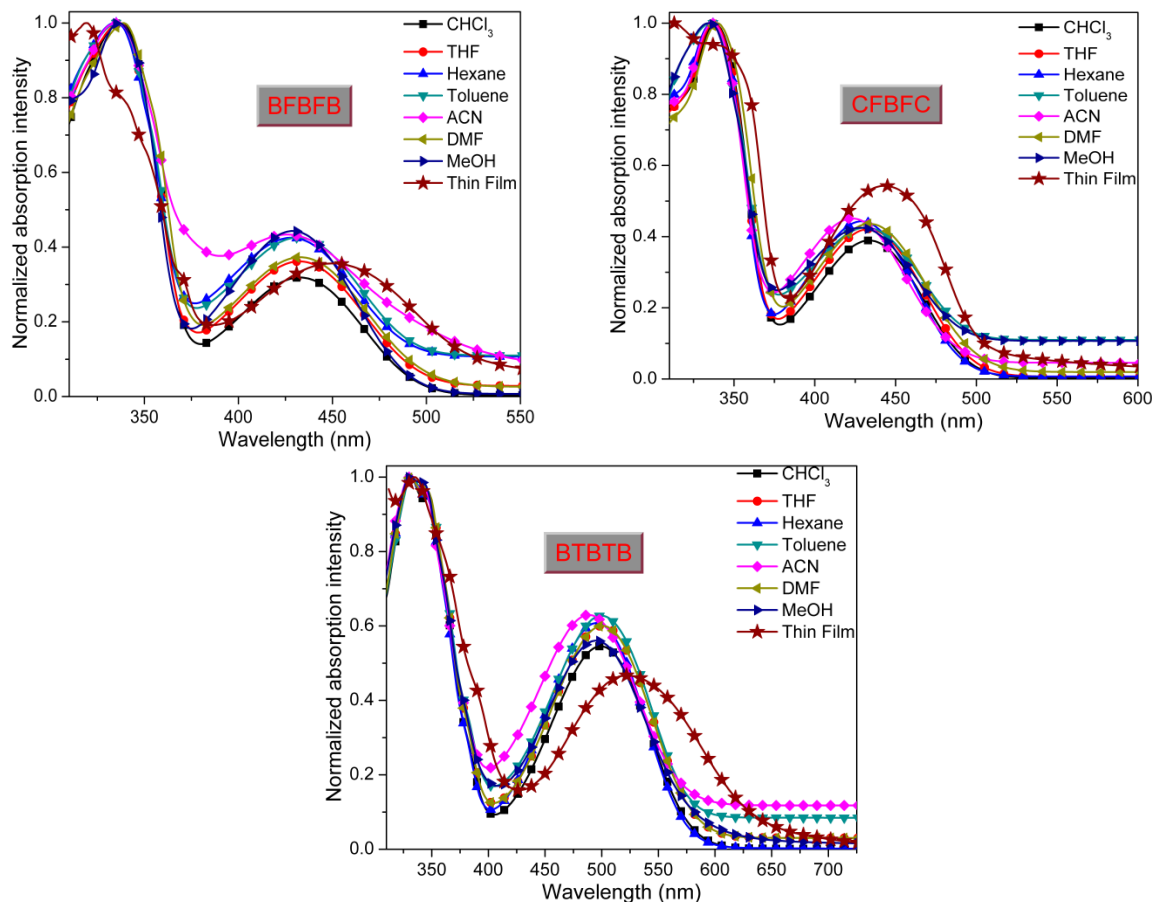


## Electronic Supplementary Information

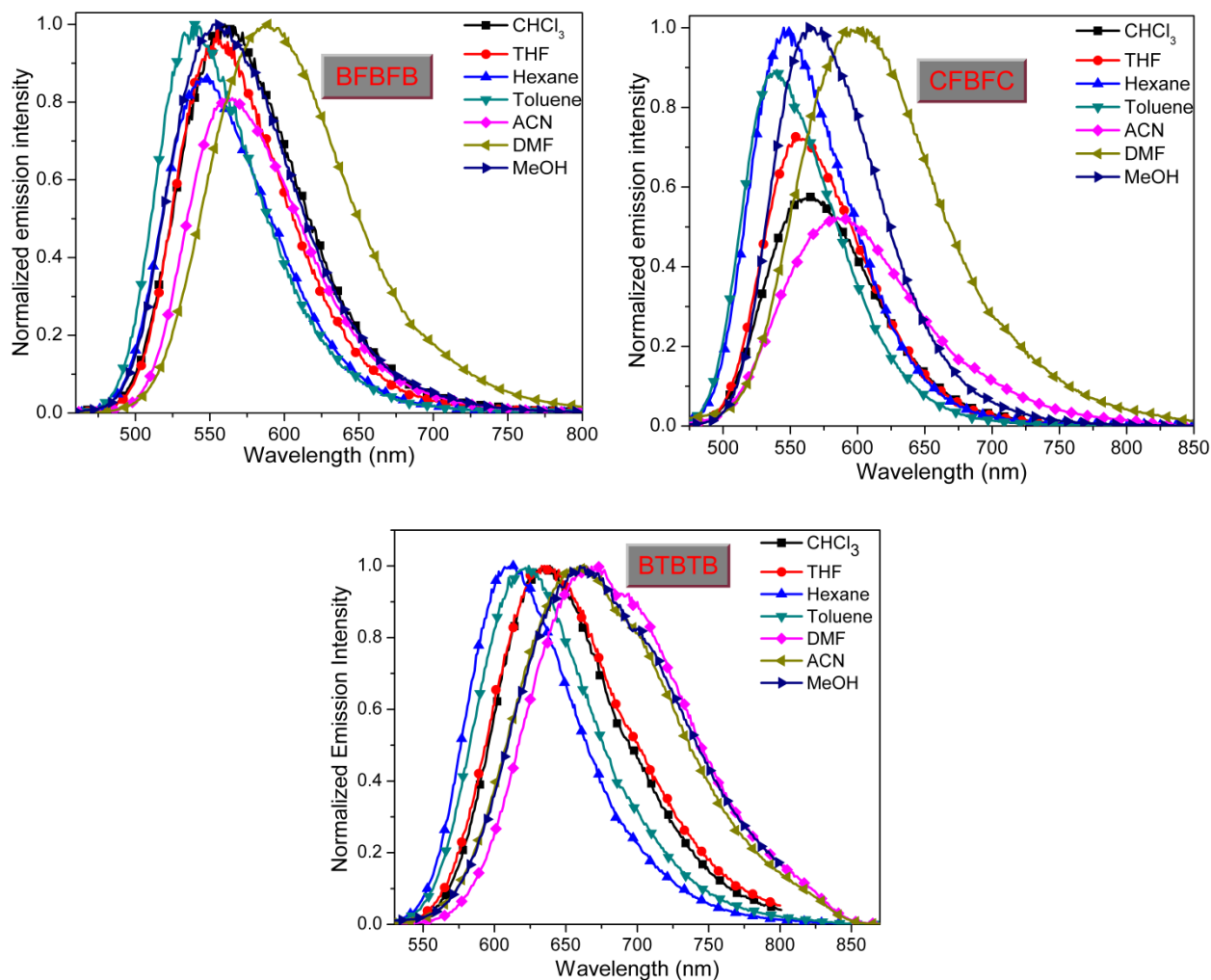
**Figure S1** Absorption maxima of compounds in different solvents and thin film state.



**Table S1** Absorption maxima of compounds in different solvents (units in nm).

| Compound | CHCl <sub>3</sub> | THF | Hexane | Toluene | ACN | DMF | MeOH |
|----------|-------------------|-----|--------|---------|-----|-----|------|
| BFBFB    | 433               | 433 | 434    | 433     | 430 | 433 | 435  |
| CFBFC    | 434               | 435 | 434    | 434     | 430 | 433 | 435  |
| BTBTB    | 500               | 501 | 499    | 500     | 498 | 501 | 498  |
| CTBTC    | 525               | 528 | 526    | 525     | 524 | 528 | 527  |

**Figure S2** Emission maxima of compounds in different solvents.



**Table S2** Emission maxima of compounds in different solvents (units in nm).

| Compound | $\text{CHCl}_3$ | THF | Hexane | Toluene | ACN | DMF | MeOH |
|----------|-----------------|-----|--------|---------|-----|-----|------|
| BFBFB    | 560             | 555 | 547    | 540     | 565 | 589 | 567  |
| CFBFC    | 564             | 554 | 545    | 540     | 589 | 593 | 570  |
| BTBTB    | 639             | 639 | 624    | 613     | 660 | 672 | 676  |
| CTBTC    | 663             | 657 | 645    | 635     | 693 | 706 | 714  |

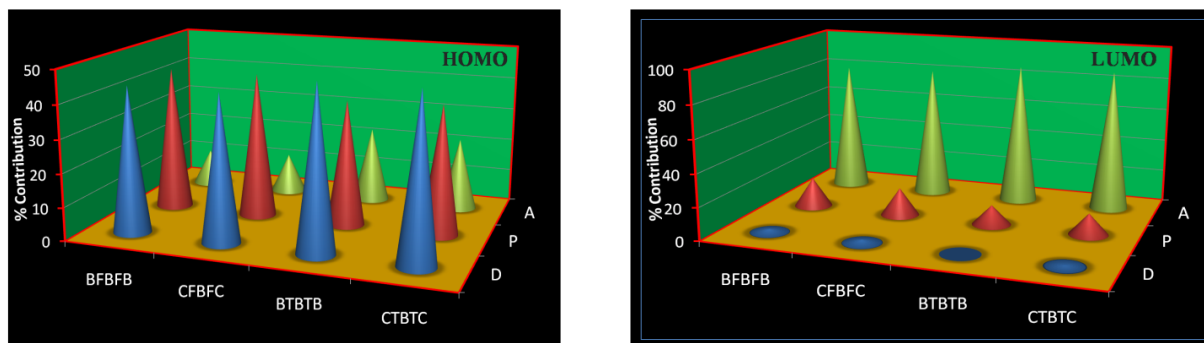
**Table S3** Stokes shift of compounds in different solvents (units in  $\text{cm}^{-1}$ ).

| Compound | $\text{CHCl}_3$ | THF  | Hexane | Toluene | ACN  | DMF  | MeOH |
|----------|-----------------|------|--------|---------|------|------|------|
| BFBFB    | 5238            | 5077 | 4760   | 4576    | 5555 | 6117 | 5352 |
| CFBFC    | 5311            | 4938 | 4693   | 4523    | 6279 | 6231 | 5446 |
| BTBTB    | 4352            | 4311 | 4015   | 3687    | 4929 | 5079 | 5387 |
| CTBTC    | 3965            | 3719 | 3508   | 3300    | 4654 | 4775 | 4970 |

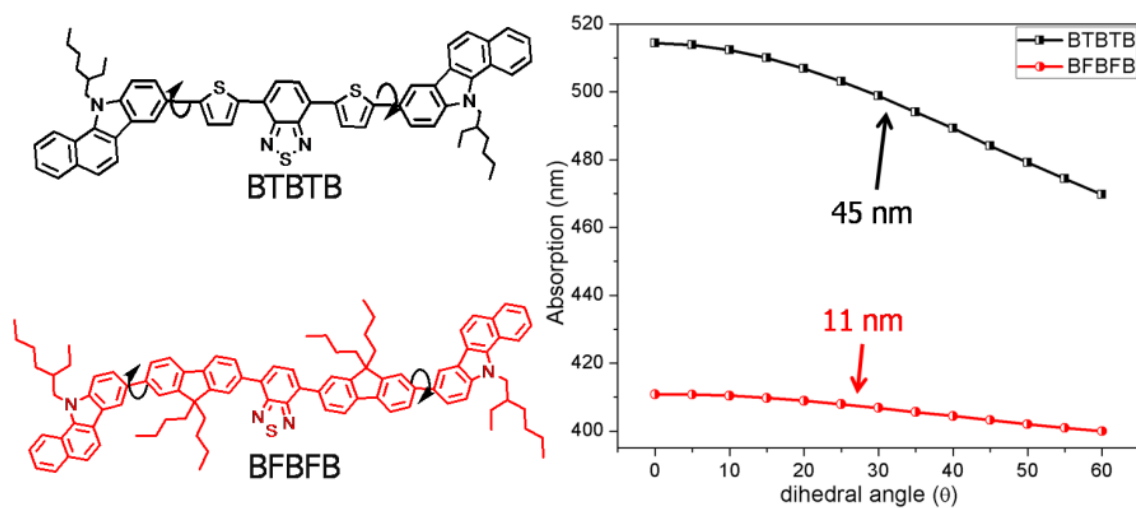
**Table S4** The computed energies of the vertical excitations along with oscillator strengths, dipole moments and configurations in terms of molecular orbitals from various functionals.

| Dye          | $\lambda_{\text{max}}^a$<br>(nm) | B3LYP (gas)                    |     |             | PBE ( gas)                     |     |                            | m062X ( gas)                   |     |                                            |
|--------------|----------------------------------|--------------------------------|-----|-------------|--------------------------------|-----|----------------------------|--------------------------------|-----|--------------------------------------------|
|              |                                  | $\lambda_{\text{max}}$<br>(nm) | f   | Composition | $\lambda_{\text{max}}$<br>(nm) | f   | Composition                | $\lambda_{\text{max}}$<br>(nm) | f   | Composition                                |
| <b>BFBFB</b> | 433                              | 528<br>(2.35eV)                | 0.7 | H->L (92%)  | 494<br>(2.51eV)                | 0.9 | H->L (86%)<br>H-2->L (11%) | 403<br>(3.07eV)                | 1.5 | H->L (62%)<br>H-2->L (19%)<br>H-4->L (12%) |
| <b>CFBFC</b> | 434                              | 530<br>(2.34eV)                | 0.7 | H->L (96%)  | 496<br>(2.50eV)                | 0.8 | H->L (93%)<br>H-2->L (6%)  | 403<br>(3.04eV)                | 1.4 | H->L (69%)<br>H-2->L (21%)                 |
| <b>BTBTB</b> | 499                              | 623<br>(1.99eV)                | 0.9 | H->L (99%)  | 589<br>(2.11eV)                | 0.9 | H->L (98%)                 | 491<br>(2.53eV)                | 1.2 | H->L (92%)                                 |
| <b>CTBTC</b> | 525                              | 627<br>(1.98eV)                | 0.7 | H->L (99%)  | 593<br>(2.09eV)                | 0.8 | H->L (98%)                 | 493<br>(2.52eV)                | 1.0 | H->L (93%)                                 |

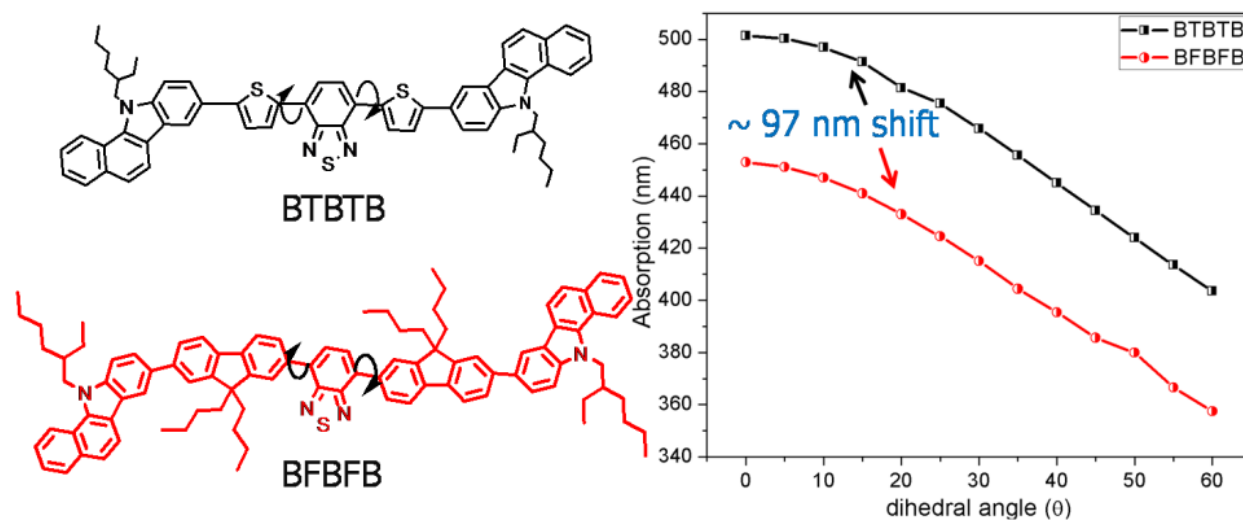
**Figure S3** Percentage contributions of individual segments in HOMO and LUMO levels of the compounds.

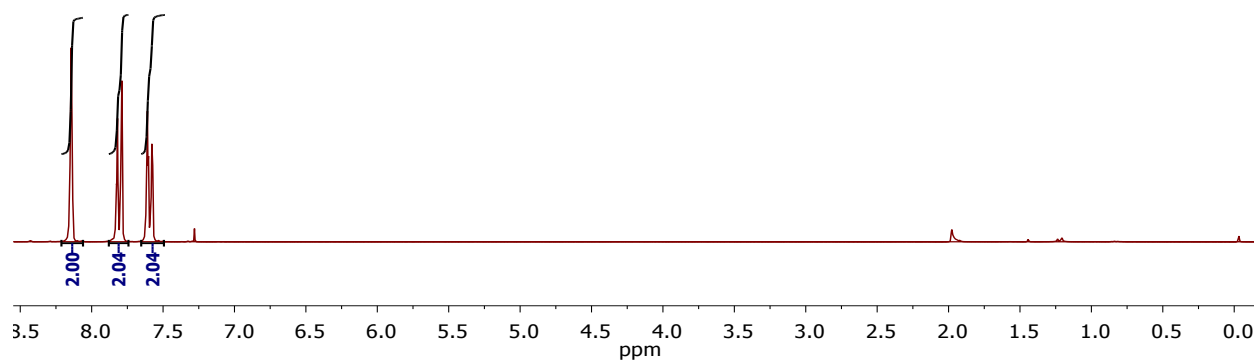
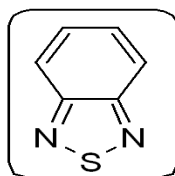


**Figure S4** Computed absorption vs. variation of dihedral angle ( $\theta$ ) between the donor-spacer segments in the dyes (in  $^\circ$ )

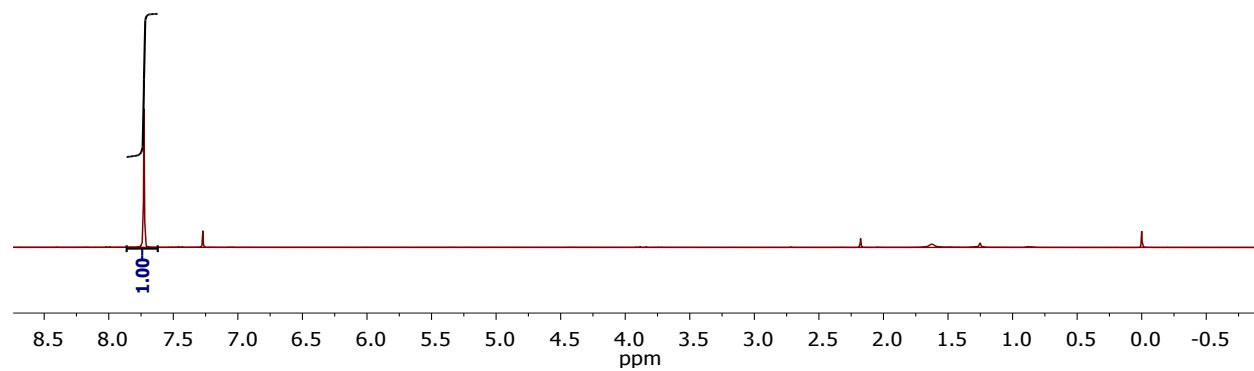
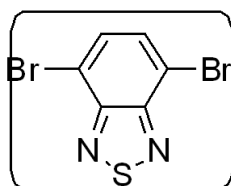


**Figure S5** Computed absorption vs. variation of dihedral angle ( $\theta$ ) between the acceptor-spacer segments in the dyes (in  $^\circ$ )

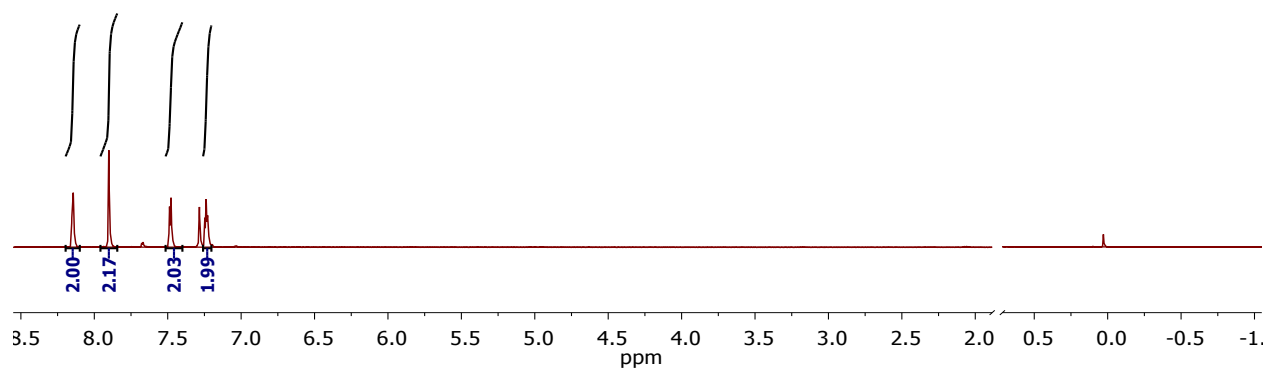
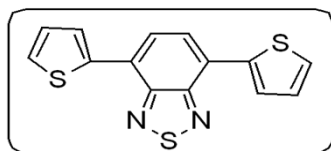




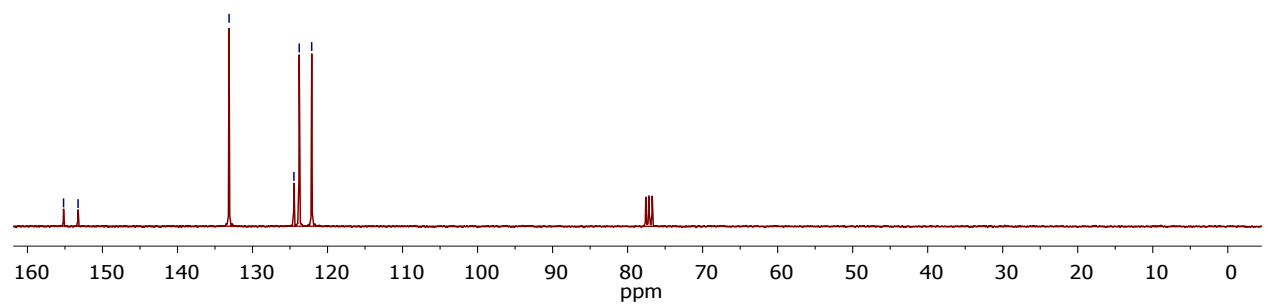
<sup>1</sup>H spectrum of molecule 1



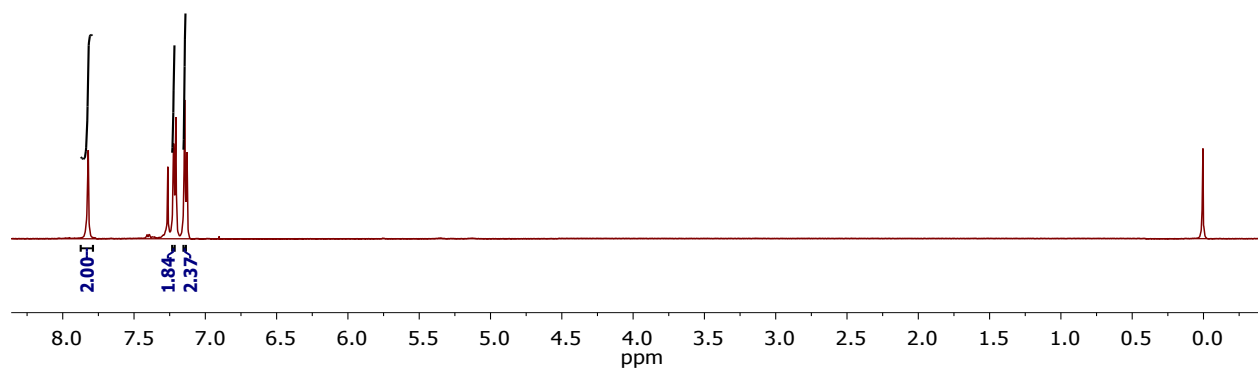
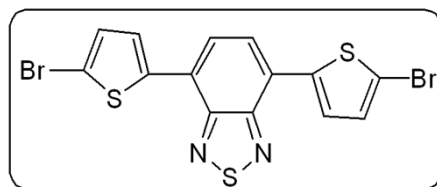
<sup>1</sup>H spectrum of molecule 2



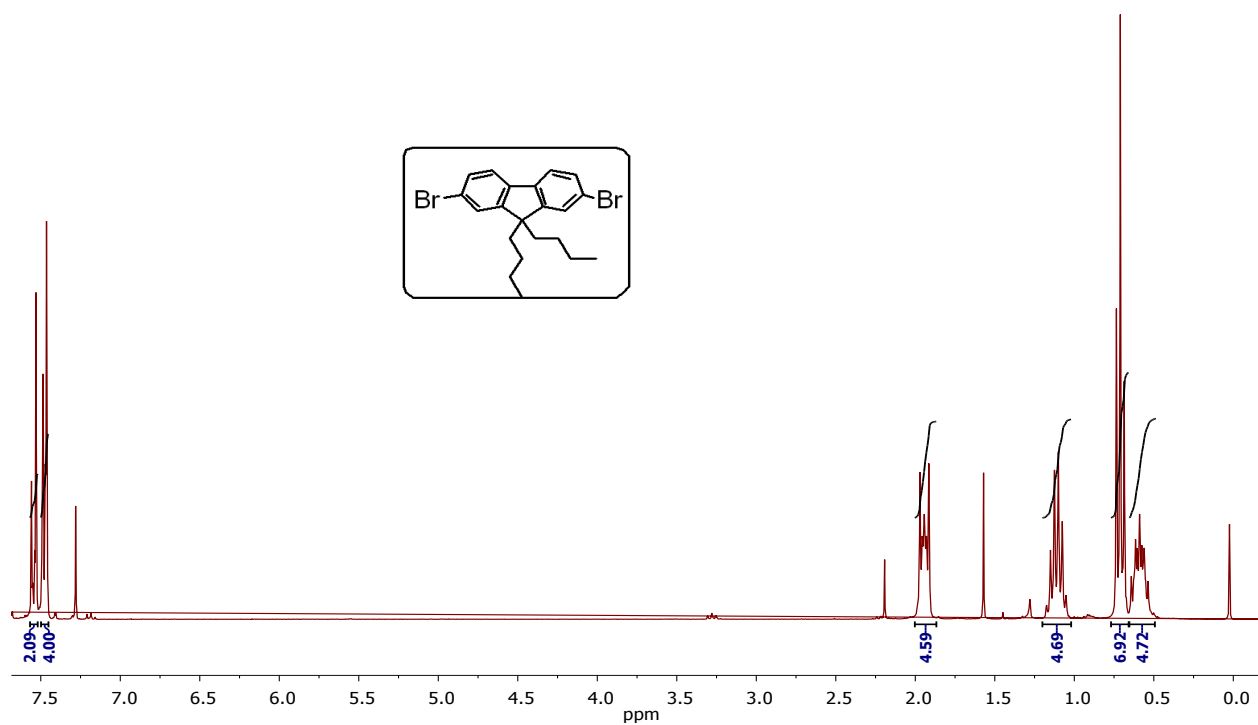
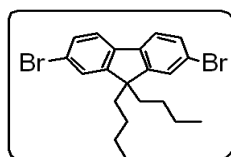
<sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>) of molecule 3. The x-axis ranges from 160 to 0 ppm. The spectrum shows several peaks in the aromatic region (122-156 ppm) and one peak at 77.0 ppm (TMS).



**<sup>1</sup>H and <sup>13</sup>C spectra of molecule 3**

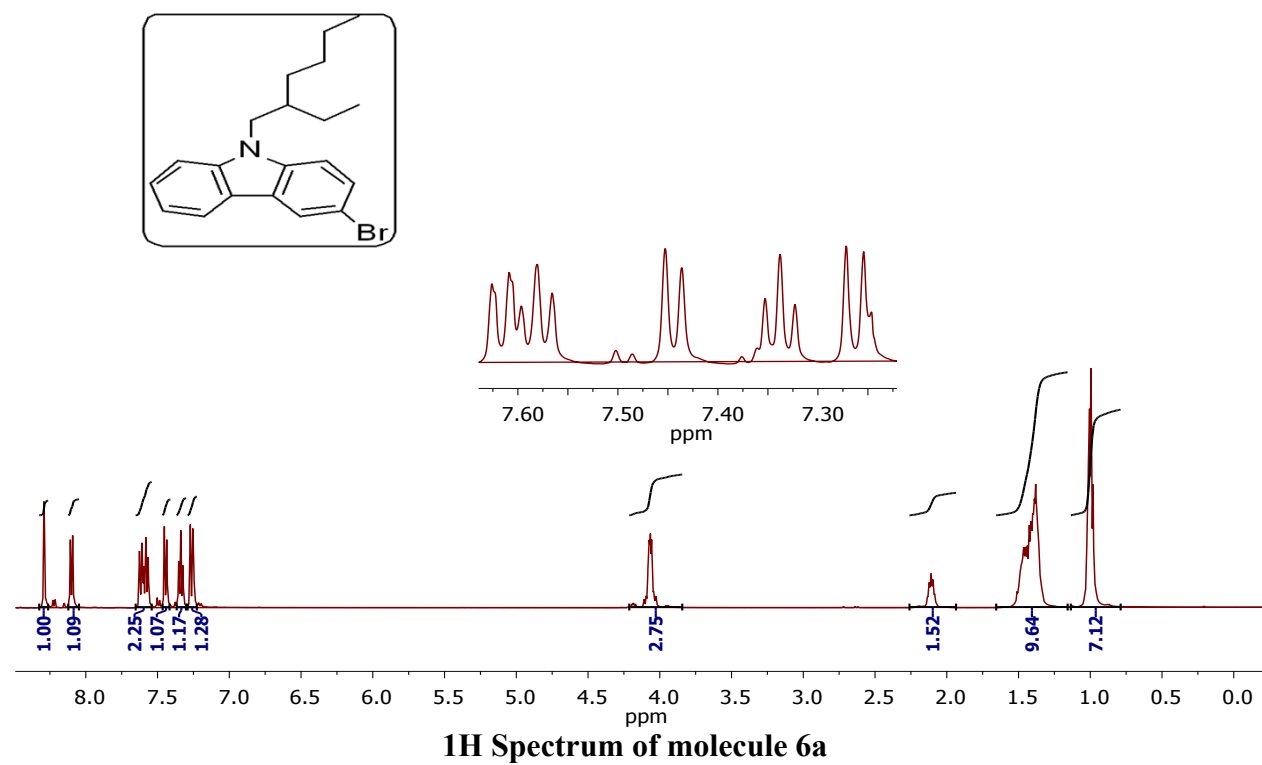
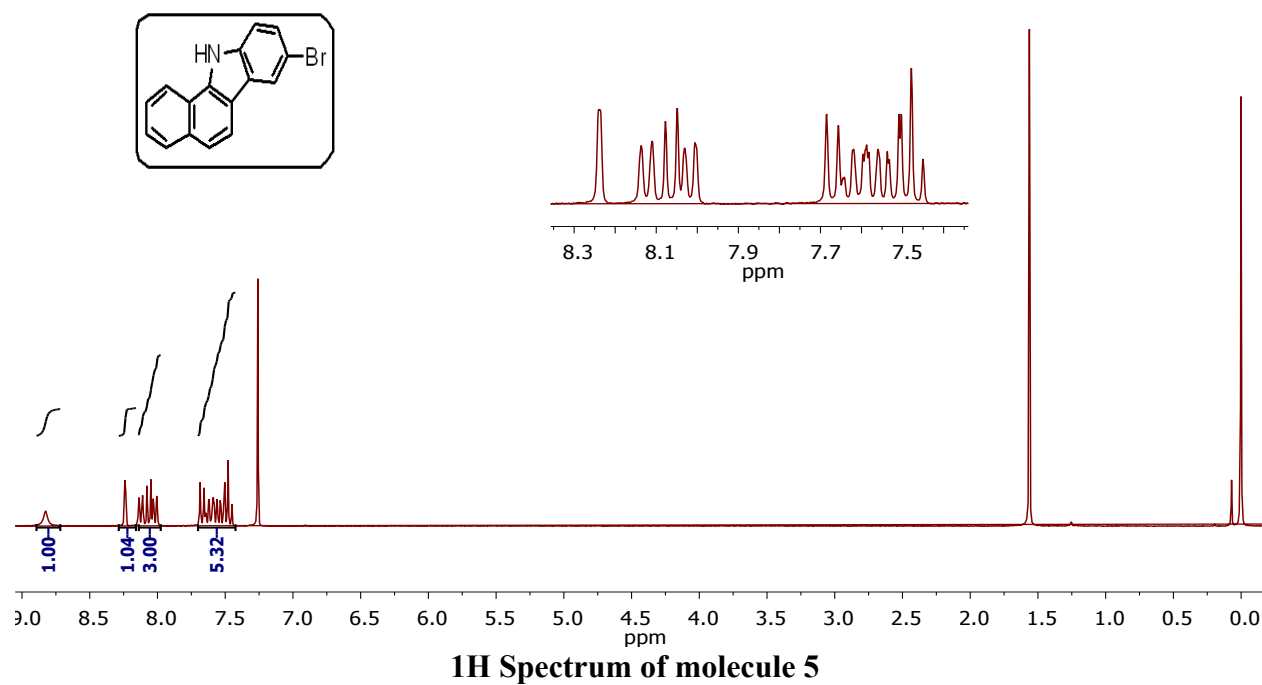


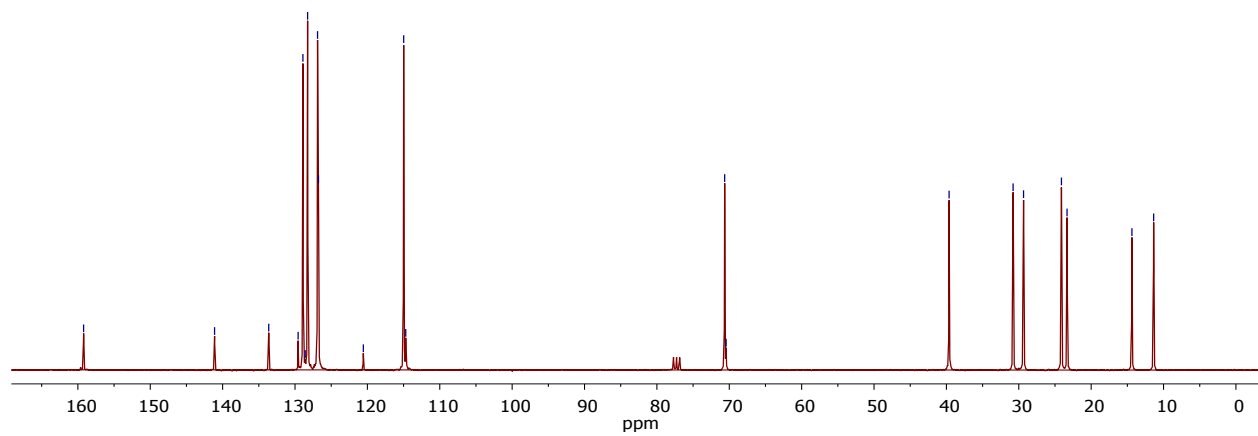
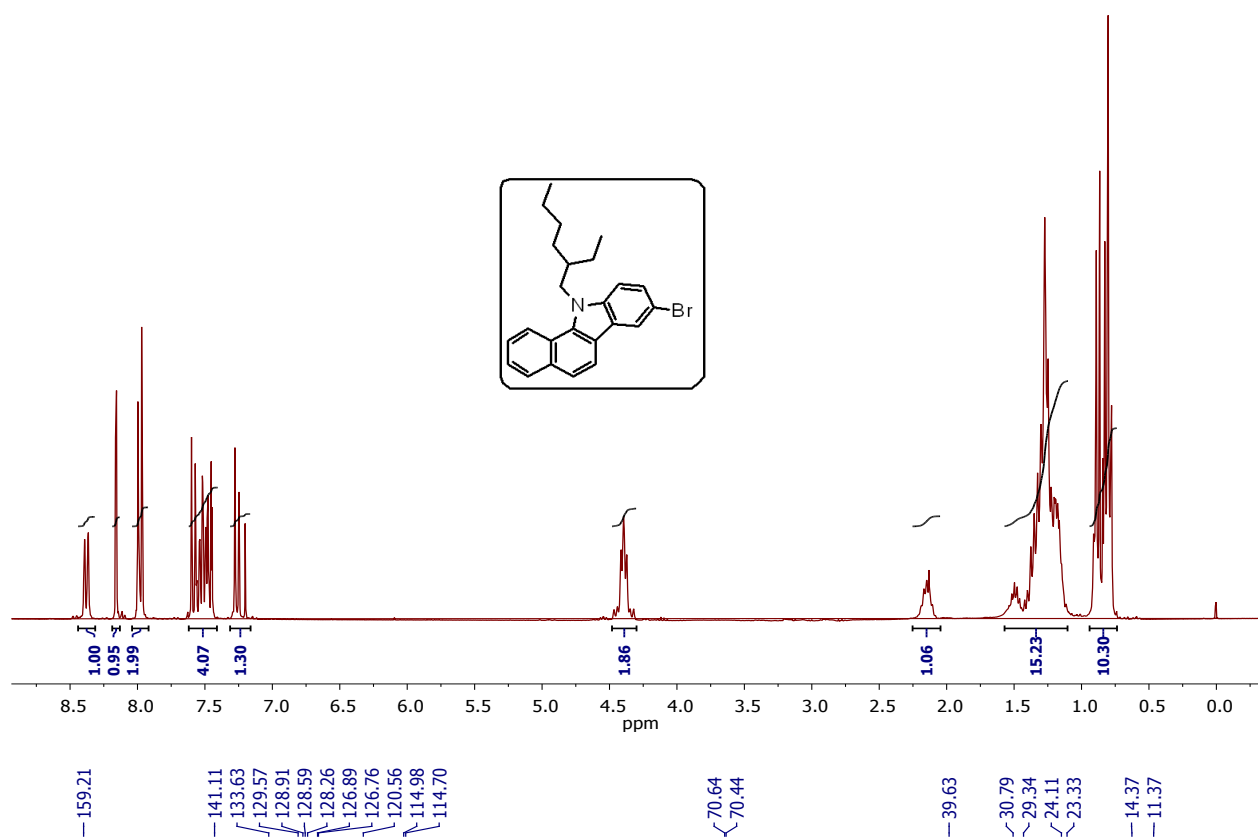
**$^1\text{H}$  spectrum of molecule 4**



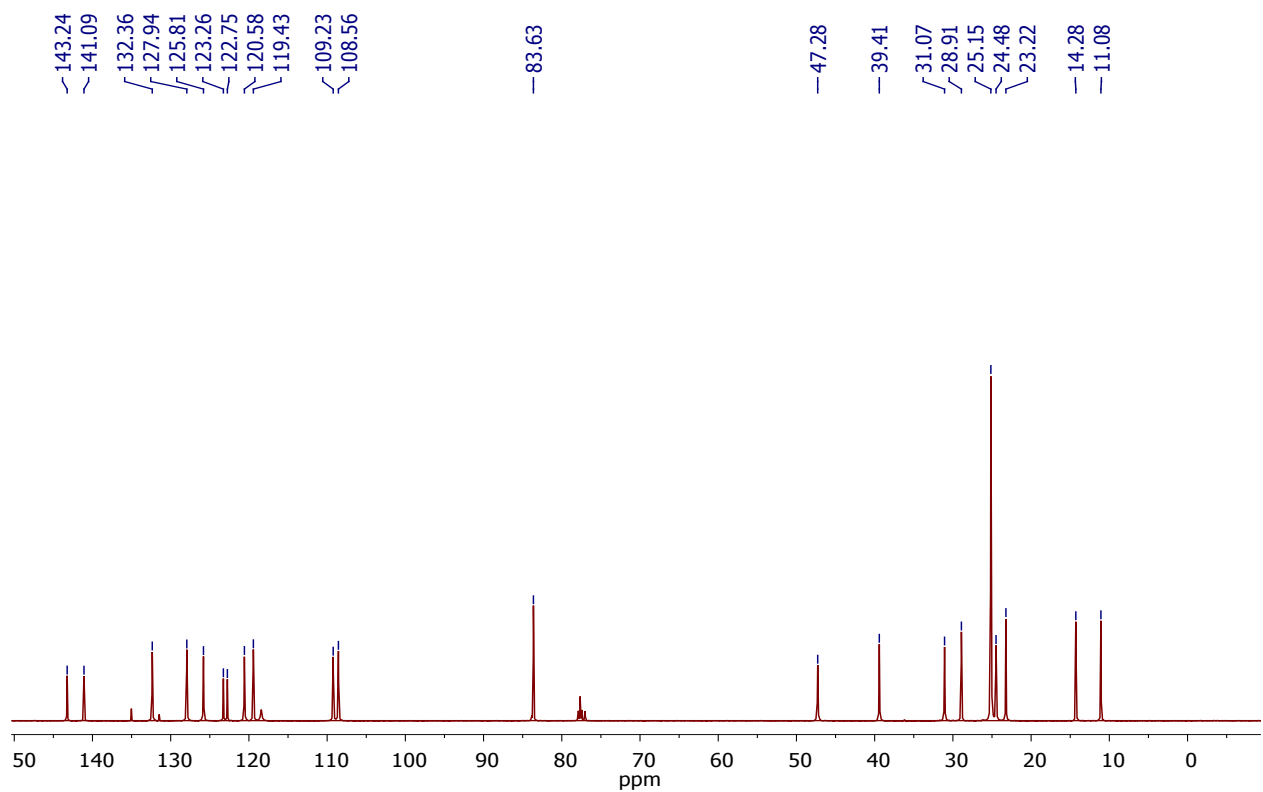
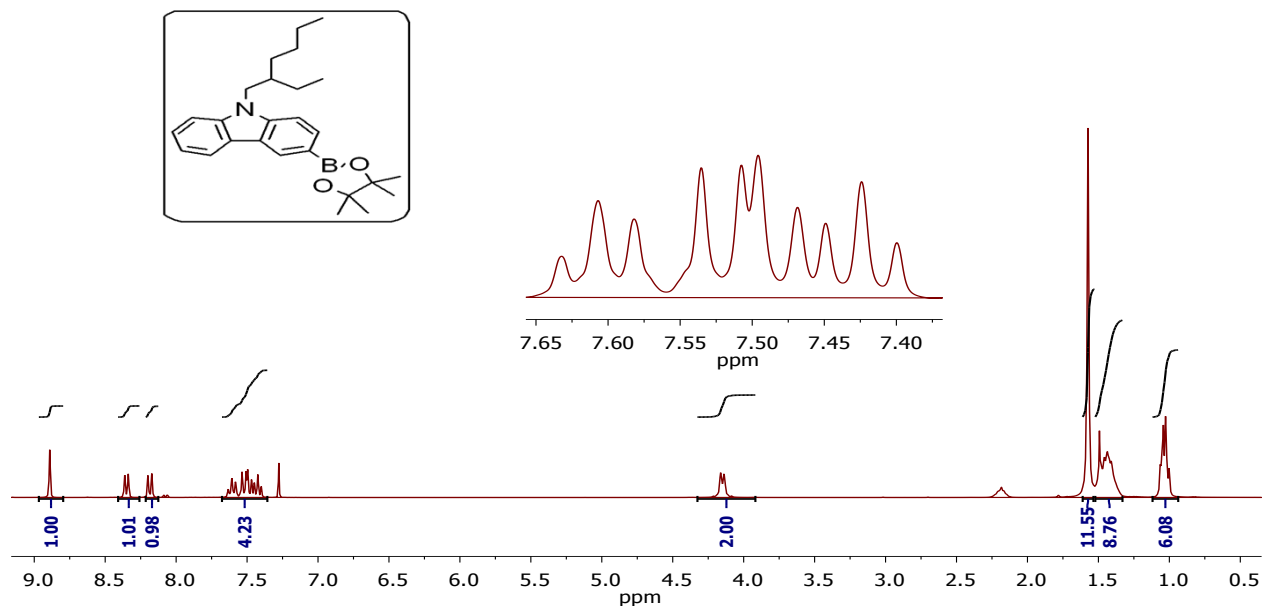
**$^1\text{H}$  Spectrum of 2,7-dibromo-9,9-dibutyl-9H-fluorene**



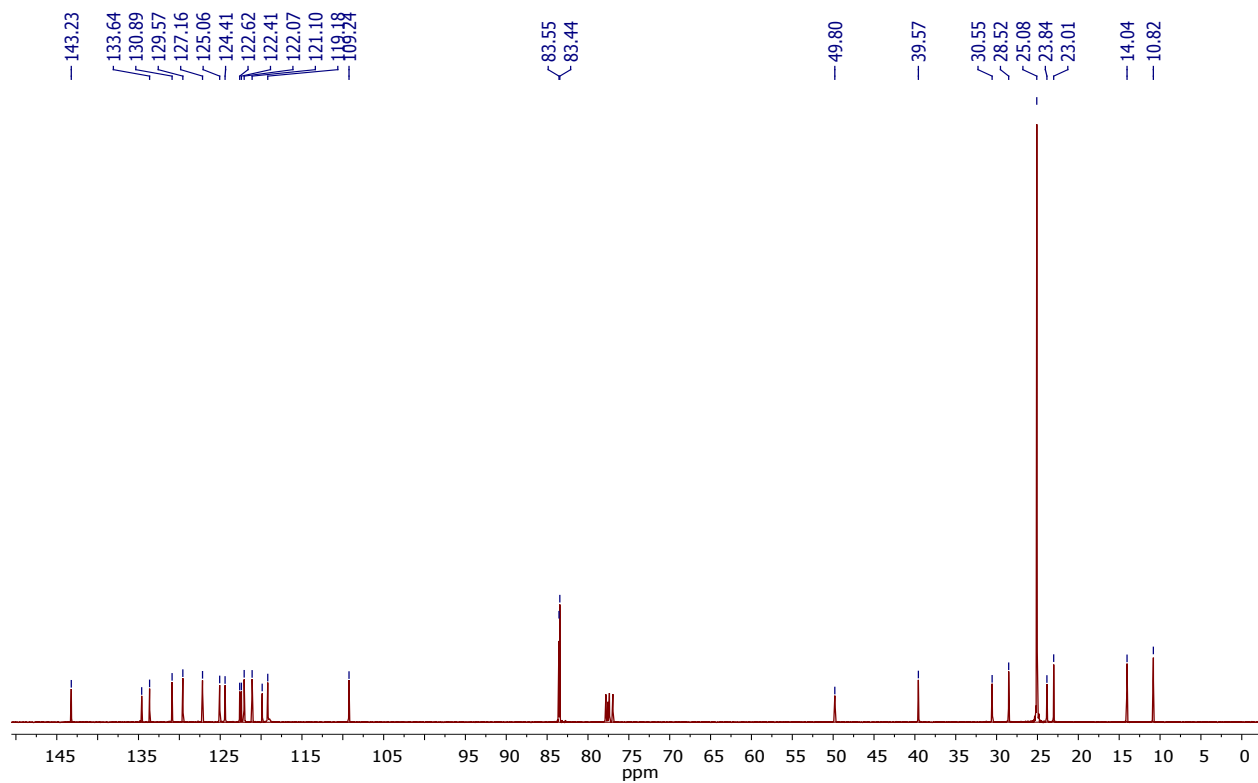
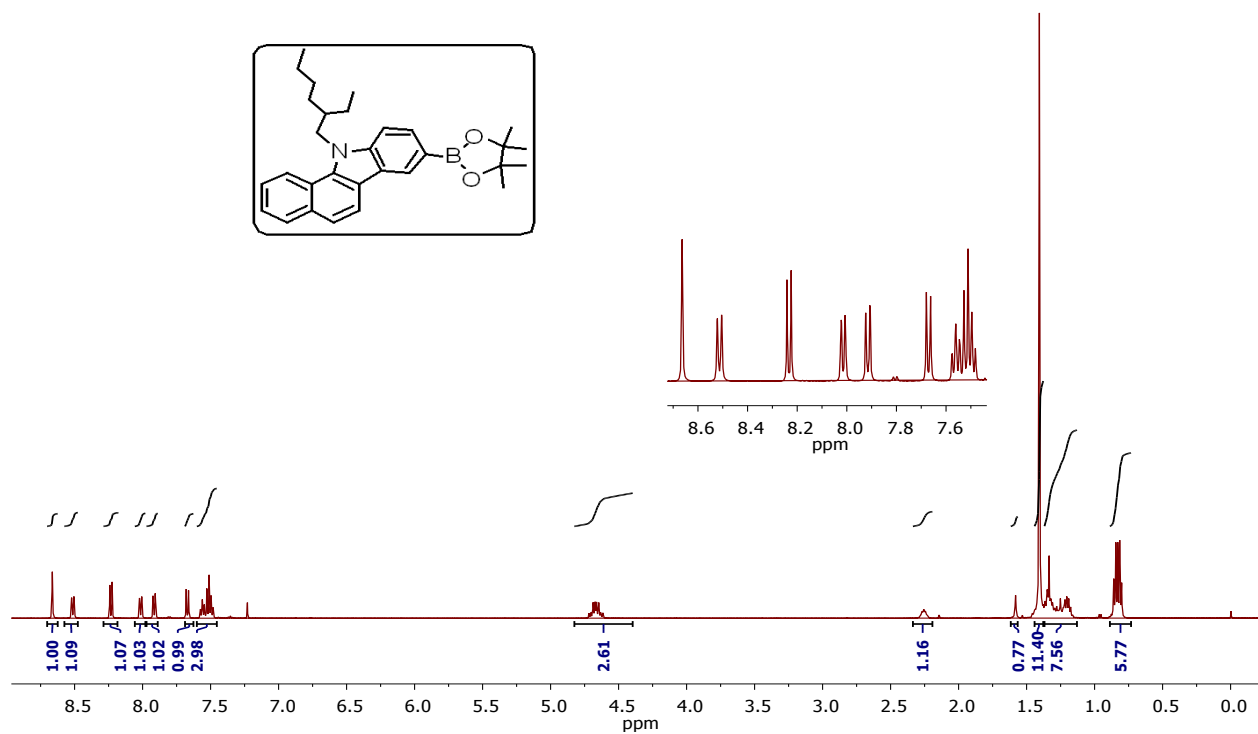
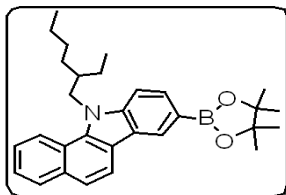




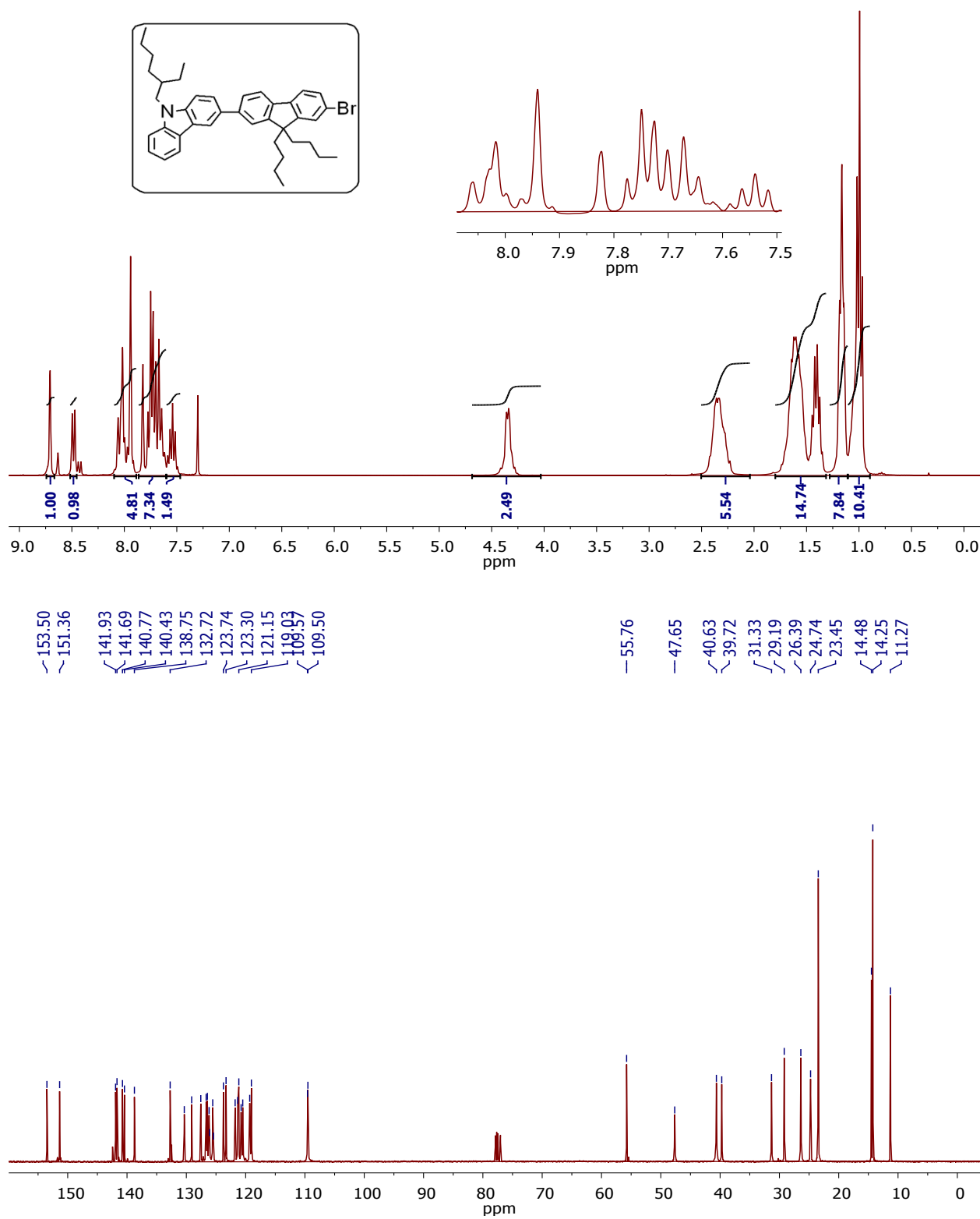
<sup>1</sup>H and <sup>13</sup>C spectra of molecule 6b



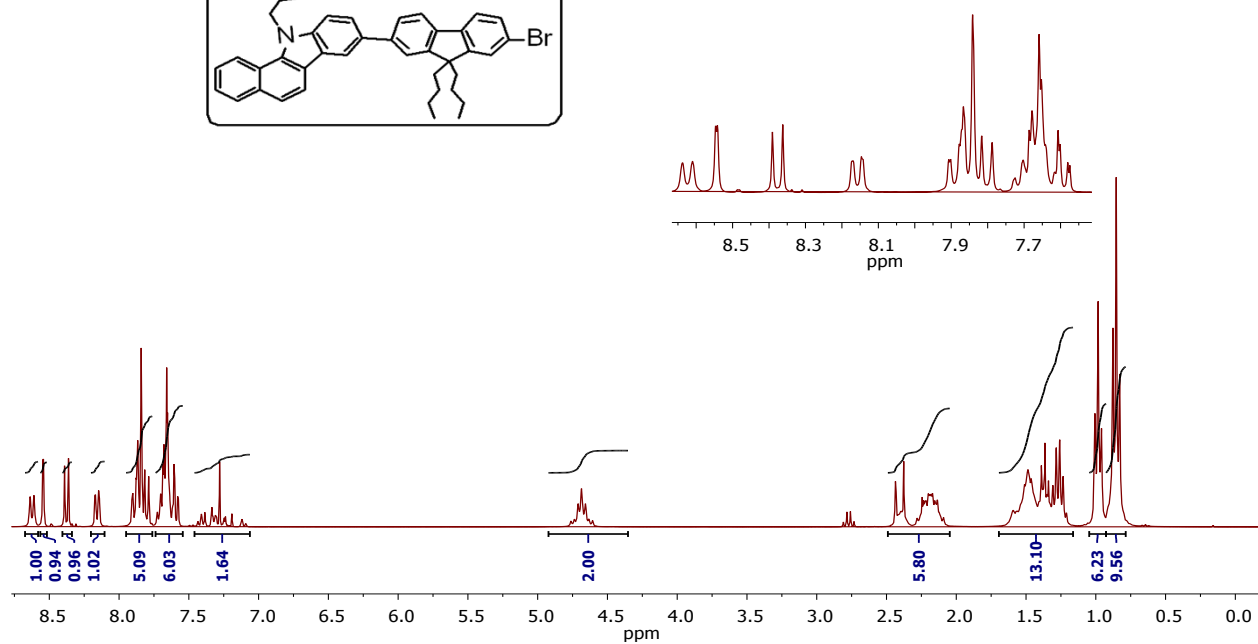
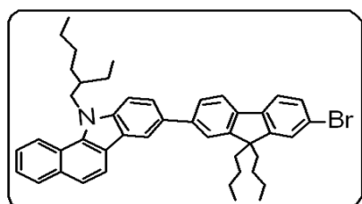
<sup>1</sup>H and <sup>13</sup>C spectra of molecule 7a



<sup>1</sup>H and <sup>13</sup>C spectra of molecule 7b

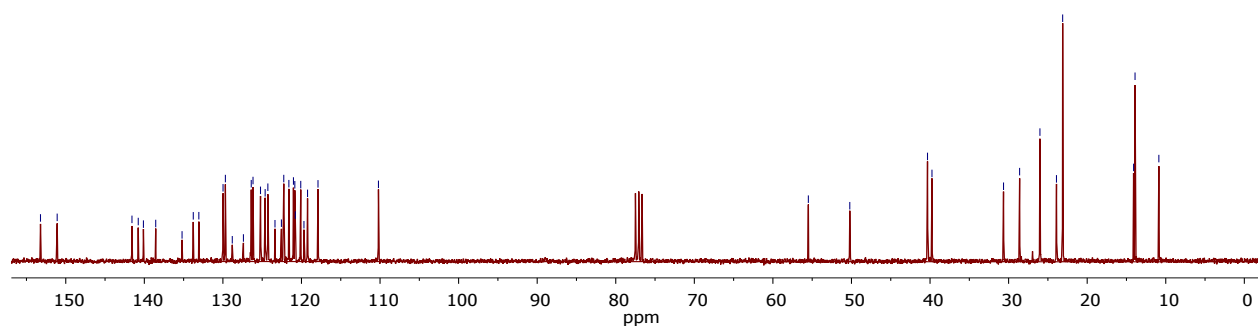
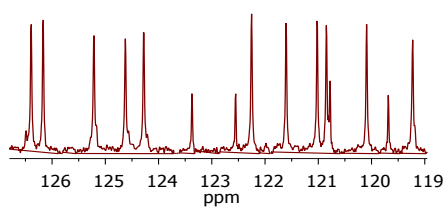


**$^1\text{H}$  and  $^{13}\text{C}$  spectra of molecule 8a**

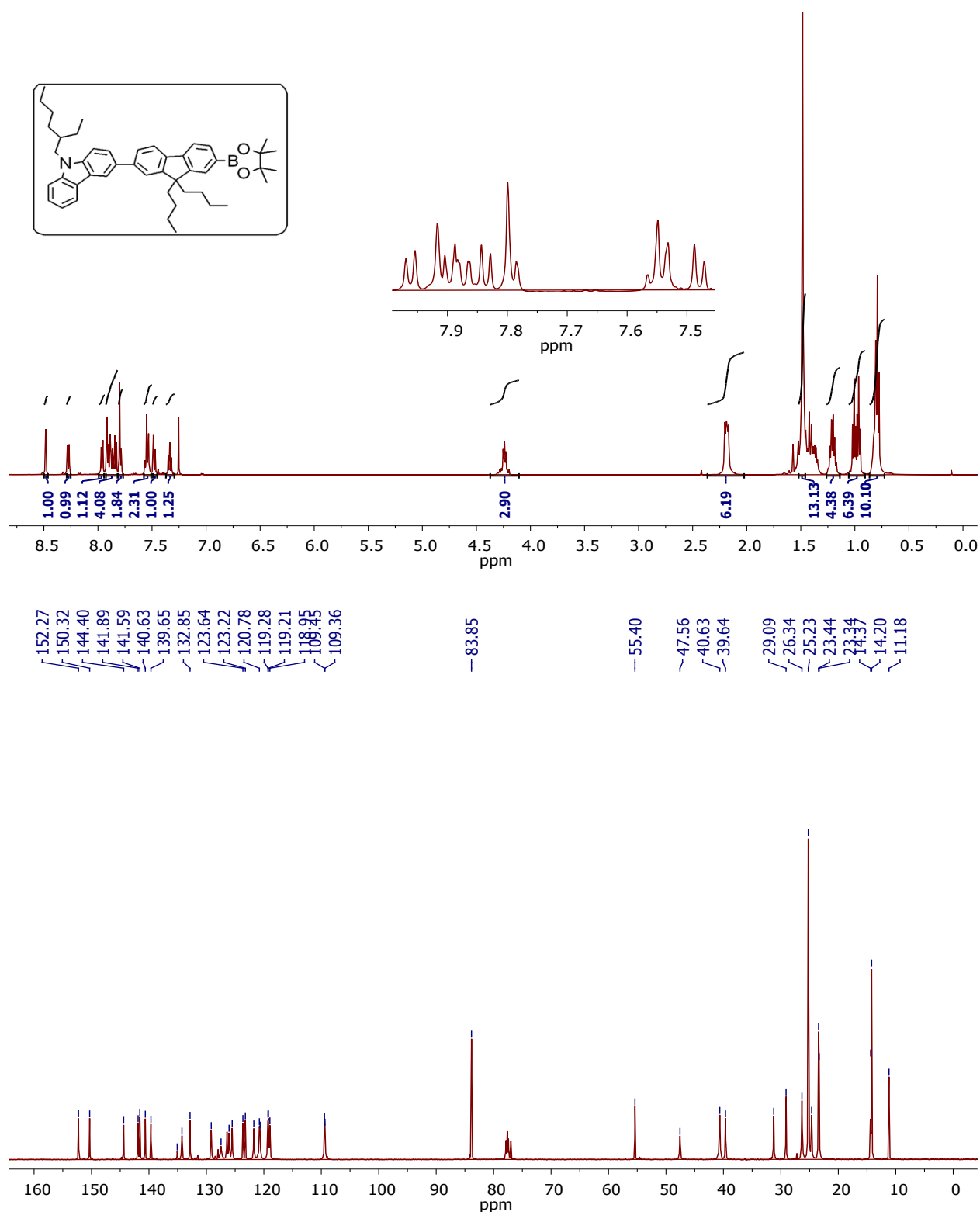


<sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>) of molecule 8b. The x-axis represents chemical shift in ppm, ranging from 117.90 to 153.22. The spectrum shows several sharp peaks in the aromatic region (118-153 ppm) and aliphatic region (14-55 ppm).

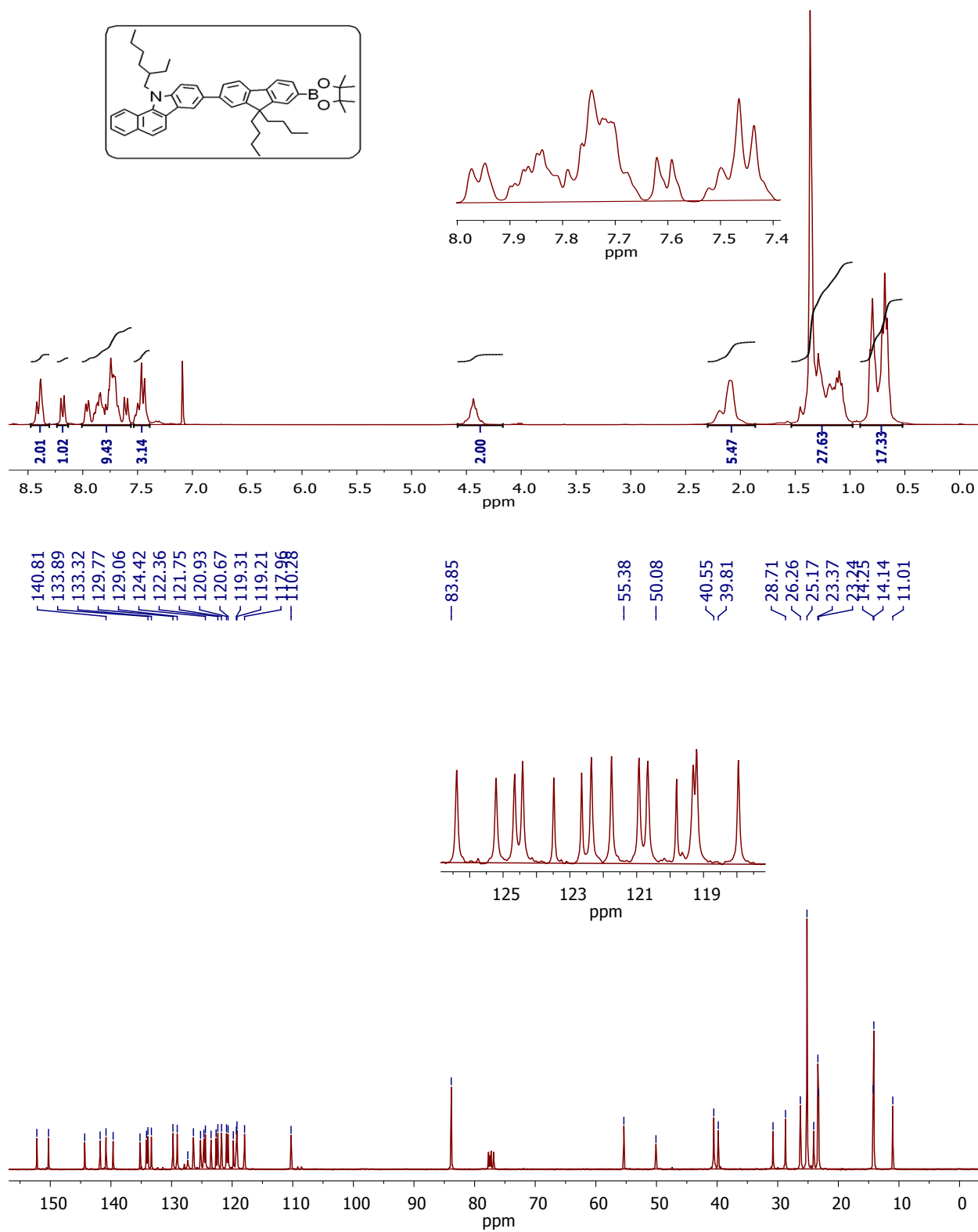
<sup>13</sup>C NMR spectrum (CDCl<sub>3</sub>) of molecule 8b. The x-axis represents chemical shift in ppm, ranging from 10.88 to 55.49. The spectrum shows several sharp peaks in the aliphatic region (14-55 ppm).



**<sup>1</sup>H and <sup>13</sup>C spectra of molecule 8b**

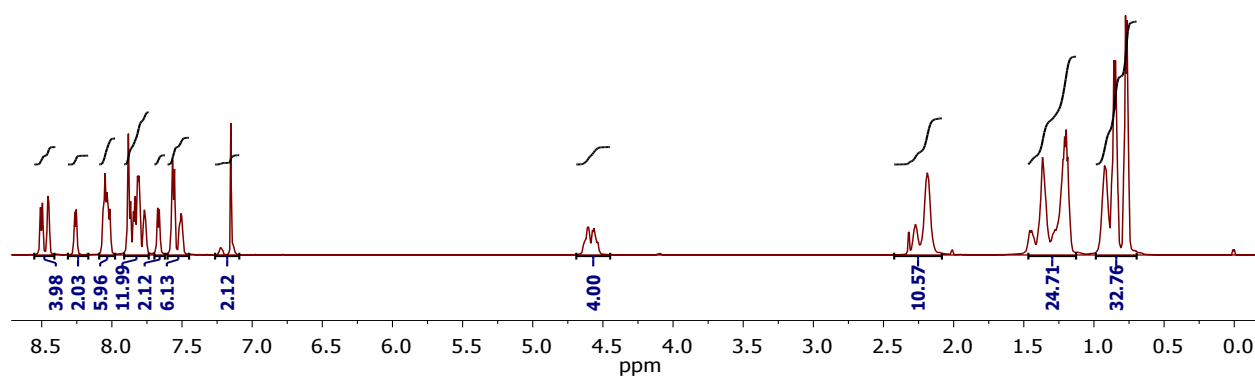
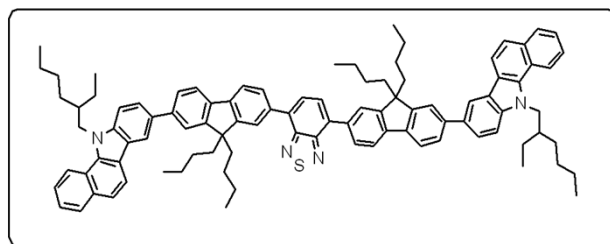


<sup>1</sup>H and <sup>13</sup>C spectra of molecule 9a



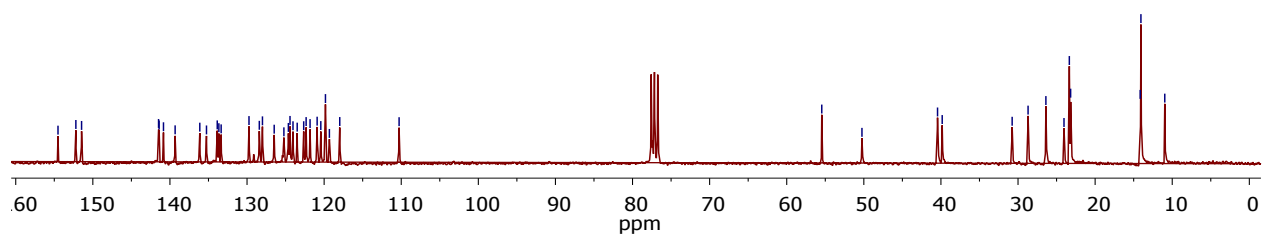
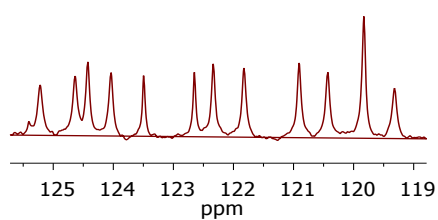
<sup>1</sup>H and <sup>13</sup>C spectra of molecule 9b



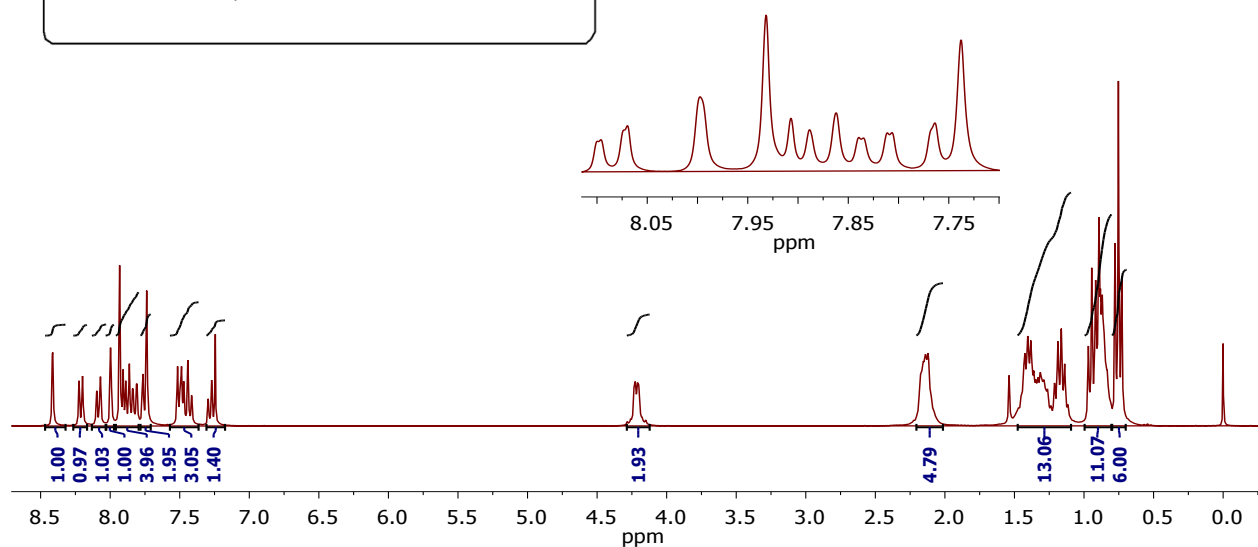
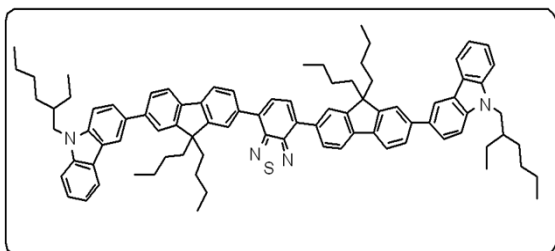


154.52  
152.20  
151.46  
141.48  
133.86  
129.75  
128.00  
124.43  
122.34  
121.82  
120.91  
119.83  
117.97  
116.28

55.46  
50.24  
40.44  
39.83  
30.76  
28.70  
26.39  
23.34  
22.18  
14.06  
10.97

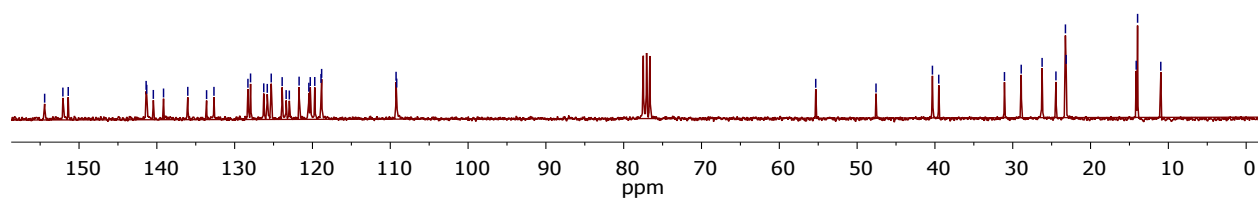
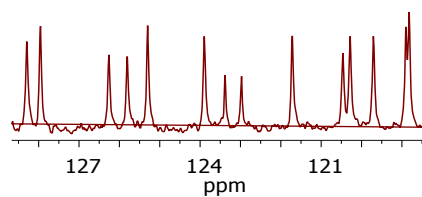


<sup>1</sup>H and <sup>13</sup>C spectra of molecule BFBFB

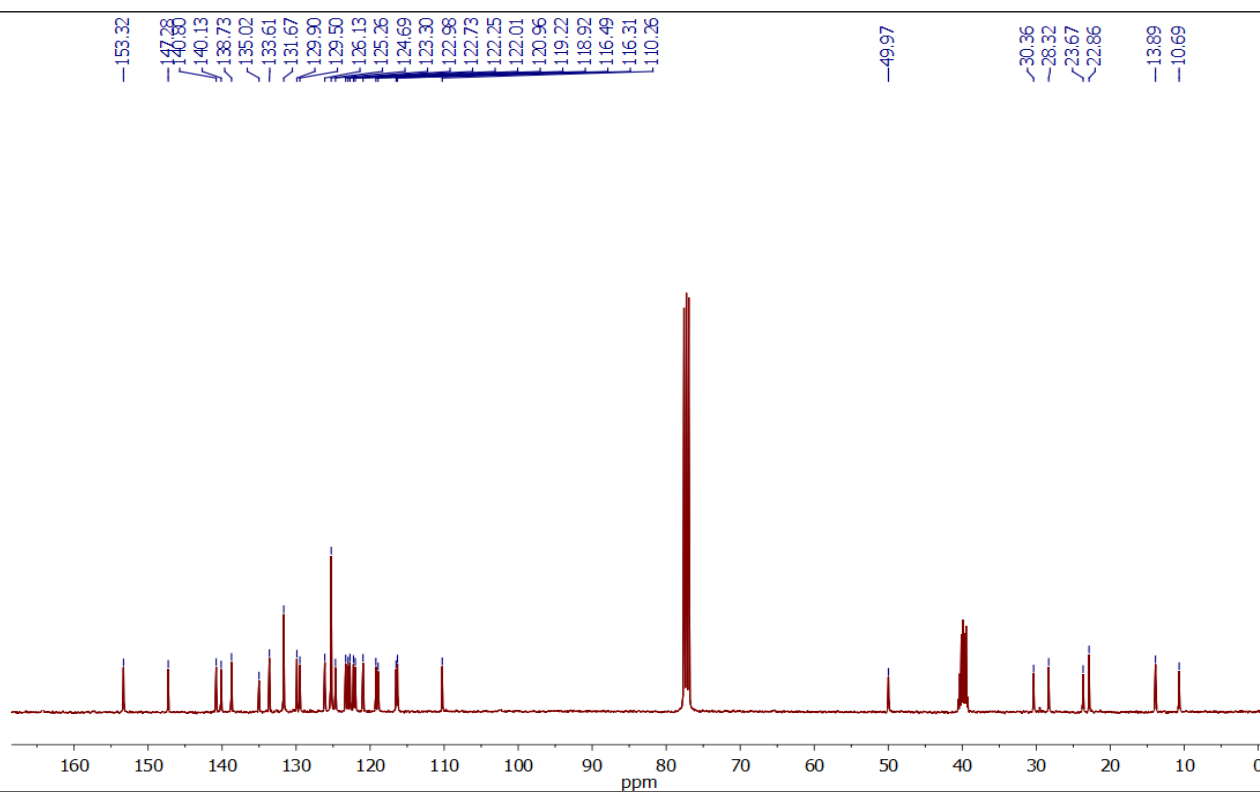
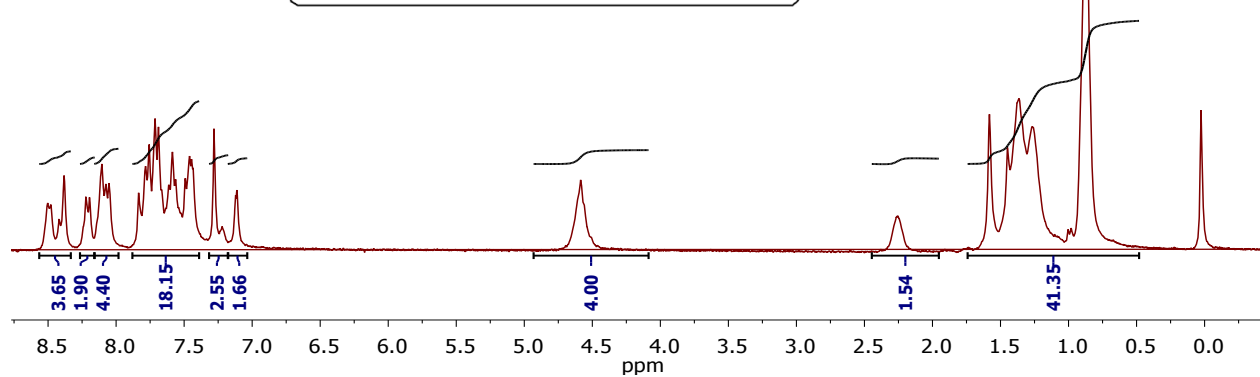
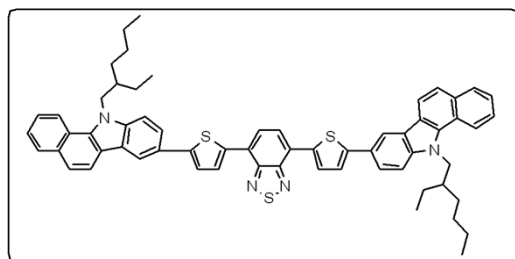


154.42  
152.08  
151.39  
141.38  
128.29  
127.96  
125.30  
123.89  
121.72  
120.28  
119.70  
118.90  
118.82  
109.25  
109.17

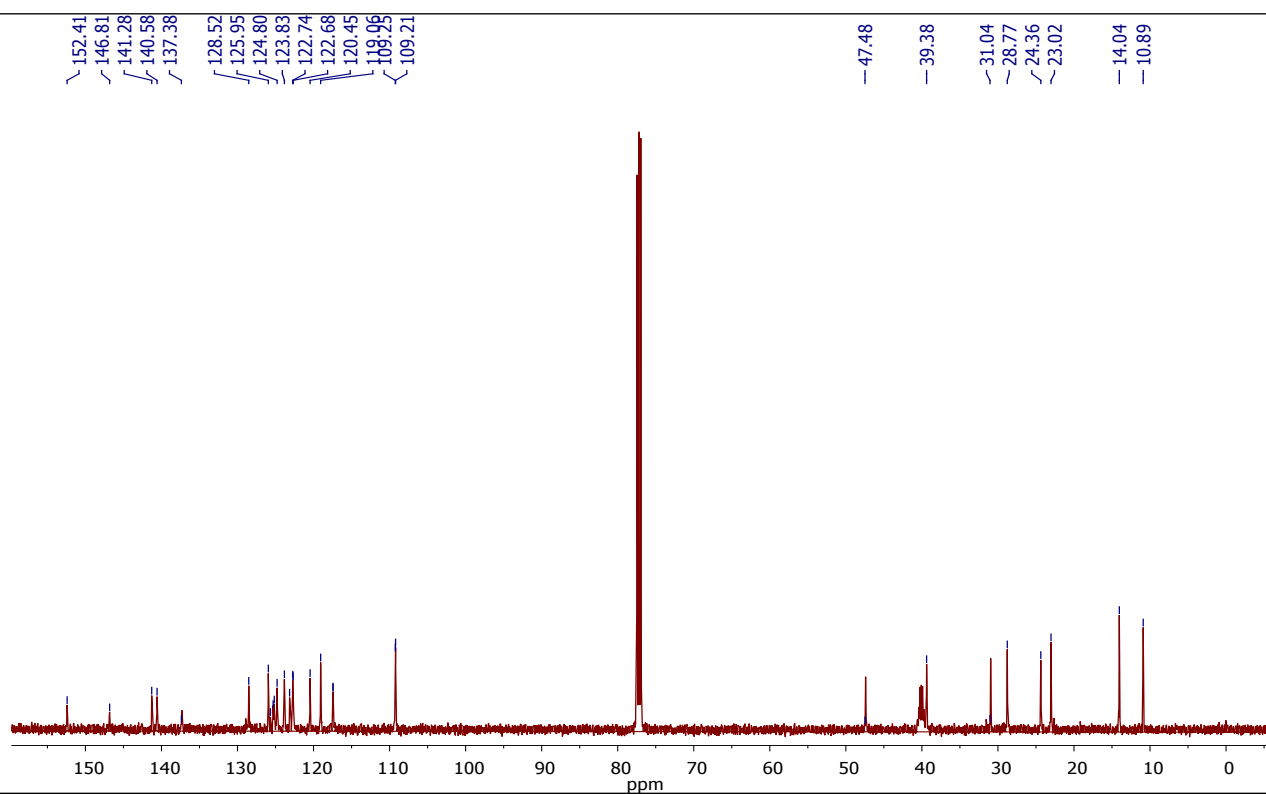
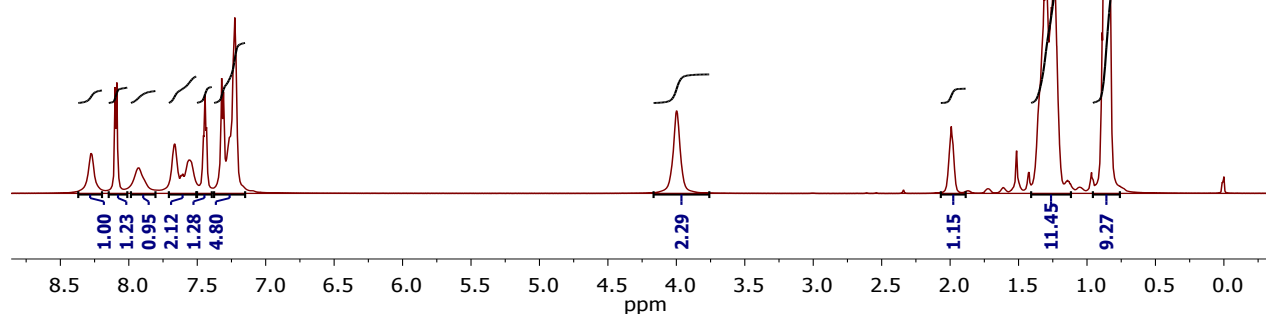
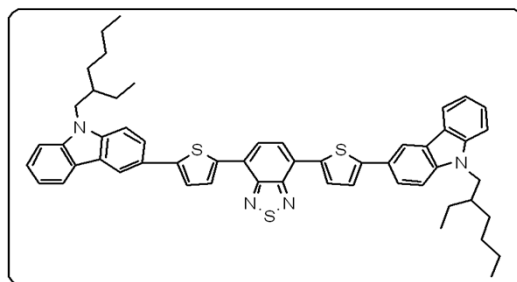
55.32  
47.57  
40.32  
39.51  
28.91  
26.23  
24.45  
23.23  
22.13  
14.13  
13.95  
10.97



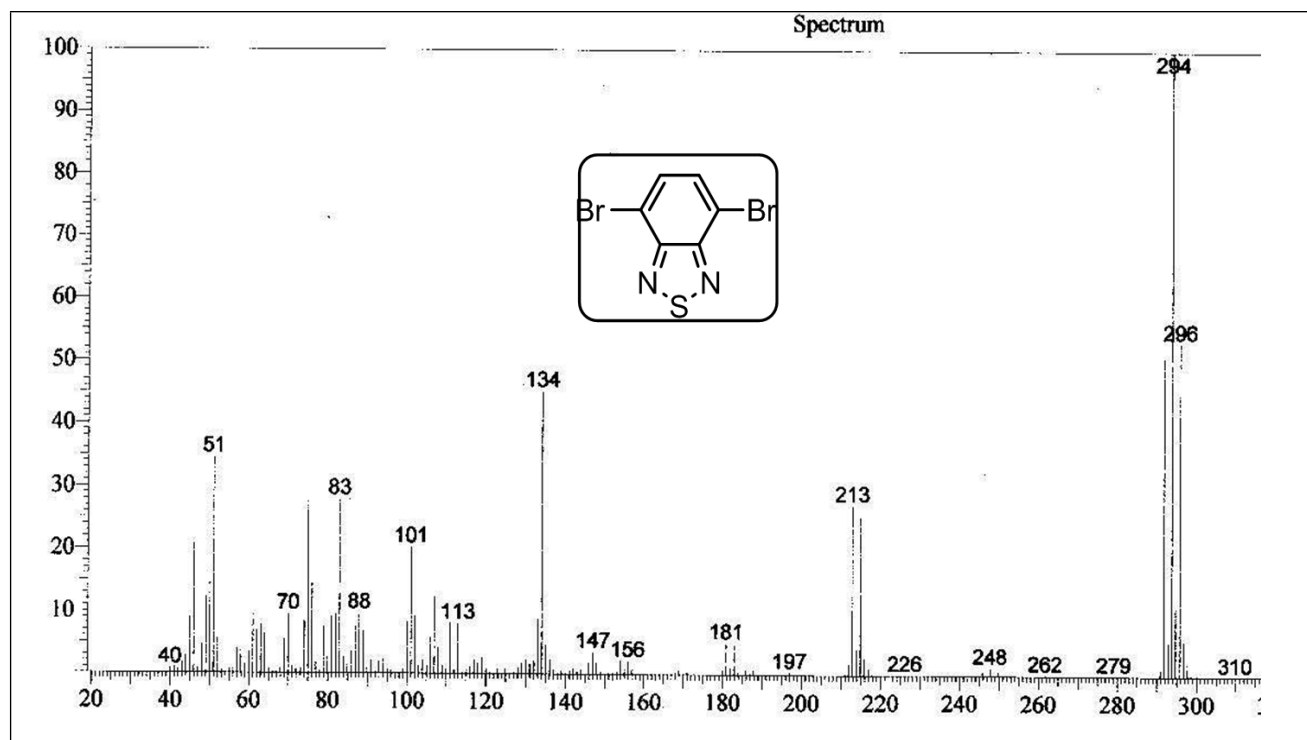
**<sup>1</sup>H and <sup>13</sup>C spectra of molecule CFBFC**



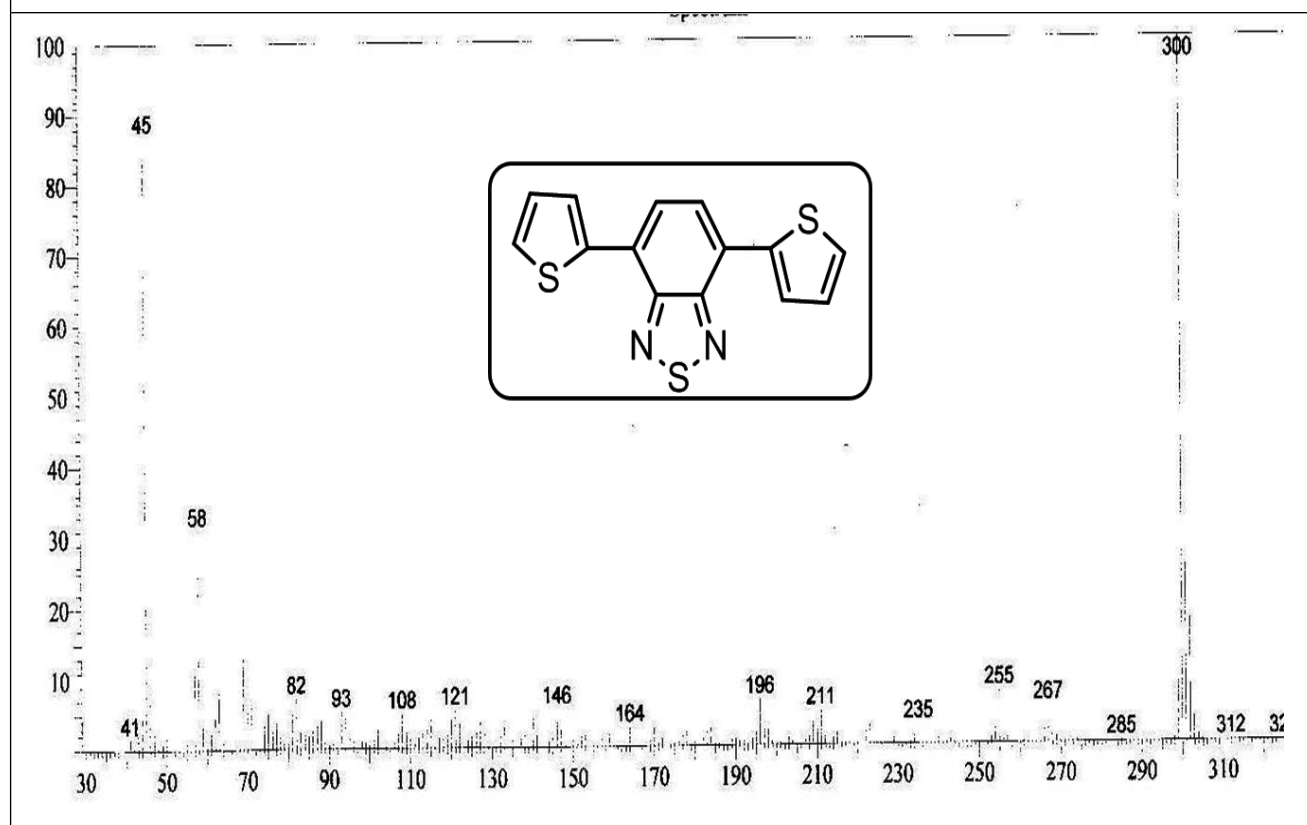
**<sup>1</sup>H and <sup>13</sup>C spectra of molecule BTBTB**



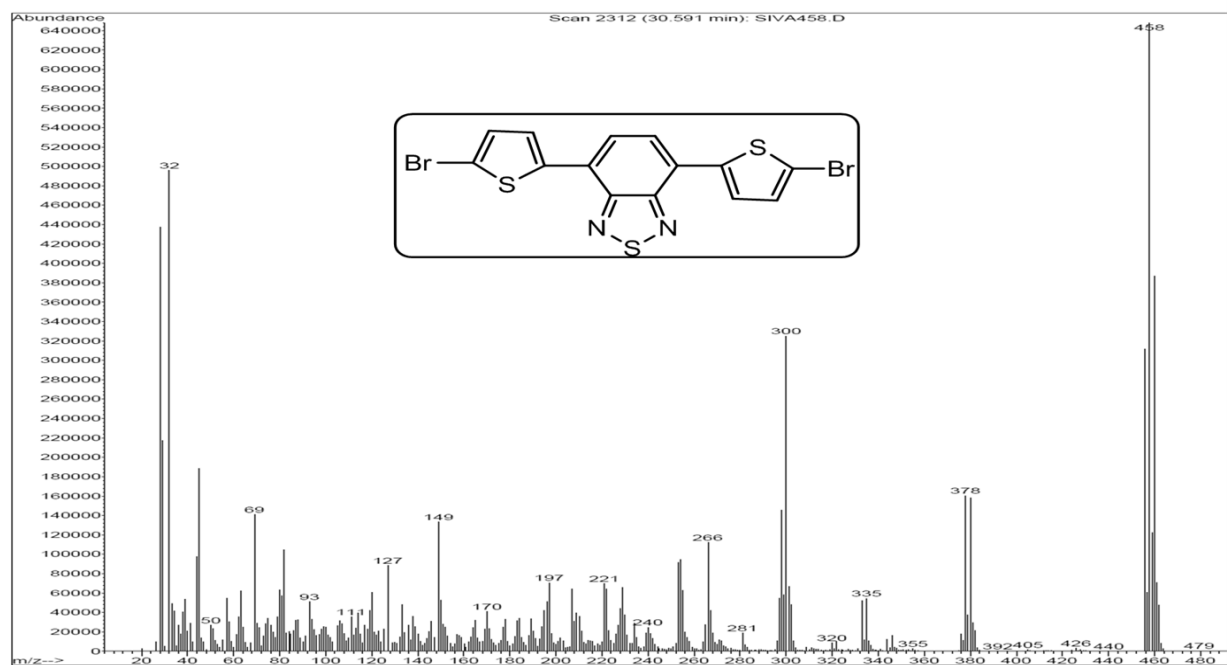
<sup>1</sup>H and <sup>13</sup>C spectra of molecule CTBTC



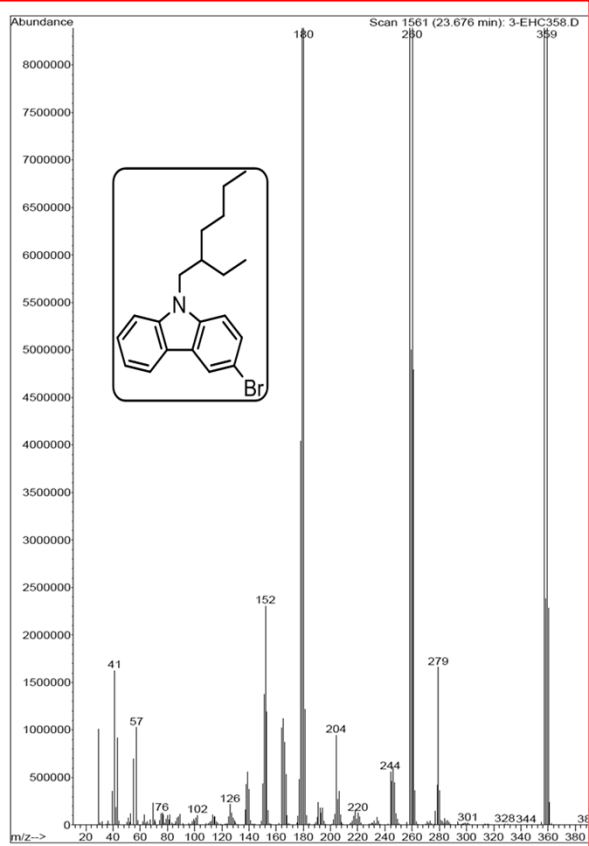
EI-Mass spectrum of molecule 2



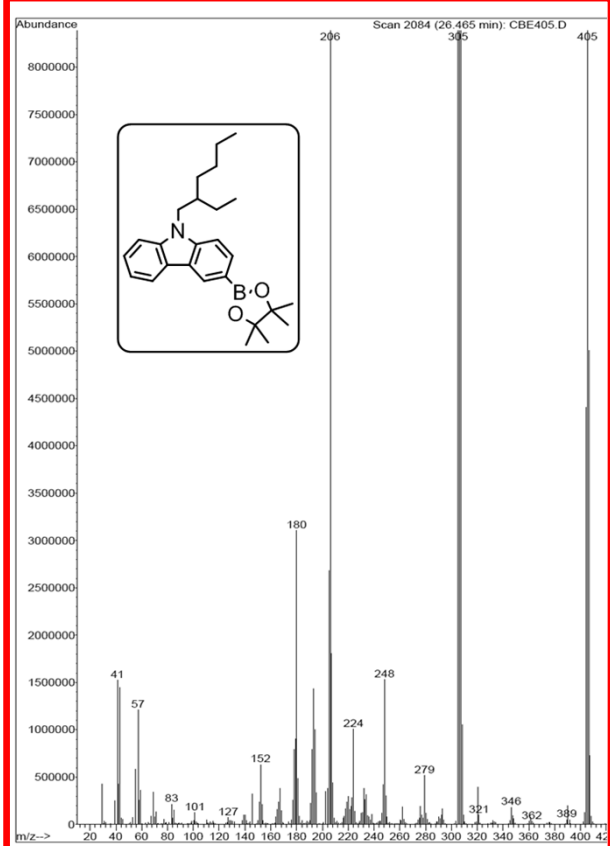
EI-Mass spectrum of molecule 3



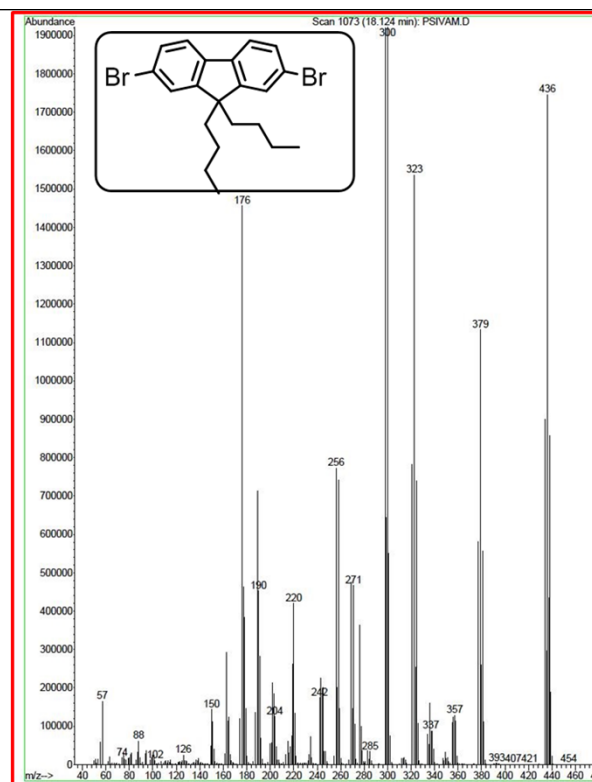
GC-Mass spectrum of molecule 4



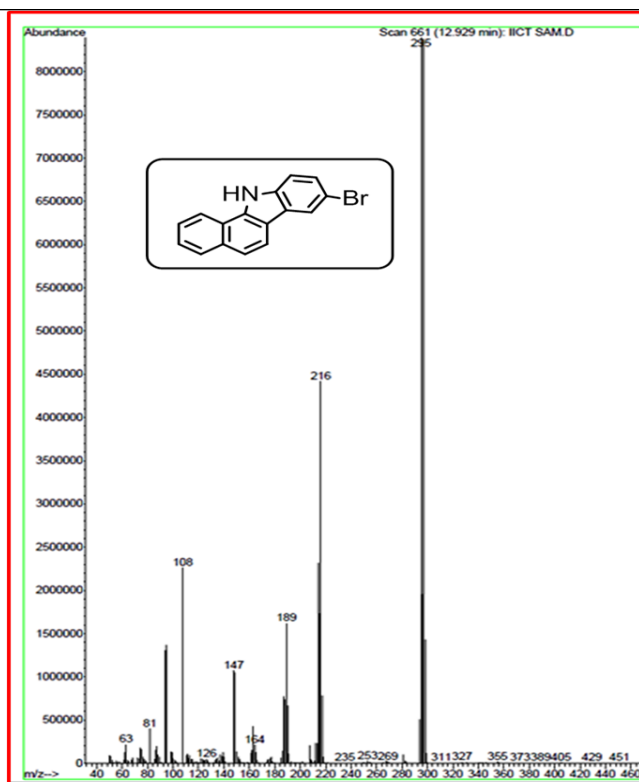
GC-Mass spectrum of molecule 6a



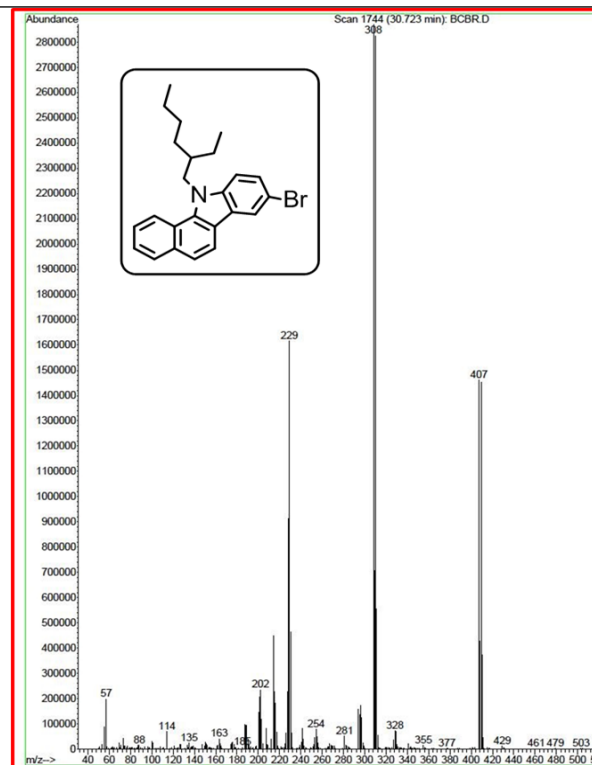
GC-Mass spectrum of molecule 7a



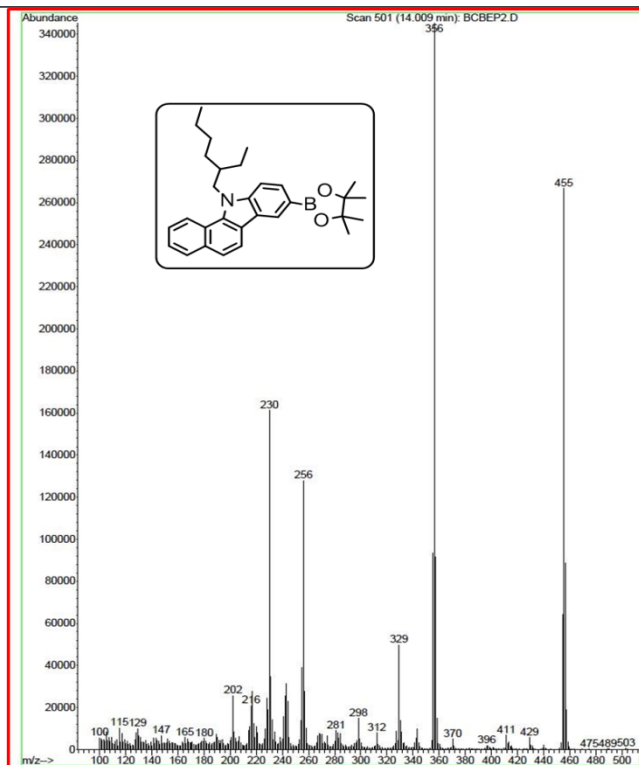
**GC-MS Spectrum of  
2,7-dibromo-9,9-dibutyl-9H-fluorene**



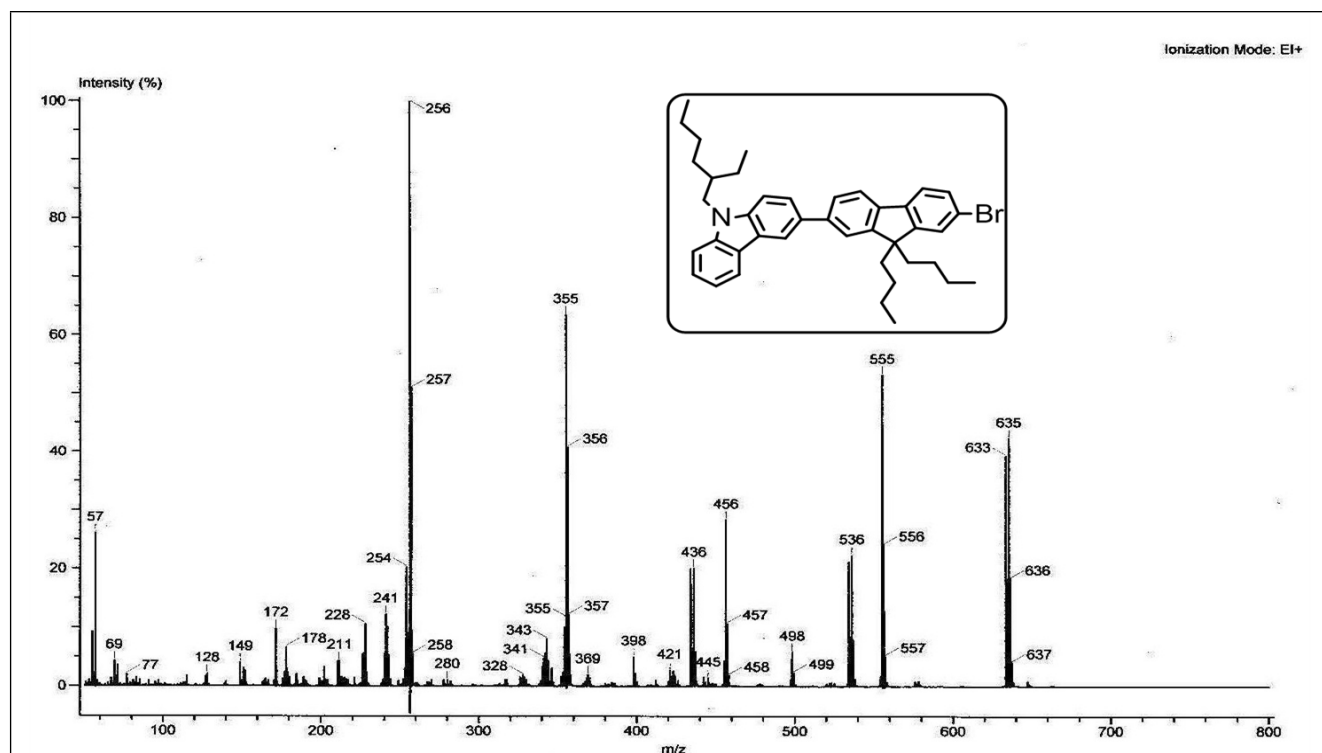
**GC-MS Spectrum of 5**



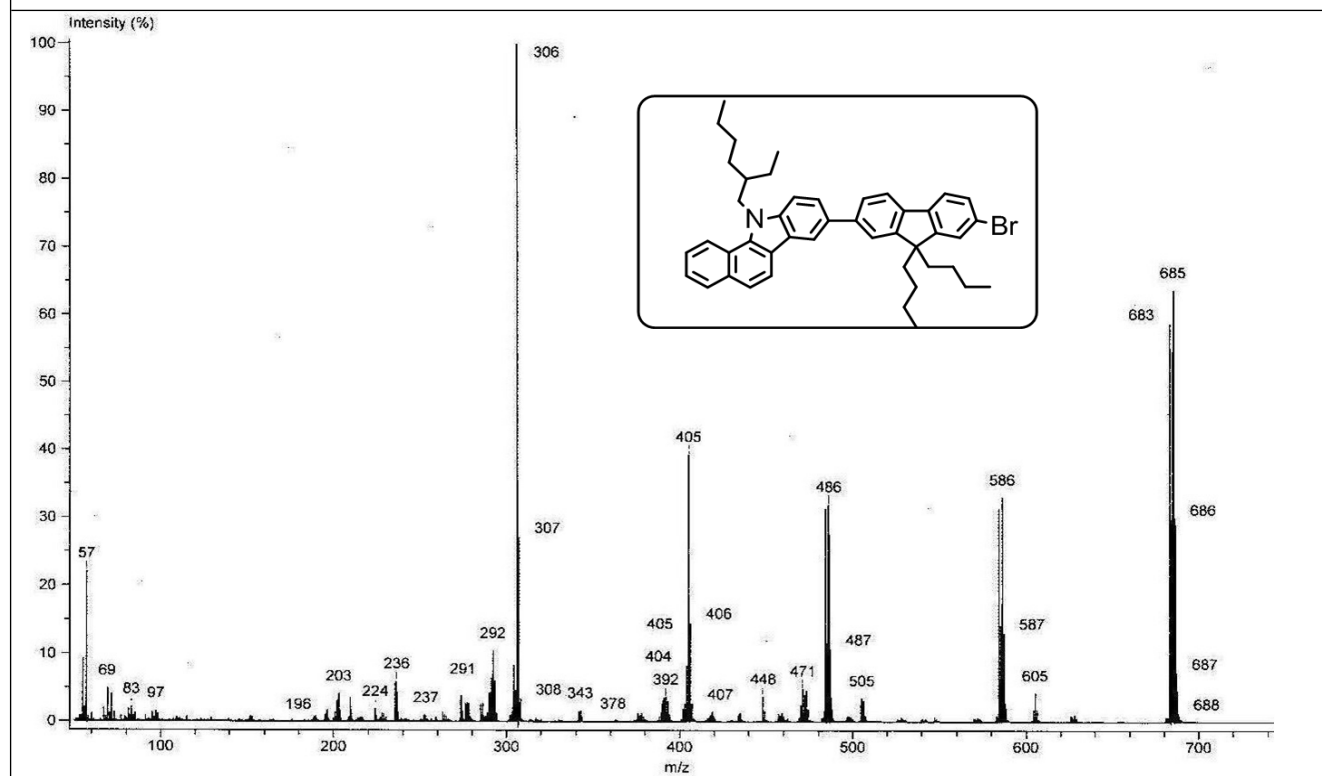
**GC-MS Spectrum of 6b**



**GC-MS Spectrum of 7b**

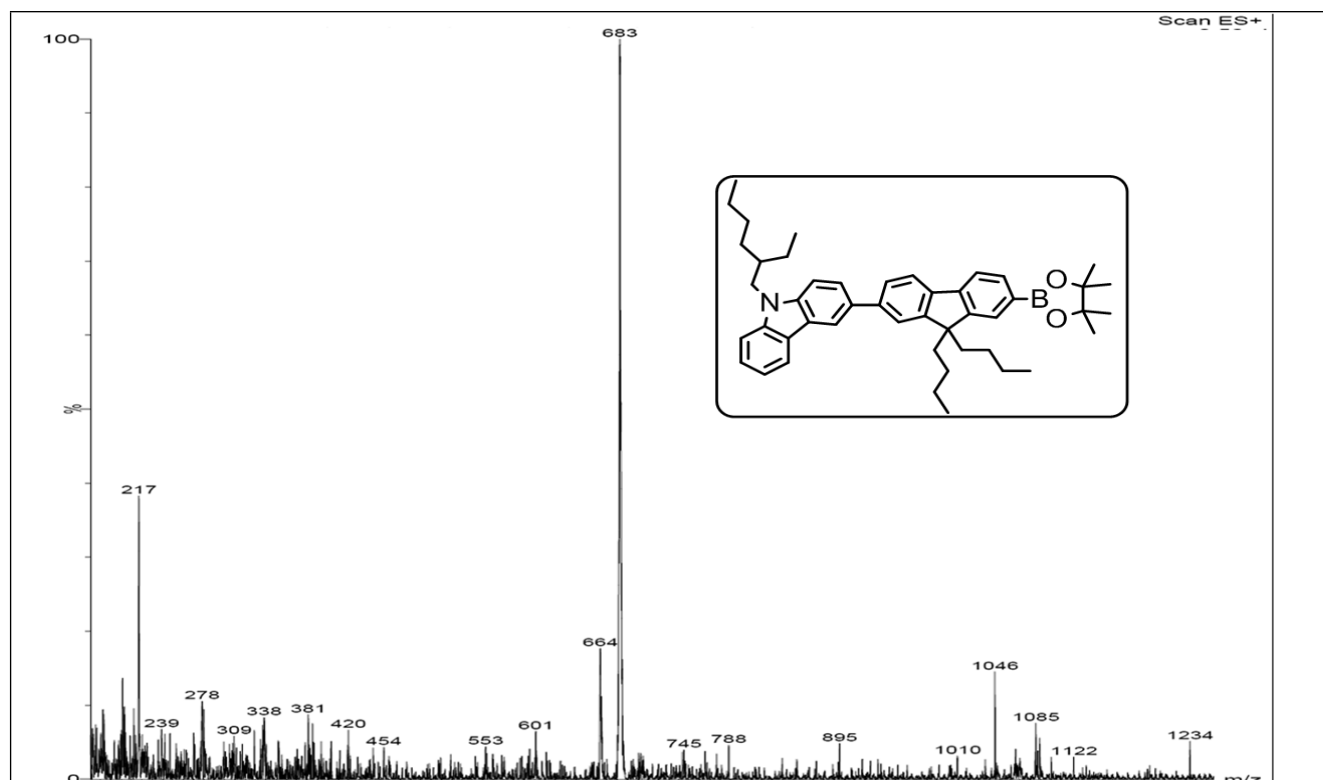


EI-MS spectrum of 8a

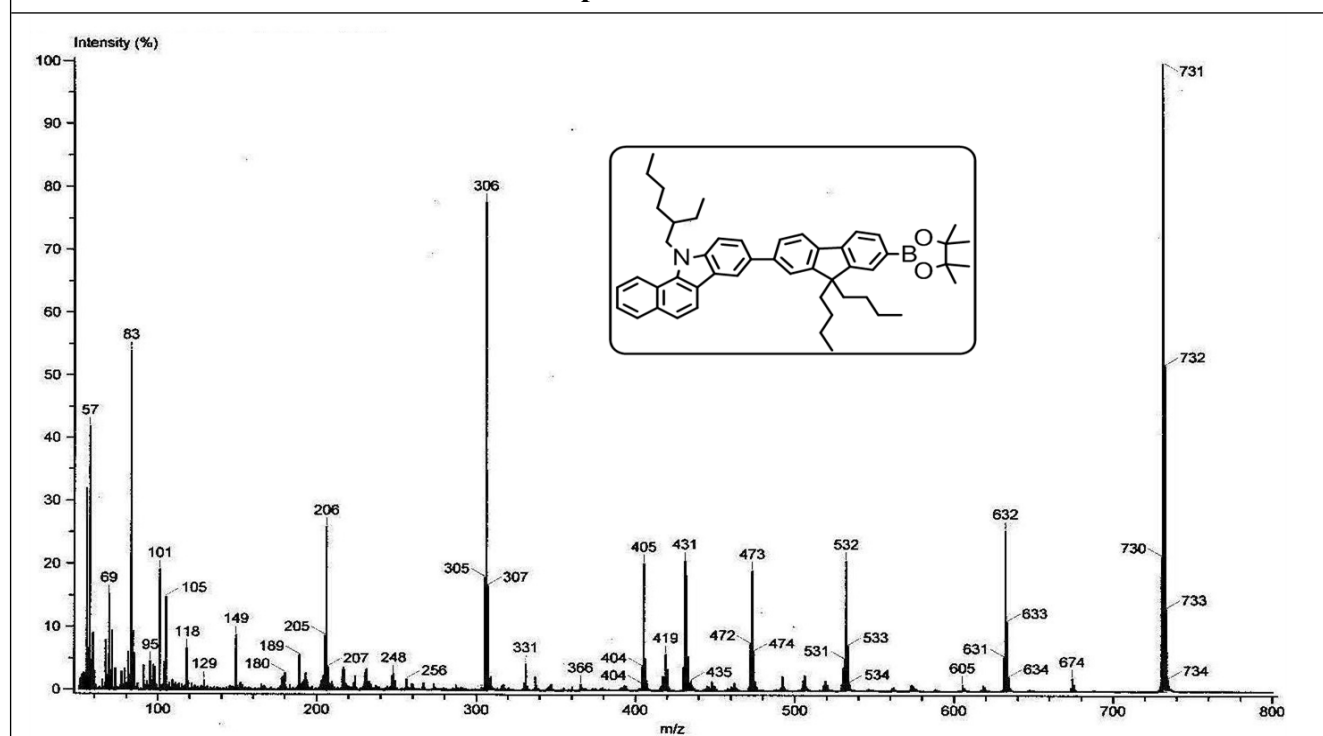


EI-MS spectrum of 8b

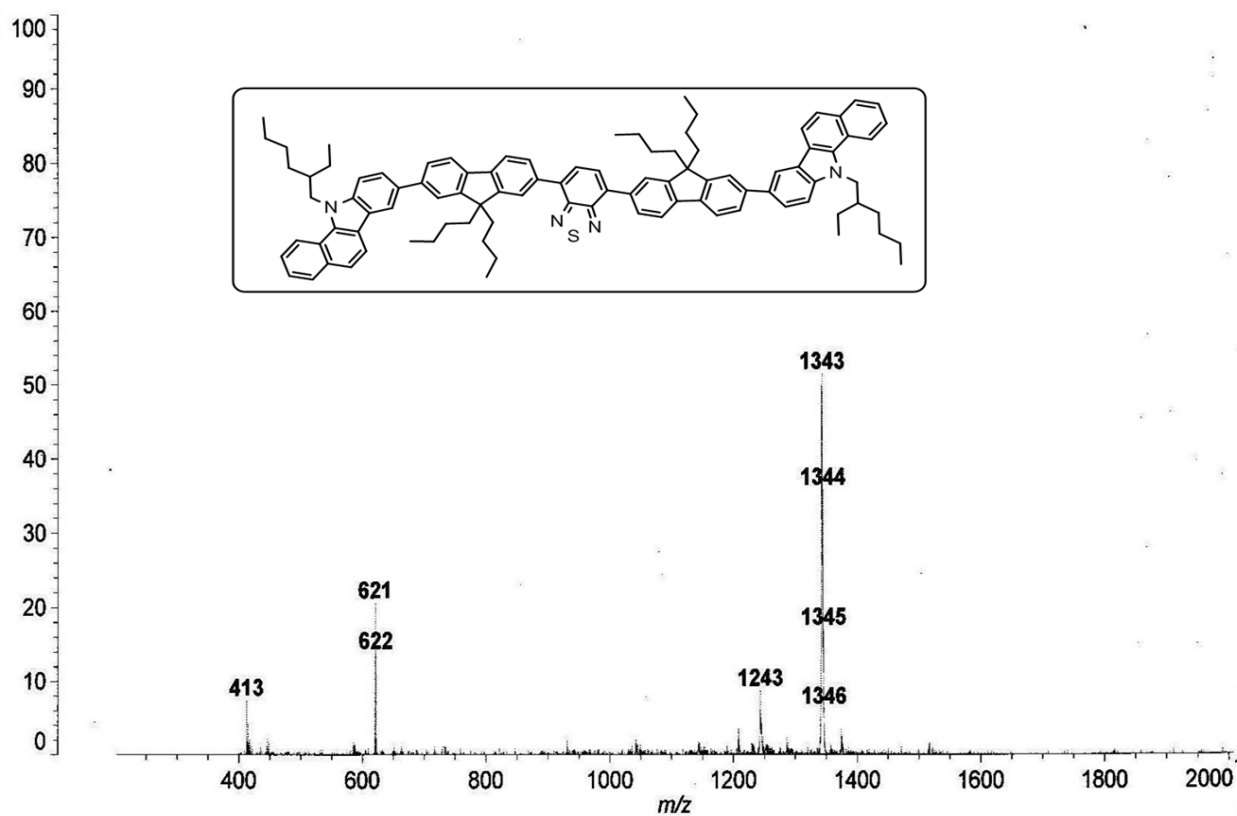




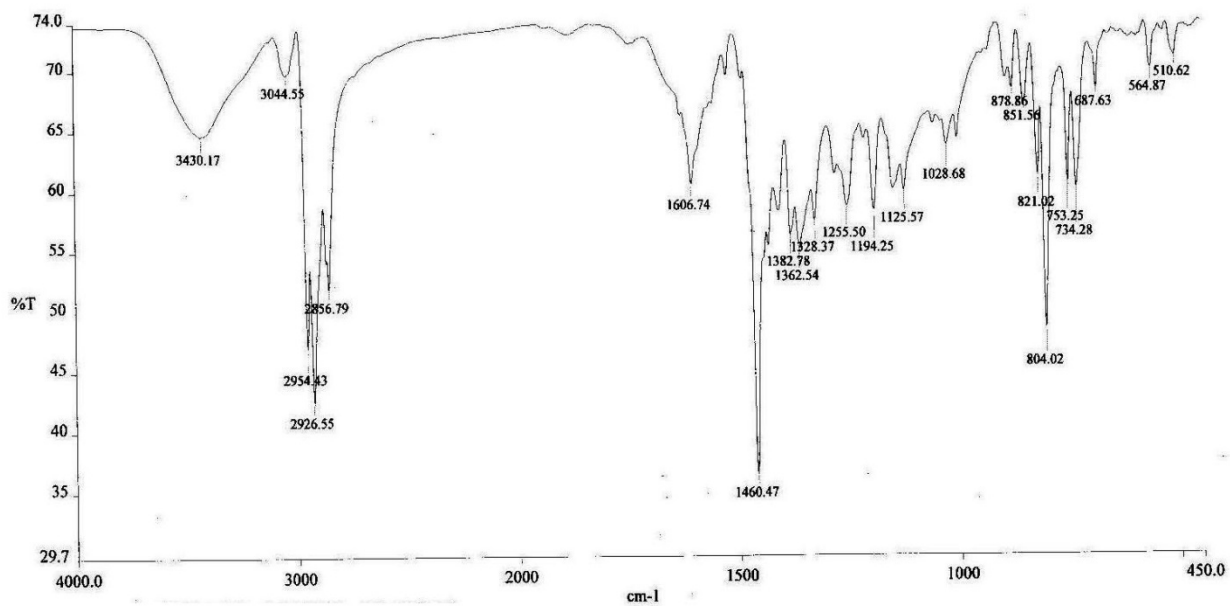
EI-Mass spectrum of molecule 9a



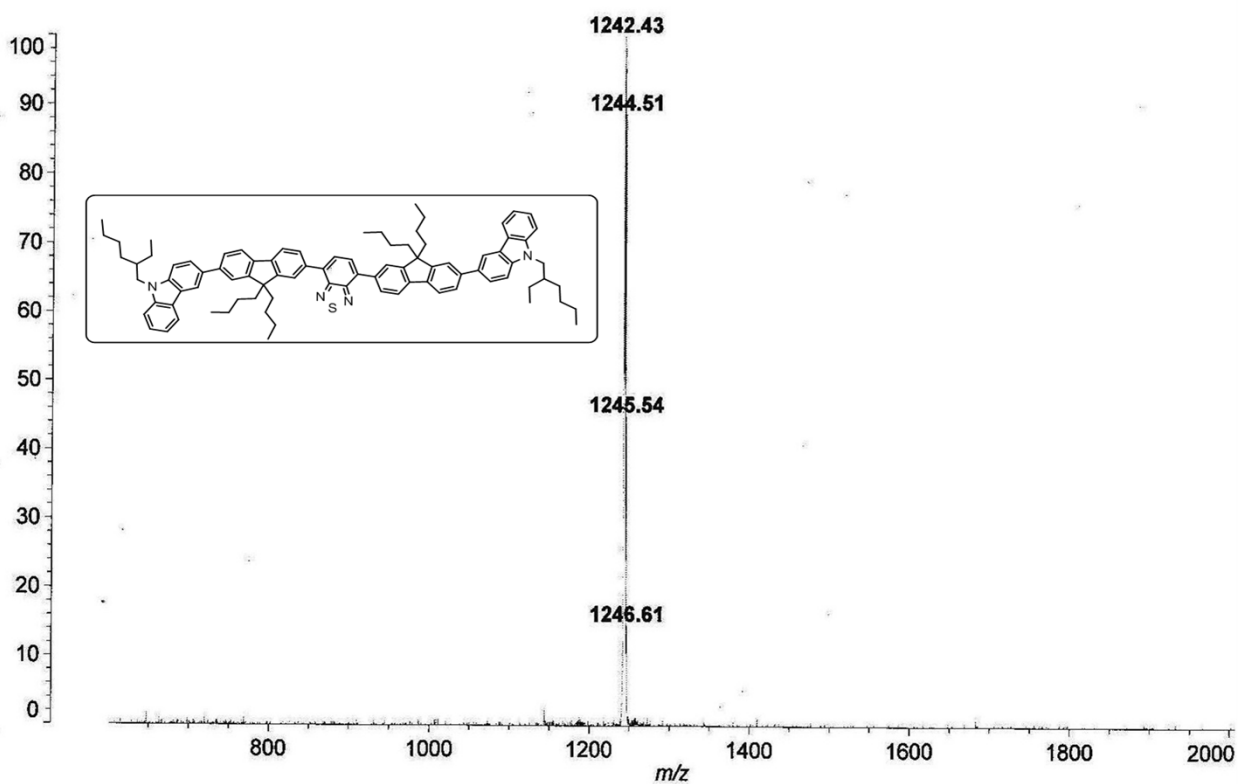
EI-Mass spectrum of molecule 9b



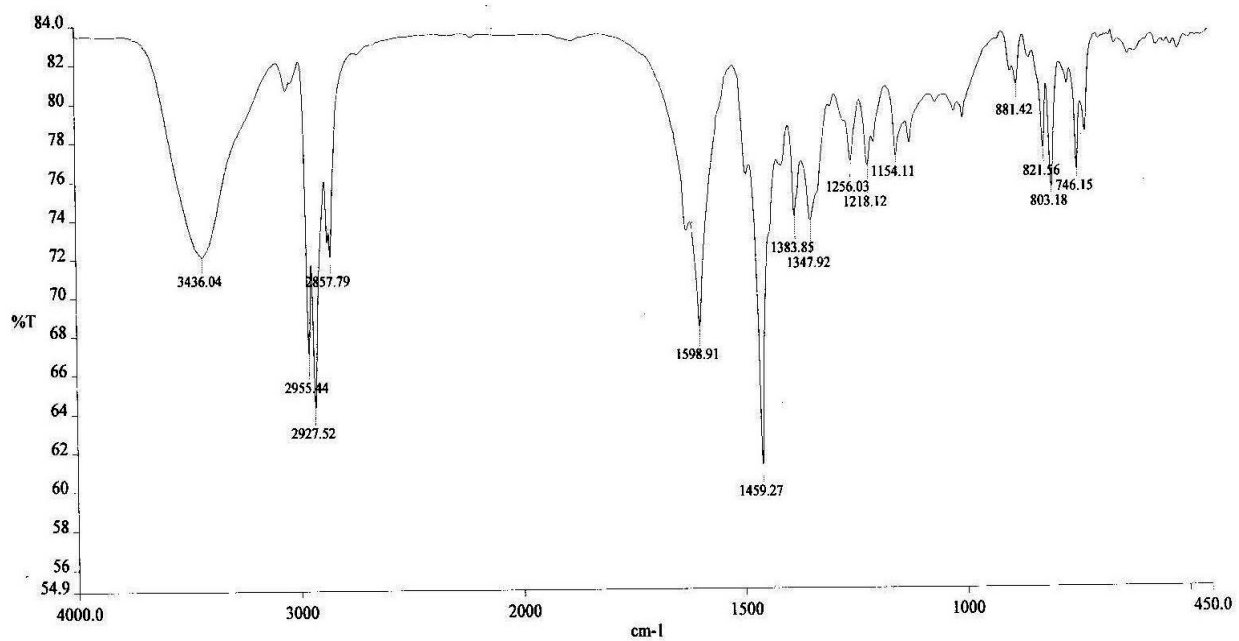
**MALDI-TOF mass Spectrum of BFBFB**



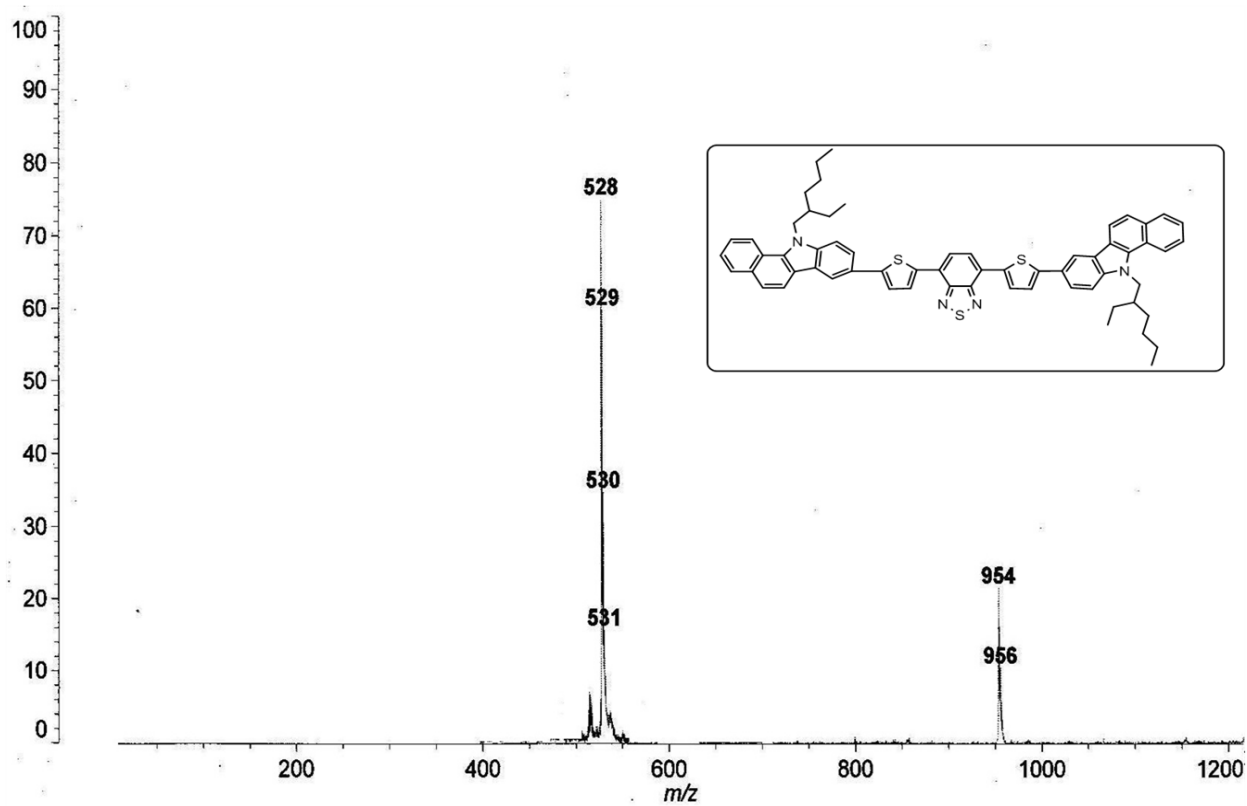
**IR Spectrum of BFBFB**



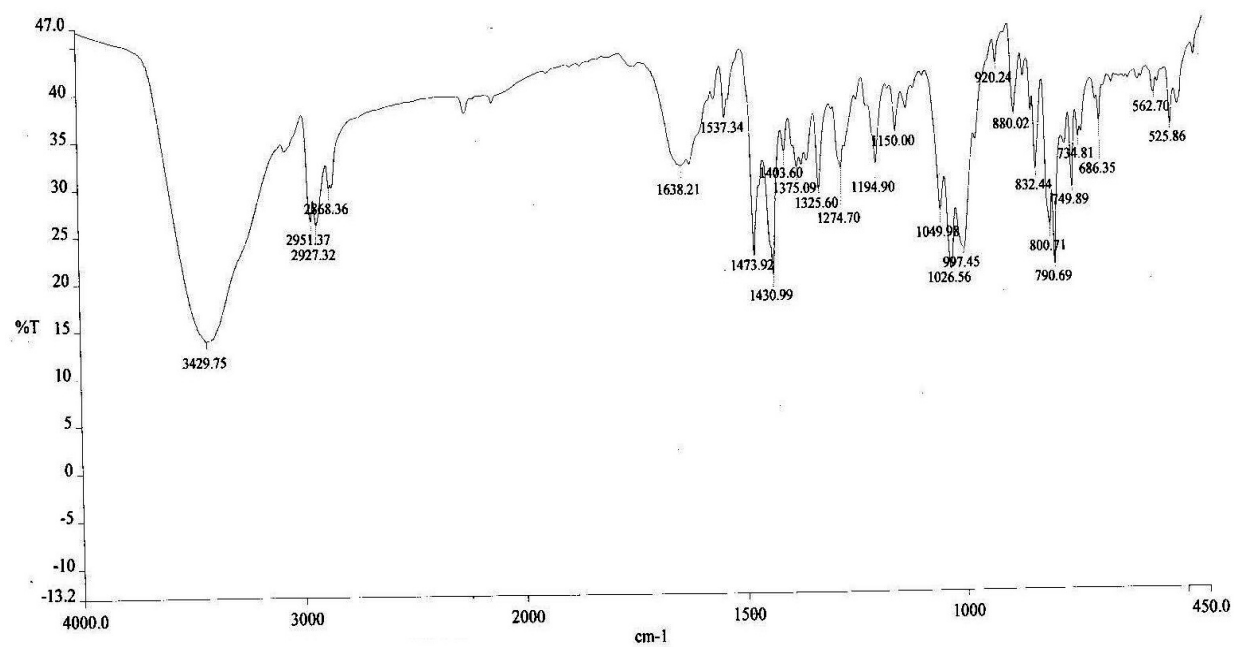
**MALDI-TOF mass Spectrum of CFBFC**



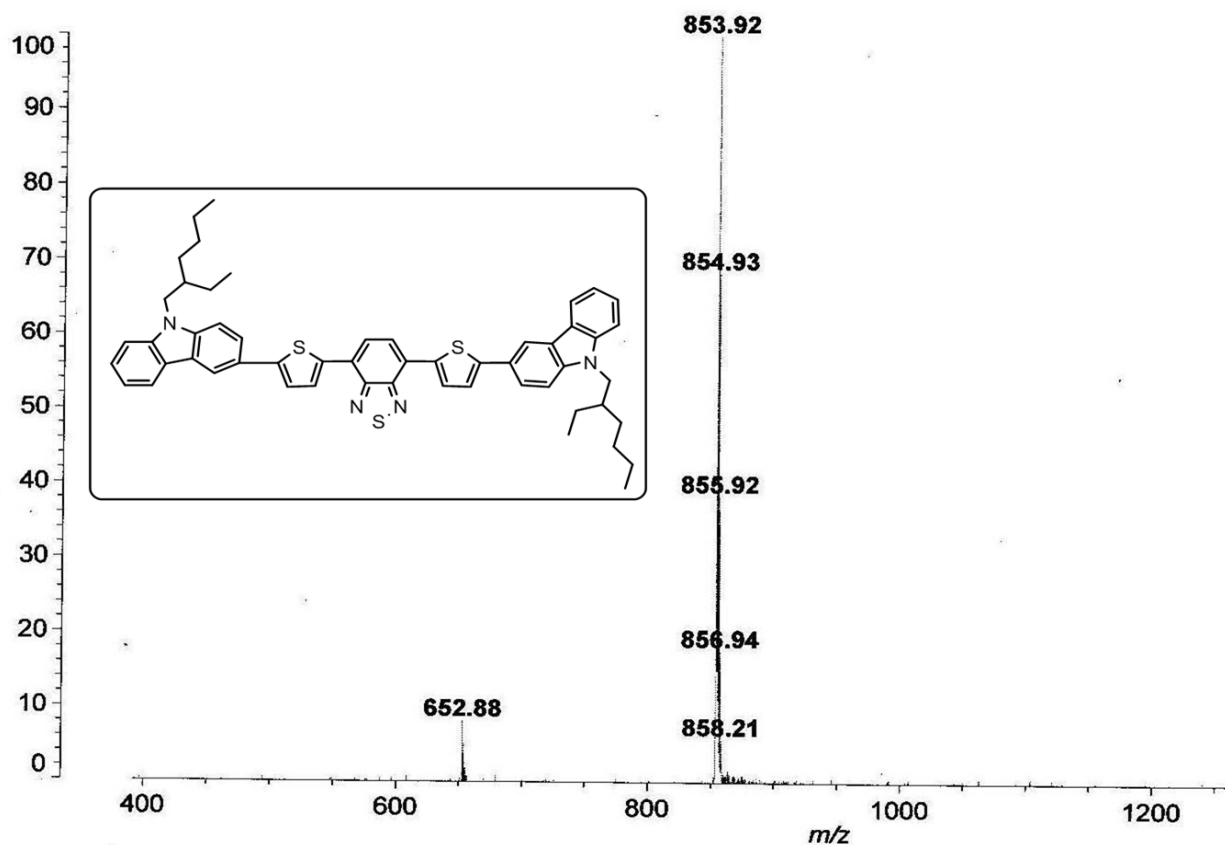
**IR Spectrum of CFBFC**



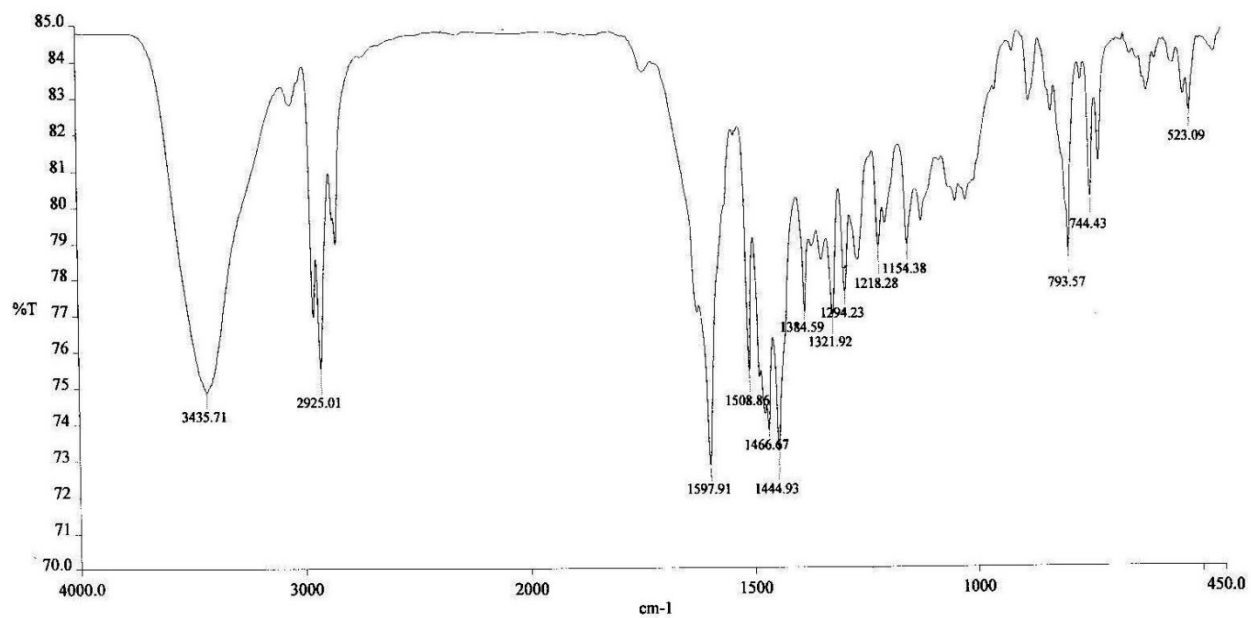
**MALDI-TOF mass Spectrum of BTBTB**



**IR Spectrum of BTBTB**



**MALDI-TOF mass Spectrum of CTBTC**



**IR Spectrum of CTBTC**