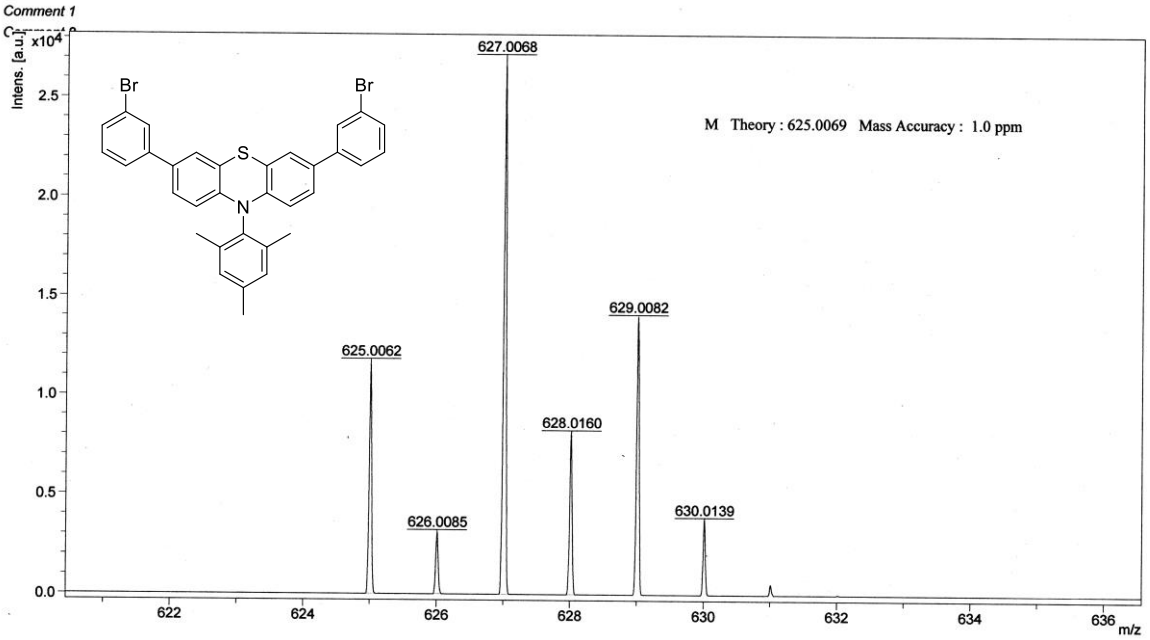
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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629.0082
628.0160
626.0085
630.0139
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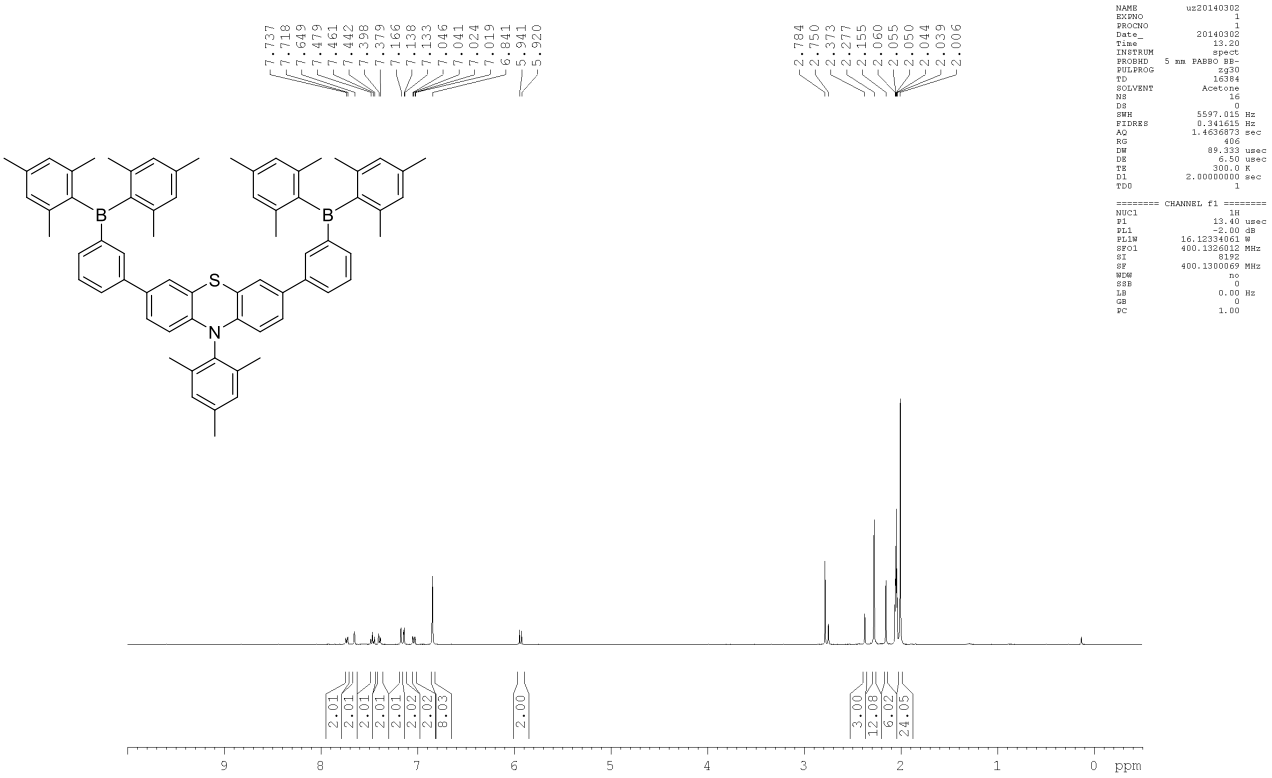
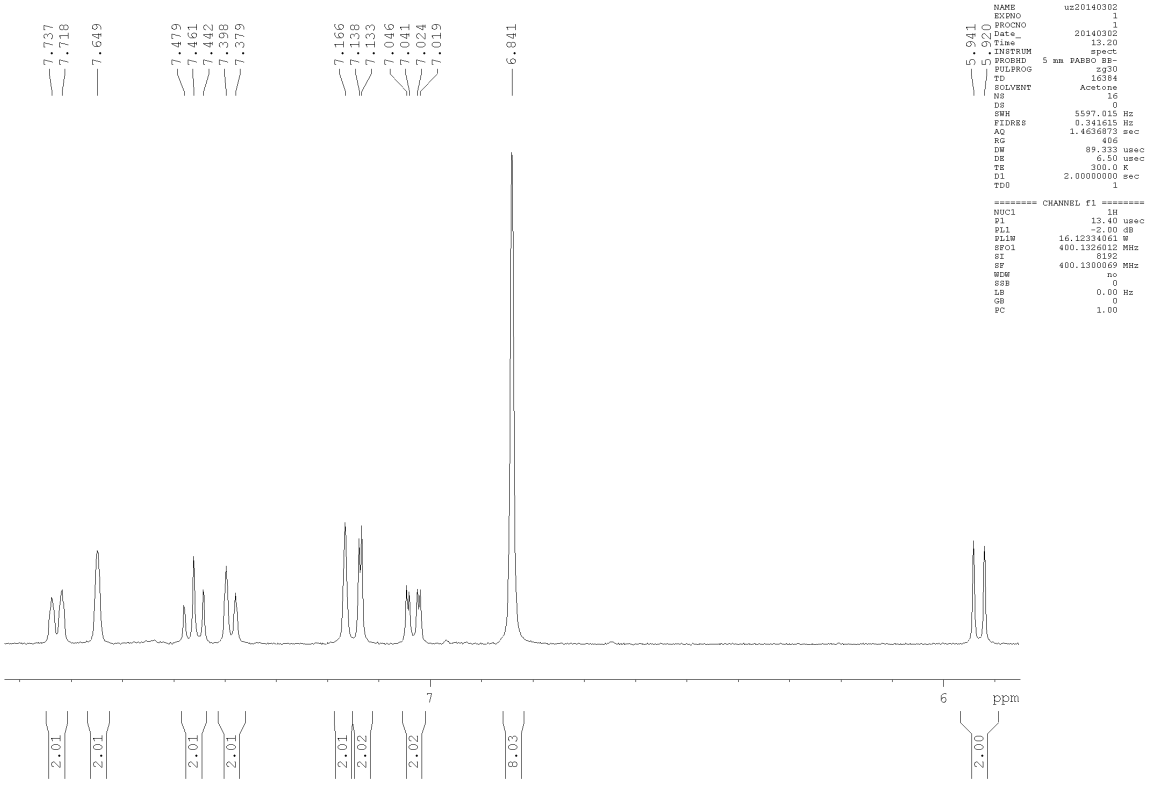
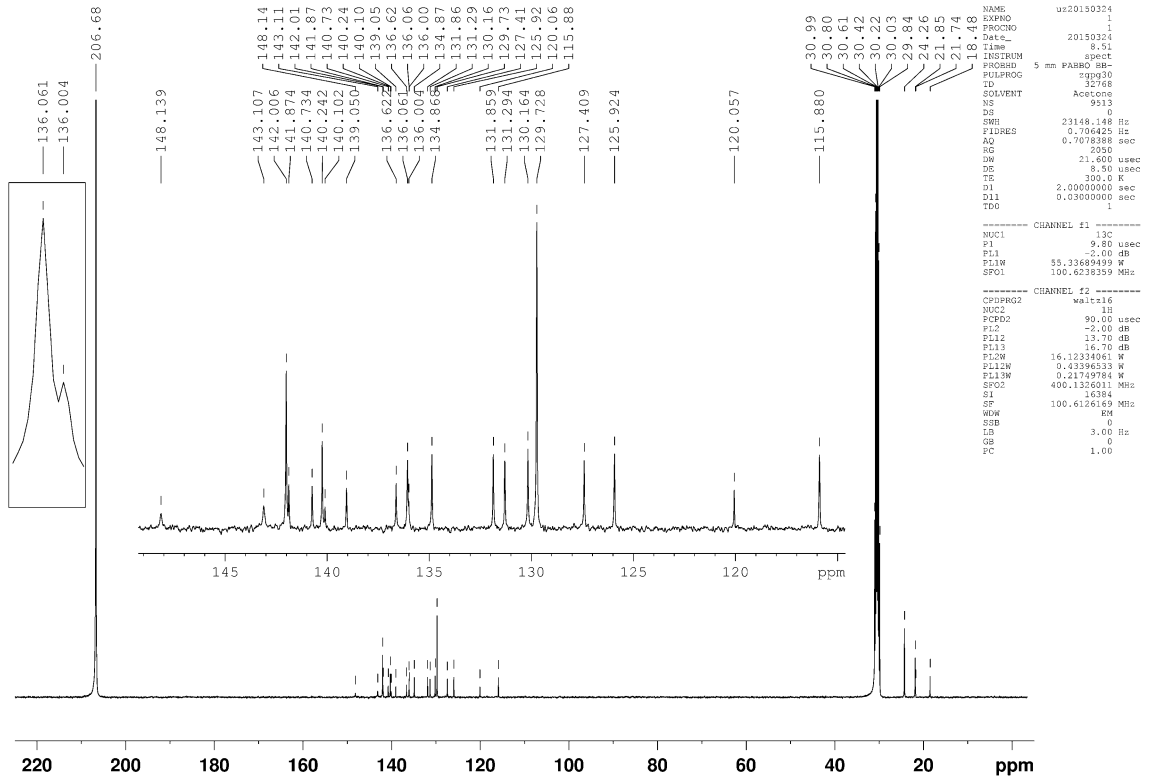
^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **CC-MP1**:



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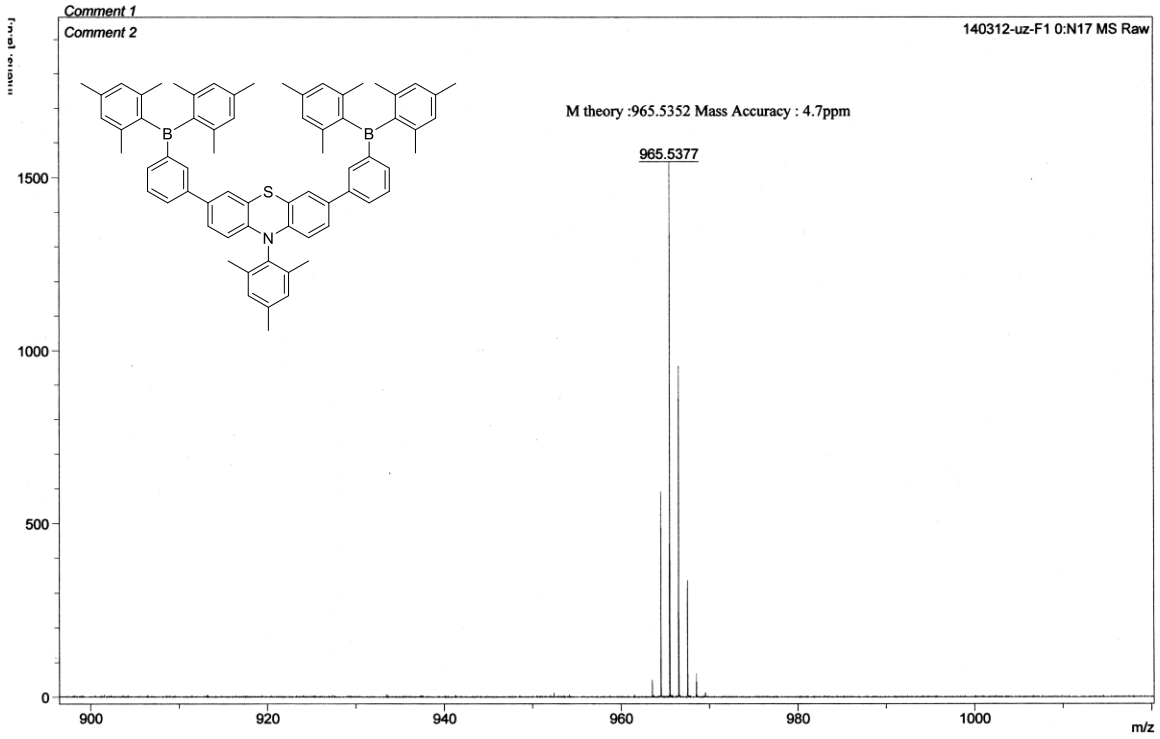
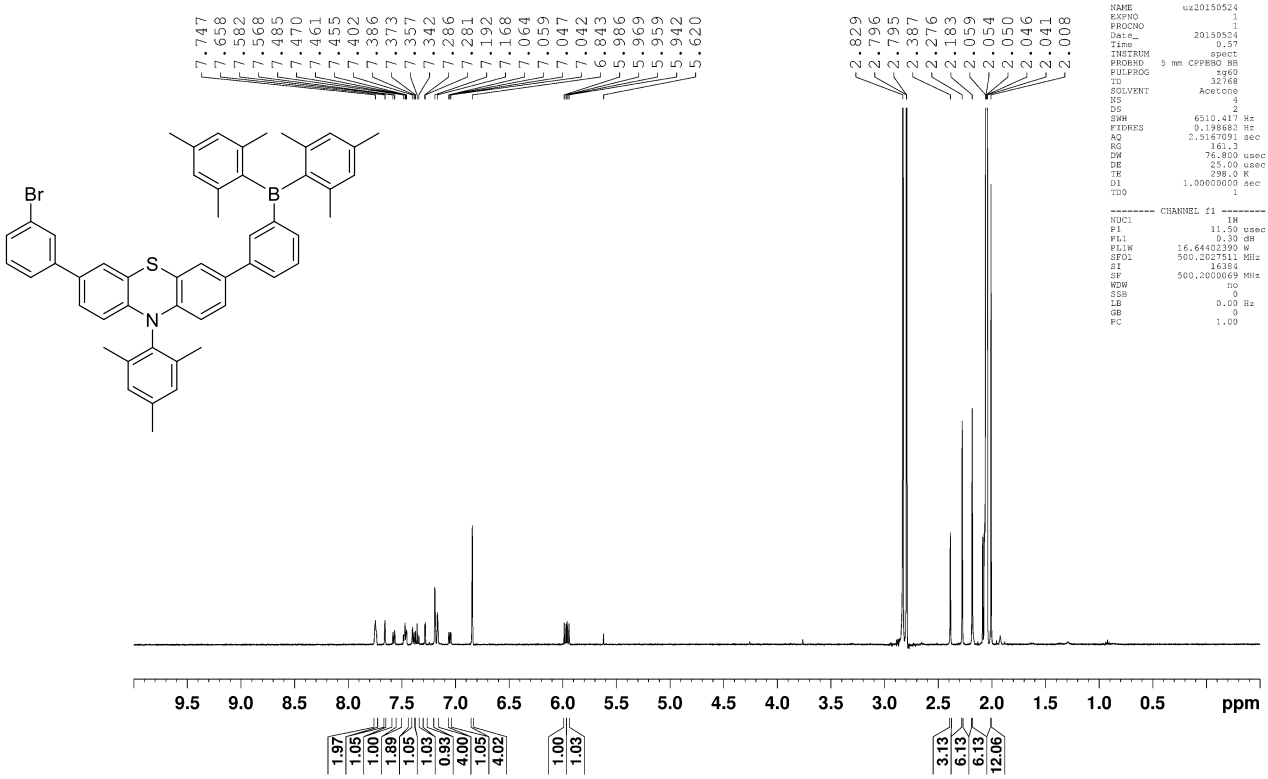
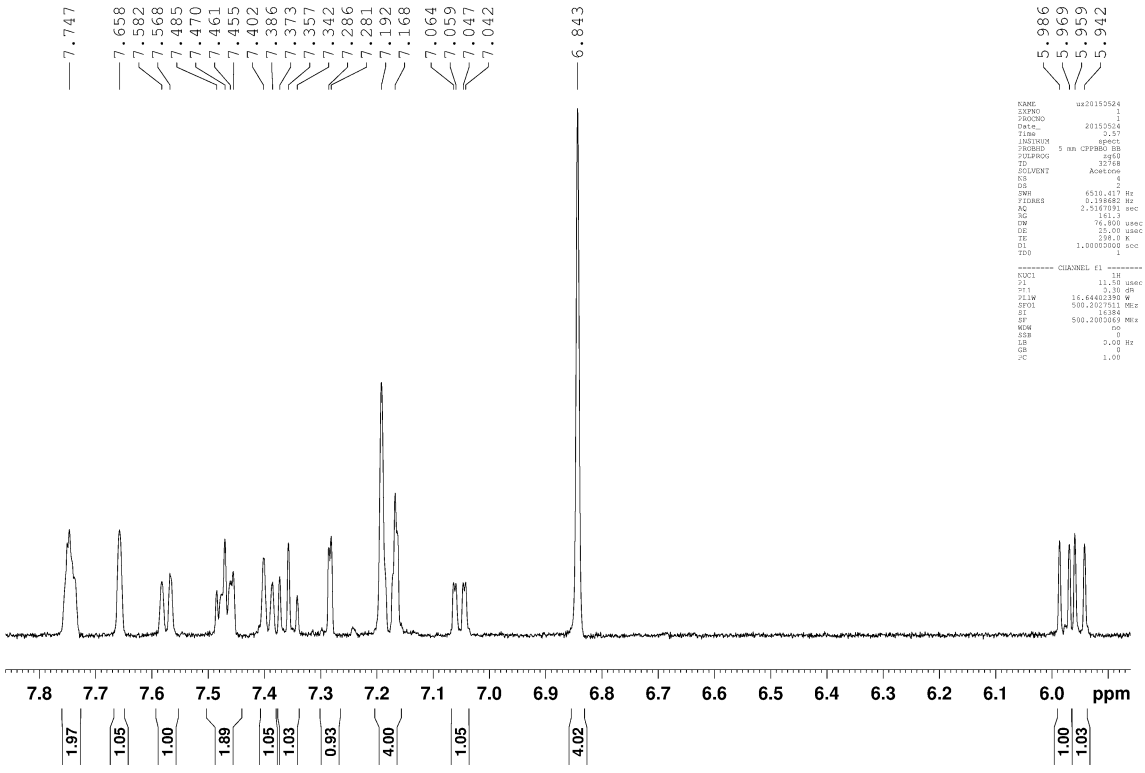
127.41
125.92
120.06
115.88
143.107
142.006
141.874
140.734
140.242
140.102
139.050
136.622
136.061
136.004
134.866
131.859
131.294
130.164
129.728
127.409
125.924
120.057
115.880
30.99
30.80
30.61
30.42
30.22
30.03
29.84
24.26
21.85
21.74
18.48
ppm


Comment 1
Comment 2
140312-uz-F1 0:N17 MS Raw
M theory :965.5352 Mass Accuracy : 4.7ppm
965.5377
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **5**:



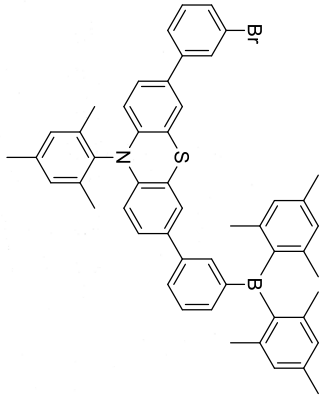


pro-MP2

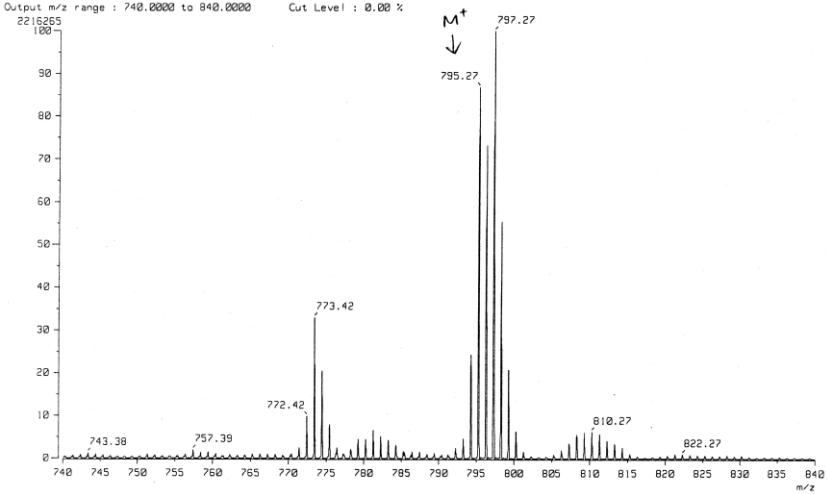
[Elemental Composition] Page: 1

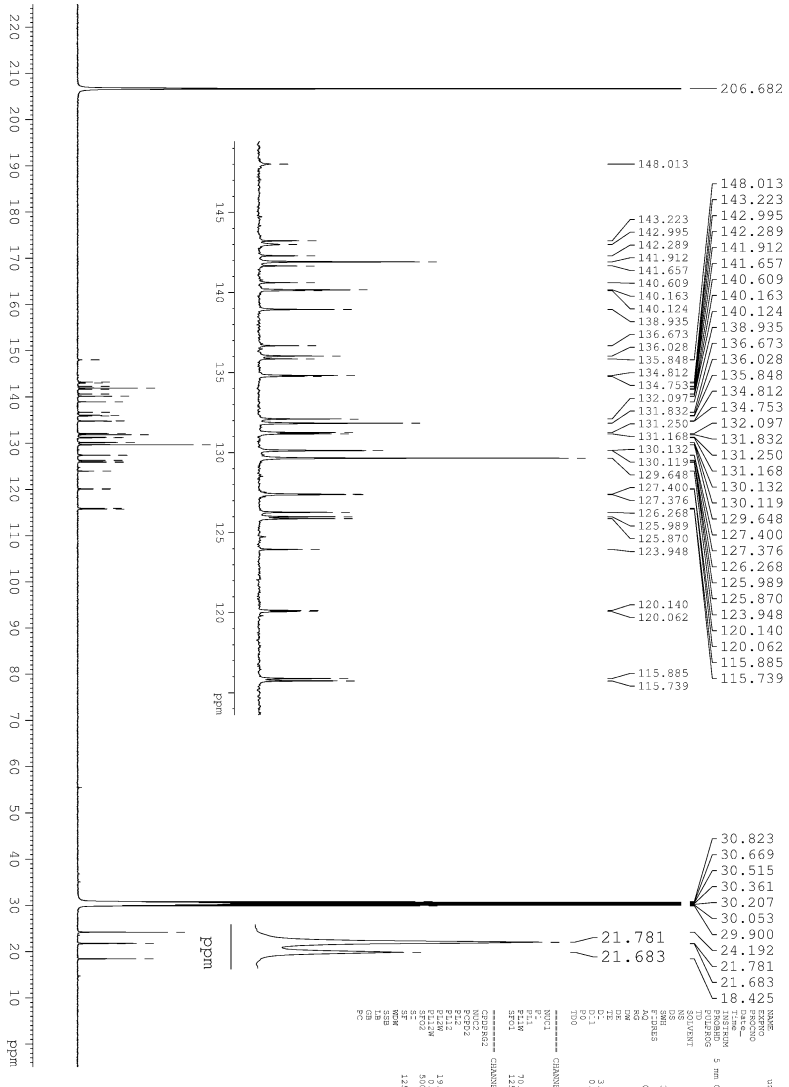
Data : 15May08_09-001 Date : 08-May-2015 18:29
Sample: pro-MP2
Note : NBA
Inlet : Direct Ion Mode : FAB+
RT : 0.14 min Scan#: (1,7)
Elements : C 1000/0, H 1000/0, N 1/1, Br 1/1(79Br 1/0, 81Br 1/0), S 1/1, B 1/1
Mass Tolerance : 10mmu
Unsaturation (U.S.) : -0.5 - 1000.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
795.2718	86.9	+1.5 / +1.2	30.0	C 51 H 47 N 79Br S B = 795.2706
797.2676	100.0	-1.1 / -0.9	30.0	C 51 H 47 N 81Br S B

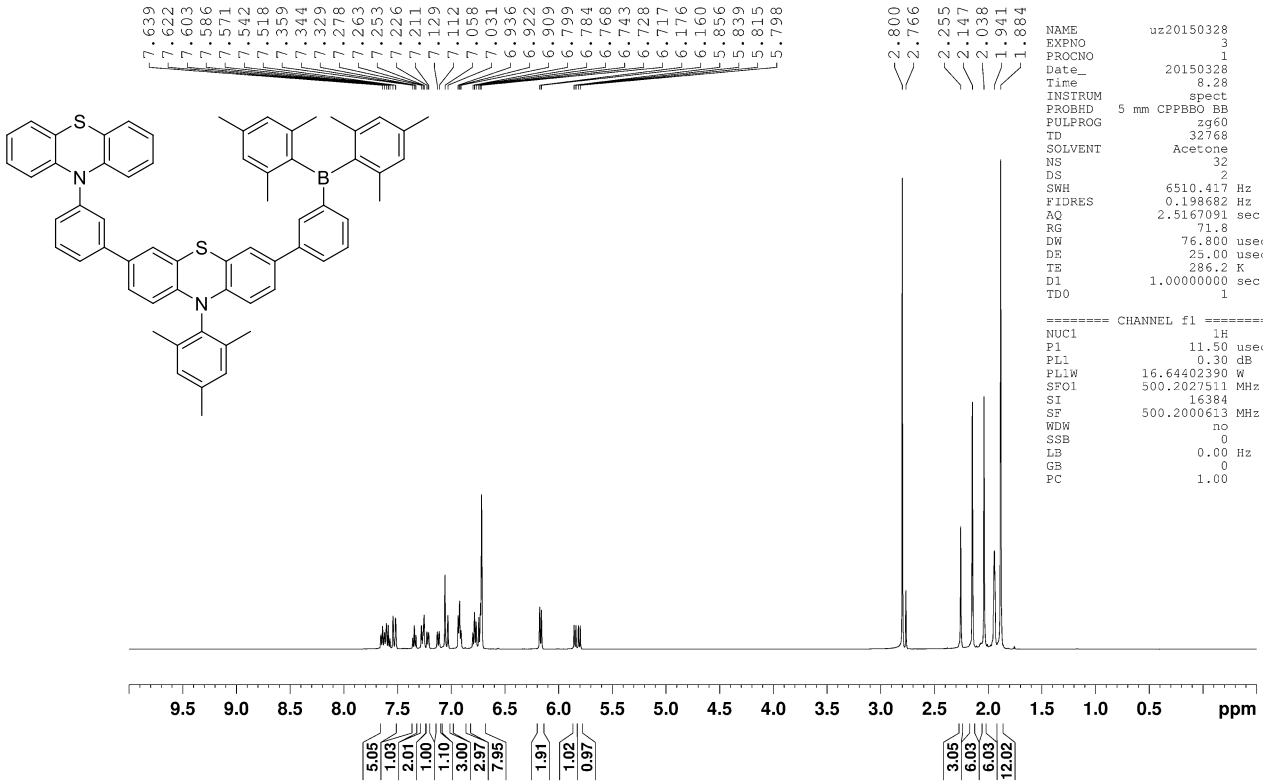


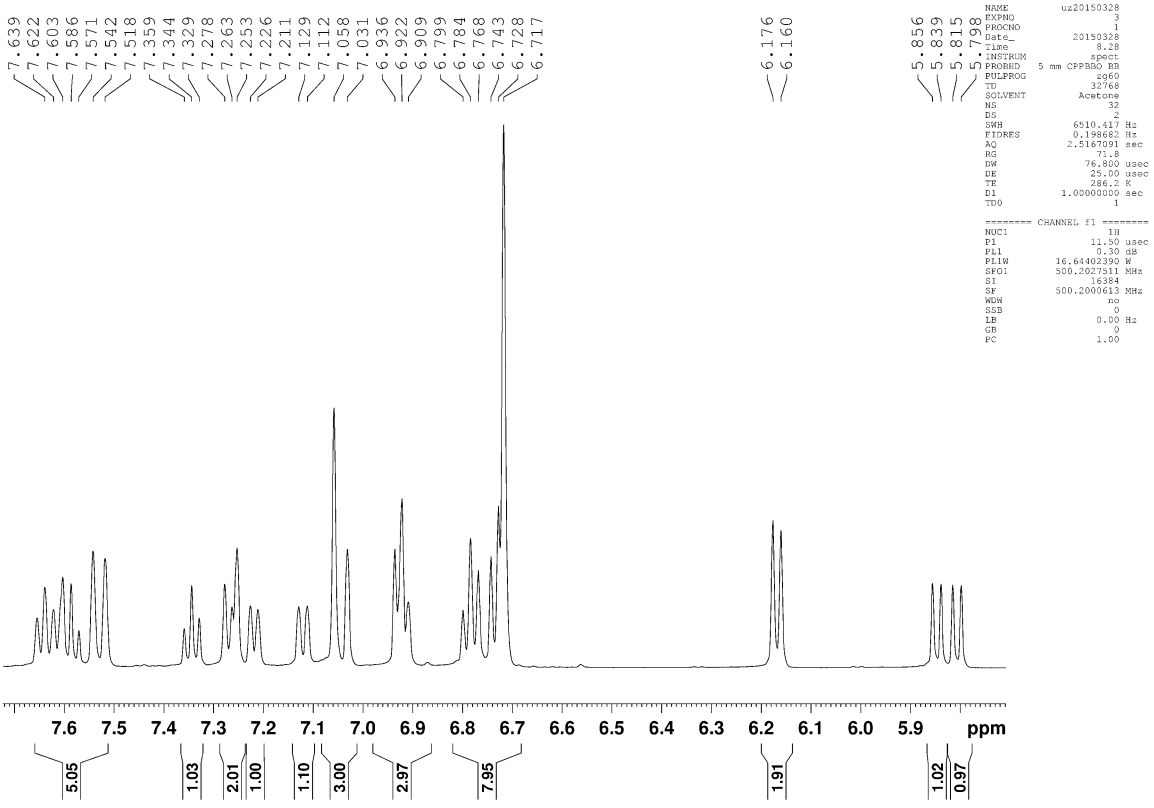
[Mass Spectrum]
Data : 15May08_09-001 Date : 08-May-2015 18:29
Sample: pro-MP2
Note : NBA
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.14 min Scan# : (1,7)
BP : m/z 797.2676 Int. : 30.19
Output m/z range : 740.0000 to 840.0000 Cut Level : 0.00 %

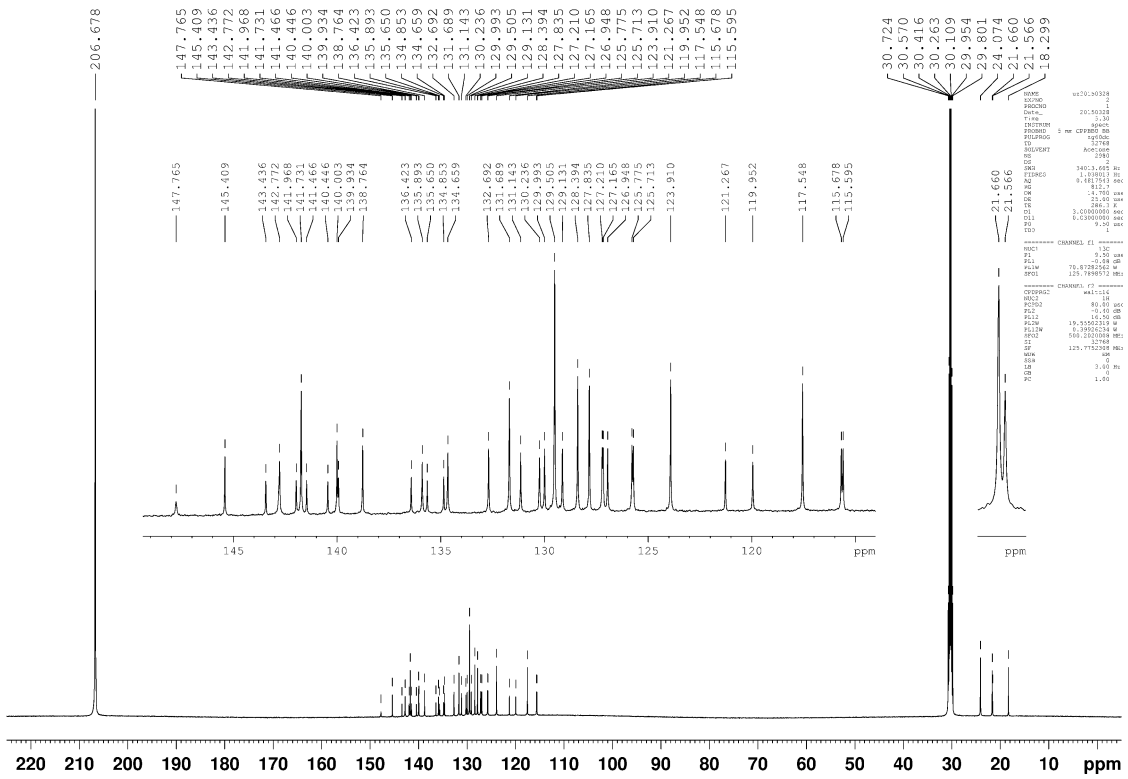


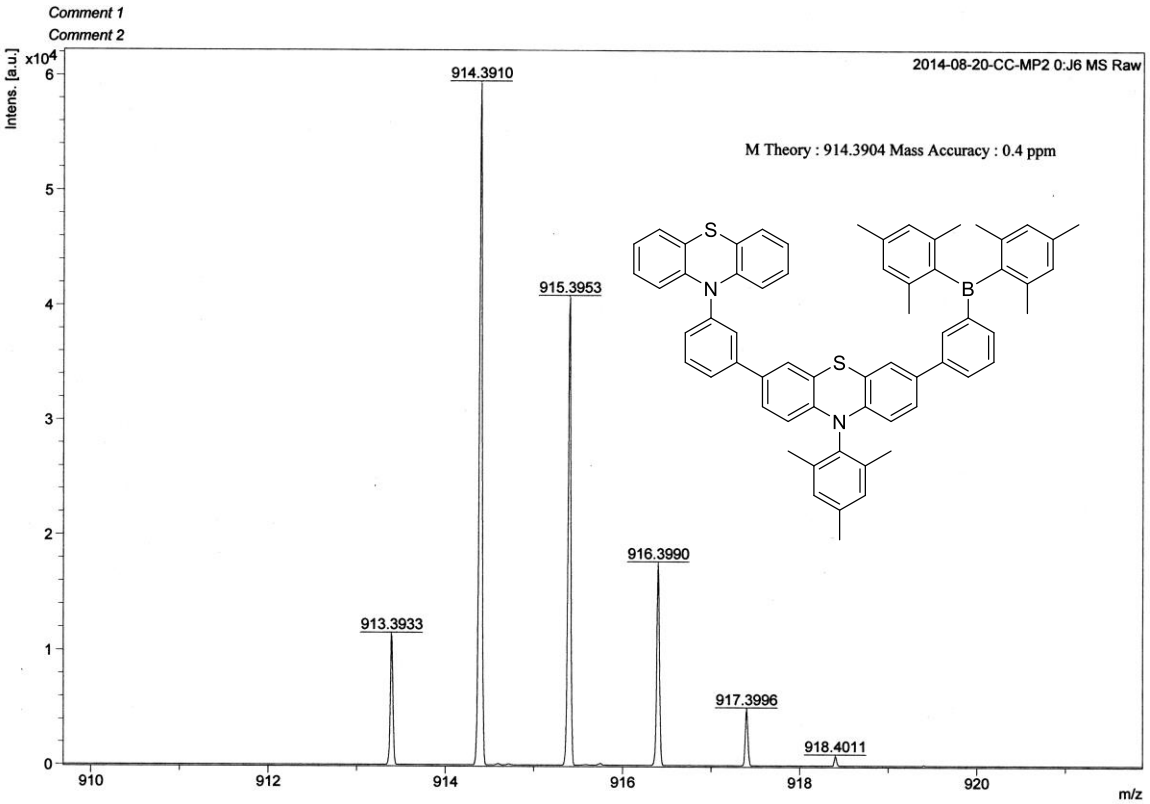


^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **CC-MP2**:

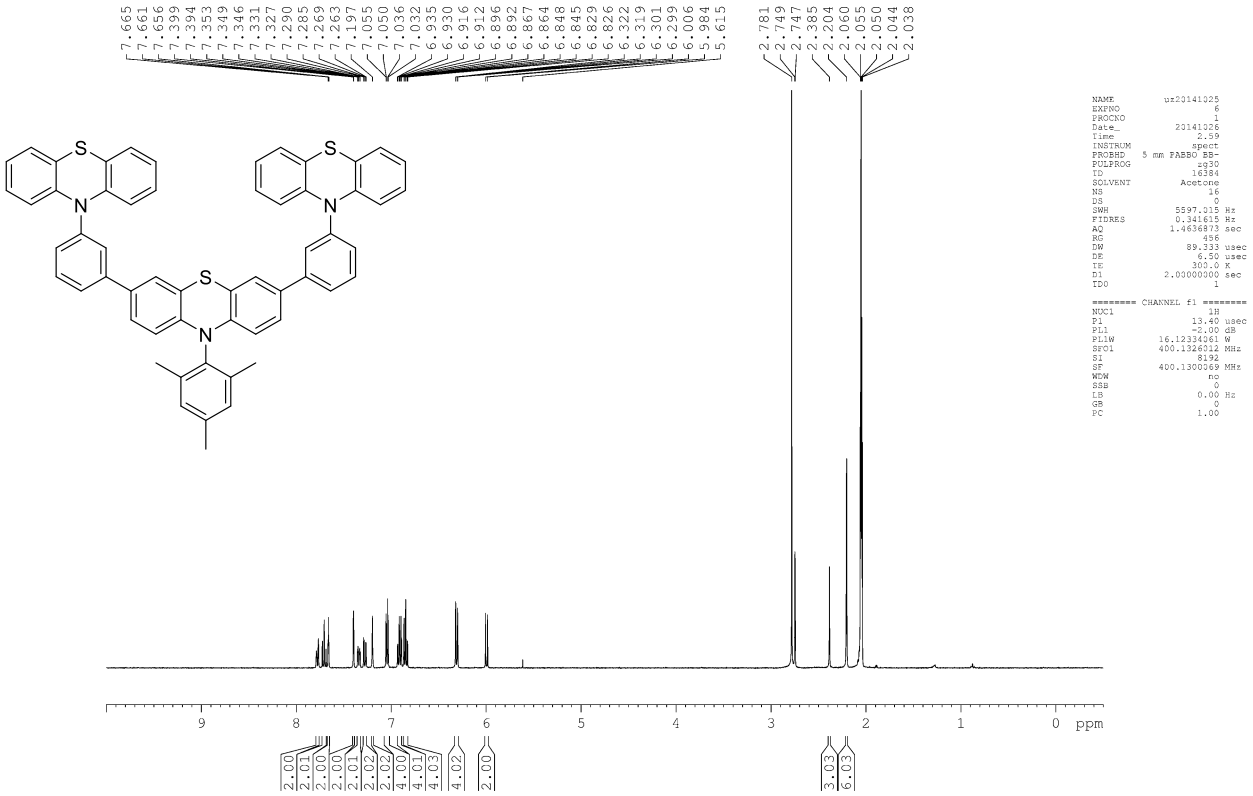


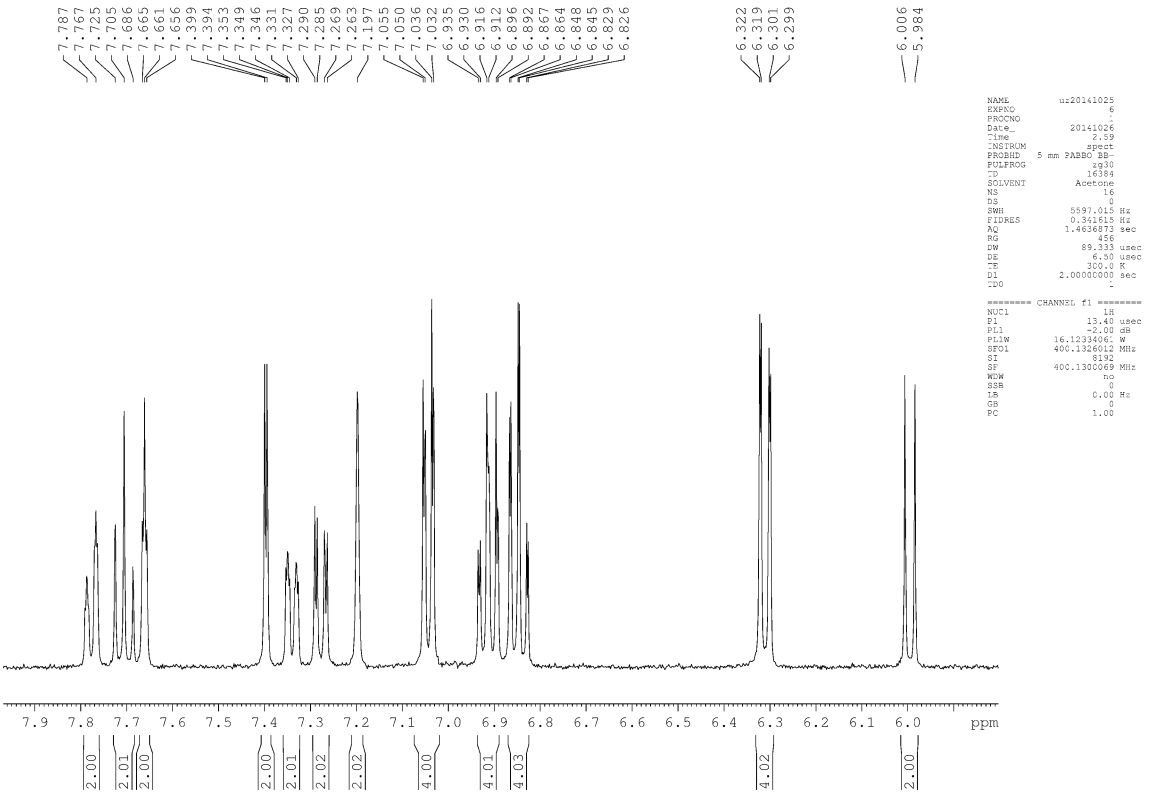


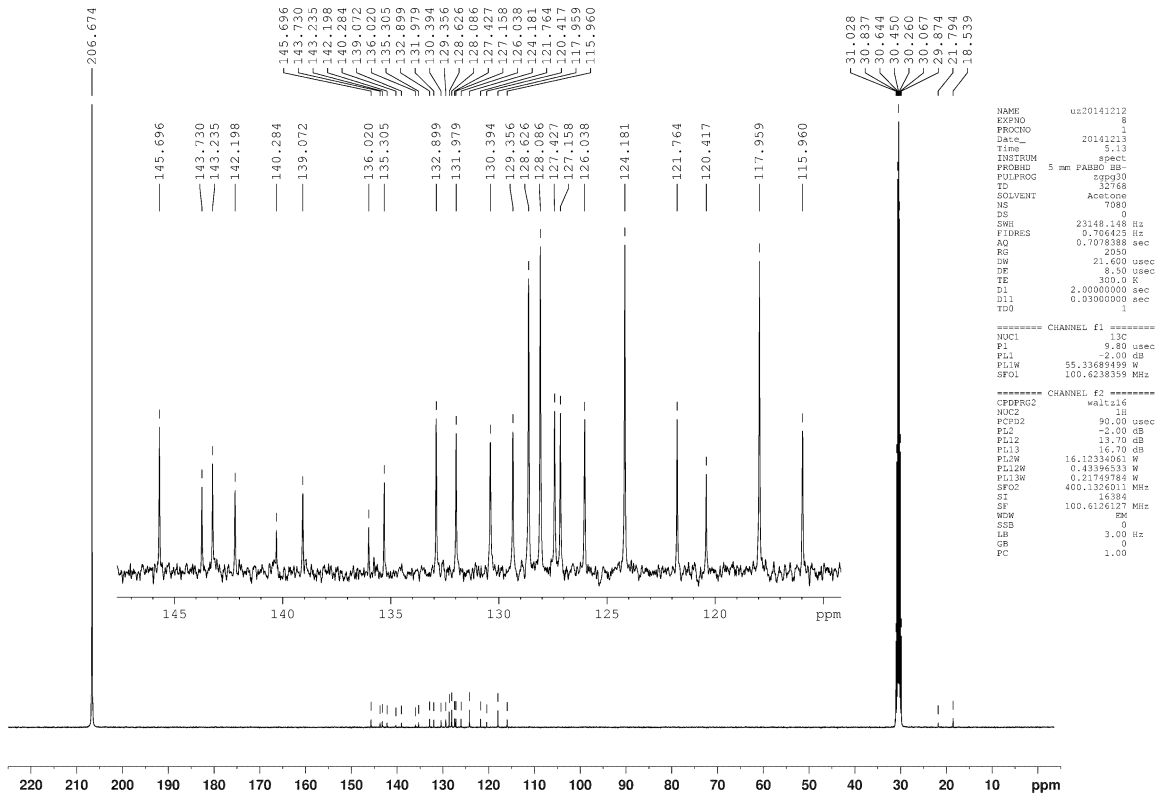

206.678
147.765
145.409
143.436
142.772
141.968
141.731
141.466
140.446
140.003
139.934
138.764
136.423
135.893
135.650
134.853
134.659
132.692
131.689
131.143
130.236
129.993
129.505
129.131
128.394
127.835
127.210
127.165
126.948
125.775
125.713
123.910
121.267
119.952
117.548
115.678
115.595
30.724
30.570
30.416
30.263
30.109
29.954
29.801
24.074
21.660
21.566
18.299
ppm

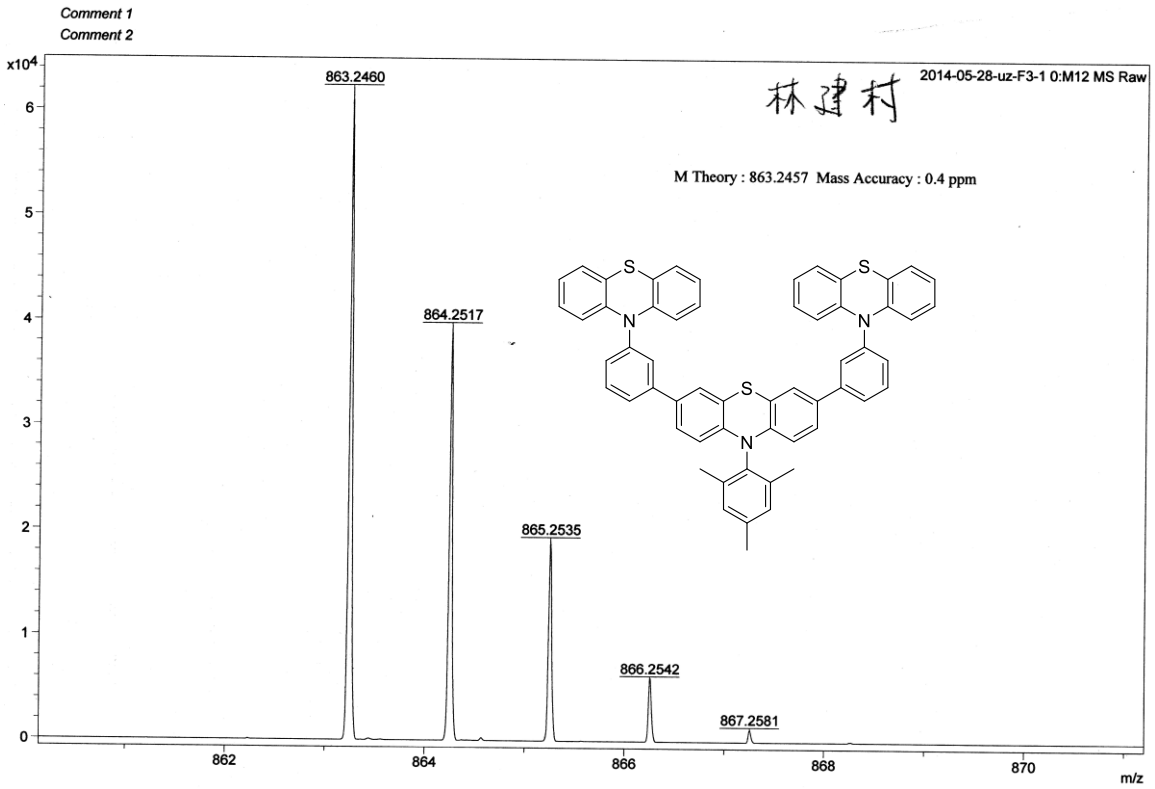

Comment 1
Comment 2
Intens. [a.u.]
x10^4
2014-08-20-CC-MP2 0:J6 MS Raw
M Theory : 914.3904 Mass Accuracy : 0.4 ppm
914.3910
915.3953
916.3990
913.3933
917.3996
918.4011
S
N
B
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **CC-MP3**:

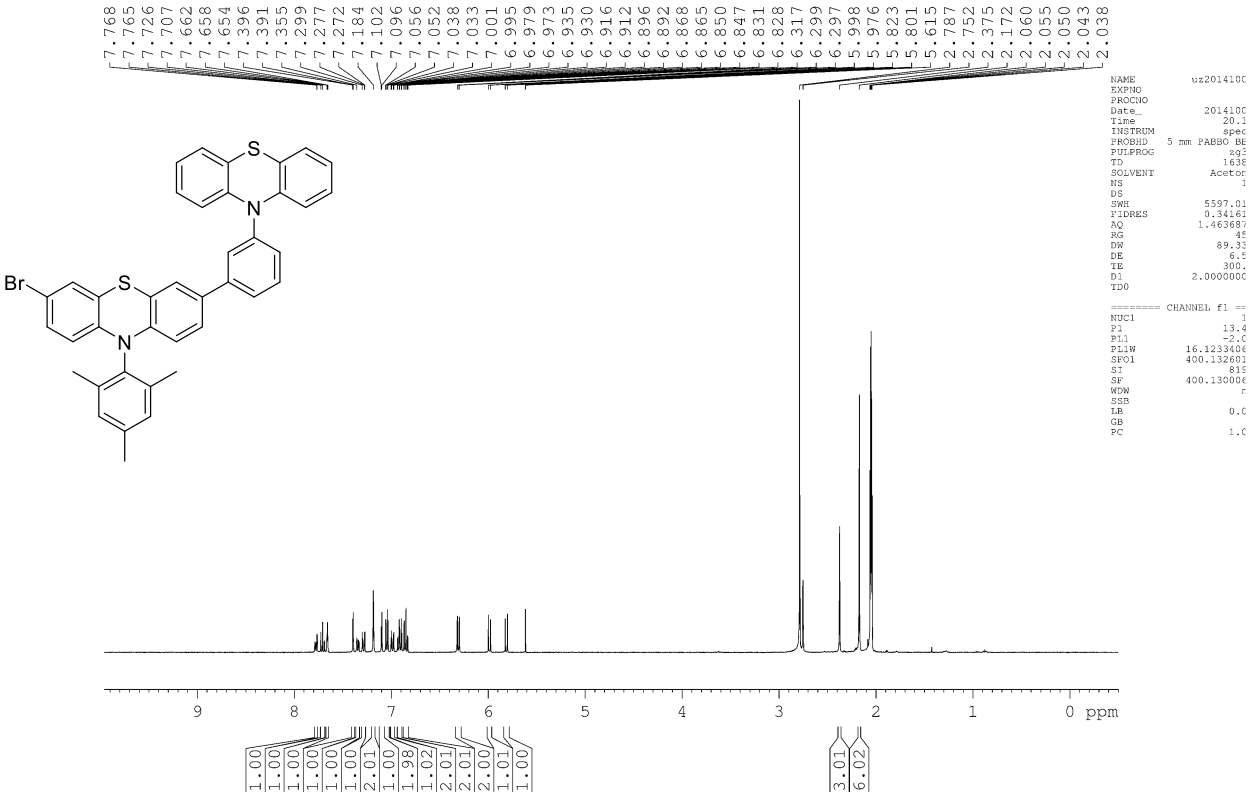


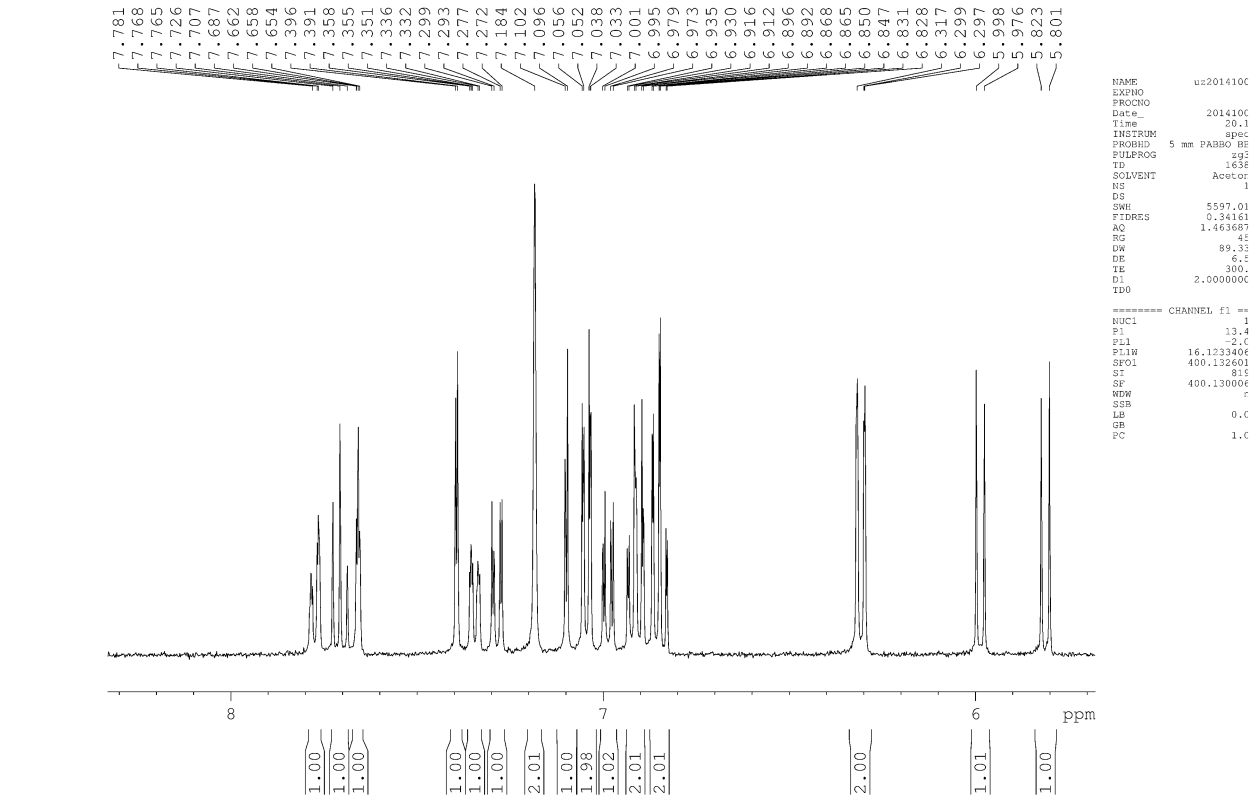


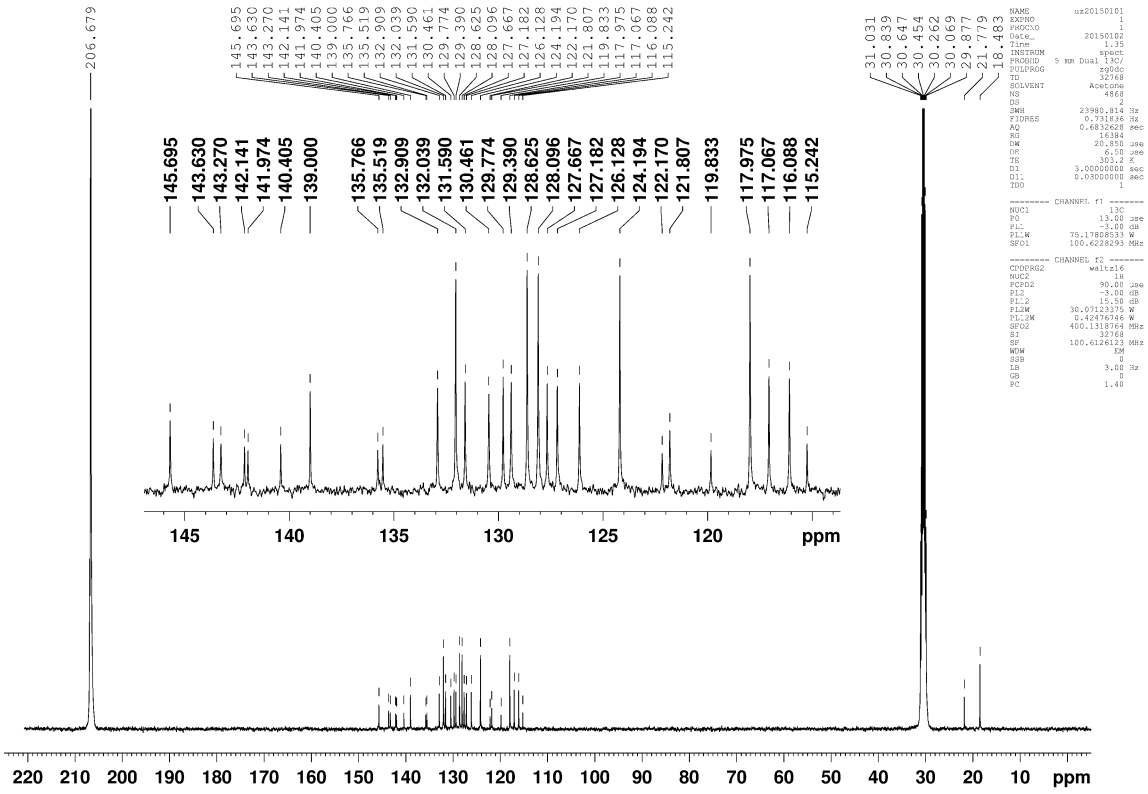

206.674
145.696
143.730
143.235
142.198
140.284
139.072
136.020
135.305
132.899
131.979
130.394
129.356
128.626
128.086
127.427
127.158
126.038
124.181
121.764
120.417
117.959
115.960
31.028
30.837
30.644
30.450
30.260
30.067
29.874
21.794
18.539
ppm
NAME uz20141212
EXPNO 8
PROCNO 1
Date_ 20141213
Time 5.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT Acetone
NS 7080
DS 0
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078388 sec
RG 2050
DW 21.600 usec
DE 8.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PL1 -2.00 dB
PL1W 55.33689499 W
SFO1 100.6238359 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 13.70 dB
PL13 16.70 dB
PL2W 16.12334061 W
PL12W 0.43396533 W
PL13W 0.21749784 W
SFO2 400.1326011 MHz
SI 16384
SF 100.6126127 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

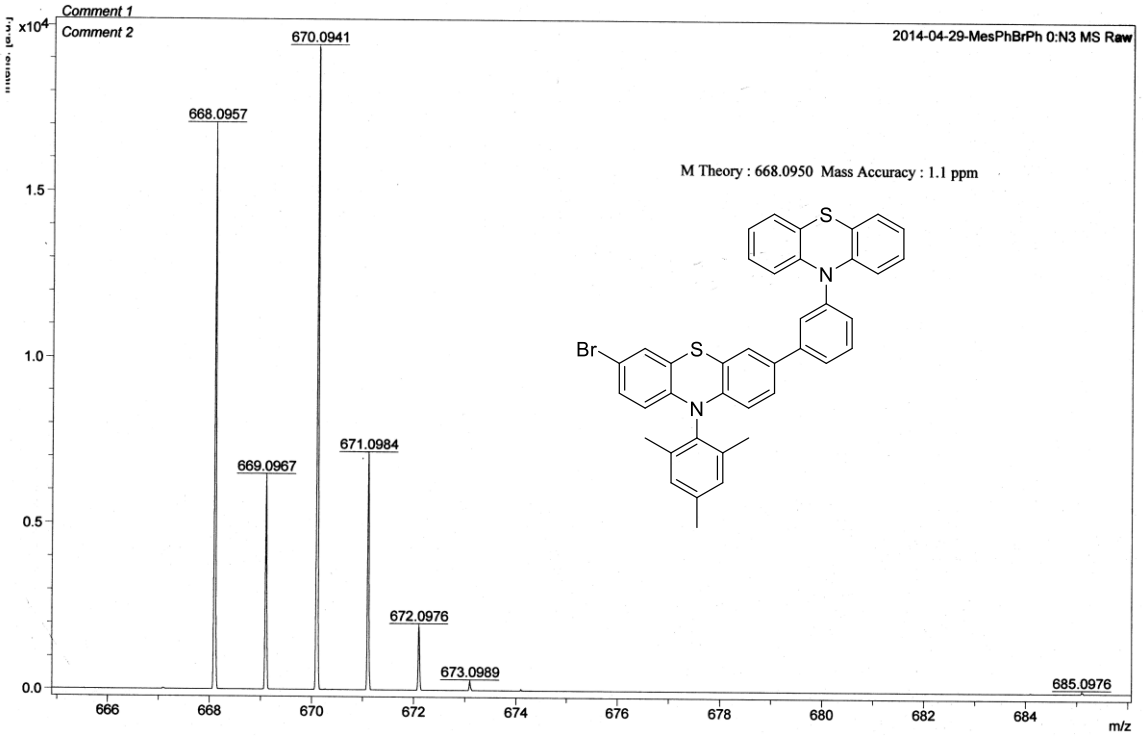

Comment 1
Comment 2
x10^4
863.2460
林建村
2014-05-28-uz-F3-1 0:M12 MS Raw
M Theory : 863.2457 Mass Accuracy : 0.4 ppm
864.2517
865.2535
866.2542
867.2581
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **7**:

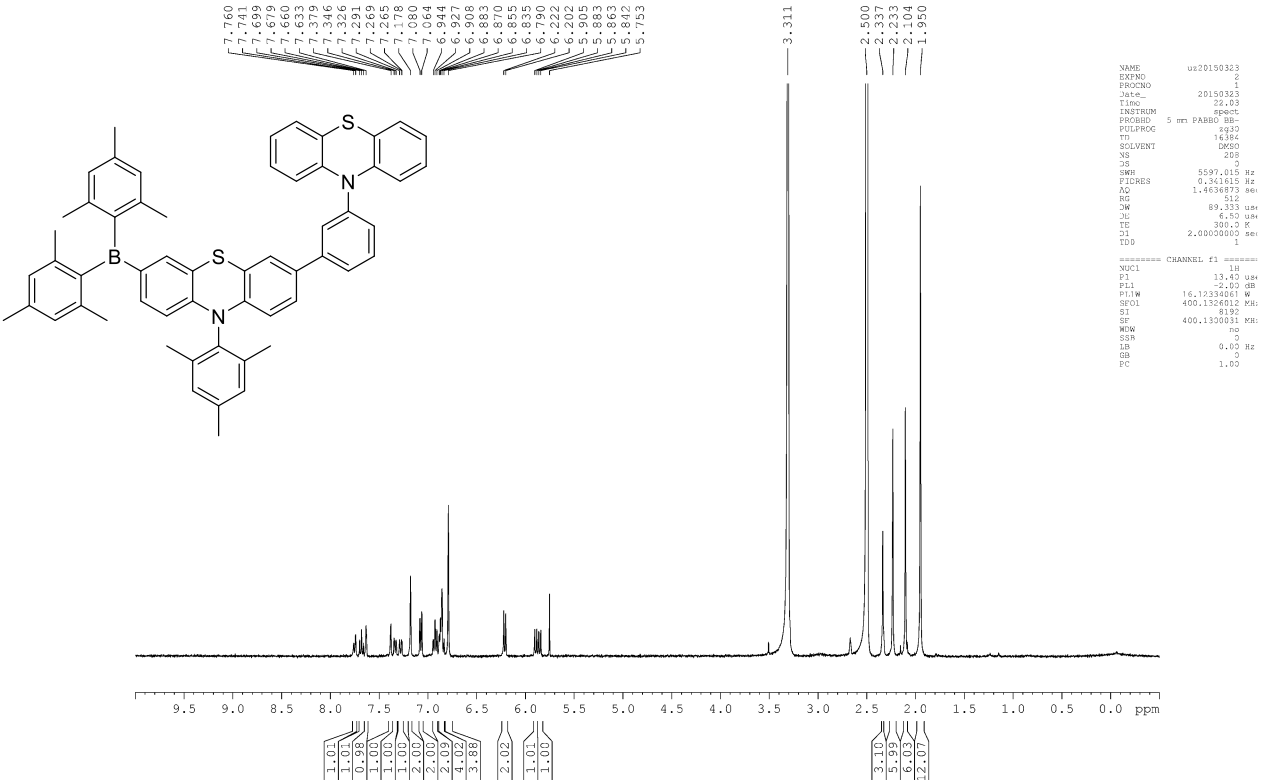


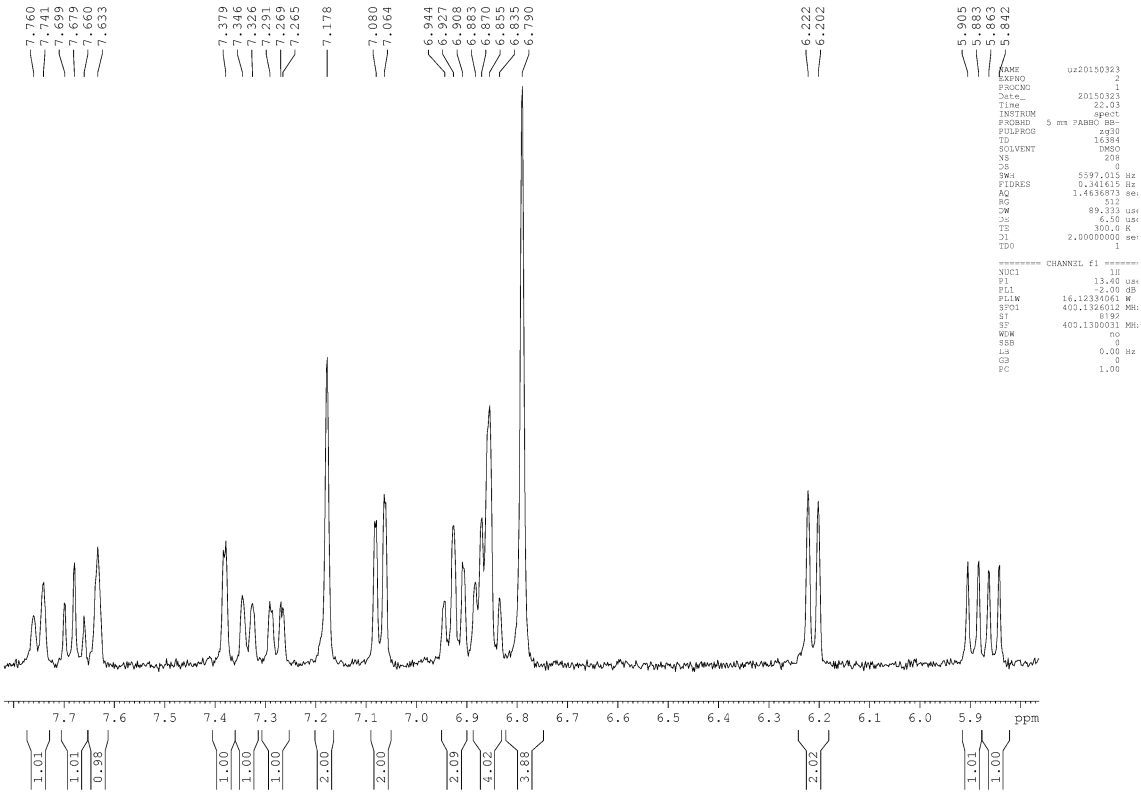


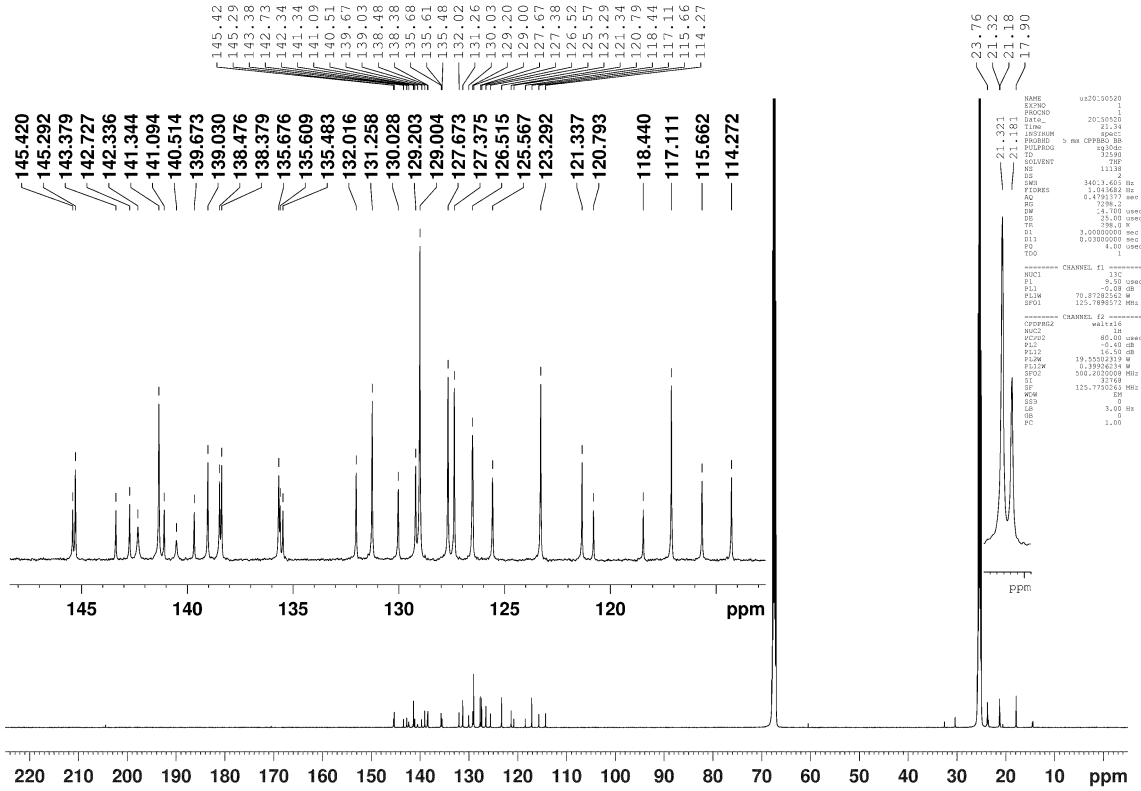

206.679
145.695
143.630
143.270
142.141
141.974
140.405
139.000
135.766
135.519
132.909
132.039
131.590
130.461
129.774
129.390
128.625
128.096
127.667
127.182
126.128
124.194
122.170
121.807
119.833
117.975
117.067
116.088
115.242
31.031
30.839
30.647
30.454
30.262
30.069
29.877
21.779
18.483
ppm

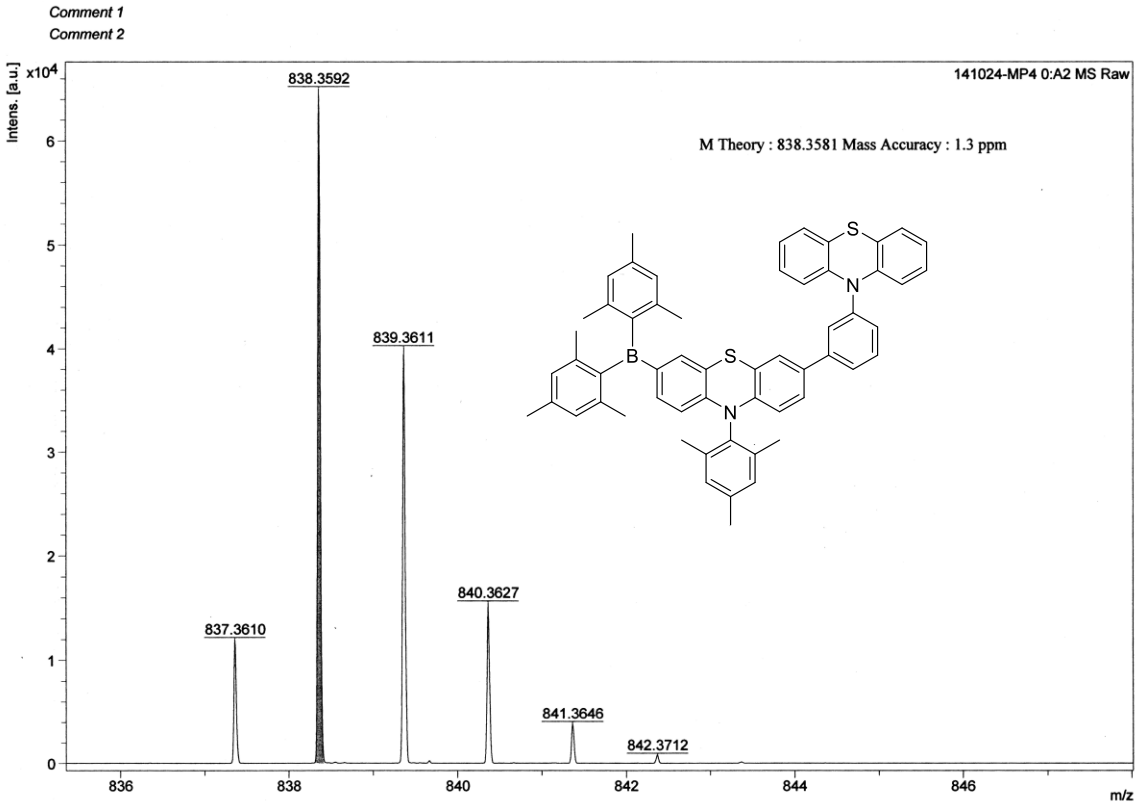

Comment 1
Comment 2
2014-04-29-MesPhBrPh 0:N3 MS Raw
x10^4
670.0941
668.0957
669.0967
671.0984
672.0976
673.0989
685.0976
M Theory : 668.0950 Mass Accuracy : 1.1 ppm
Br
S
N
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **CC-MP4**:

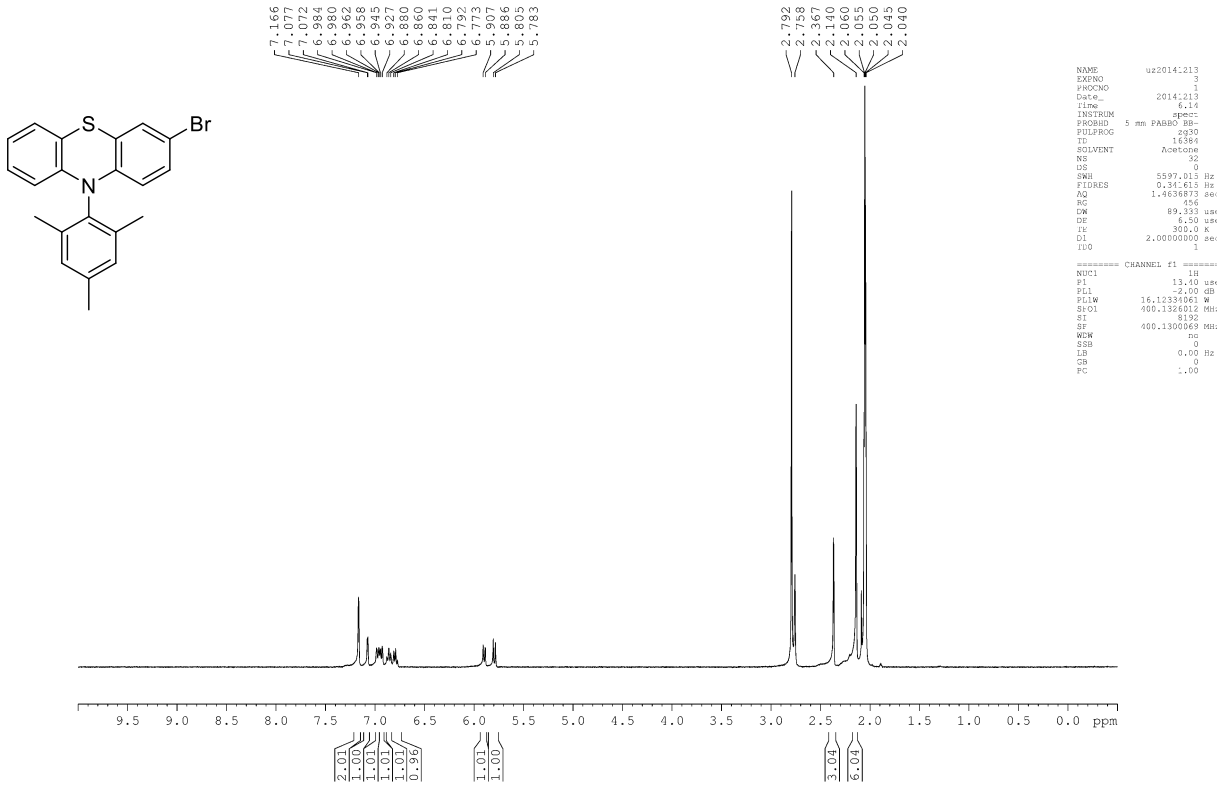


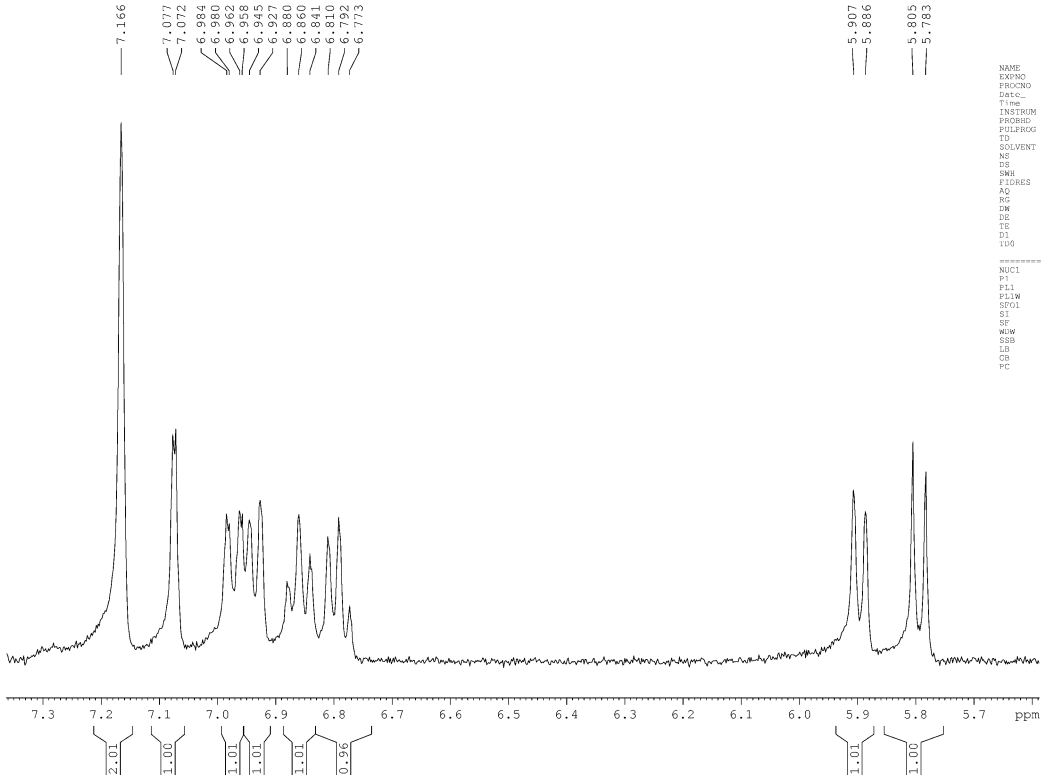


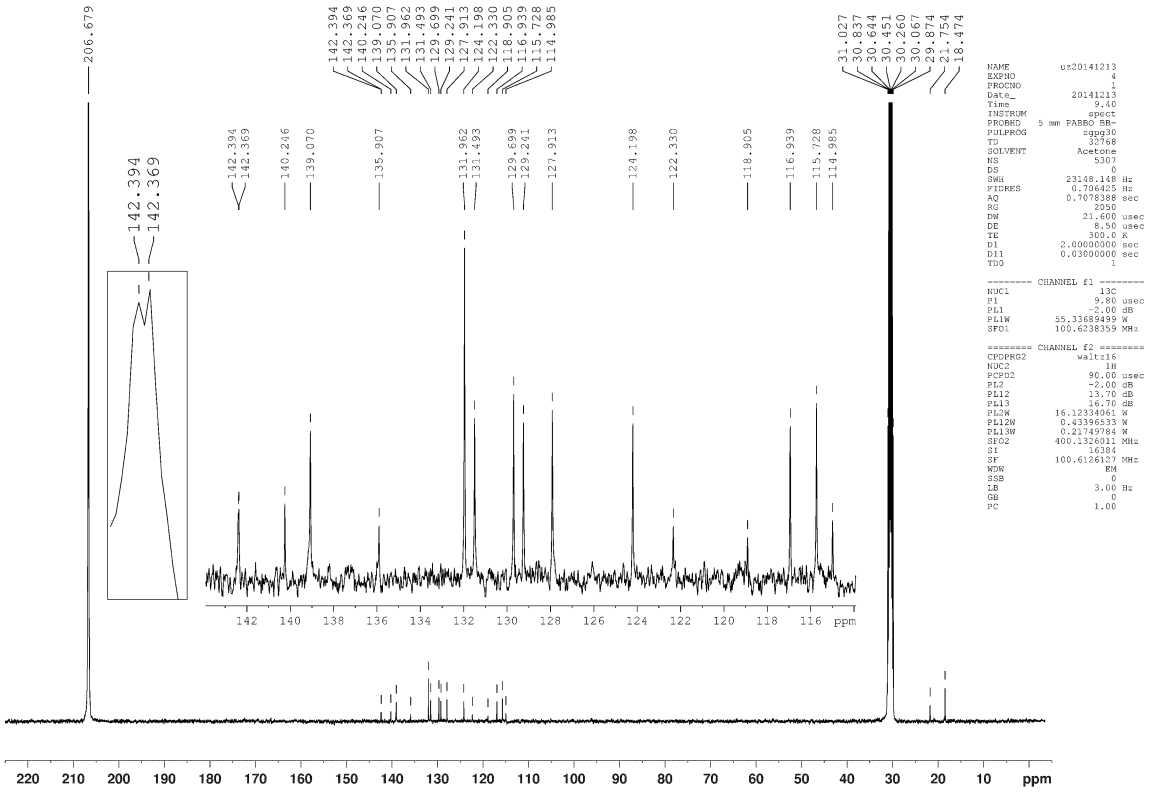

145.420
145.292
143.379
142.727
142.336
141.344
141.094
140.514
139.673
139.030
138.476
138.379
135.676
135.609
135.483
132.016
131.258
130.028
129.203
129.004
127.673
127.375
126.515
125.567
123.292
121.337
120.793
118.440
117.111
115.662
114.272
23.76
21.32
21.18
17.90
21.321
21.181
145
140
135
130
125
120
ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

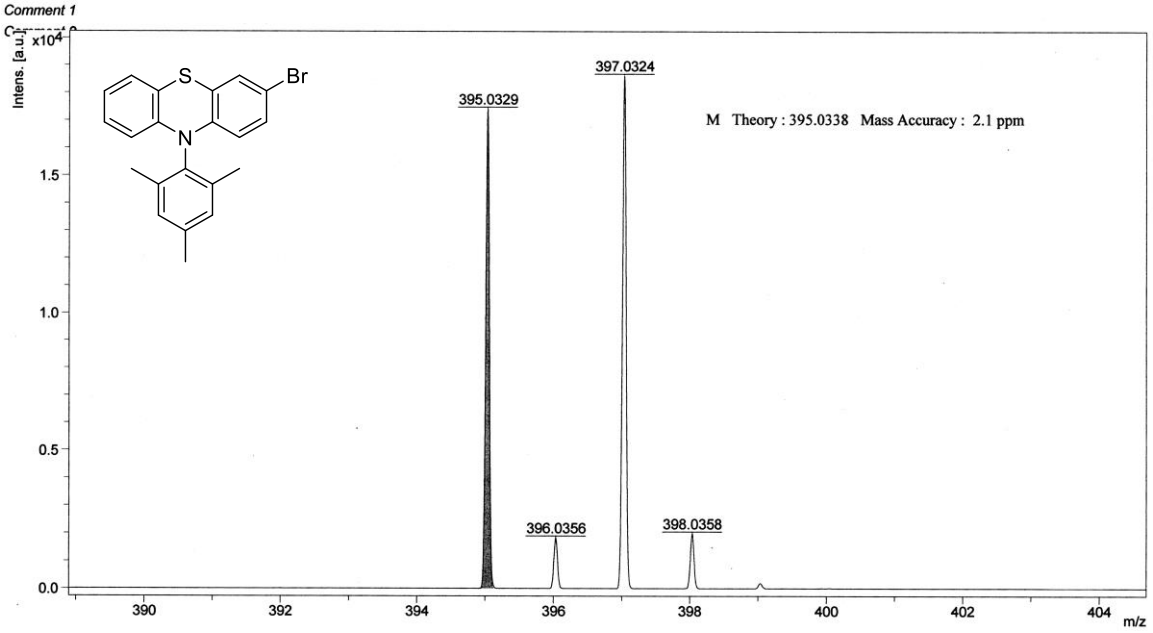

Comment 1
Comment 2
141024-MP4 0:A2 MS Raw
Intens. [a.u.]
x10^4
838.3592
839.3611
840.3627
837.3610
841.3646
842.3712
M Theory : 838.3581 Mass Accuracy : 1.3 ppm
S
N
B
S
N
836
838
840
842
844
846
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **8**:

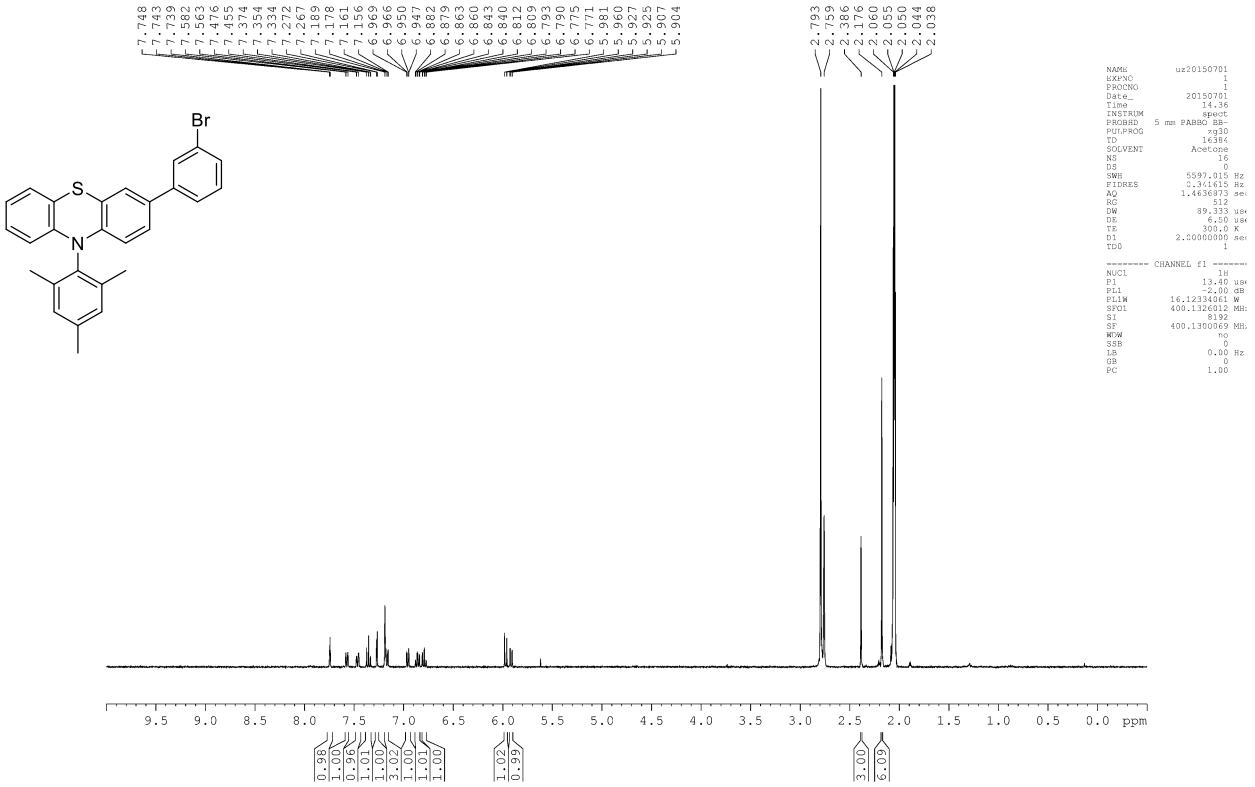


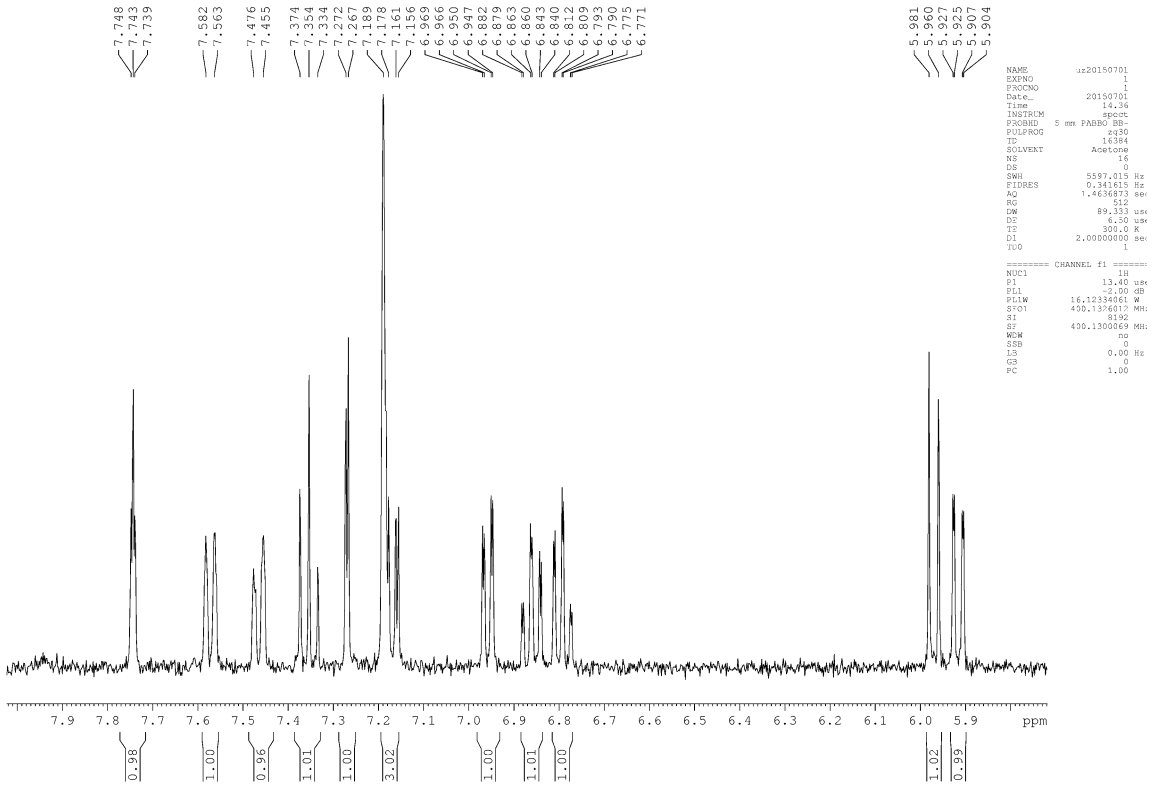


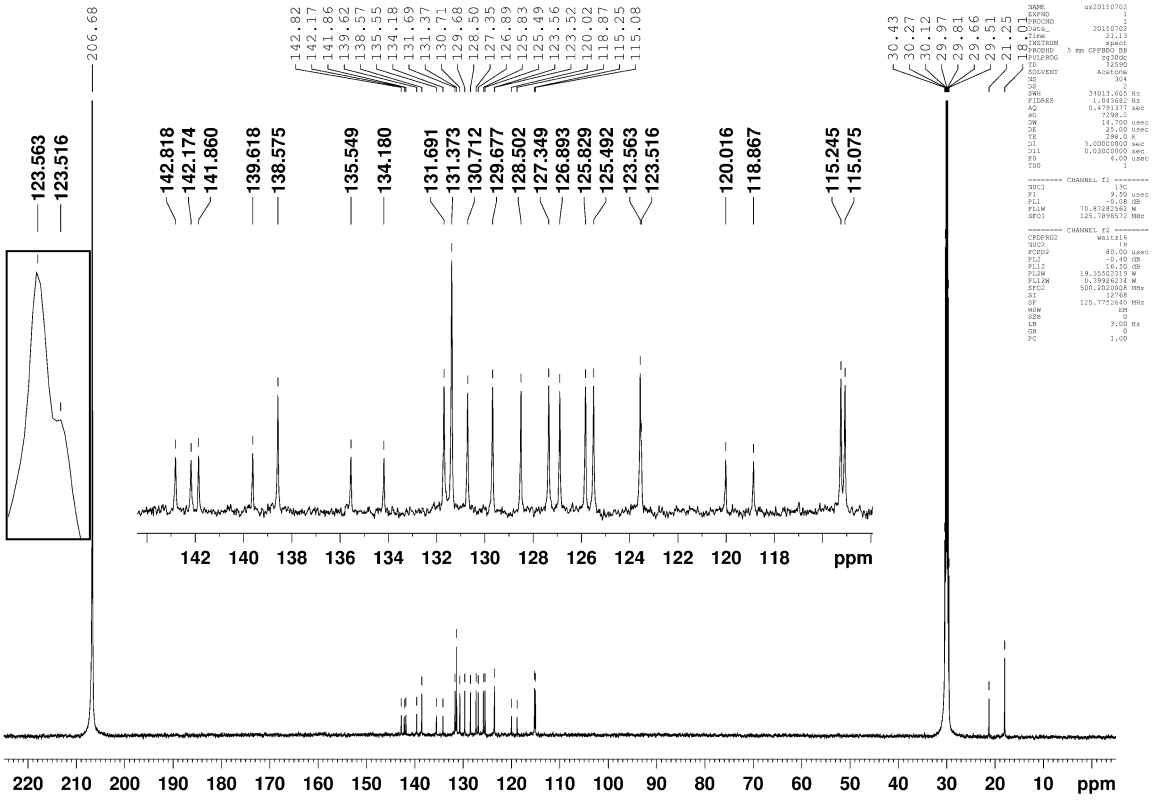

206.679
142.394
142.369
140.246
139.070
135.907
131.962
131.493
129.699
129.241
127.913
124.198
122.330
118.905
116.939
115.728
114.985
31.027
30.837
30.644
30.451
30.260
30.067
29.874
21.754
18.474
ppm

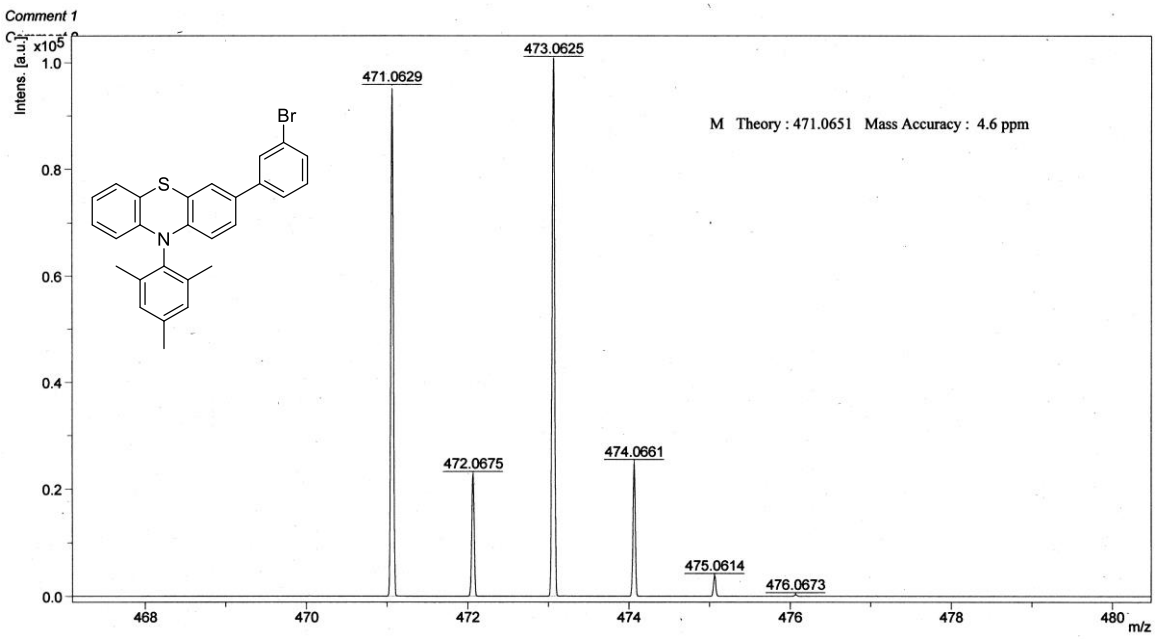

Comment 1
x10^4
Intens. [a.u.]
395.0329
397.0324
396.0356
398.0358
M Theory : 395.0338 Mass Accuracy : 2.1 ppm
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **10**:

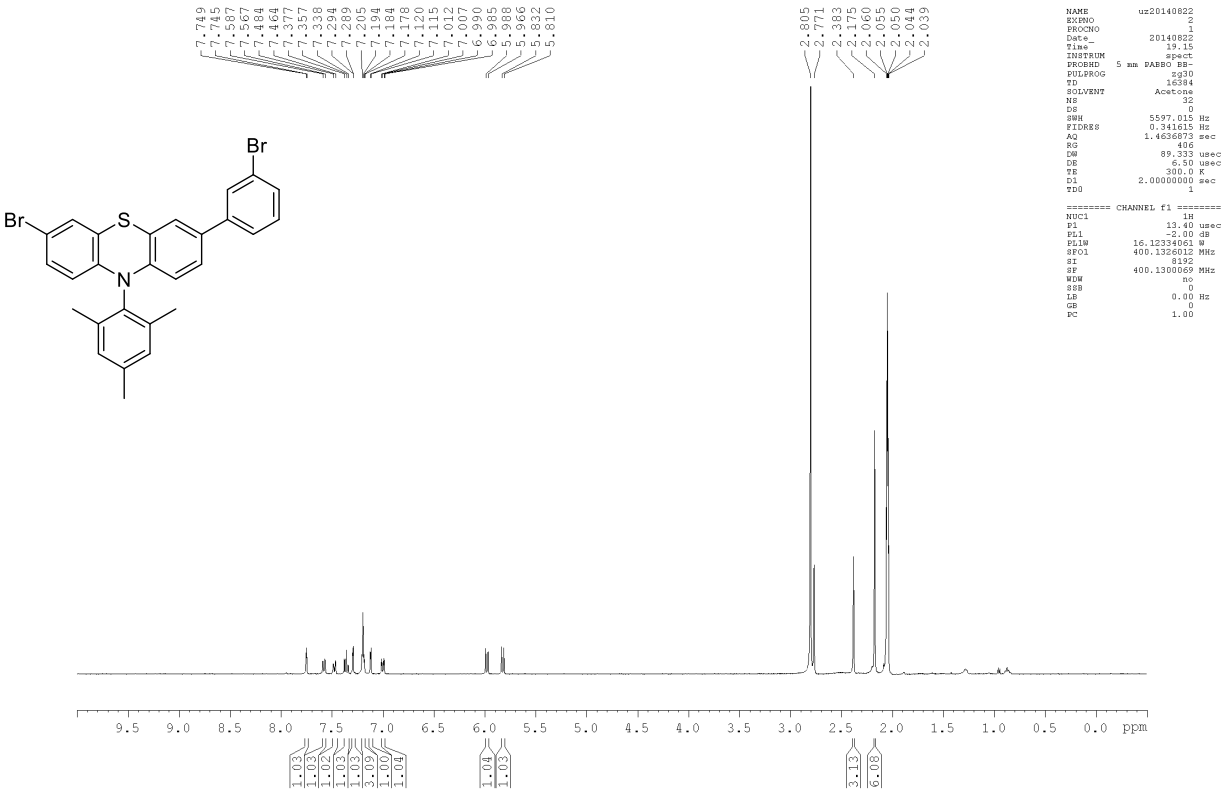


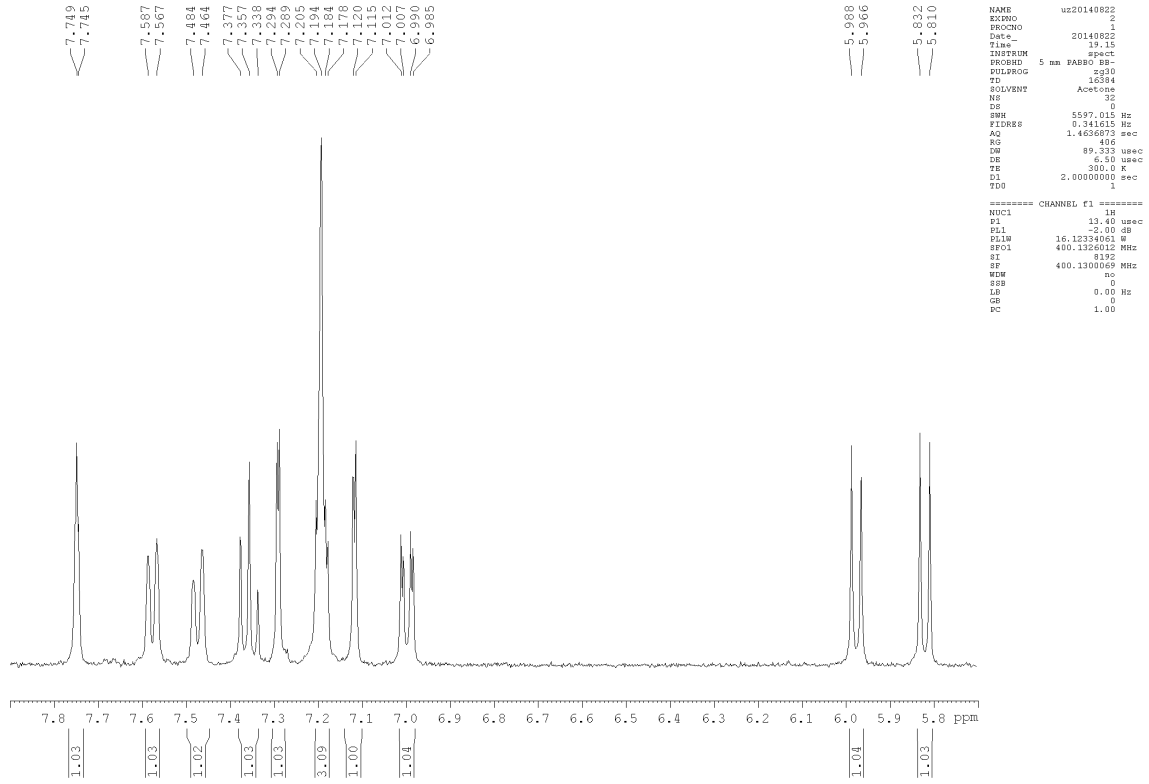


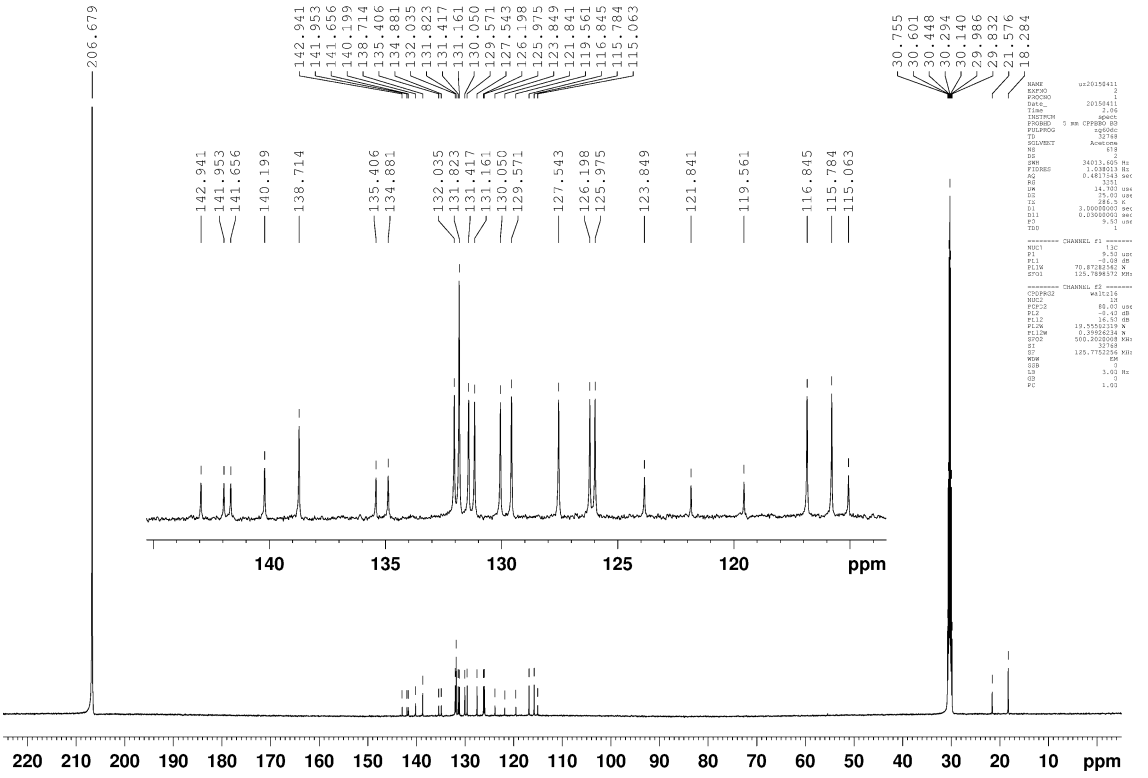

206.68
142.82
142.17
141.86
139.62
138.57
135.55
134.18
131.69
131.37
130.71
129.68
128.50
127.35
126.89
125.83
125.49
123.56
123.52
120.02
118.87
115.25
115.08
30.43
30.27
30.12
29.97
29.81
29.66
29.51
21.25
18.01
123.563
123.516
142.818
142.174
141.860
139.618
138.575
135.549
134.180
131.691
131.373
130.712
129.677
128.502
127.349
126.893
125.829
125.492
123.563
123.516
120.016
118.867
115.245
115.075
142 140 138 136 134 132 130 128 126 124 122 120 118 ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

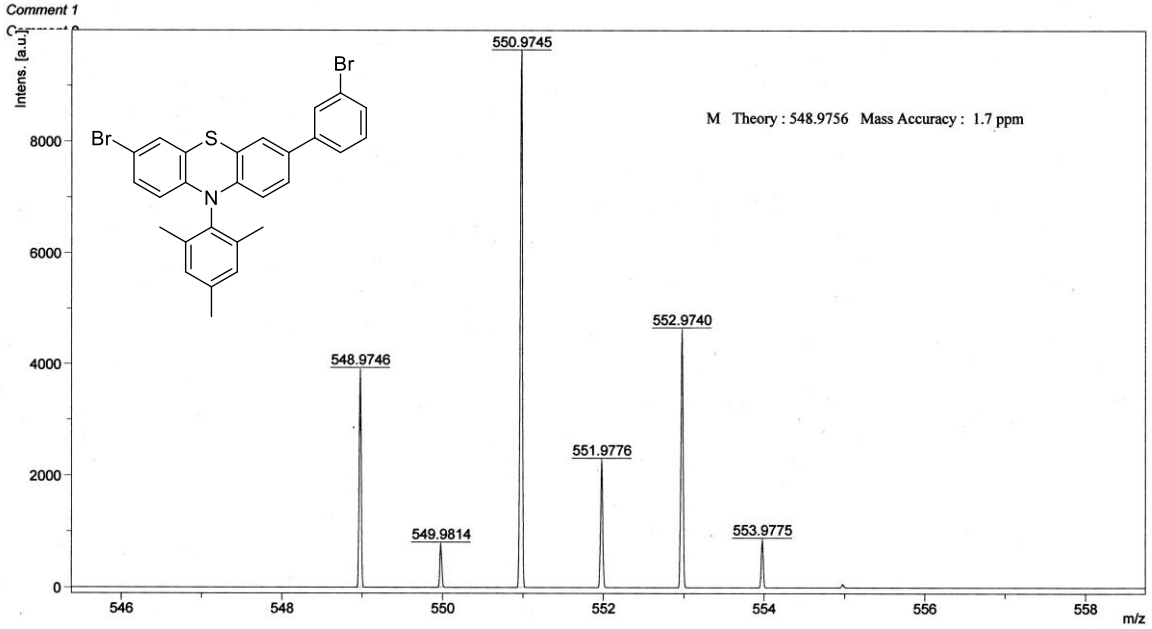

Comment 1
Intens. [a.u.]
x10^5
1.0
0.8
0.6
0.4
0.2
0.0
471.0629
473.0625
472.0675
474.0661
475.0614
476.0673
Br
S
N
M Theory : 471.0651 Mass Accuracy : 4.6 ppm
468 470 472 474 476 478 480
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **11**:

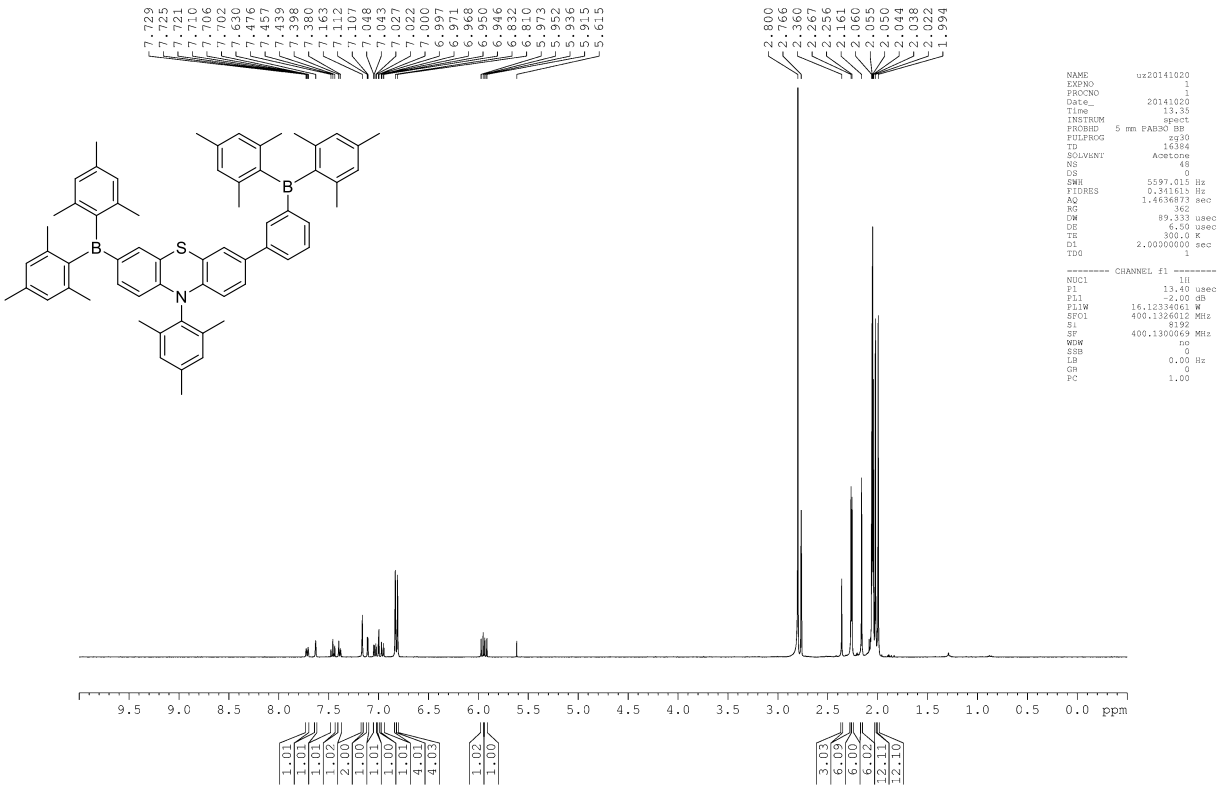


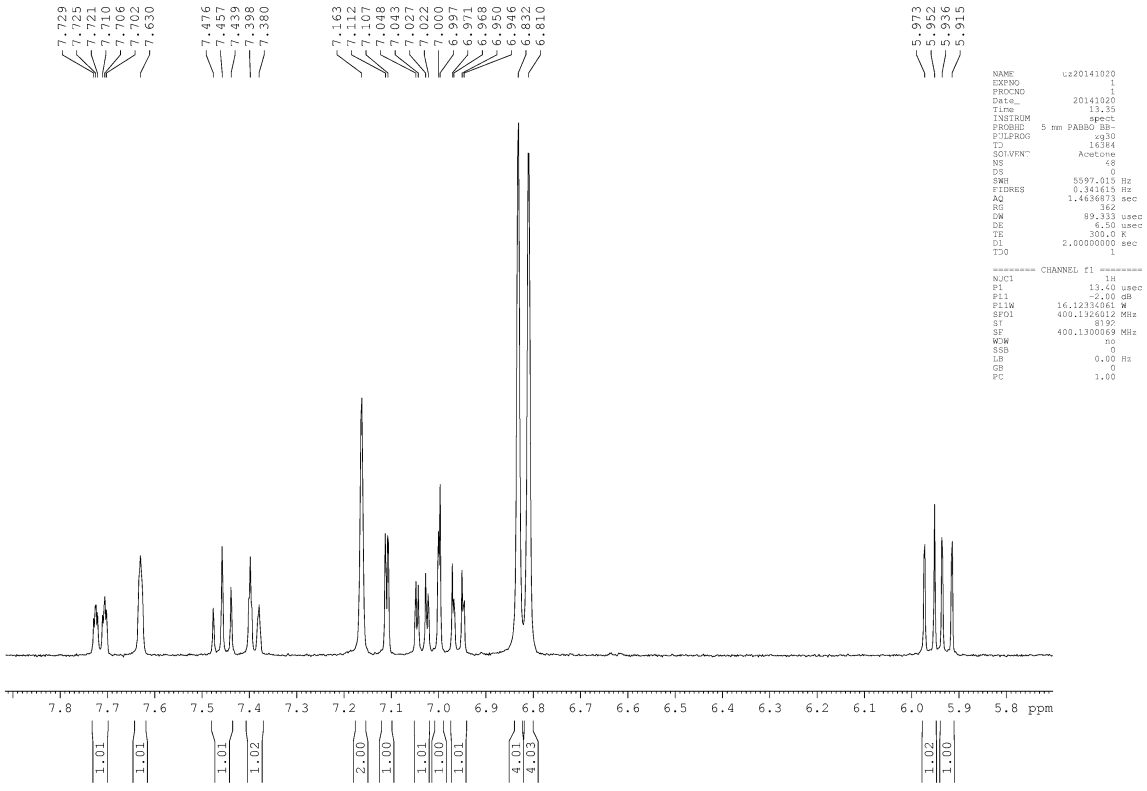


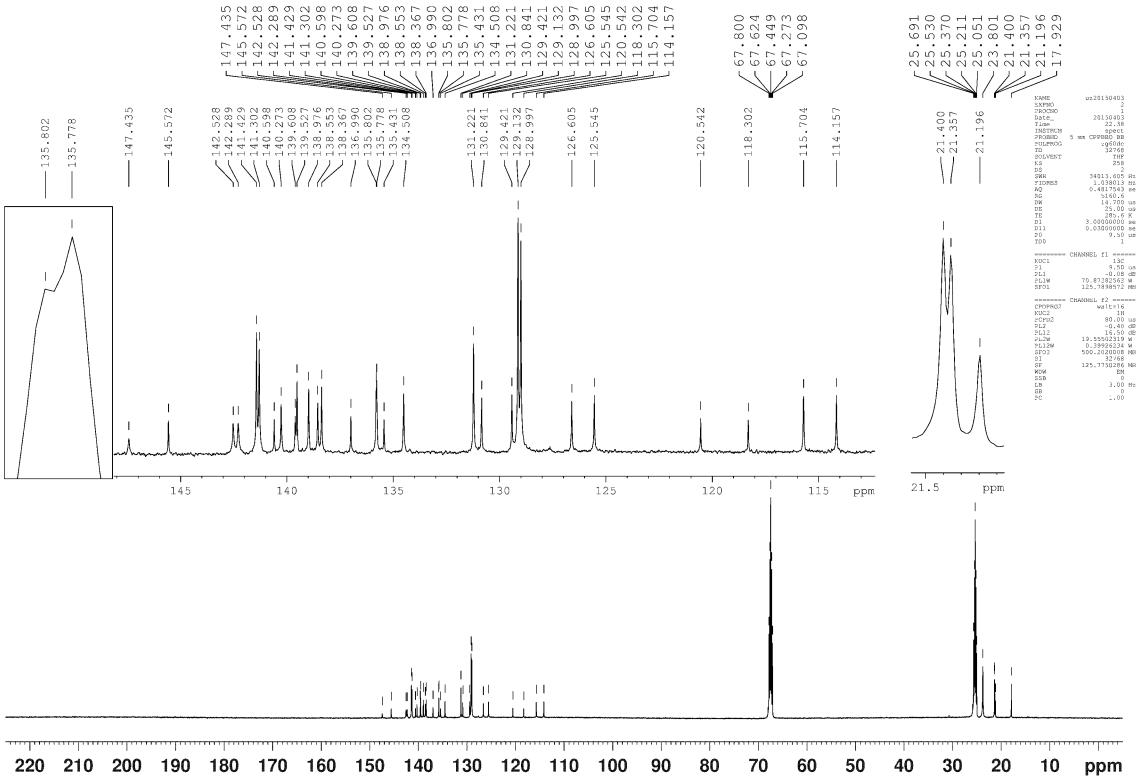

206.679
142.941
141.953
141.656
140.199
138.714
135.406
134.881
132.035
131.823
131.417
131.161
130.050
129.571
127.543
126.198
125.975
123.849
121.841
119.561
116.845
115.784
115.063
30.755
30.601
30.448
30.294
30.140
29.986
29.832
21.576
18.284
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
140 135 130 125 120 ppm

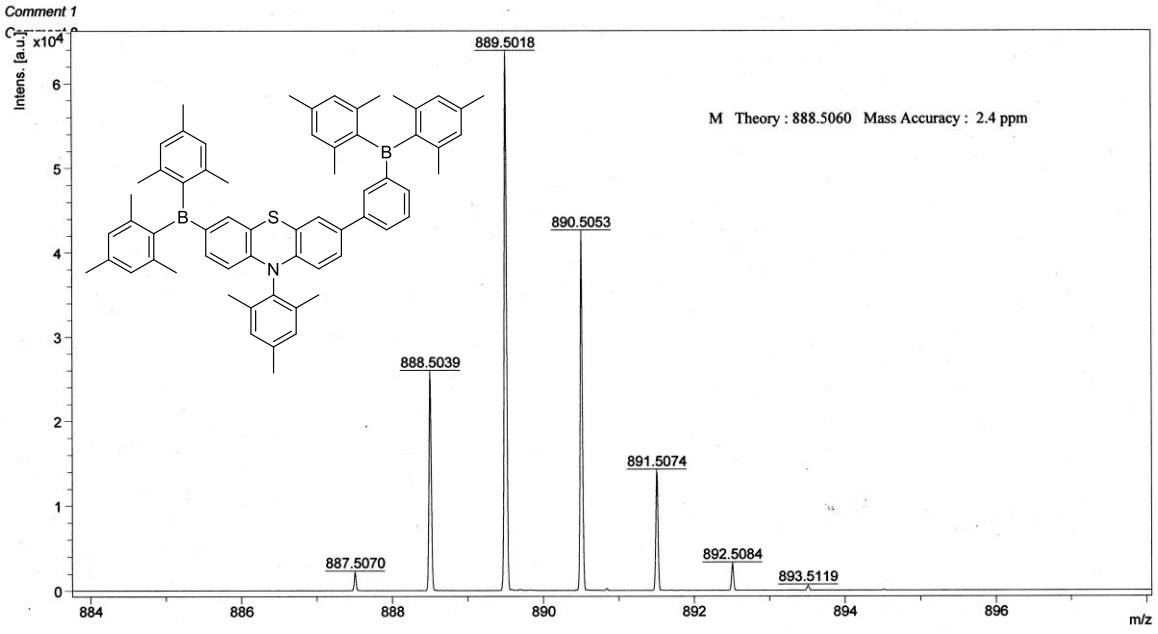

Comment 1
Intens. [a.u.]
8000
6000
4000
2000
0
Br
Br
S
N
550.9745
552.9740
548.9746
551.9776
549.9814
553.9775
M Theory : 548.9756 Mass Accuracy : 1.7 ppm
546 548 550 552 554 556 558
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **CC-MP5**:

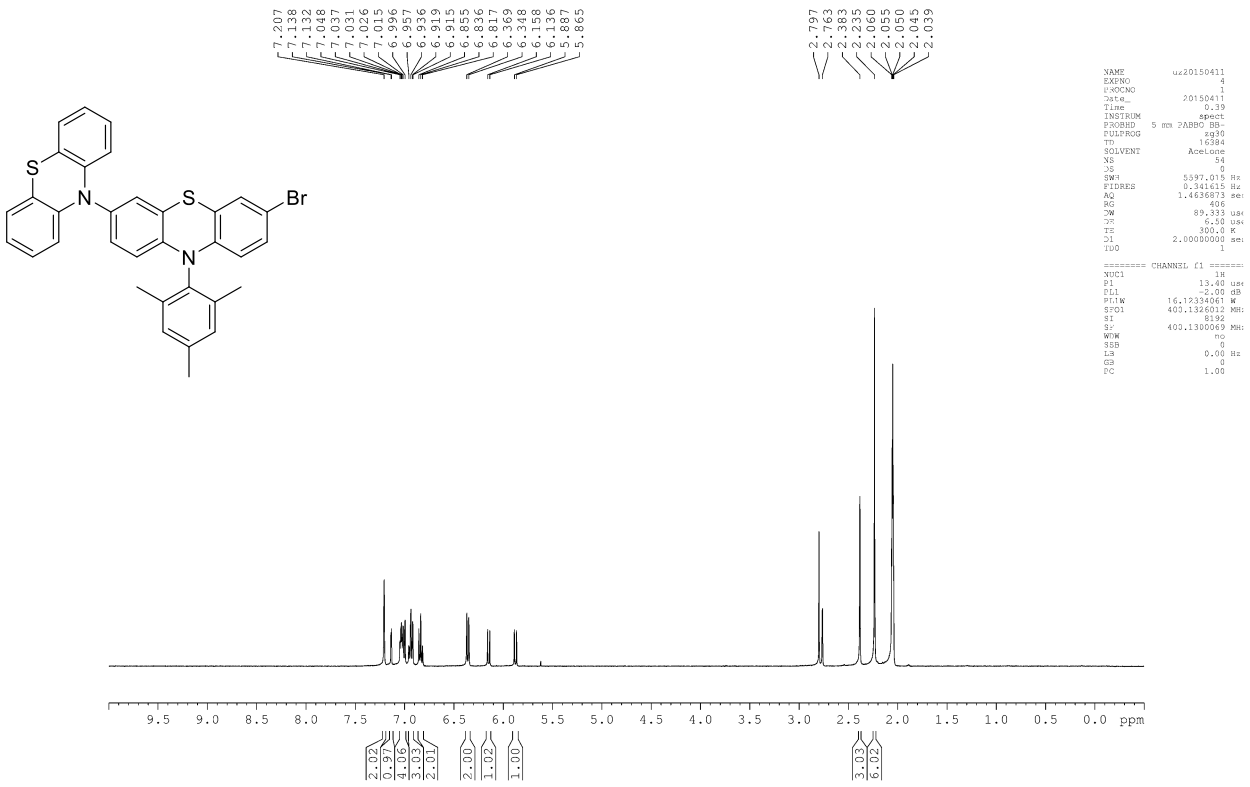


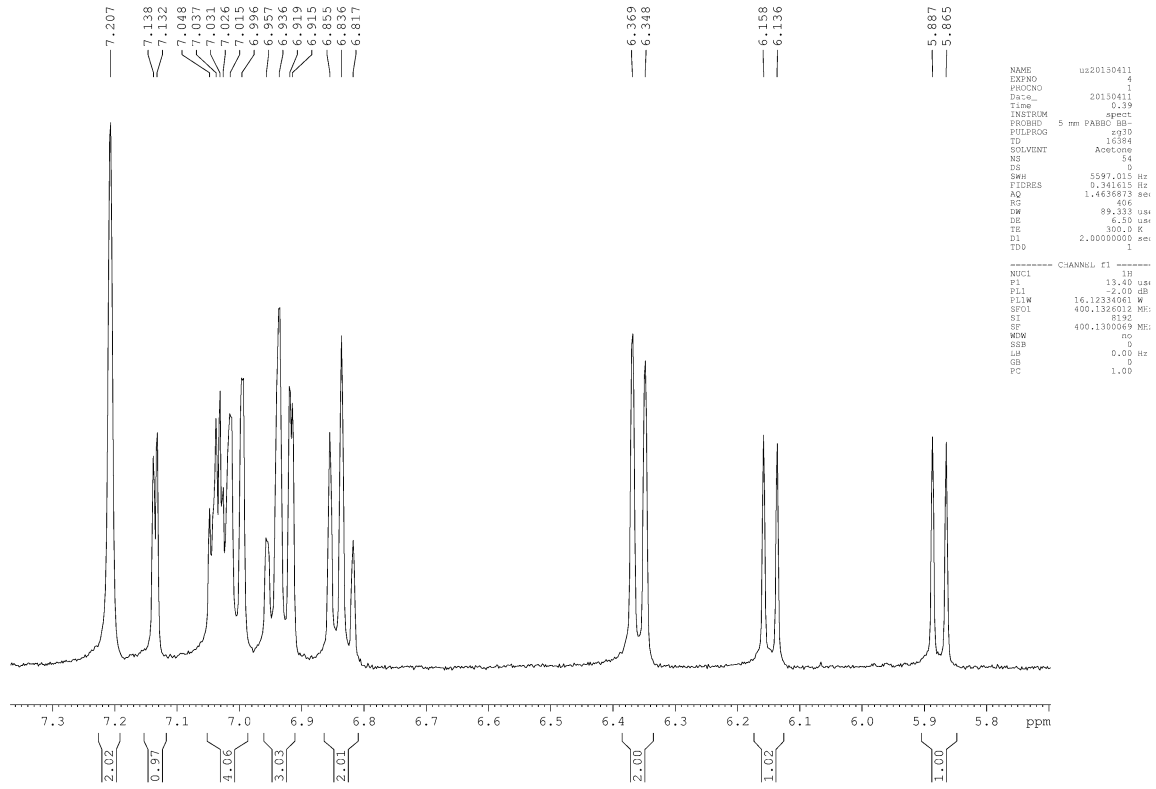



147.435
145.572
142.528
142.289
141.429
141.302
140.598
140.273
139.608
139.527
138.553
138.367
136.990
135.802
135.778
135.431
134.508
131.221
130.841
129.421
129.132
128.997
126.605
125.545
120.542
118.302
115.704
114.157
67.800
67.624
67.449
67.273
67.098
25.691
25.530
25.370
25.211
25.051
23.801
21.400
21.357
21.196
17.929
ppm
21.5
ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Comment 1
Intens. [a.u.]
x10^4
889.5018
890.5053
888.5039
891.5074
887.5070
892.5084
893.5119
M Theory : 888.5060 Mass Accuracy : 2.4 ppm
B
B
S
N
884 886 888 890 892 894 896
m/z

^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **12**:



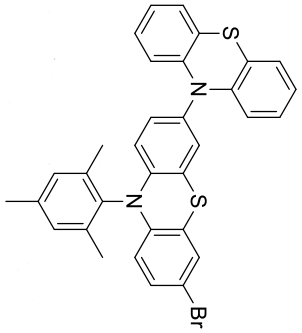


MPBrPh

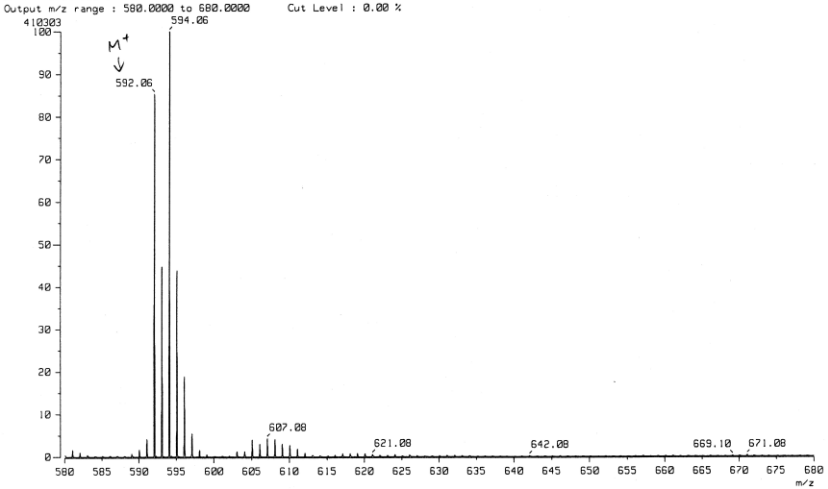
[Elemental Composition] Page: 1

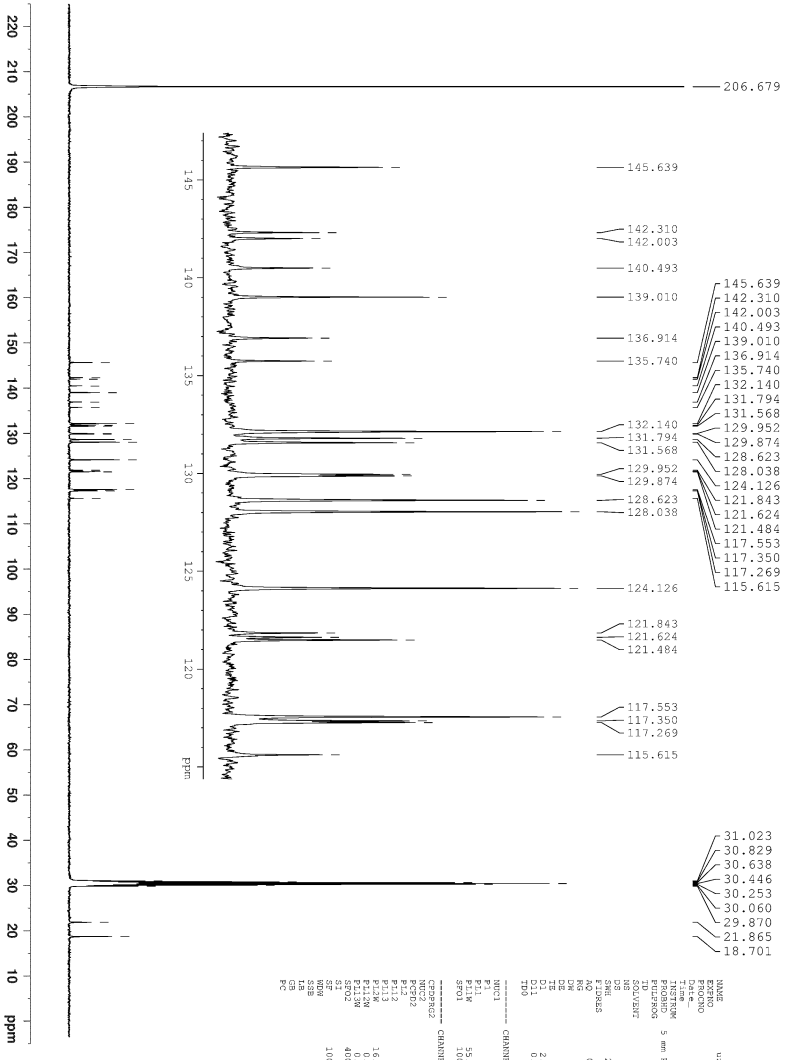
Data : 14Nov10_15-001 Date : 10-Nov-2014 18:19
Sample: MPBrPh
Note : NBA
Inlet : Direct Ion Mode : FAB+
RT : 0.00 min Scan#: 1
Elements : C 400/0, H 1000/0, N 2/2, Br 1/1(79Br 1/0, 81Br 1/0), S 2/2
Mass Tolerance : 10mmu
Unsaturation (U.S.) : -0.5 - 1000.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
592.0638	85.4	-0.7 / -0.4	24.0	C 33 H 25 N 2 79Br S 2 = 592.0643
594.0641	100.0	+3.3 / +1.9	24.0	C 33 H 25 N 2 81Br S 2

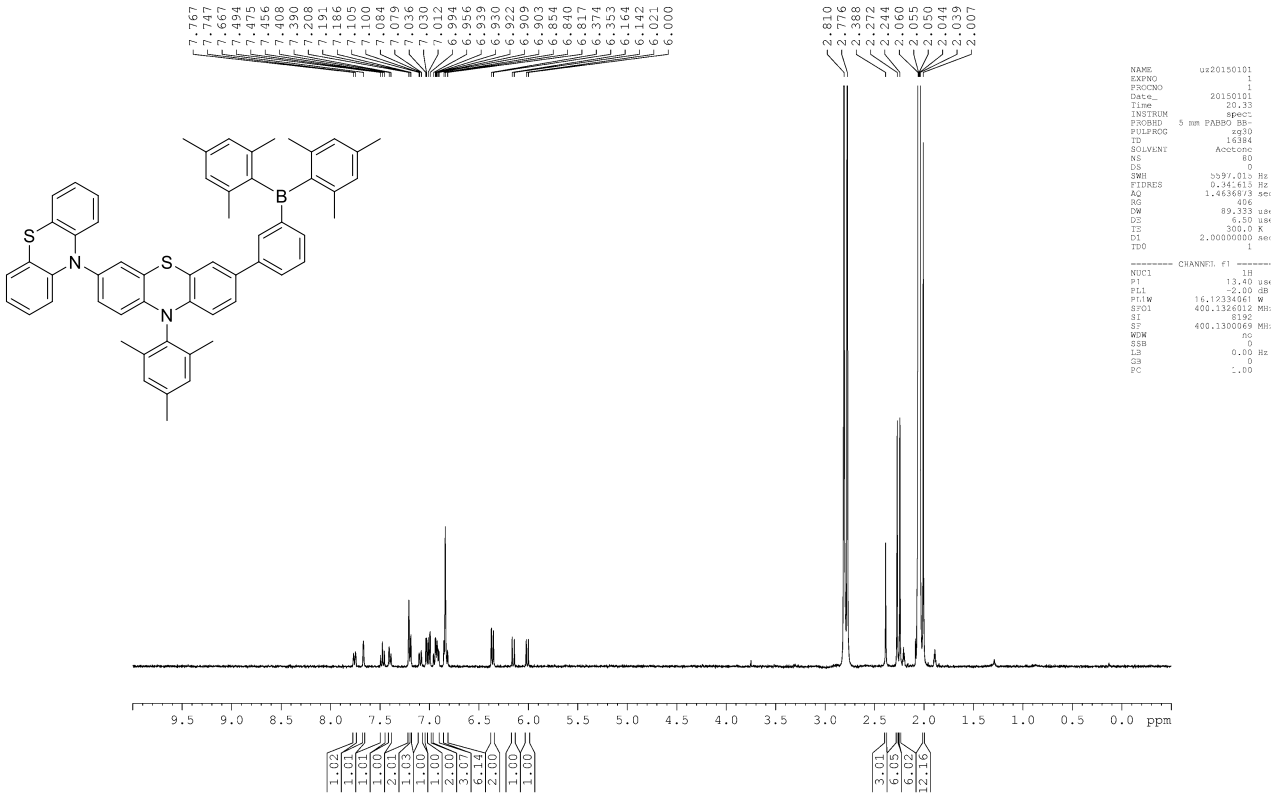


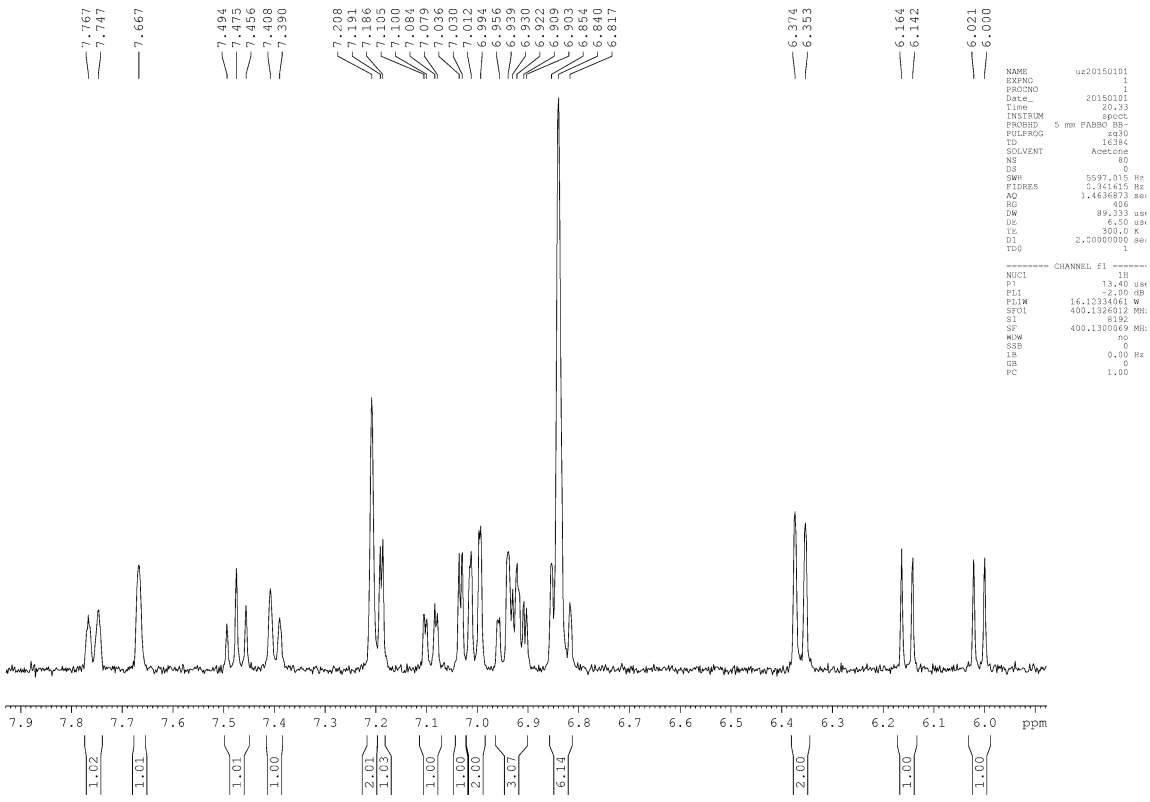
[Mass Spectrum]
Data : 14Nov10_15-001 Date : 10-Nov-2014 18:19
Sample: MPBrPh
Note : NBA
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.00 min Scan# : 1
BP : m/z 594.0641 Int. : 39.13
Output m/z range : 580.0000 to 680.0000 Cut Level : 0.00 %





^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **CC-MP6**:



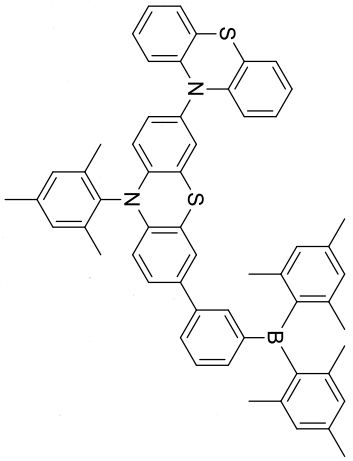


MP6

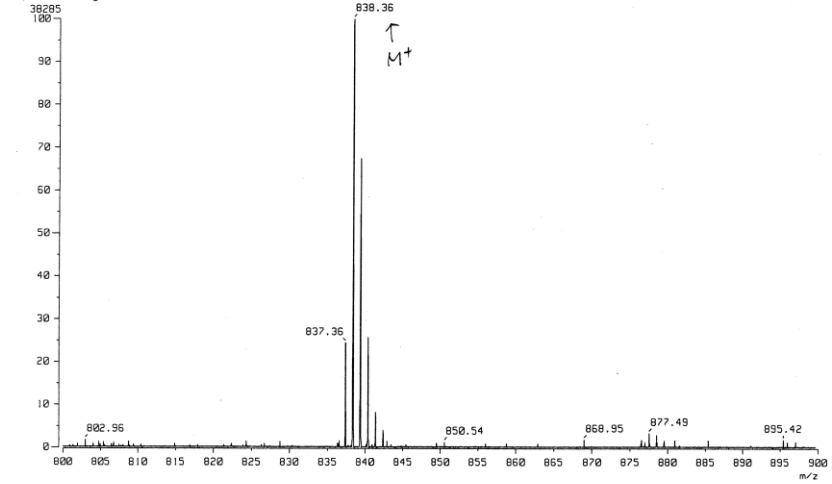
[Elemental Composition] Page: 1

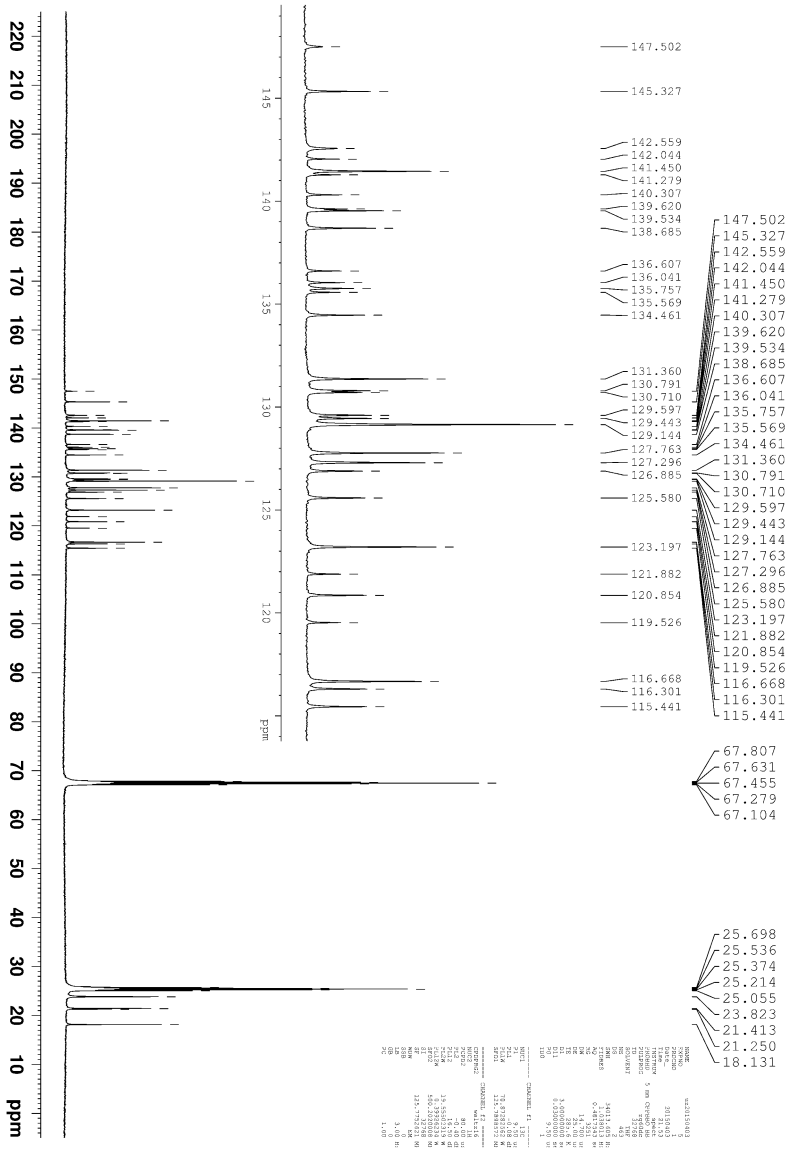
Data : 14Nov19_E23-001 Date : 19-Nov-2014 18:03
Sample: MP6
Note : 70eV
Inlet : Direct Ion Mode : EI+
RT : 1.19 min Scan#: 29
Elements : C 400/0, H 800/0, N 2/2, S 2/2, B 1/1
Mass Tolerance : 10mmu
Unsaturation (U.S.) : -0.5 - 10000.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
838.3584	100.0	-0.3 / -0.3	36.0	C 57 H 51 N 2 S 2 B = 838.3587

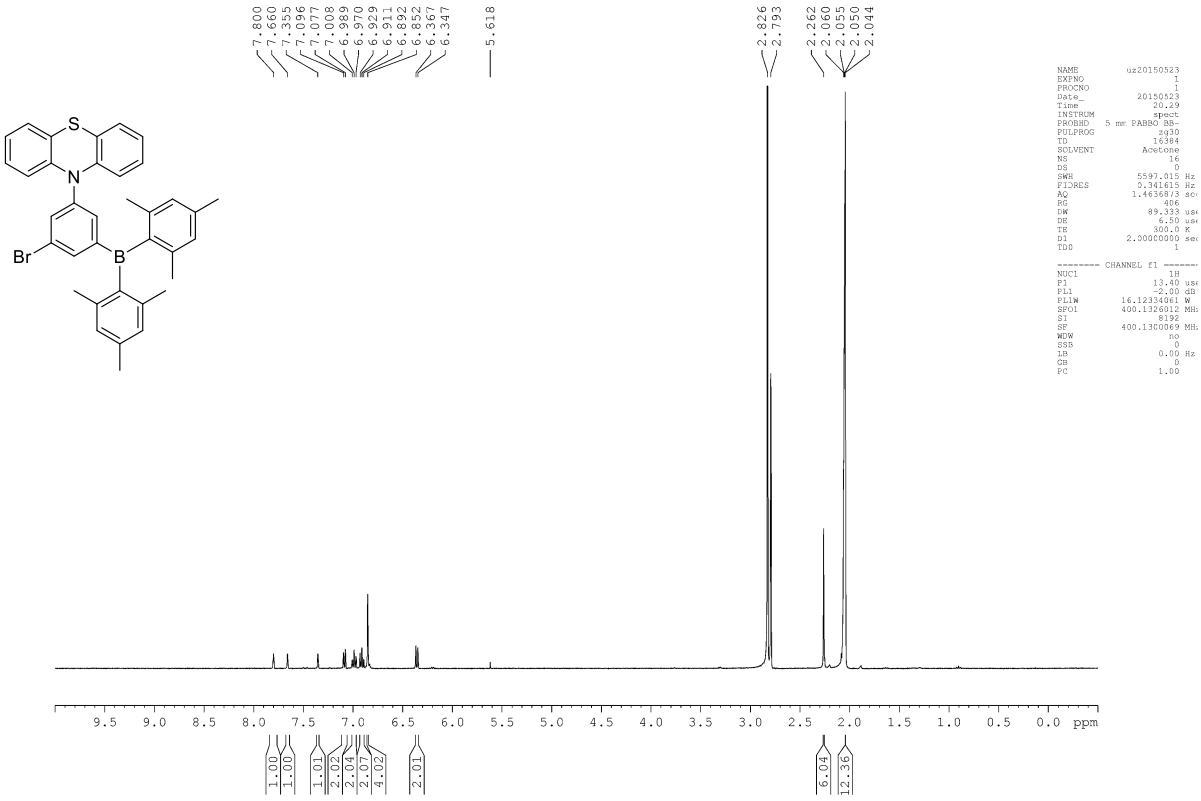


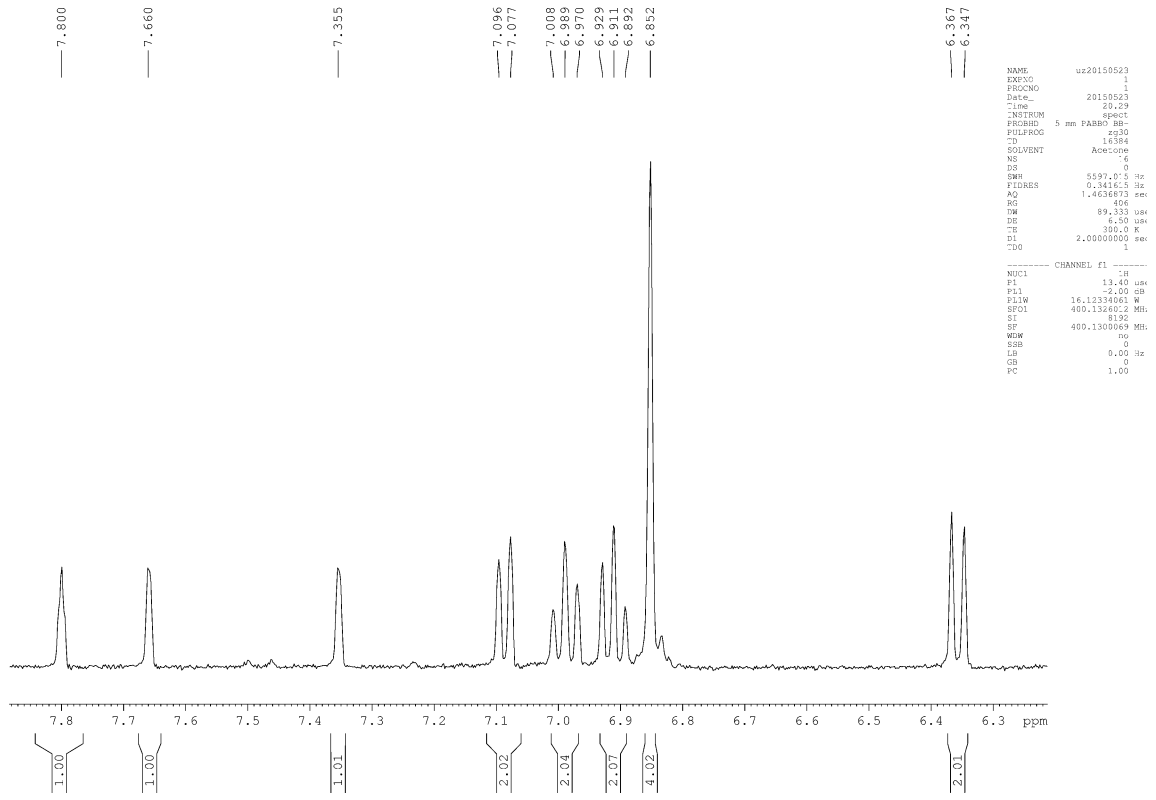
[Mass Spectrum]
Data : 14Nov19_E23-001 Date : 19-Nov-2014 18:03
Sample: MP6
Note : 70eV
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 1.19 min Scan# : 29
BP : m/z 838.3584 Int. : 3.65
Output m/z range : 800.0000 to 900.0000 Cut Level : 0.00 %





^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **14**:





MP7-C

[Elemental Composition] Page: 1

Data : 15Jan29_34-001 Date : 29-Jan-2015 17:50

Sample: MP7-C

Note : NBA

Inlet : Direct Ion Mode : FAB+

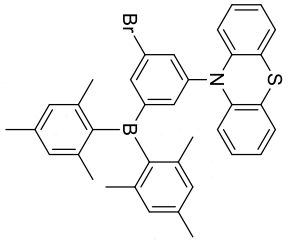
RT : 0.00 min Scan#: 1

Elements : C 1000/0, H 1000/0, N 1/1, Br 1/1(79Br 1/0, 81Br 1/0), S 1/1, B 1/1

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 1000.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
601.1613	90.5	+0.4 / +0.2	22.0	C 36 H 33 N 79Br S B = 601.1610
603.1581	100.0	-1.5 / -0.9	22.0	C 36 H 33 N 81Br S B



[Mass Spectrum]

Data : 15Jan29_34-001 Date : 29-Jan-2015 17:50

Sample: MP7-C

Note : NBA

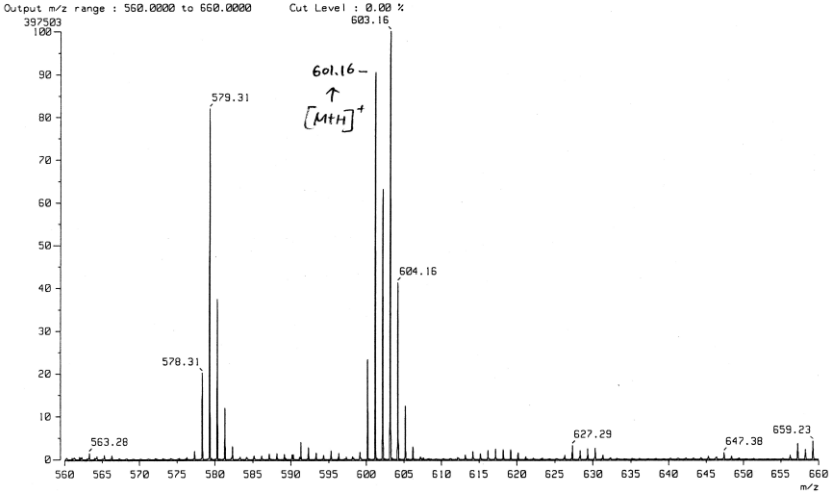
Inlet : Direct Ion Mode : FAB+

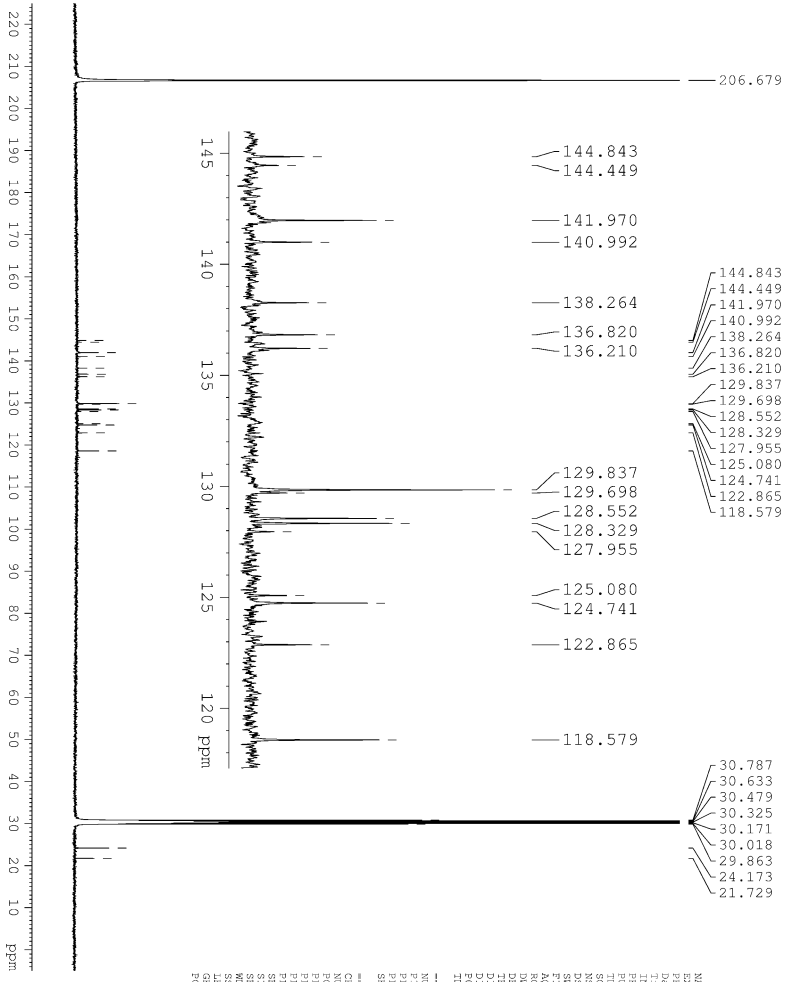
Spectrum Type : Normal Ion (EF-Linear)

RT : 0.00 min Scan# : 1

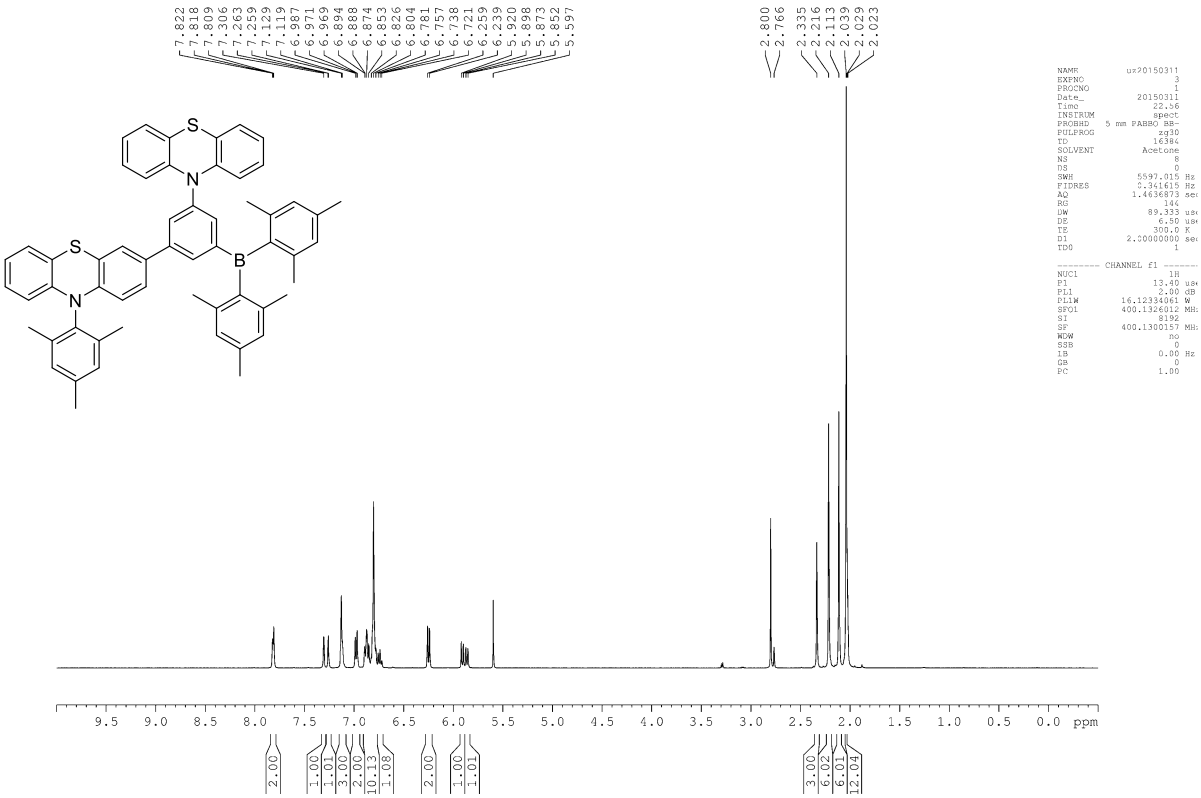
BP : m/z 603.1581 Int. : 37.91

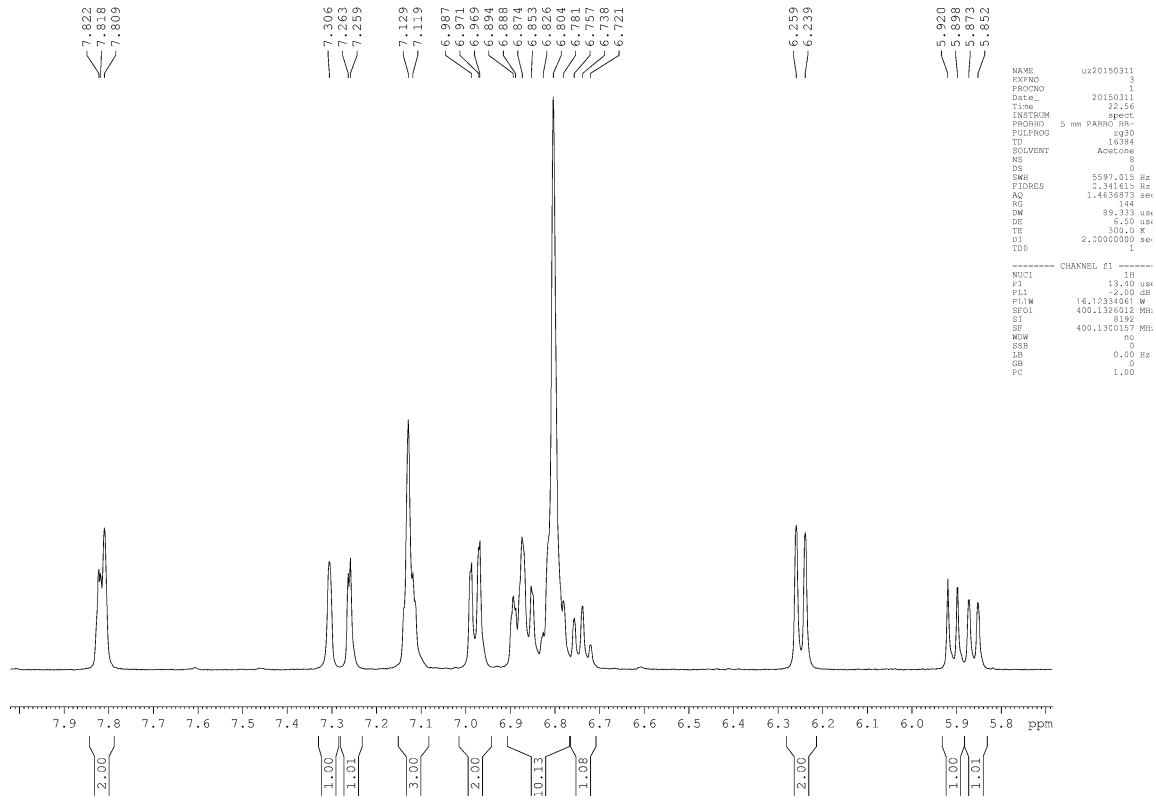
Output m/z range : 560.0000 to 660.0000 Cut Level : 0.00 %





^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **CC-MP7**:





MP7

[Elemental Composition] Page: 1

Data : 15Jan20_E16-001 Date : 20-Jan-2015 18:25

Sample: MP7

Note : 70eV

Inlet : Direct Ion Mode : EI+

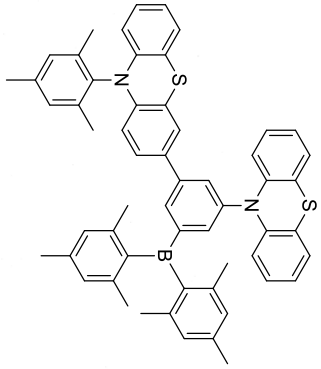
RT : 1.32 min Scan#: 32

Elements : C 400/0, H 800/0, N 2/2, S 2/2, B 1/1

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 10000.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
838.3577	100.0	-1.2 / -1.0	36.0	C 57 H 51 N 2 S 2 B = 838.3587



[Mass Spectrum]

Data : 15Jan20_E16-001 Date : 20-Jan-2015 18:25

Sample: MP7

Note : 70eV

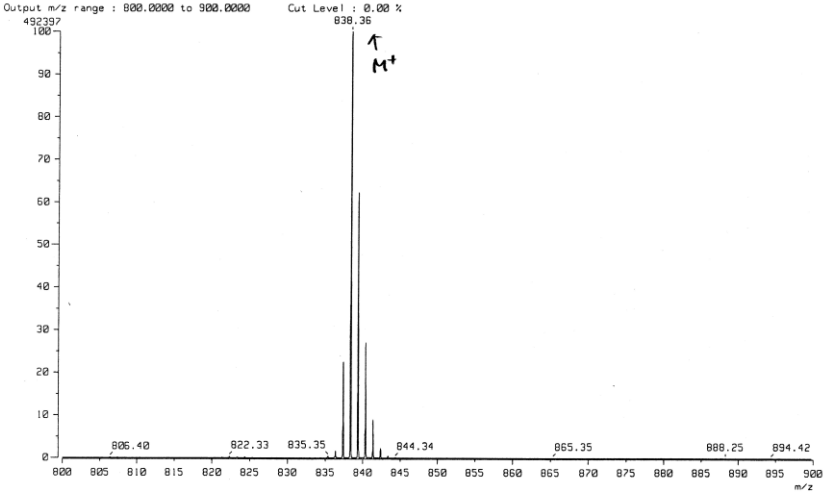
Inlet : Direct Ion Mode : EI+

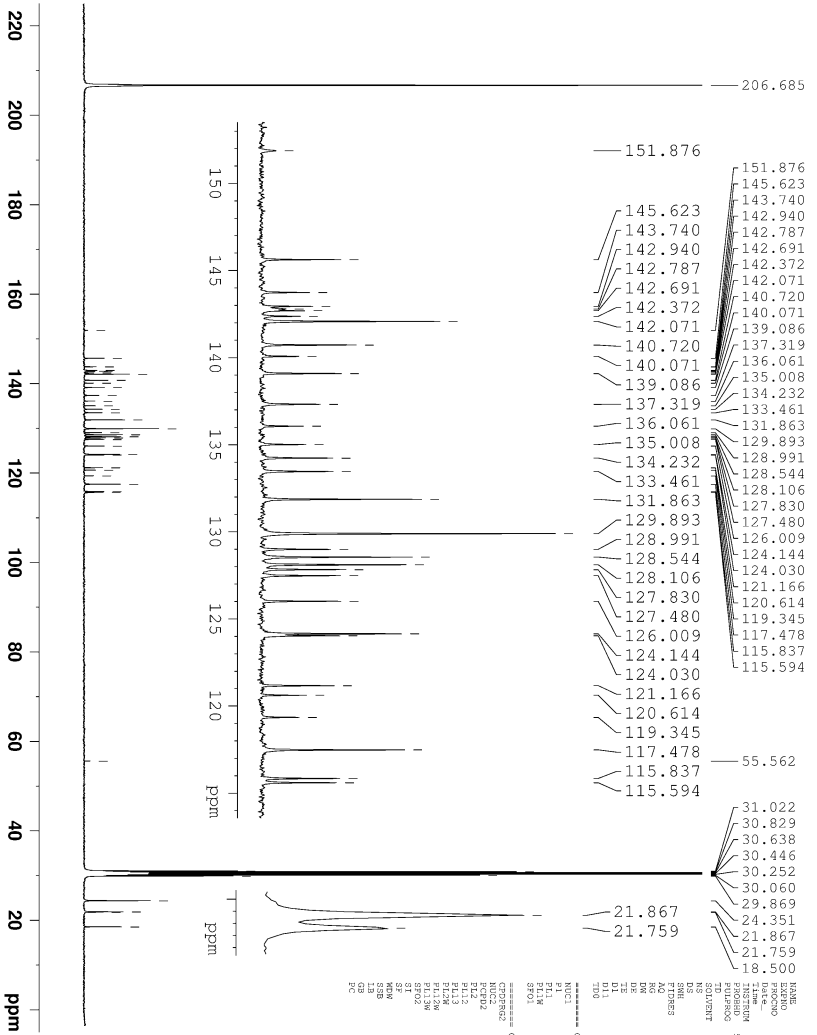
Spectrum Type : Normal Ion [EF-Linear]

RT : 1.32 min Scan# : 32

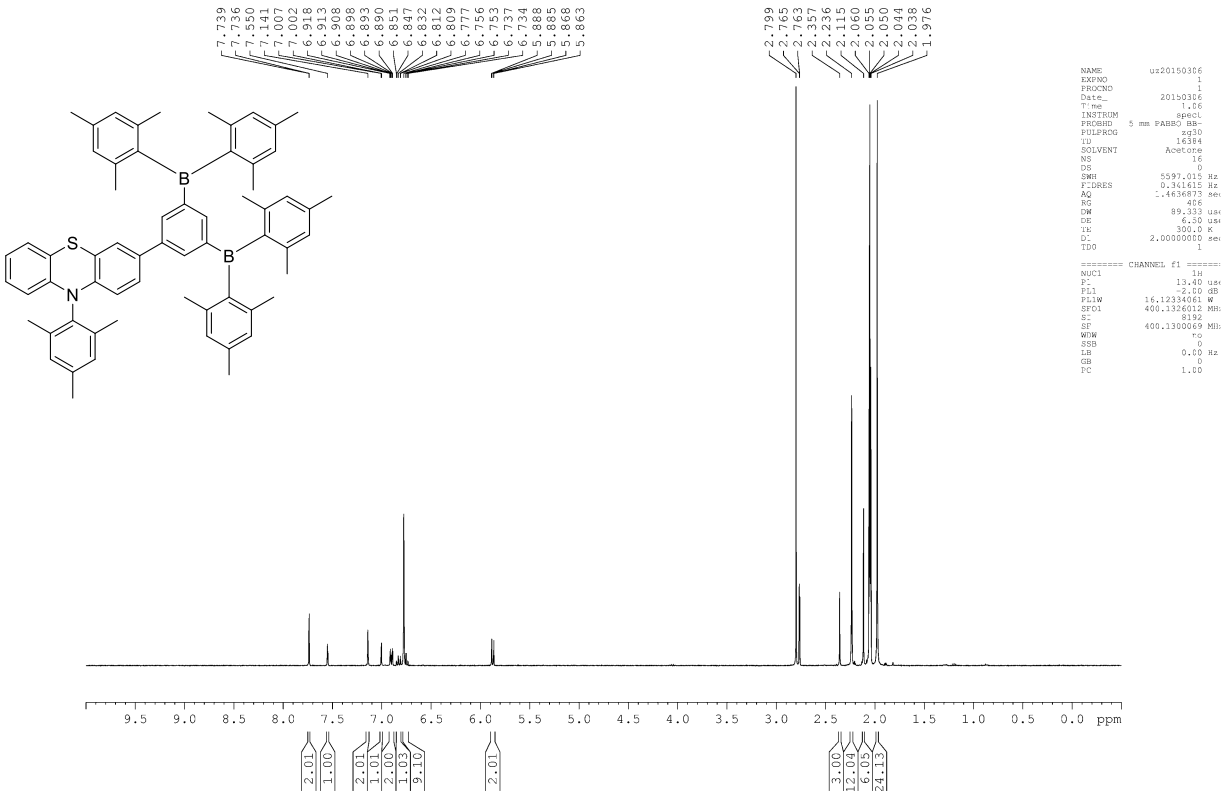
BP : m/z 838.3577 Int. : 46.96

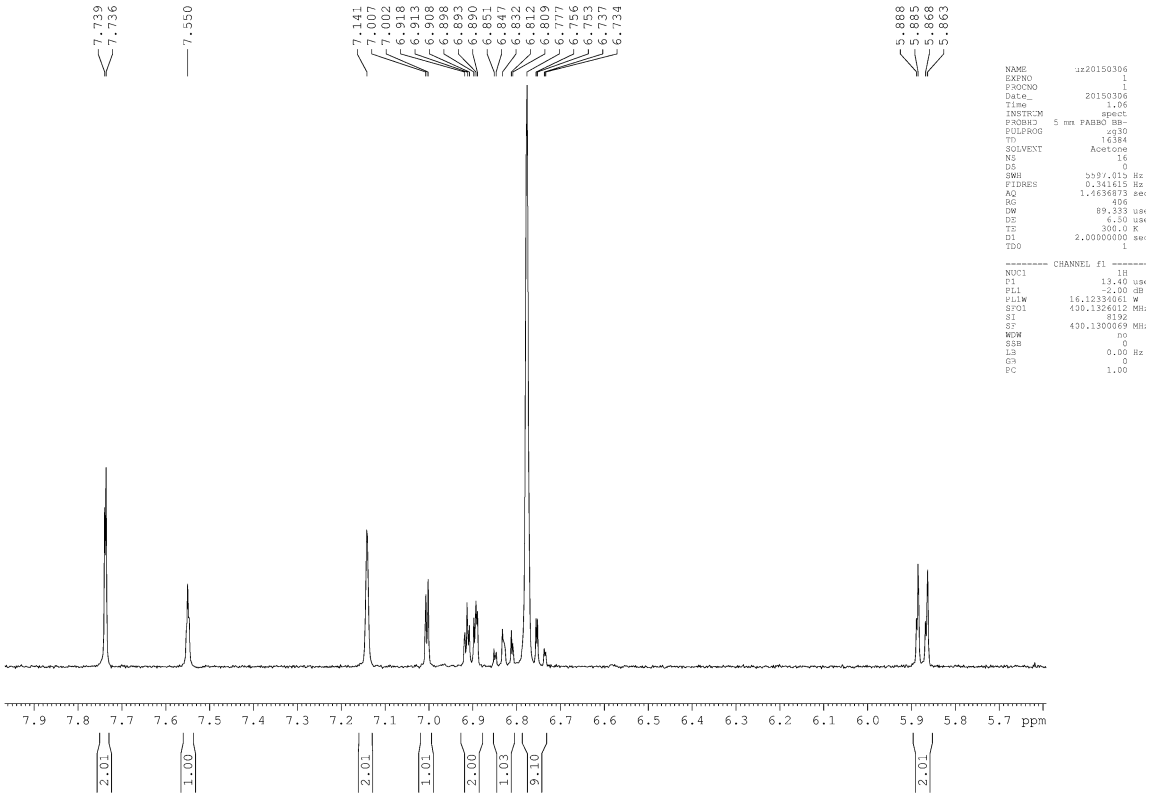
Output m/z range : 800.0000 to 900.0000 Cut Level : 0.00 %





^{1}H and ^{13}C-NMR NMR Spectra and HRMS of **CC-MP8**:



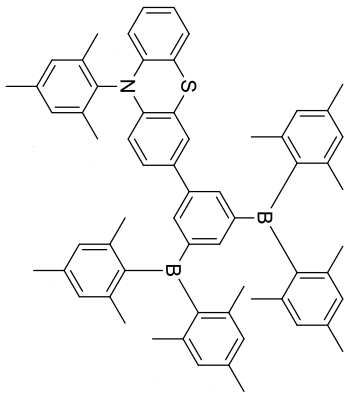


CC-MP8

[Elemental Composition] Page: 1

Data : 15Mar23_07-001 Date : 23-Mar-2015 16:40
Sample: CC-MP8
Note : NBA
Inlet : Direct Ion Mode : FAB+
RT : 0.08 min Scan#: (1,5)
Elements : C 1000/0, H 1000/0, N 1/1, S 1/1, B 2/2
Mass Tolerance : 10mmu
Unsaturation (U.S.) : -0.5 - 1000.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
889.5005	100.0	-2.1 / -1.8	34.0	C 63 H 65 N S B 2 = 889.5024



[Mass Spectrum]
Data : 15Mar23_07-001 Date : 23-Mar-2015 16:40
Sample: CC-MP8
Note : NBA
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.08 min Scan# : (1,5)
BP : m/z 889.5005 Int. : 21.06
Output m/z range : 850.0000 to 950.0000 Cut Level : 0.00 %