Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

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

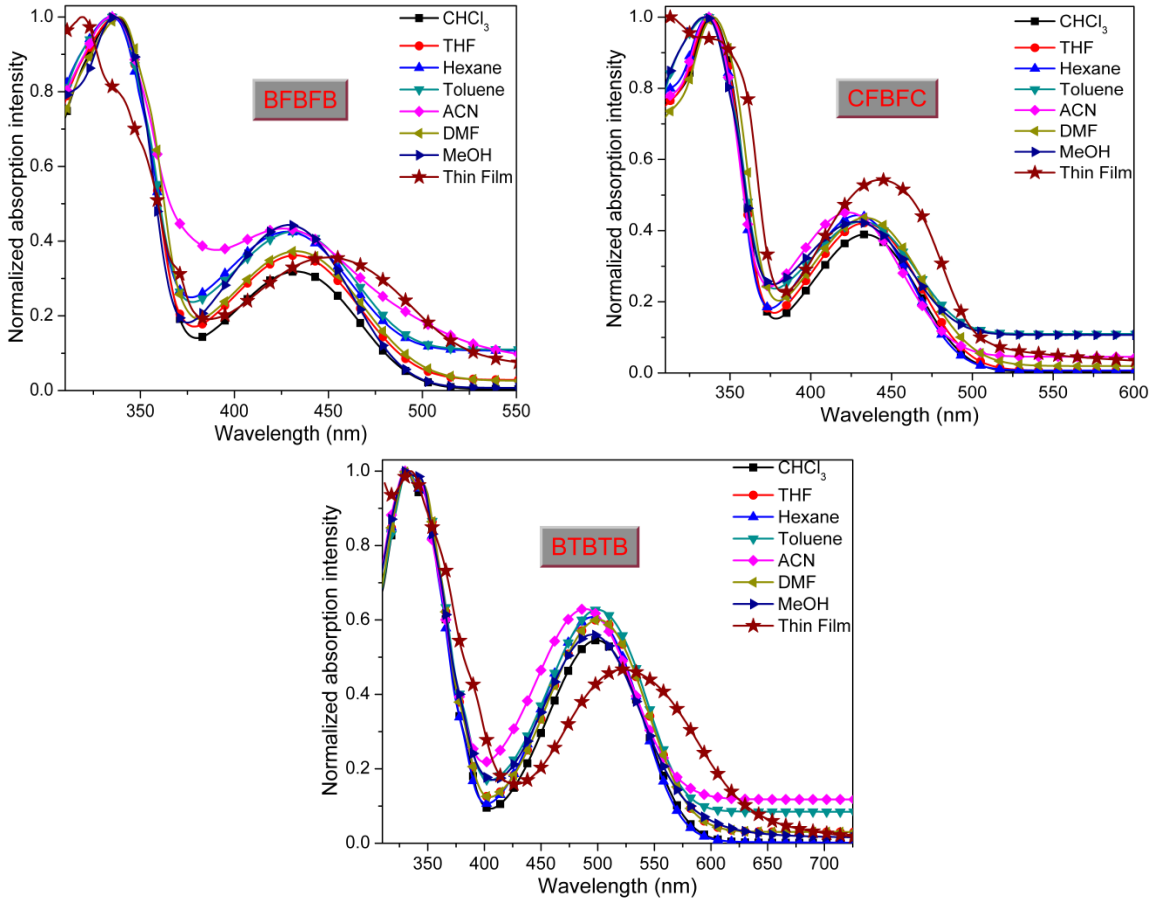


Table S1 Absorption maxima of compounds in different solvents (units in nm).

Compound	$CHCl_3$	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.

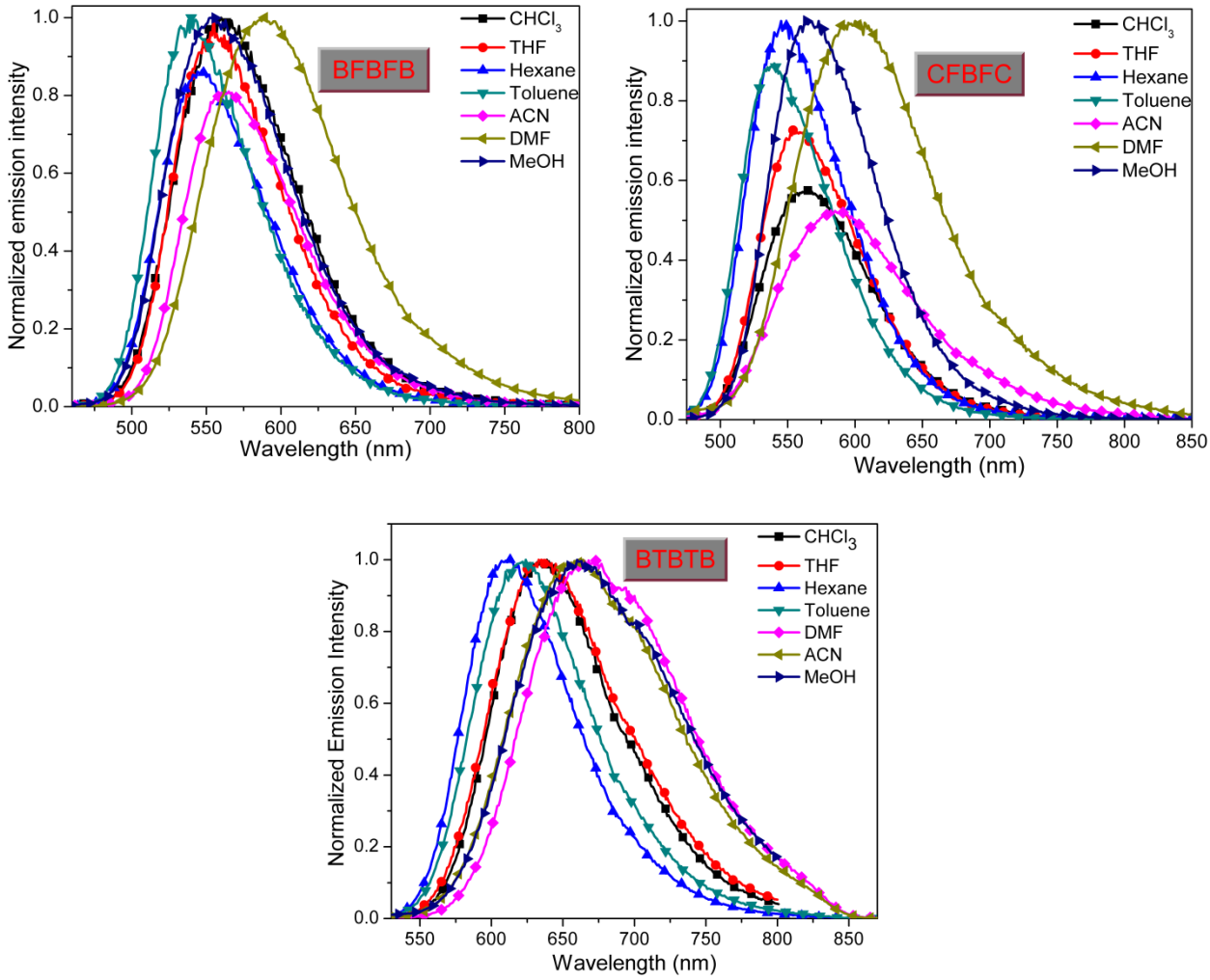


Table S2 Emission maxima of compounds in different solvents (units in nm).

Compound	$CHCl_3$	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 cm^{-1}).

Compound	$CHCl_3$	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	λ_{max}[a] (nm)	B3LYP (gas)			PBE (gas)			m062X (gas)		
		λ_{max} (nm)	f	Composition	λ_{max} (nm)	f	Composition	λ_{max} (nm)	f	Composition
BFBFB	433	528 (2.35eV)	0.7	H->L (92%)	494 (2.51eV)	0.9	H->L (86%) H-2->L (11%)	403 (3.07eV)	1.5	H->L (62%) H-2->L (19%) H-4->L (12%)
CFBFC	434	530 (2.34eV)	0.7	H->L (96%)	496 (2.50eV)	0.8	H->L (93%) H-2->L (6%)	403 (3.04eV)	1.4	H->L (69%) H-2->L (21%)
BTBTB	499	623 (1.99eV)	0.9	H->L (99%)	589 (2.11eV)	0.9	H->L (98%)	491 (2.53eV)	1.2	H->L (92%)
CTBTC	525	627 (1.98eV)	0.7	H->L (99%)	593 (2.09eV)	0.8	H->L (98%)	493 (2.52eV)	1.0	H->L (93%)

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

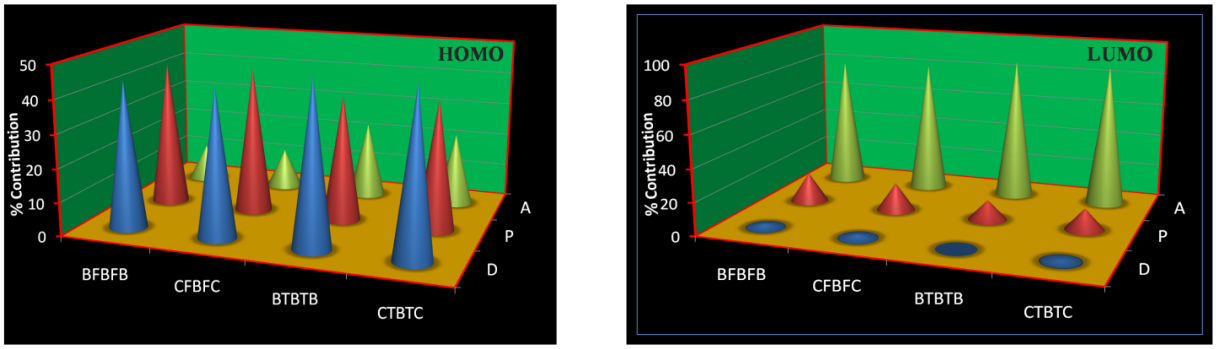


Figure S4 Computed absorption vs. variation of dihedral angle (θ) between the donor-spacer segments in the dyes (in ^{0})

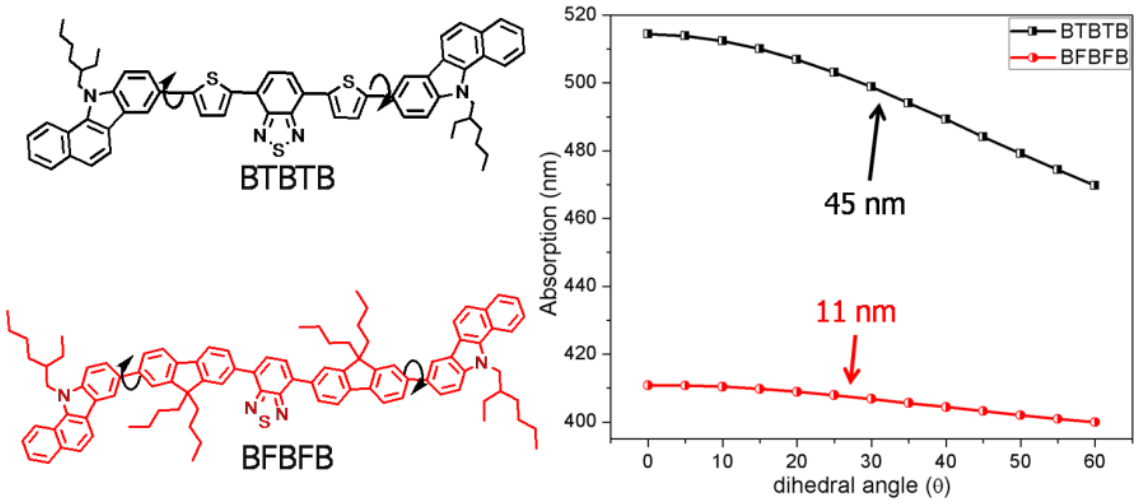
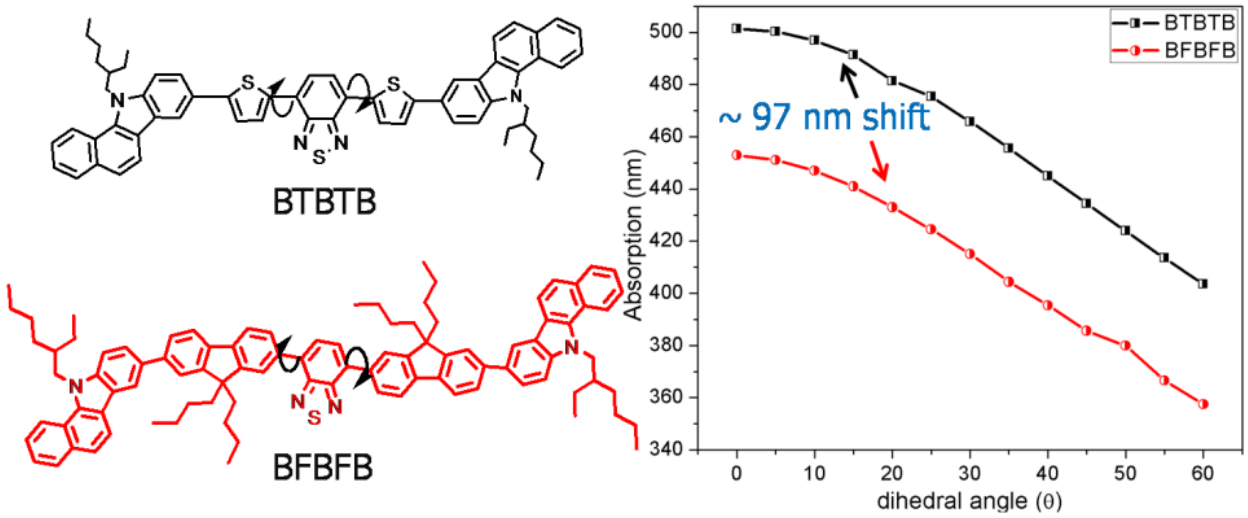
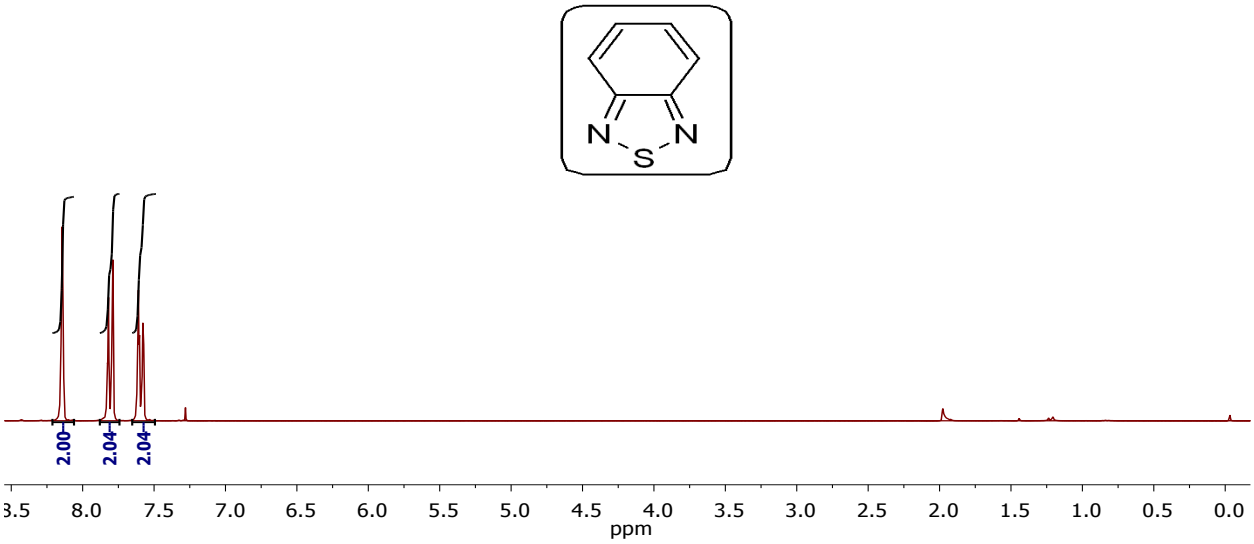
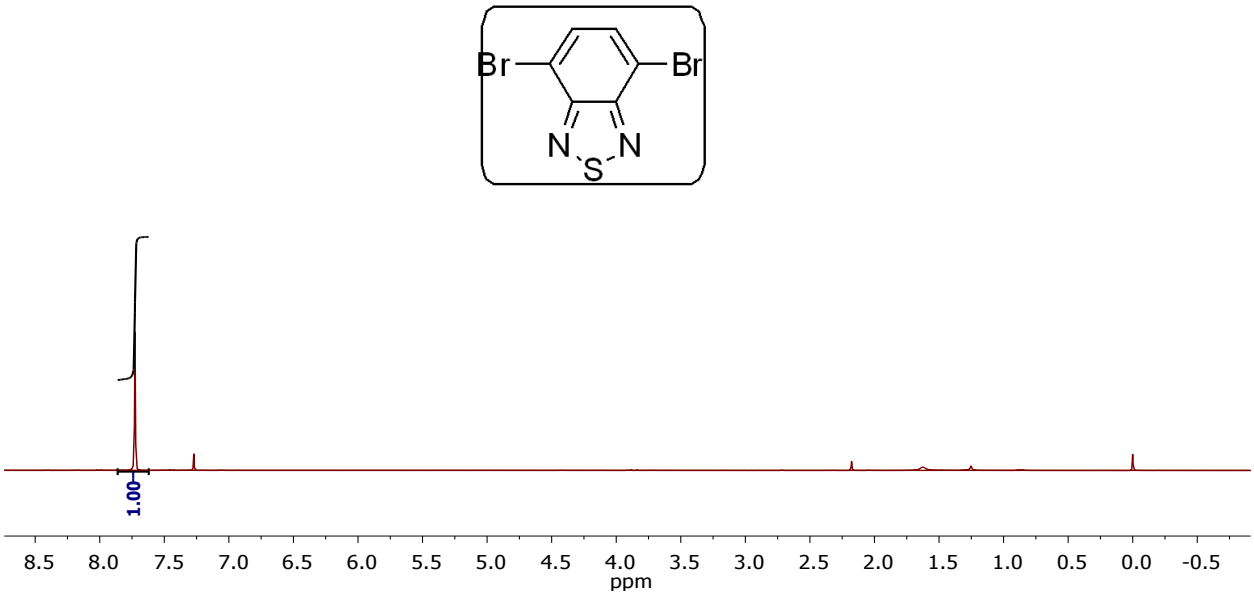


Figure S5 Computed absorption vs. variation of dihedral angle (θ) between the acceptor-spacer segments in the dyes (in ^{0})

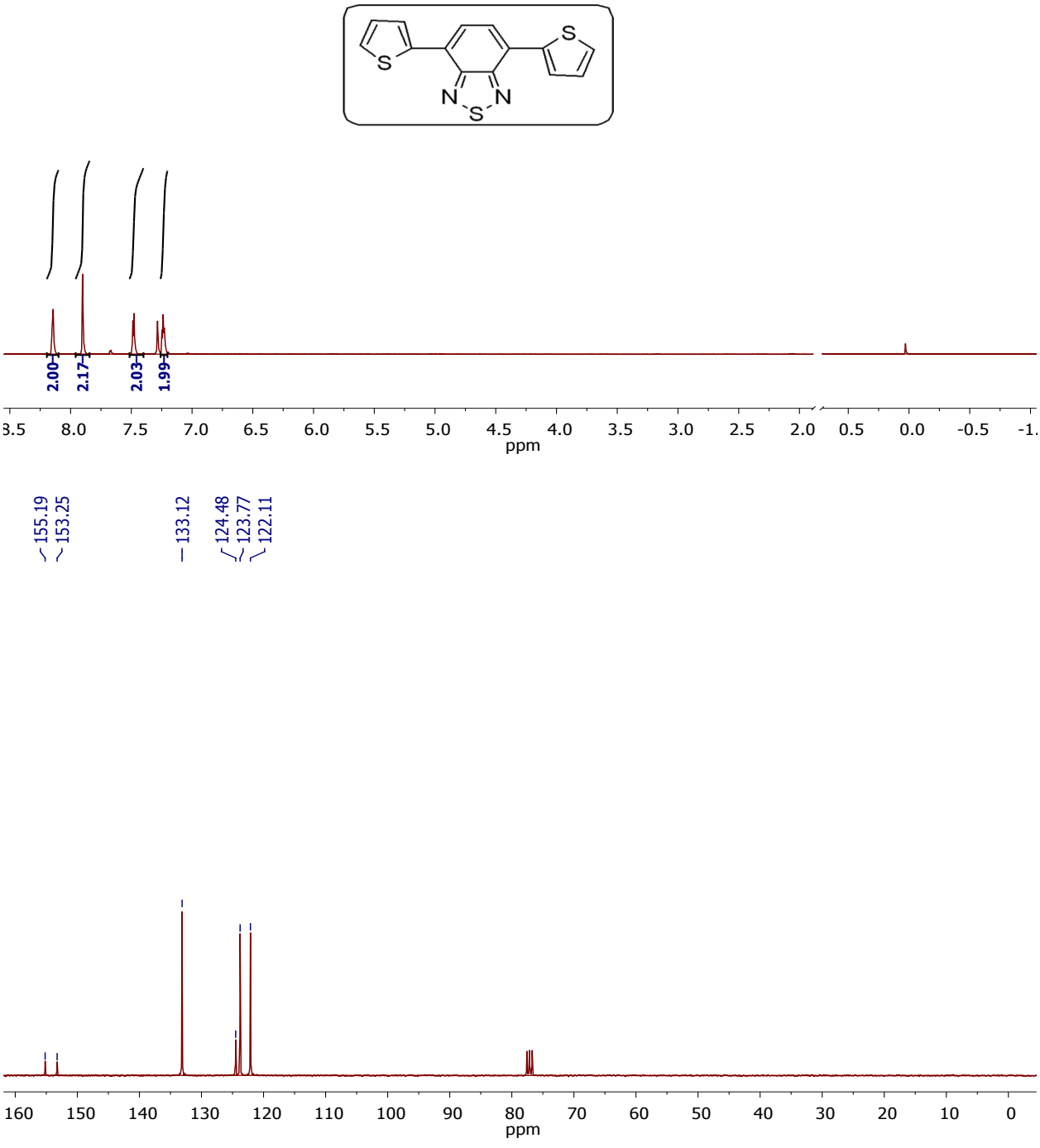




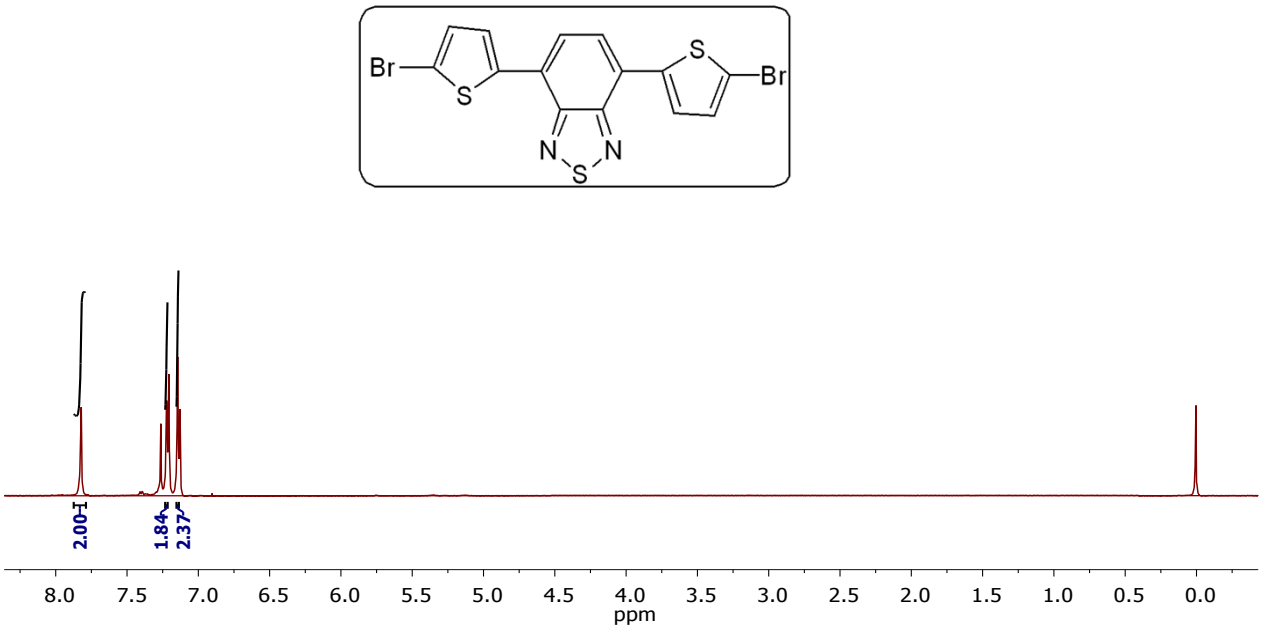
^{1}H spectrum of molecule 1



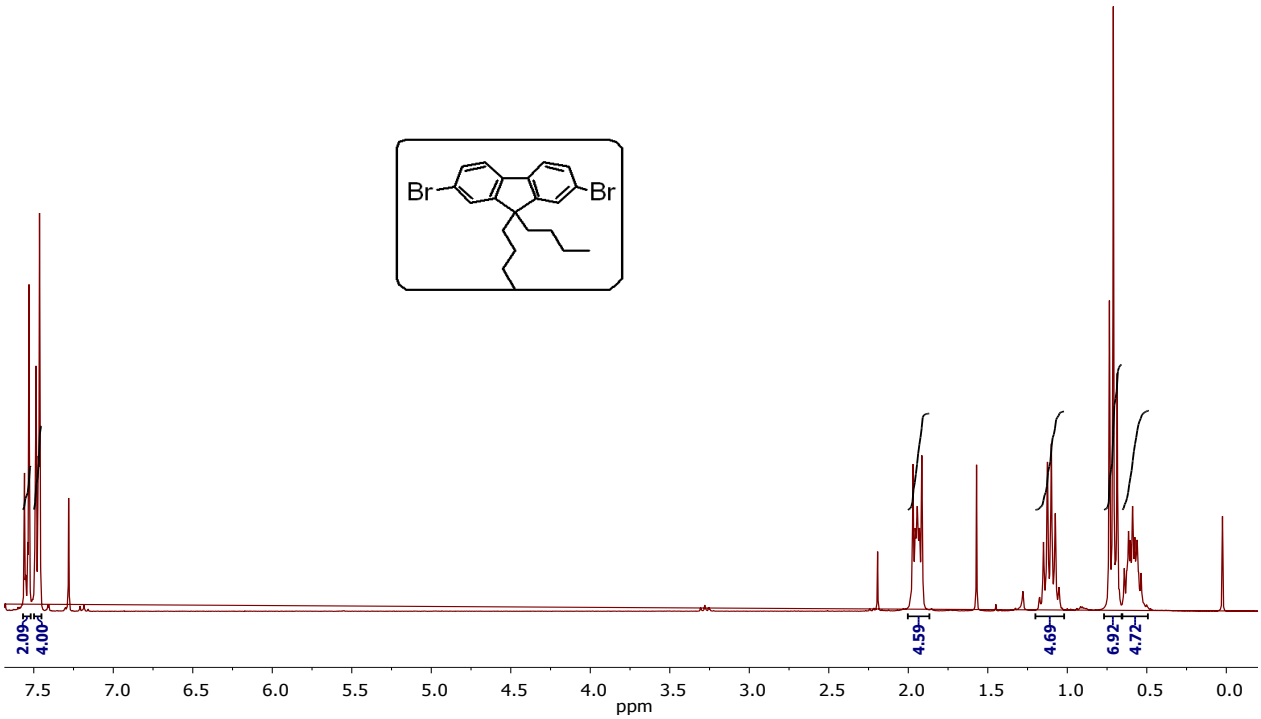
^{1}H spectrum of molecule 2



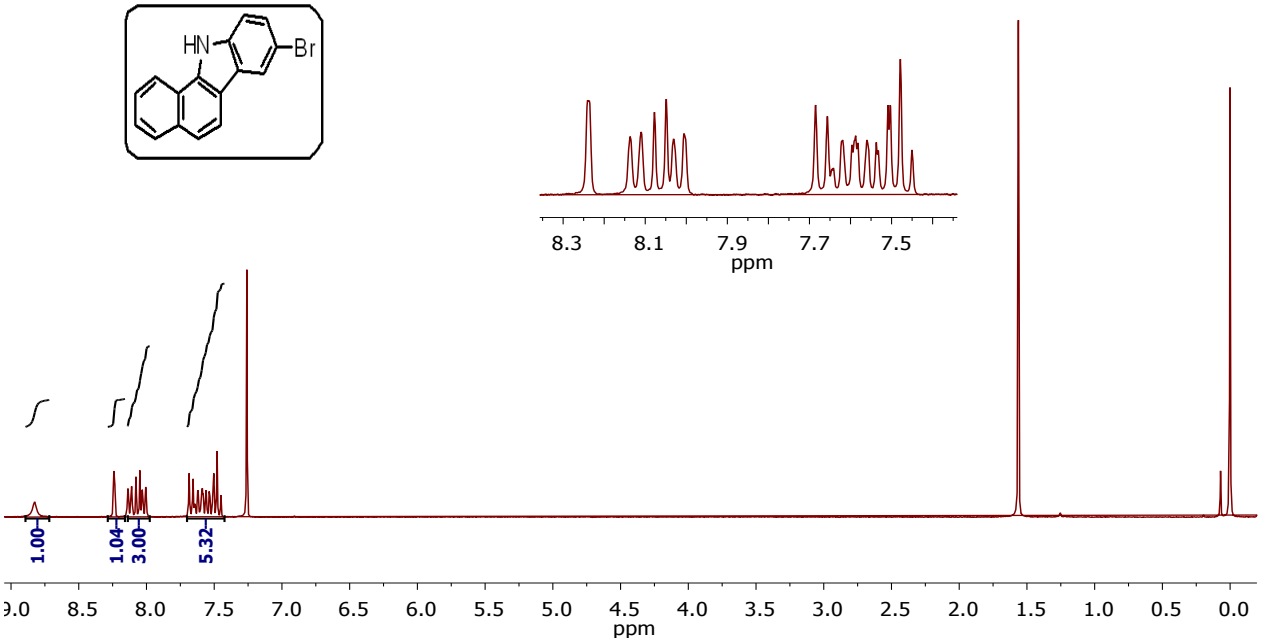
^{1}H and ^{13}C spectra of molecule 3



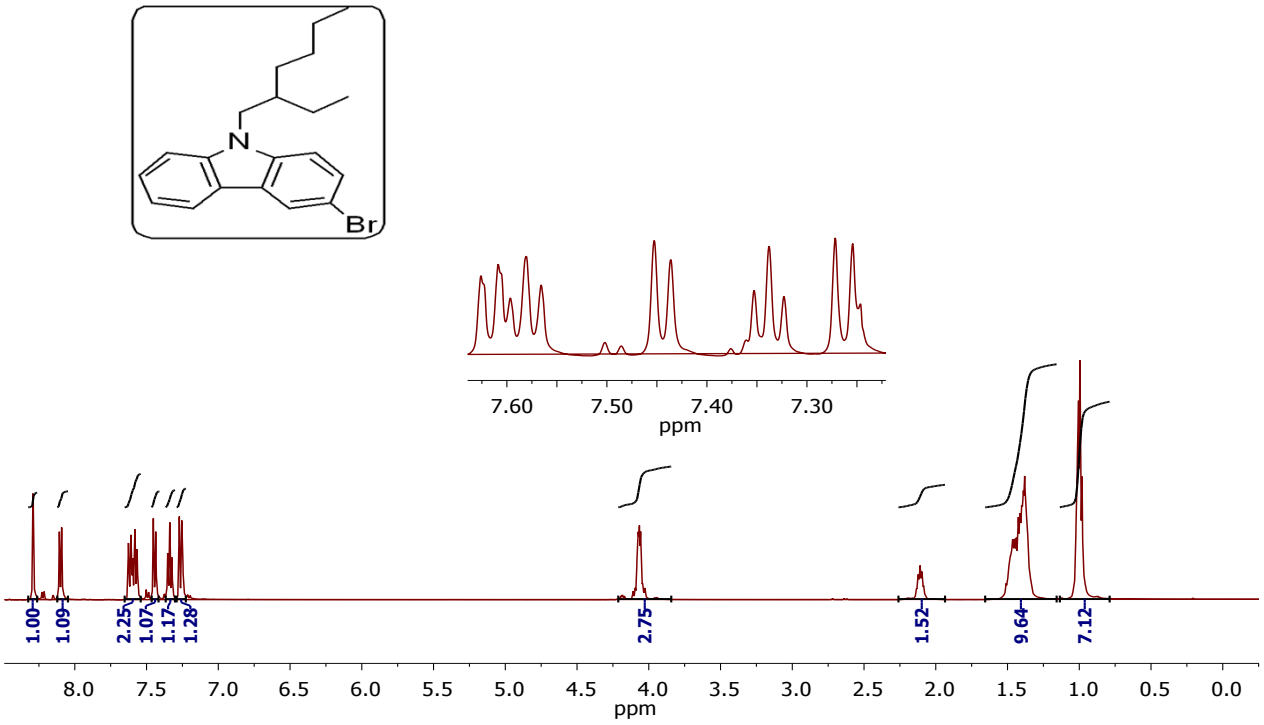
^{1}H spectrum of molecule 4



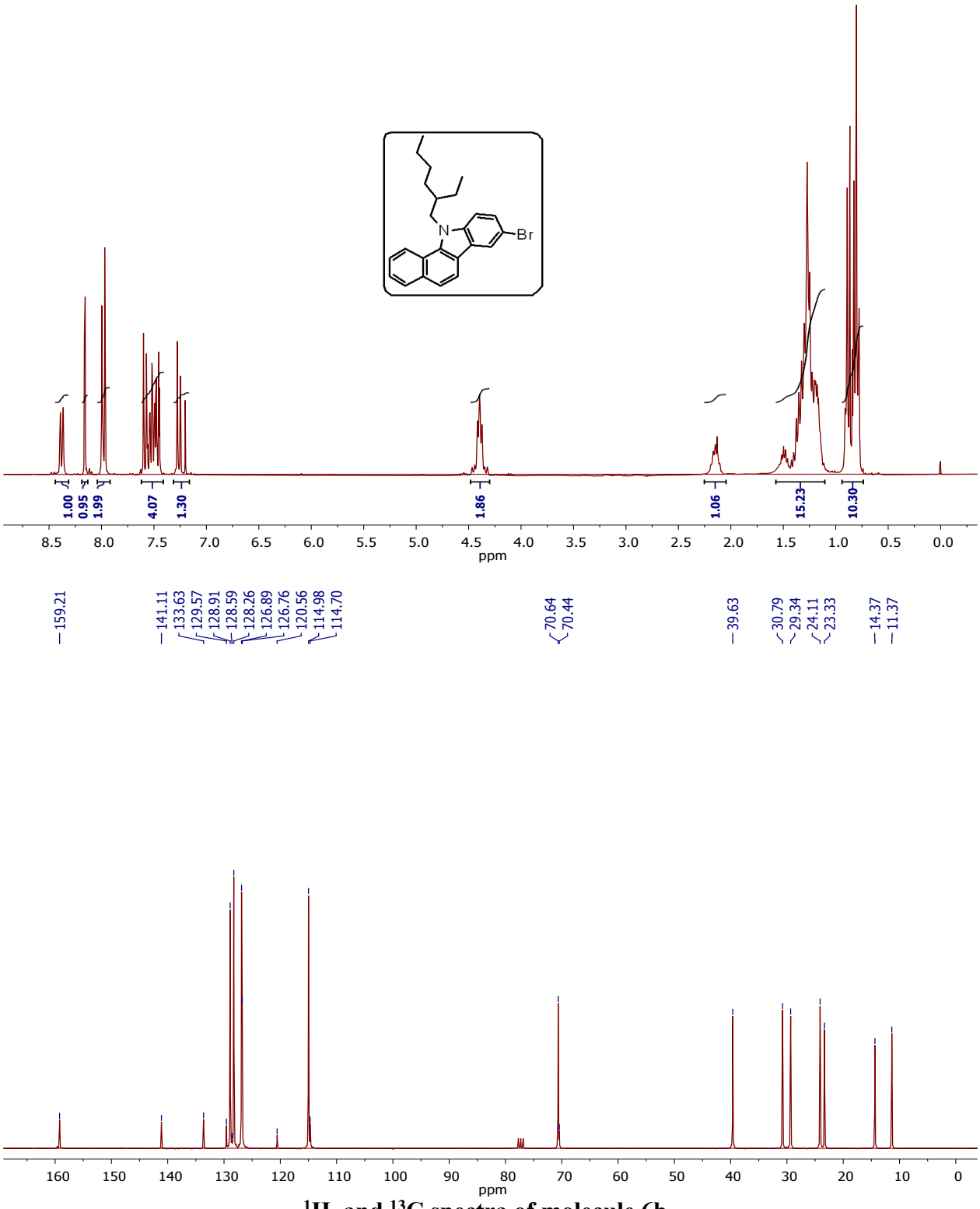
1H Spectrum of 2,7-dibromo-9,9-dibutyl-9H-fluorene



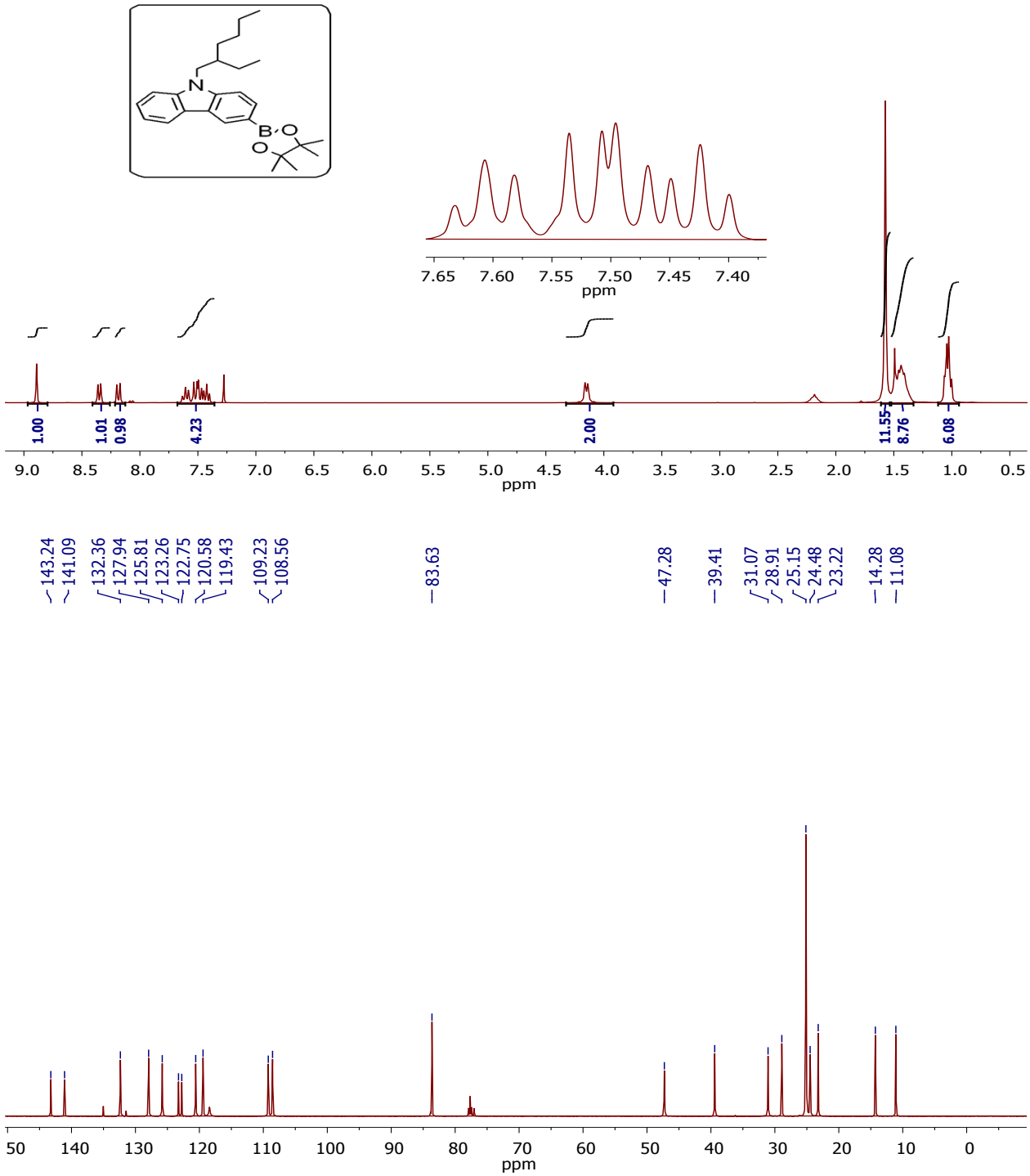
1H Spectrum of molecule 5



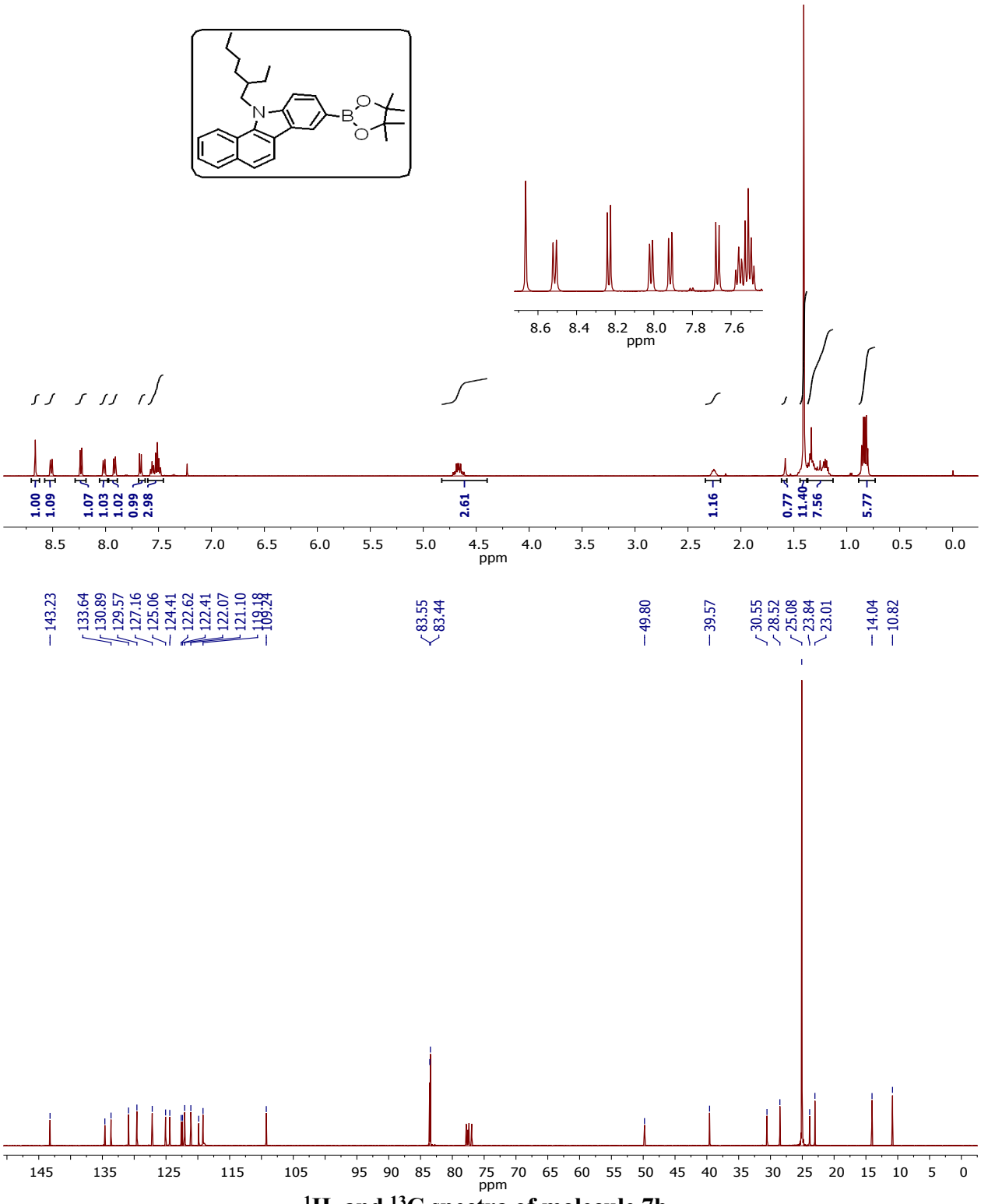
1H Spectrum of molecule 6a



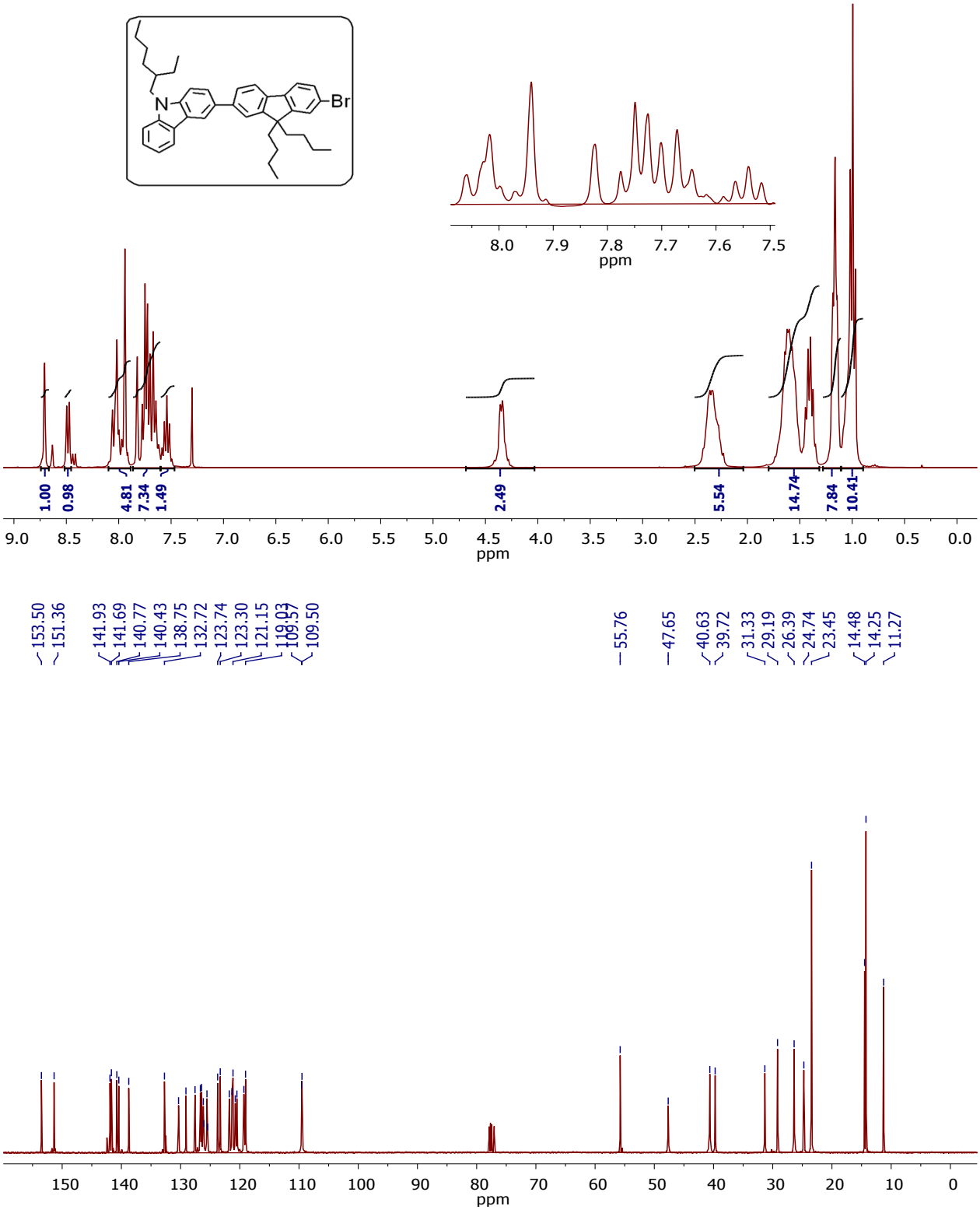
^{1}H and ^{13}C spectra of molecule 6b



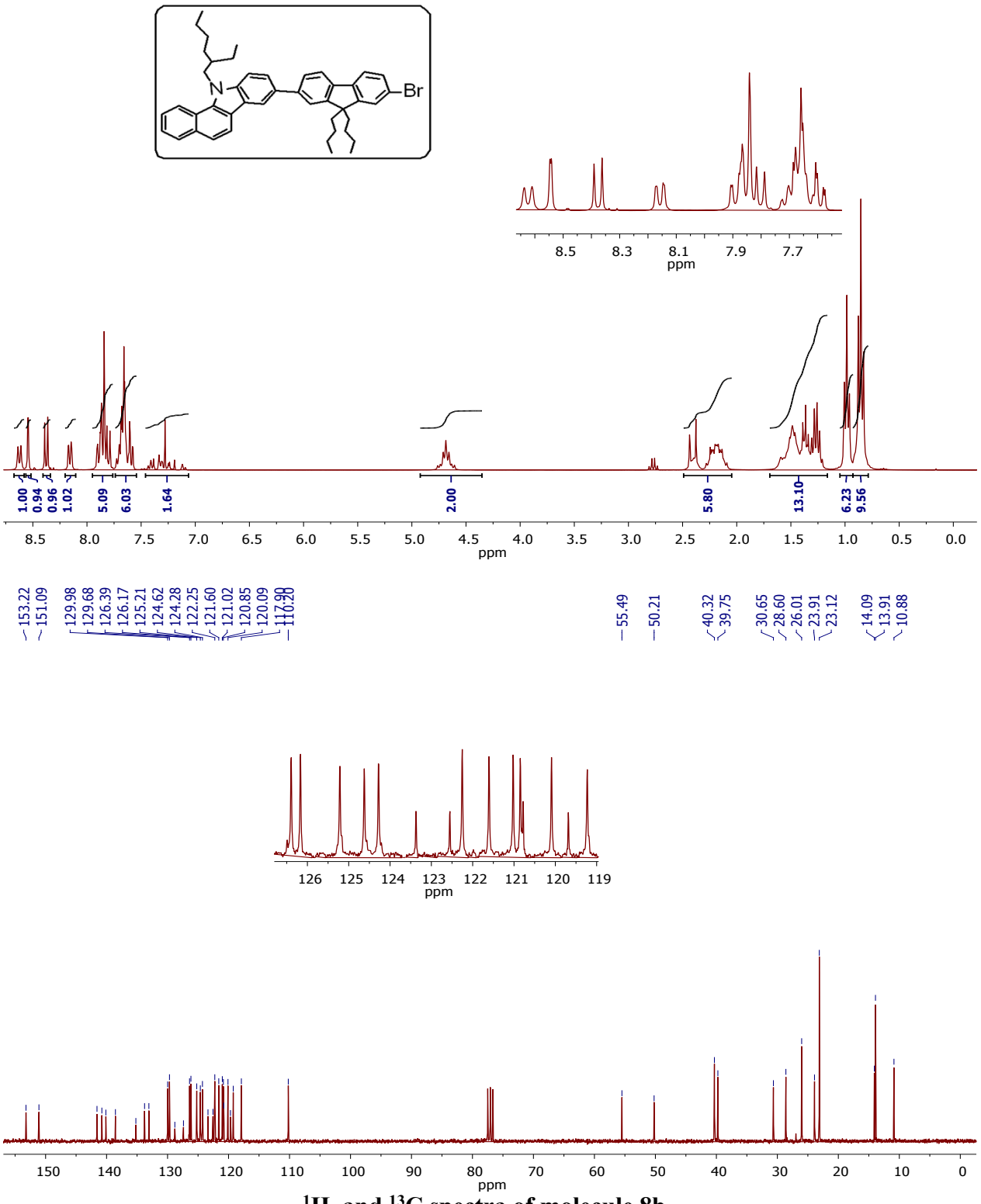
^{1}H and ^{13}C spectra of molecule 7a



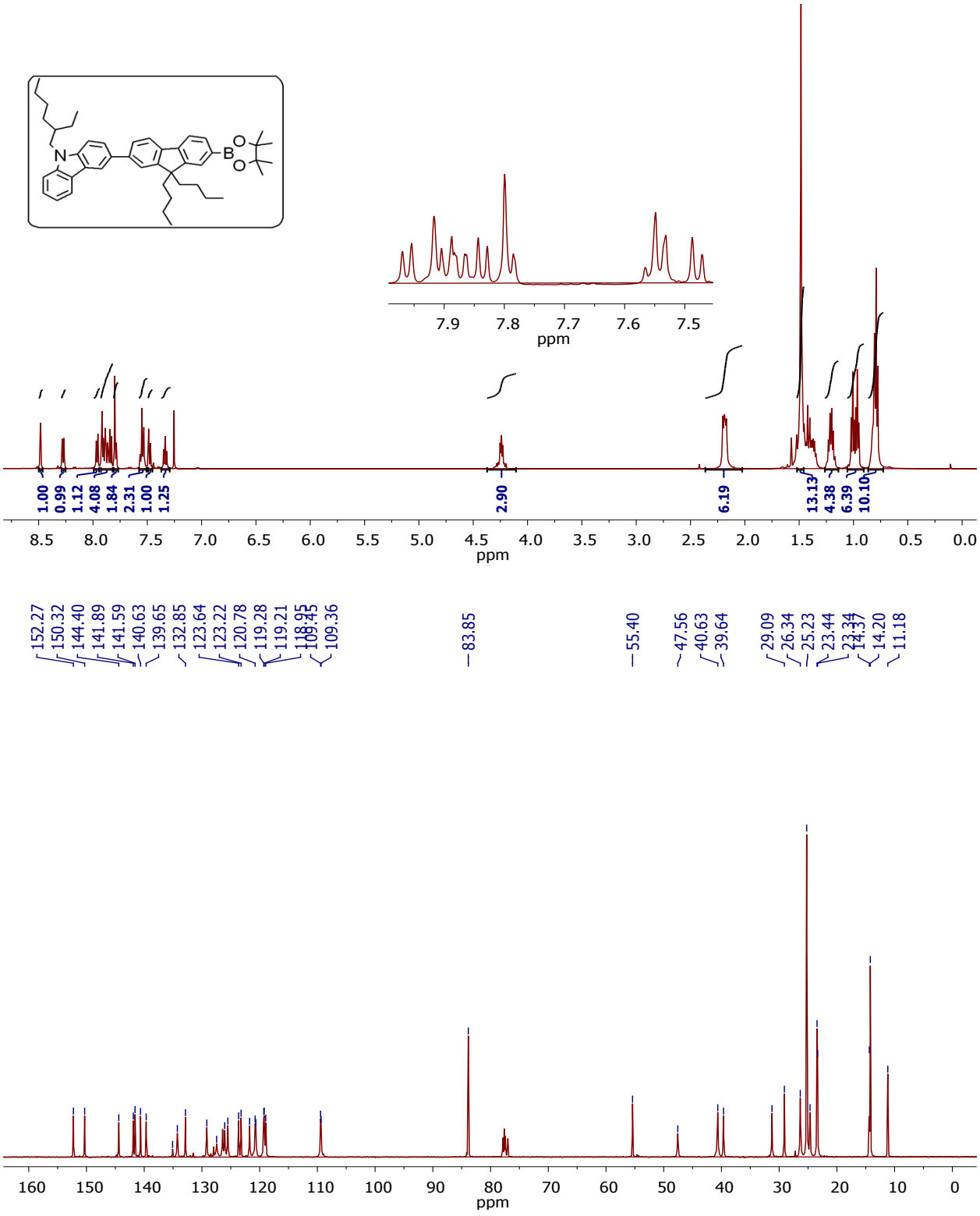
^{1}H and ^{13}C spectra of molecule 7b



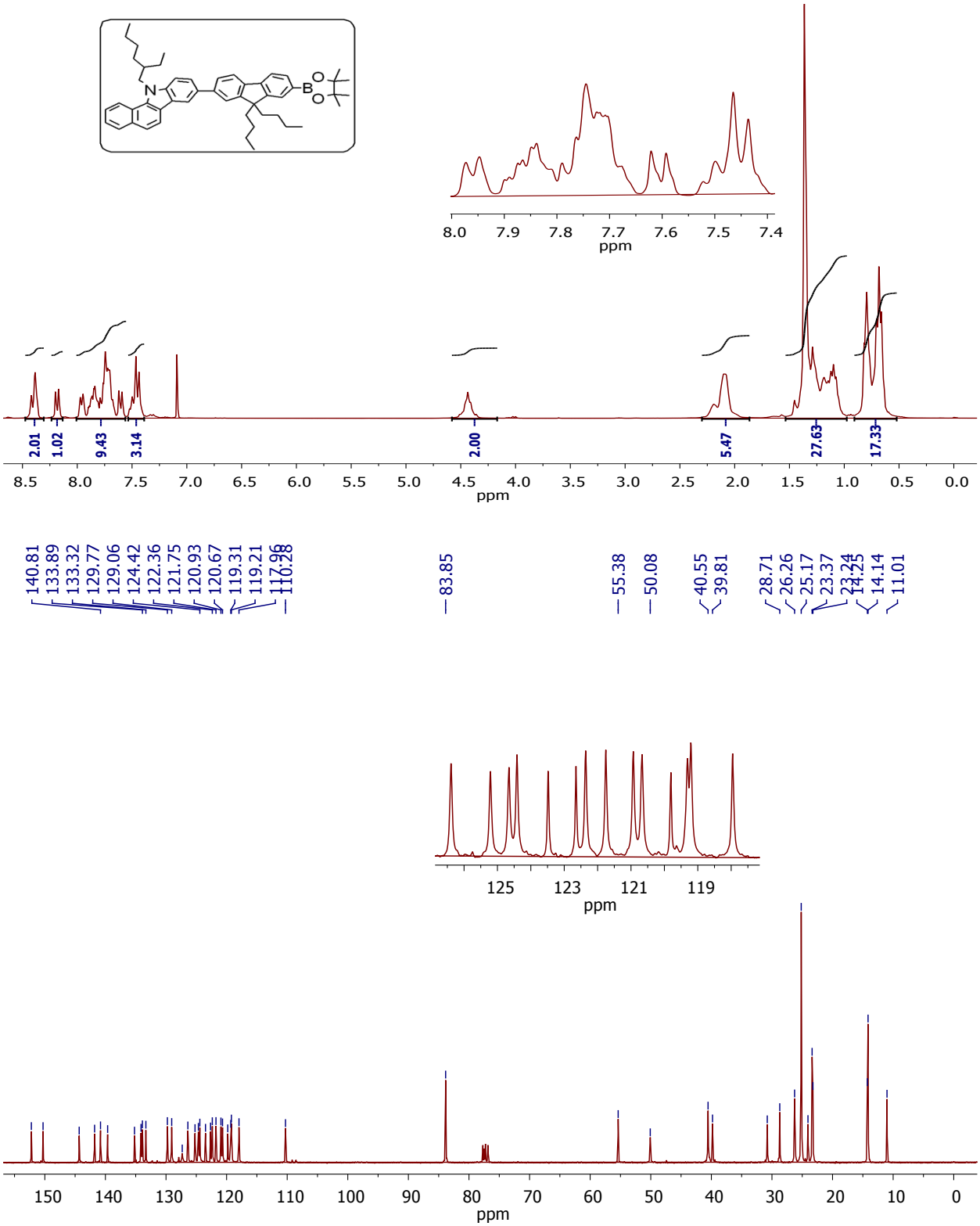
^{1}H and ^{13}C spectra of molecule 8a



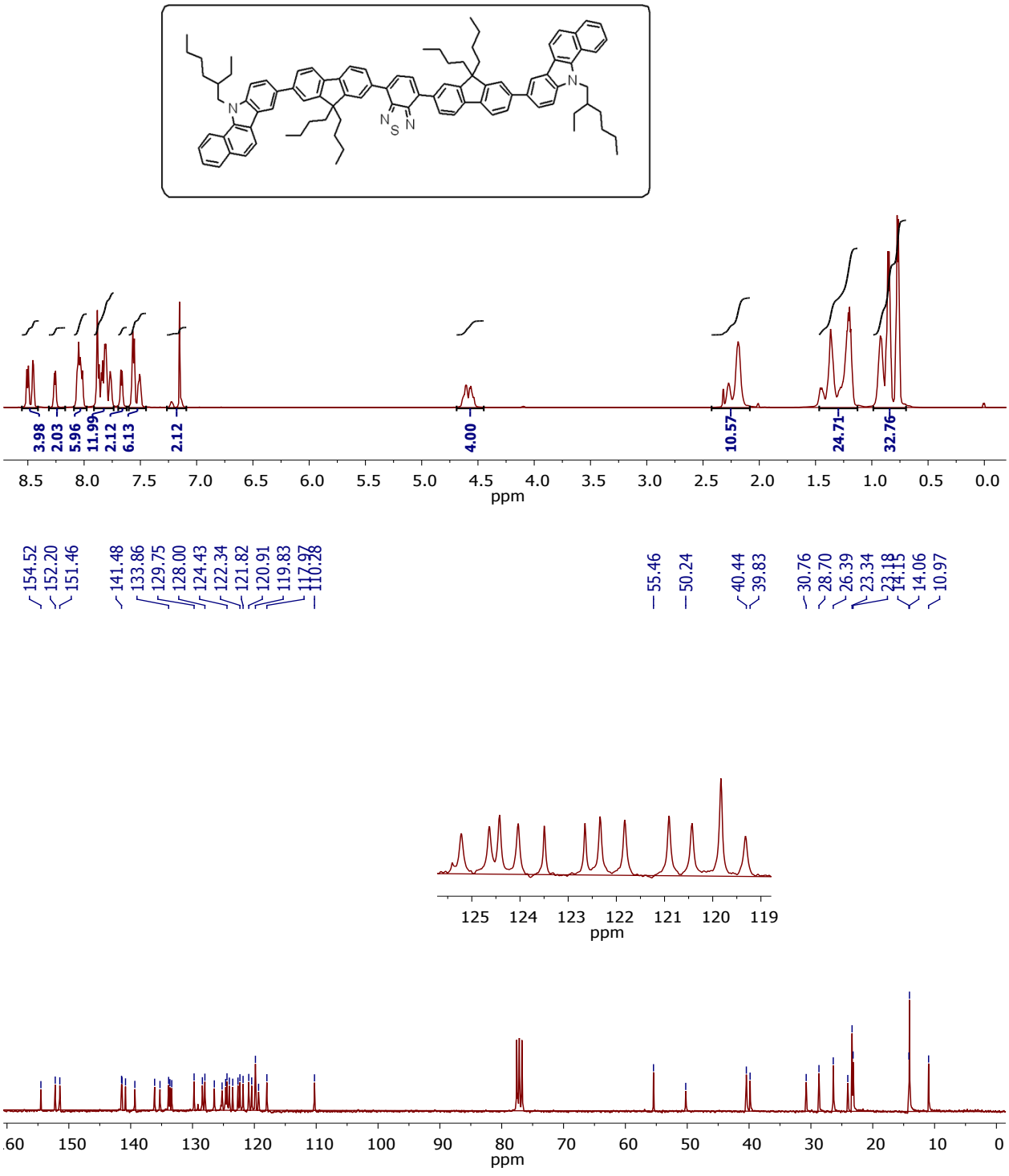
^{1}H and ^{13}C spectra of molecule 8b



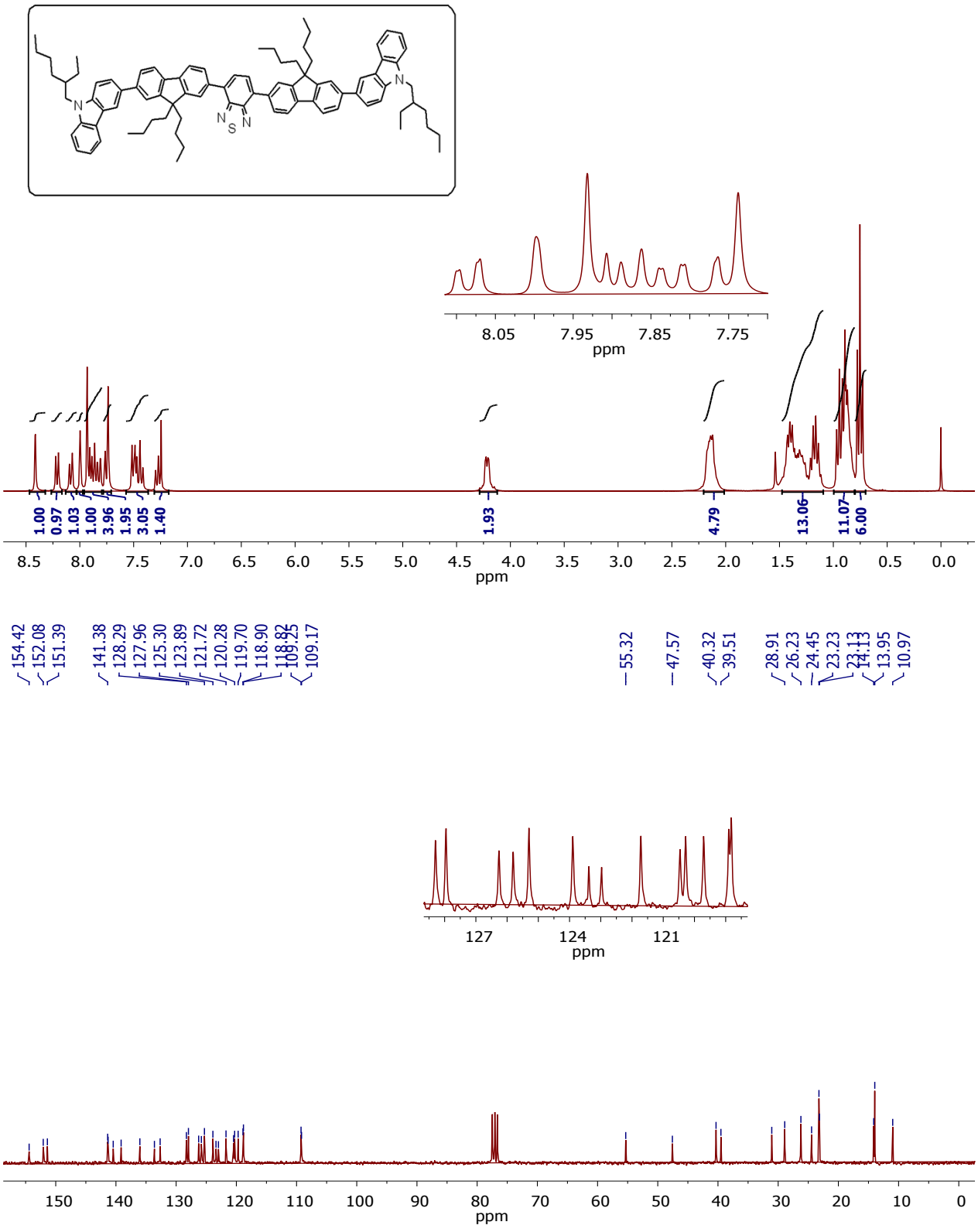
^{1}H and ^{13}C spectra of molecule 9a



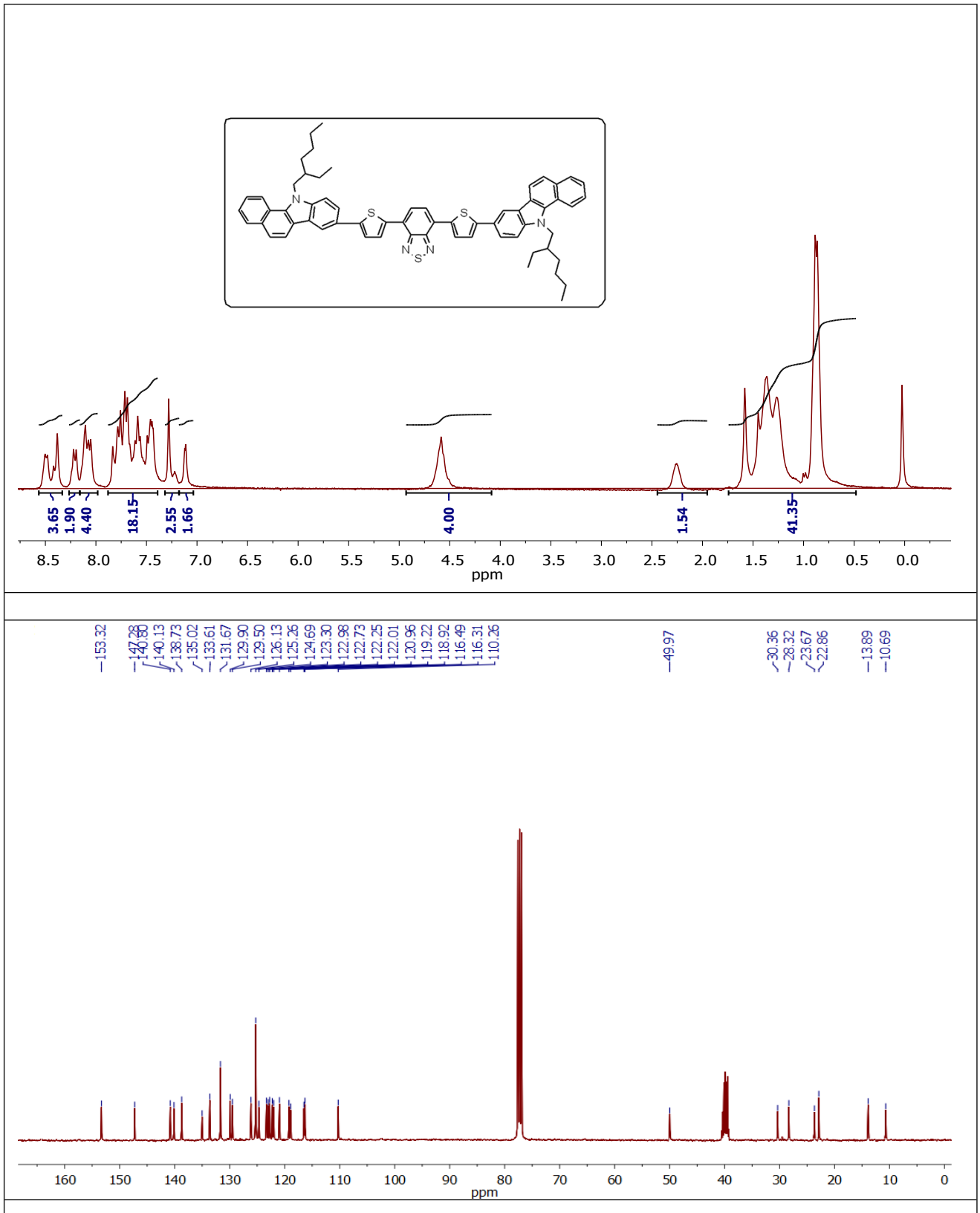
^{1}H and ^{13}C spectra of molecule 9b



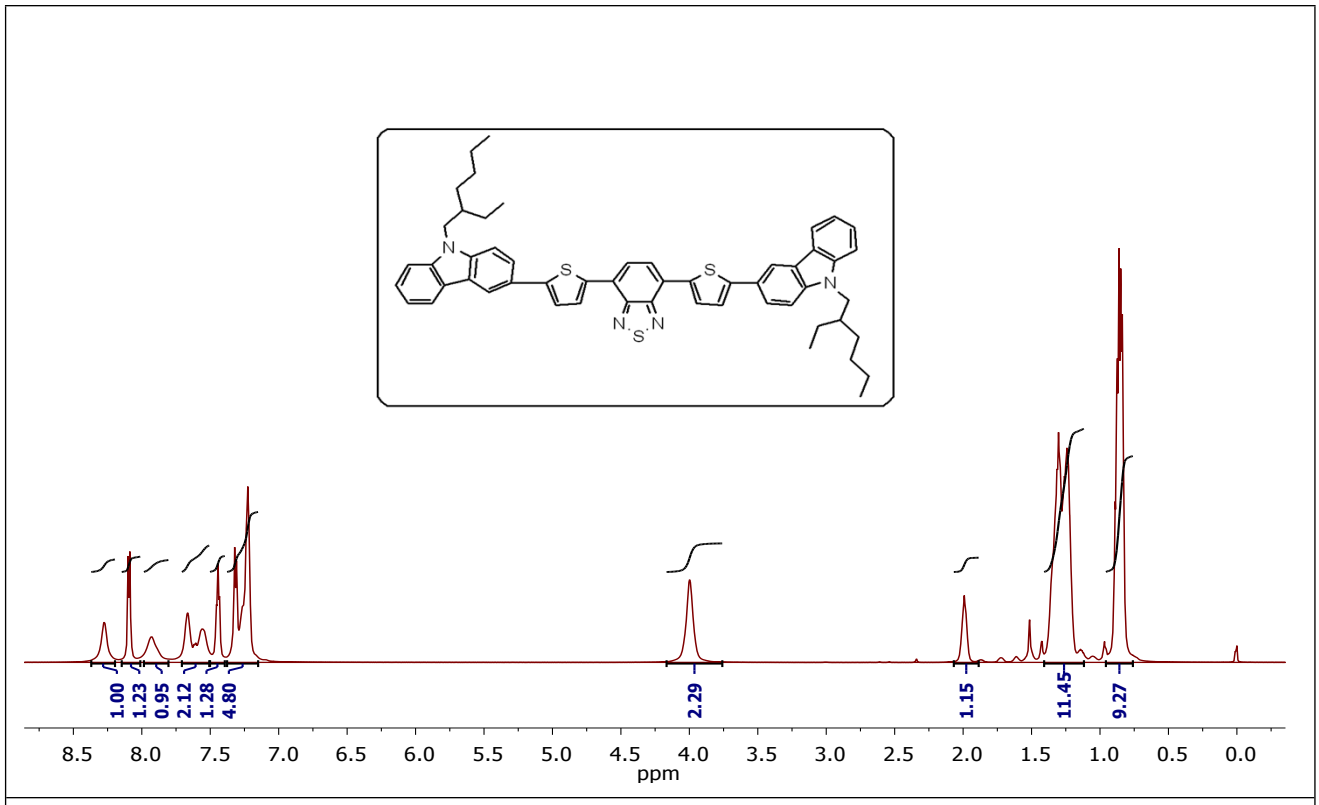
^{1}H and ^{13}C spectra of molecule BFBFB

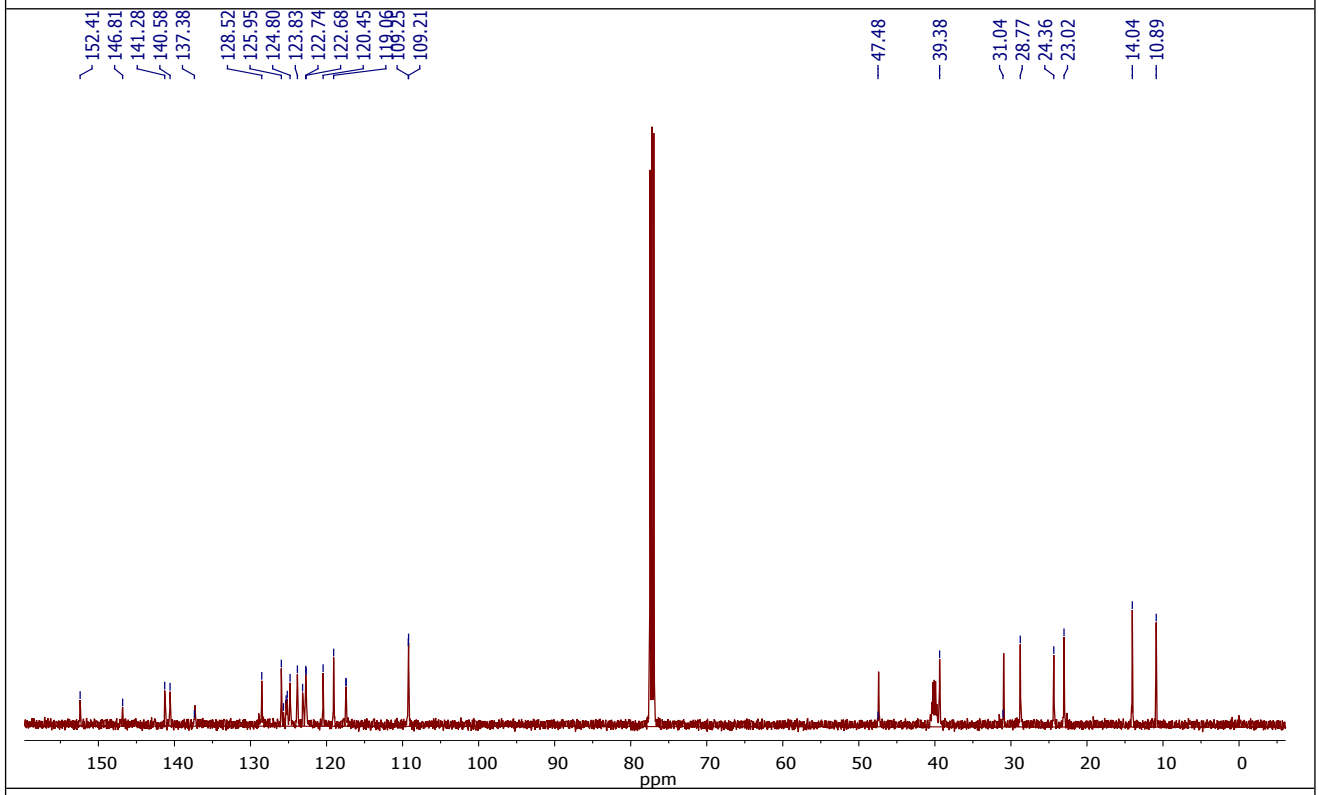


^{1}H and ^{13}C spectra of molecule CFBFC

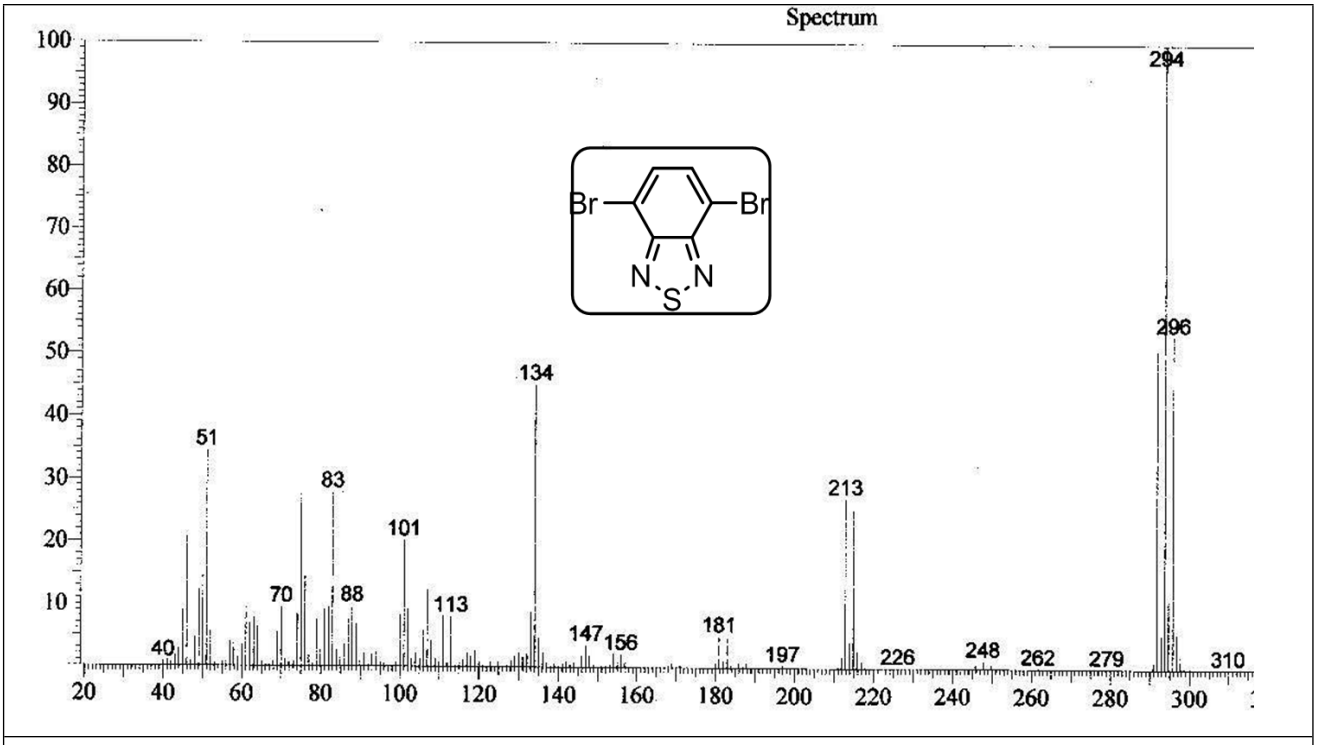


^{1}H and ^{13}C spectra of molecule BTBTB

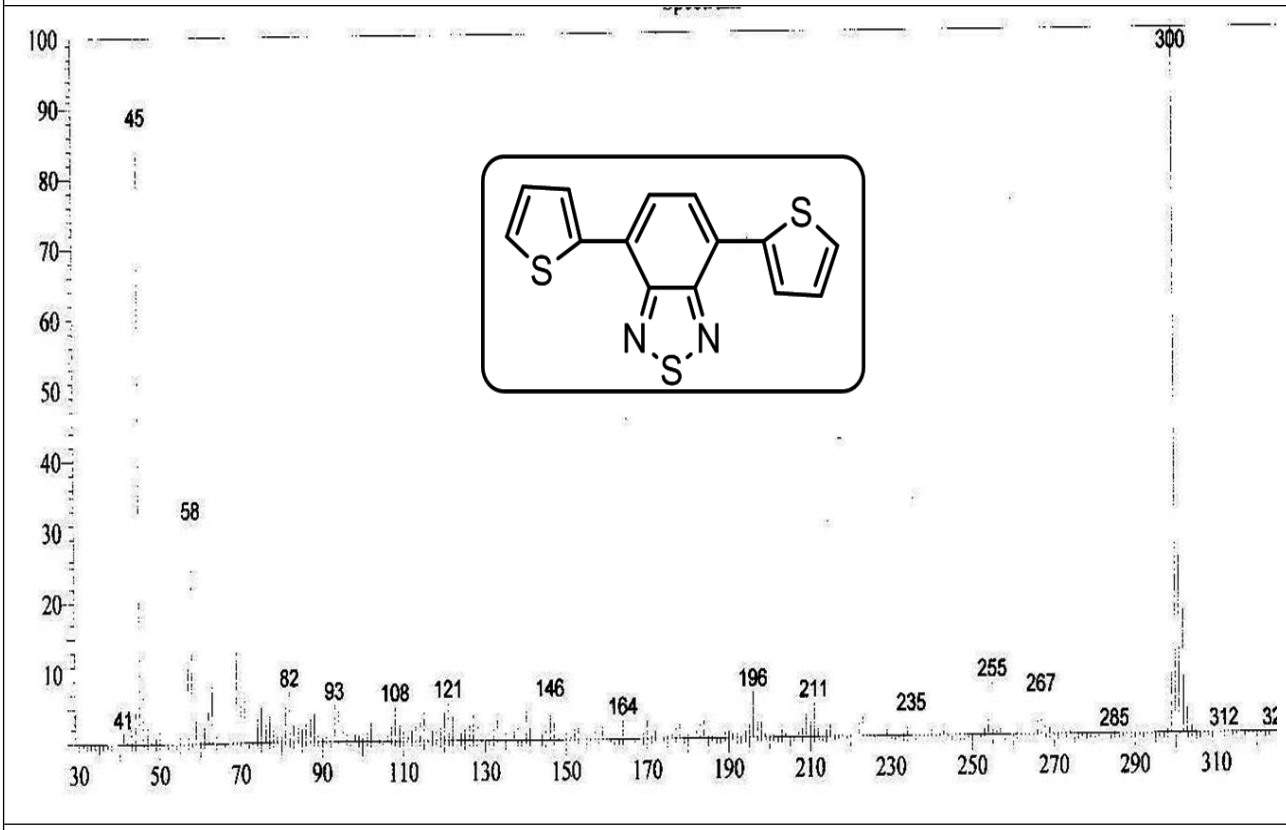




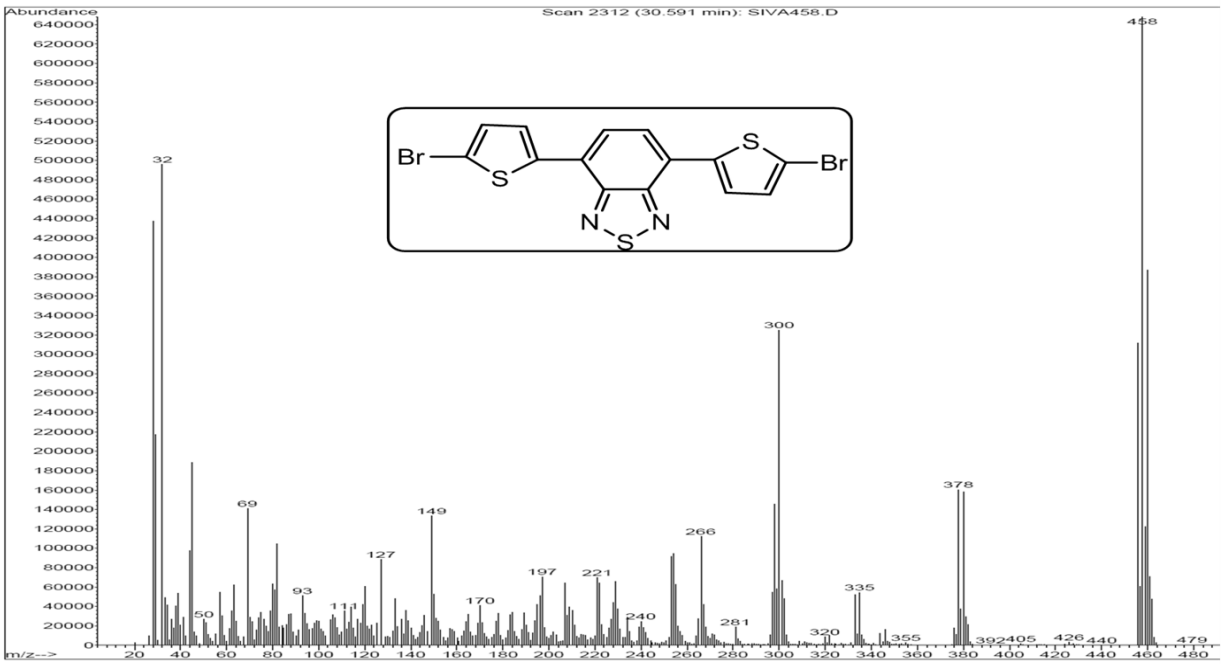
^{1}H and ^{13}C spectra of molecule CTBTC



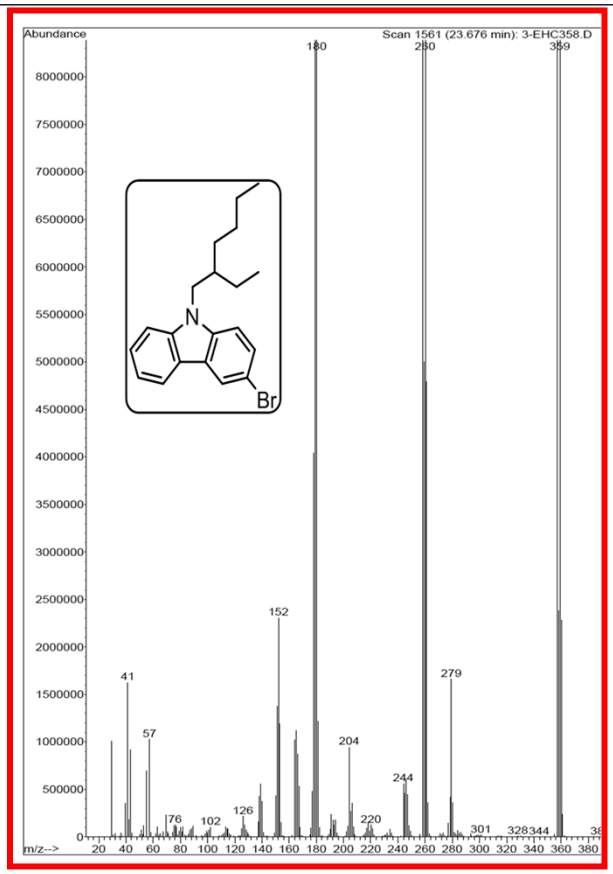
EI-Mass spectrum of molecule 2



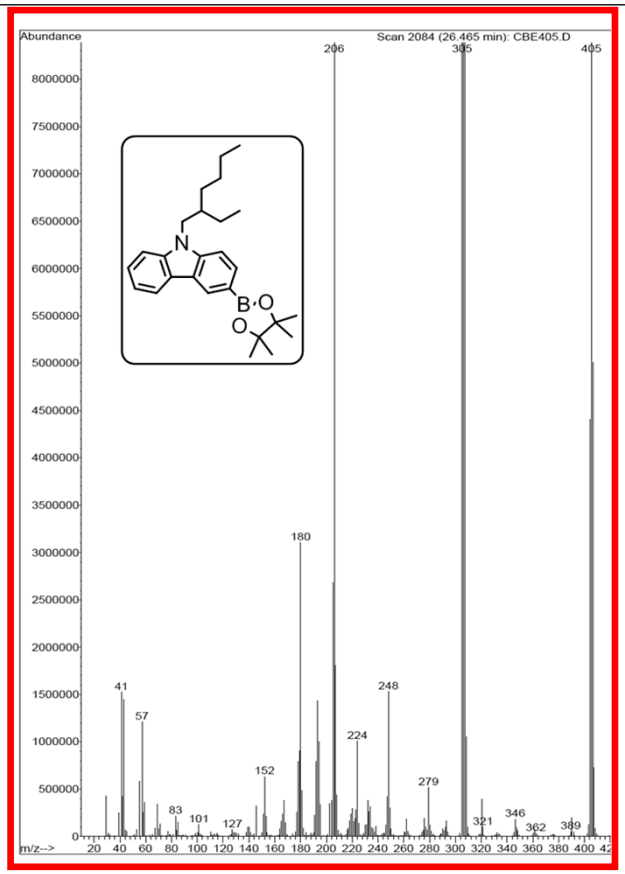
EI-Mass spectrum of molecule 3



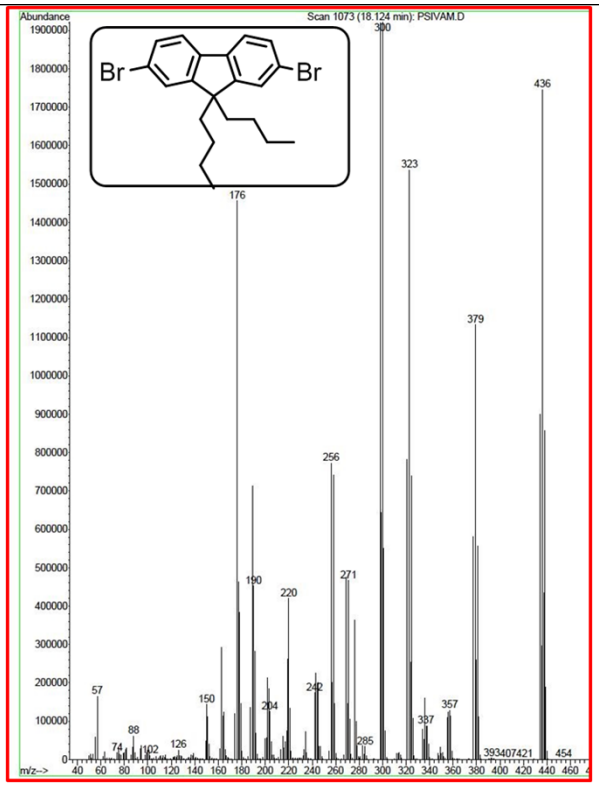
GC-Mass spectrum of molecule 4



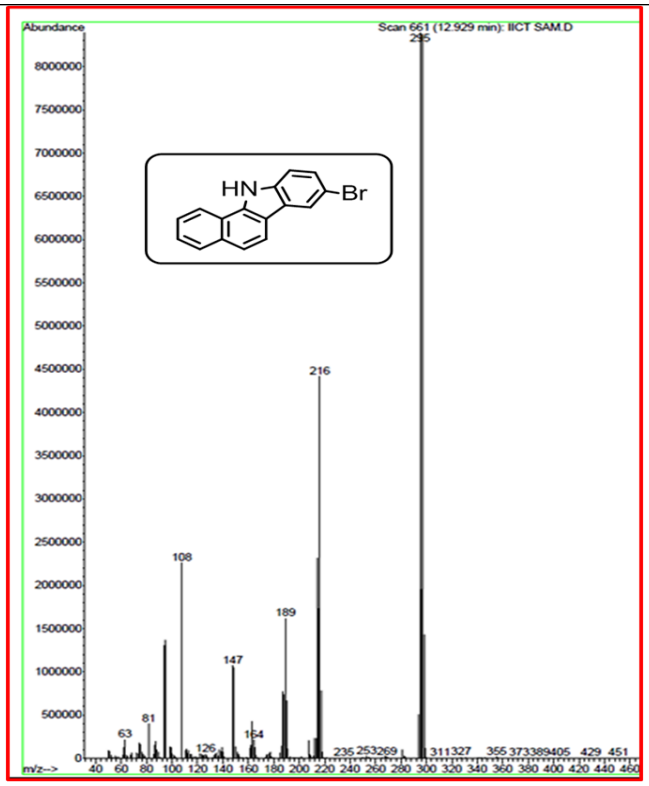
GC-Mass spectrum of molecule 6a



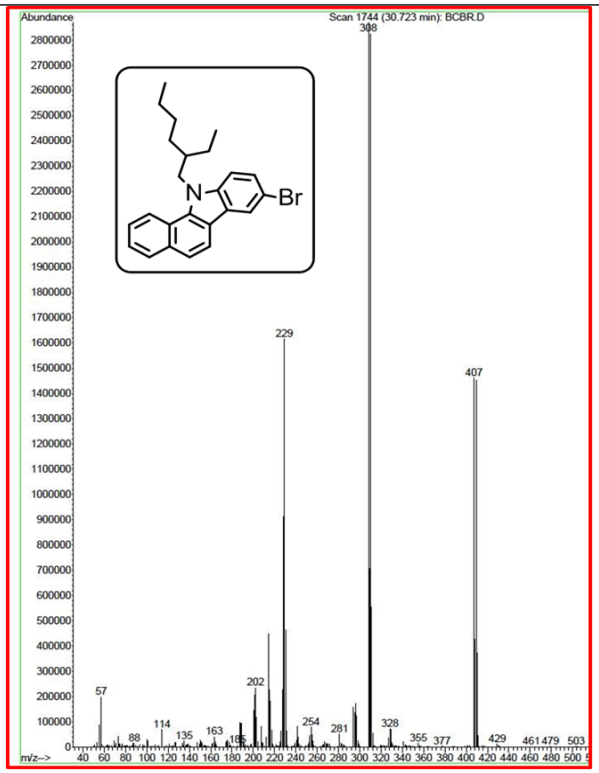
GC-Mass spectrum of molecule 7a



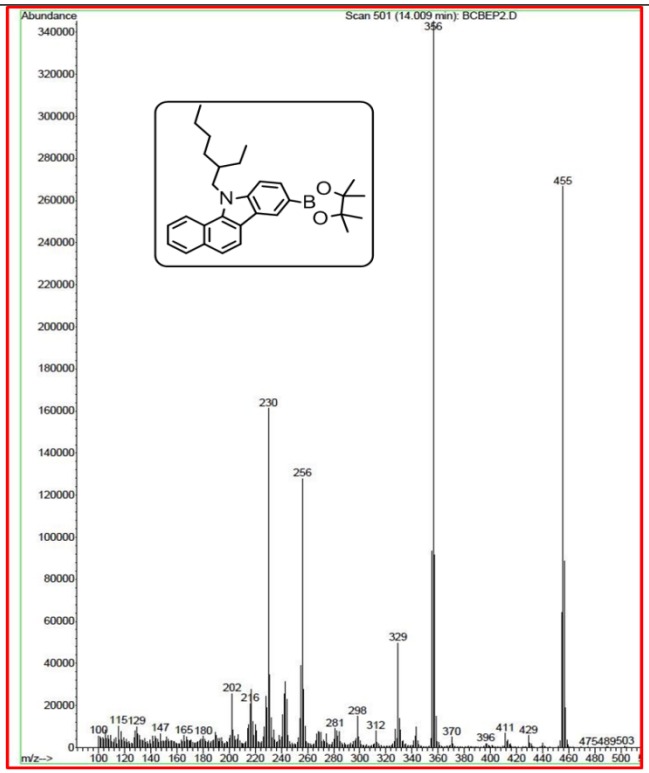
GC-MS Spectrum of 2,7-dibromo-9,9-dibutyl-9H-fluorene



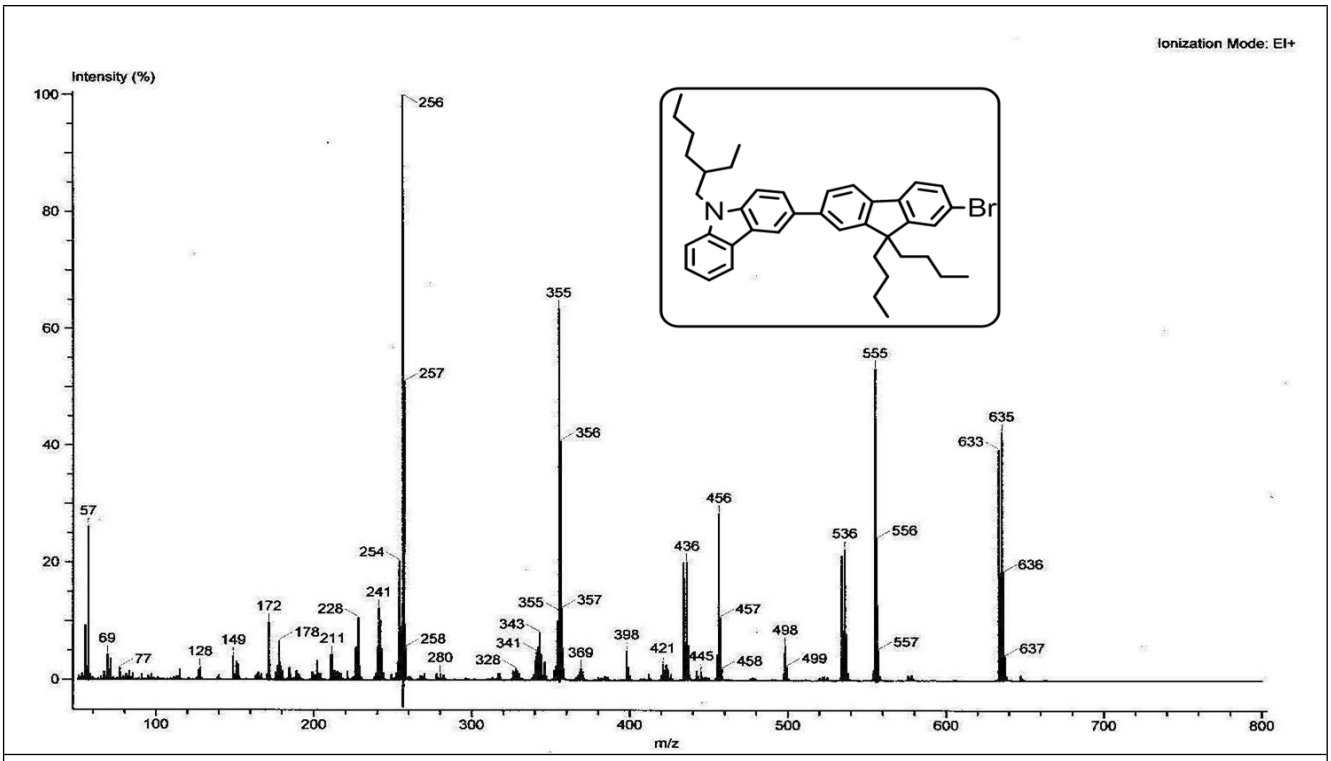
GC-MS Spectrum of 5



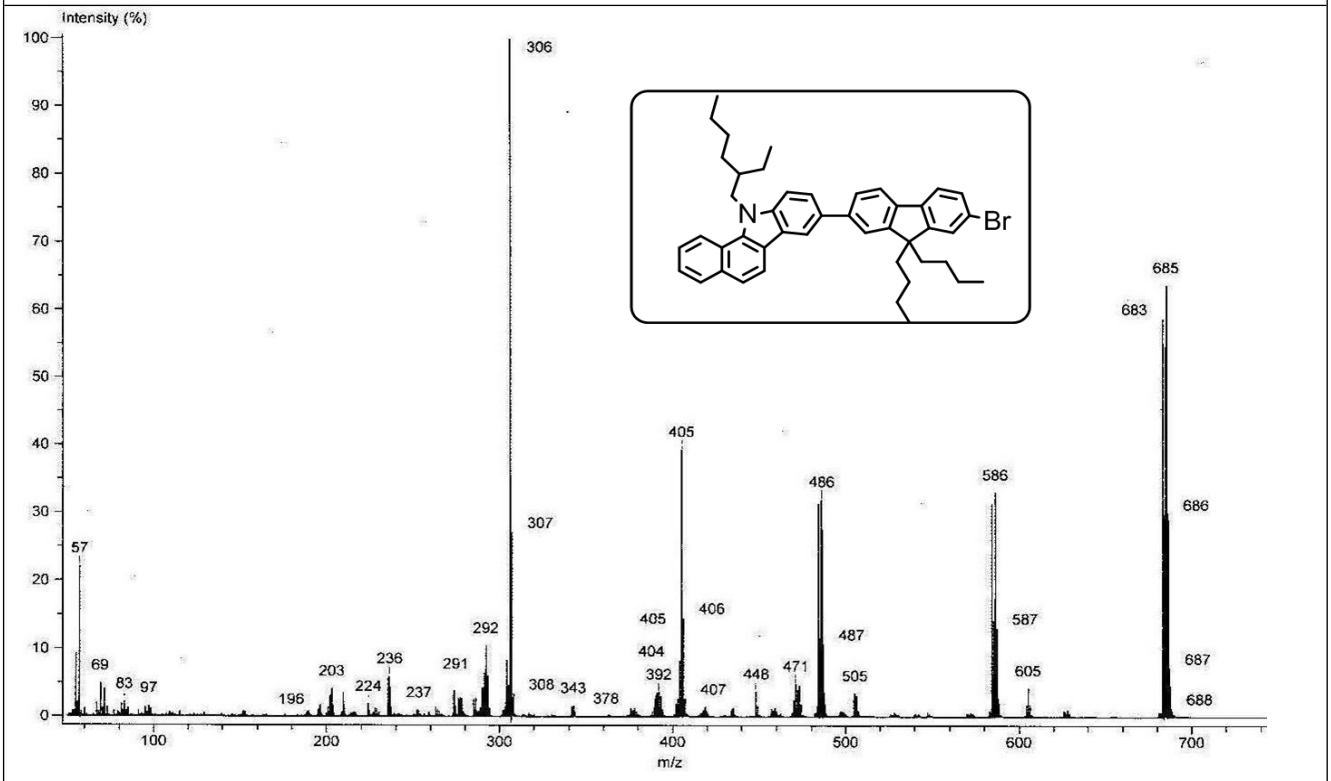
GC-MS Spectrum of 6b



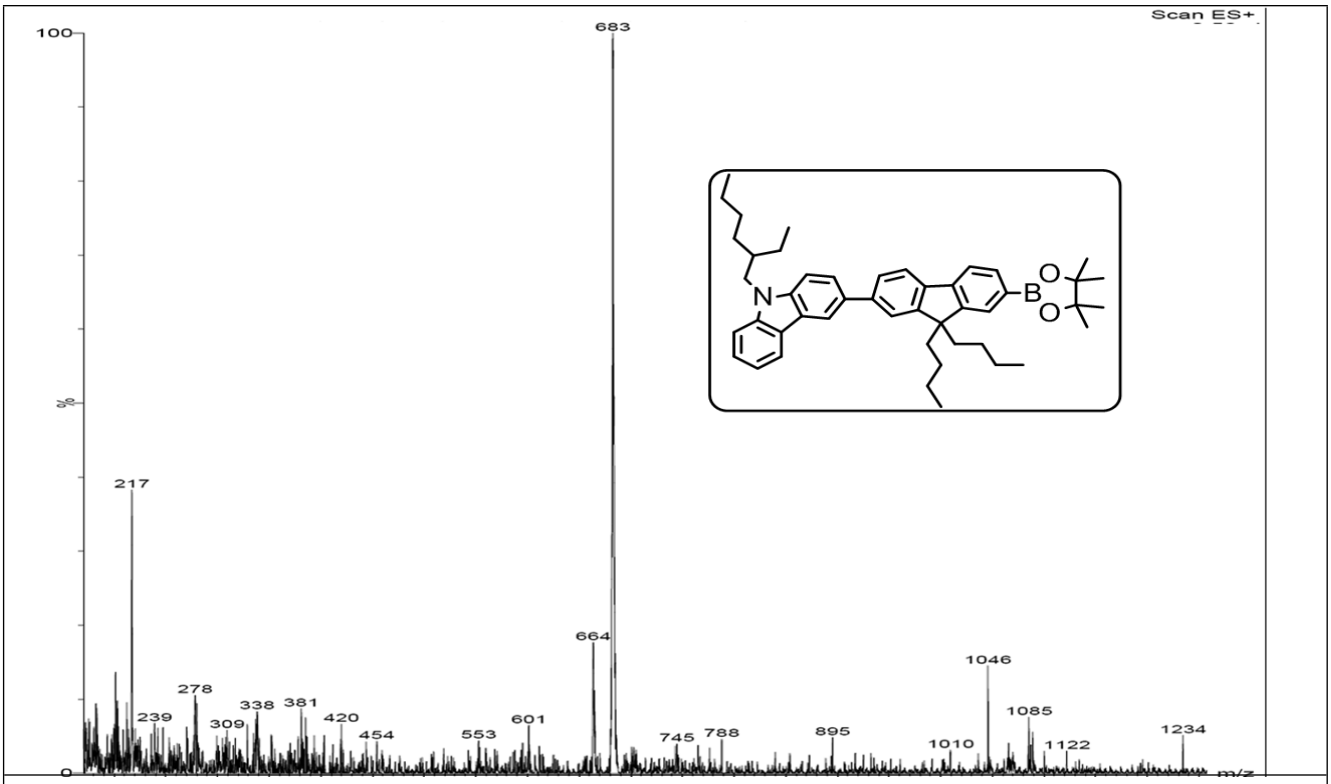
GC-MS Spectrum of 7b



EI-MS spectrum of 8a

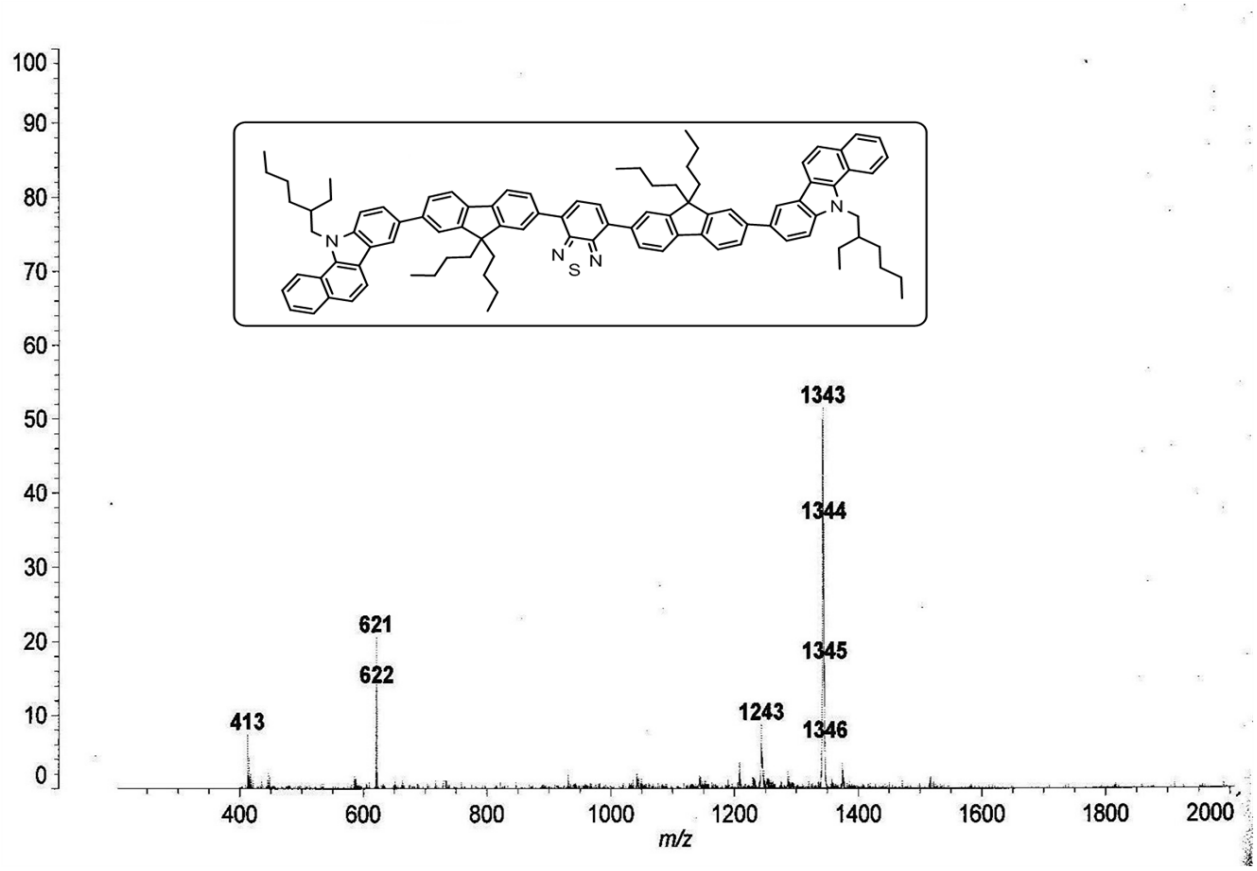


EI-MS spectrum of 8b

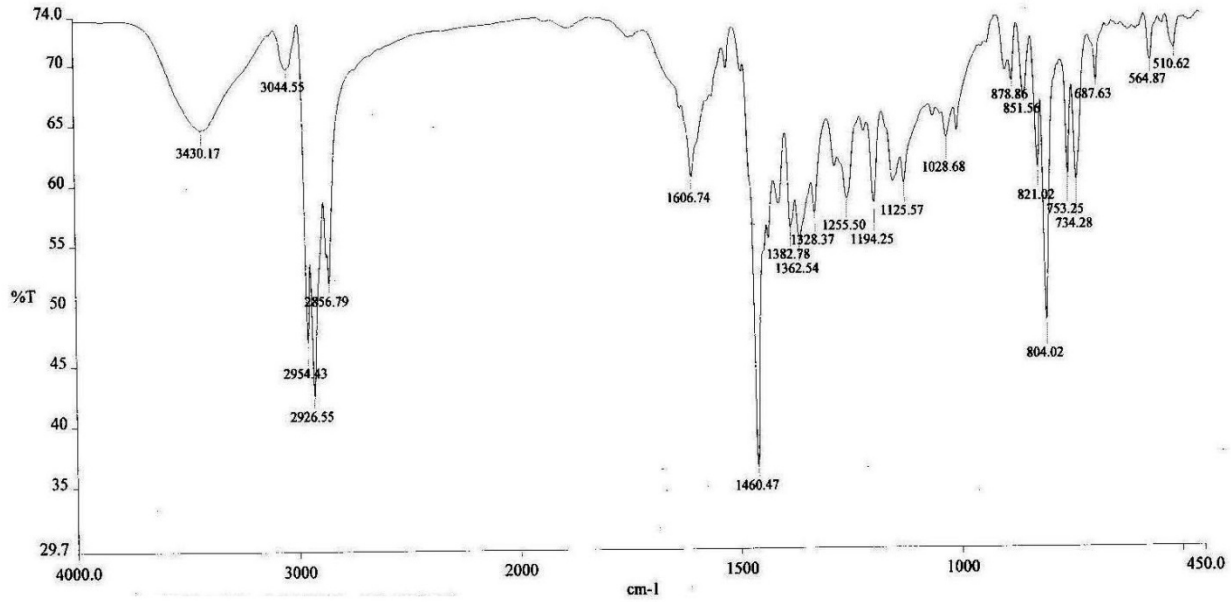


EI-Mass spectrum of molecule 9a

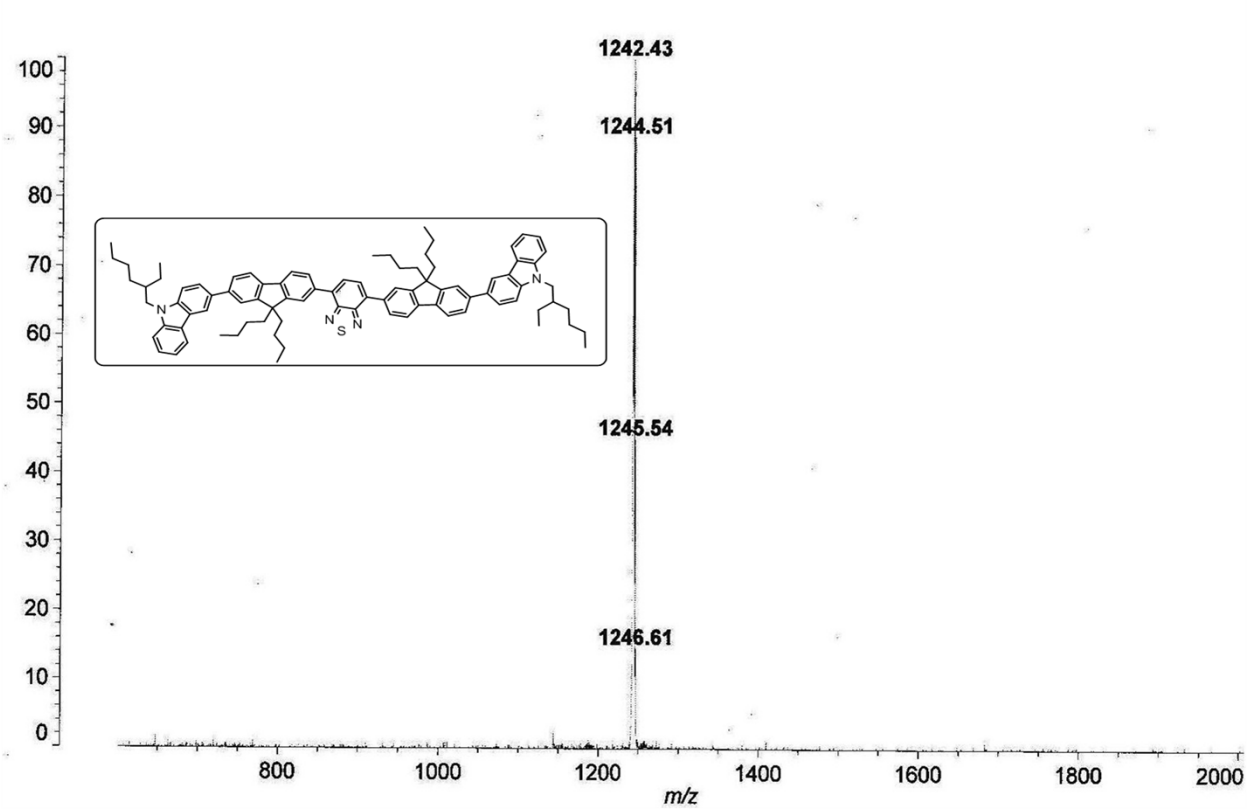
EI-Mass spectrum of molecule 9b



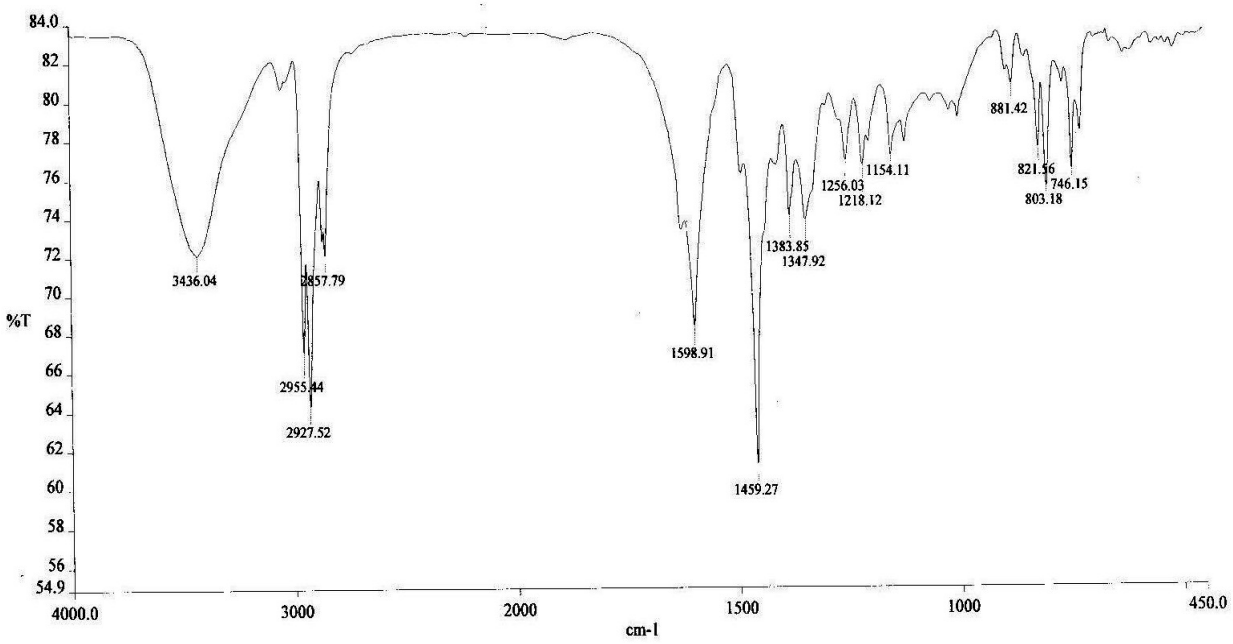
MALDI-TOF mass Spectrum of BFBFB



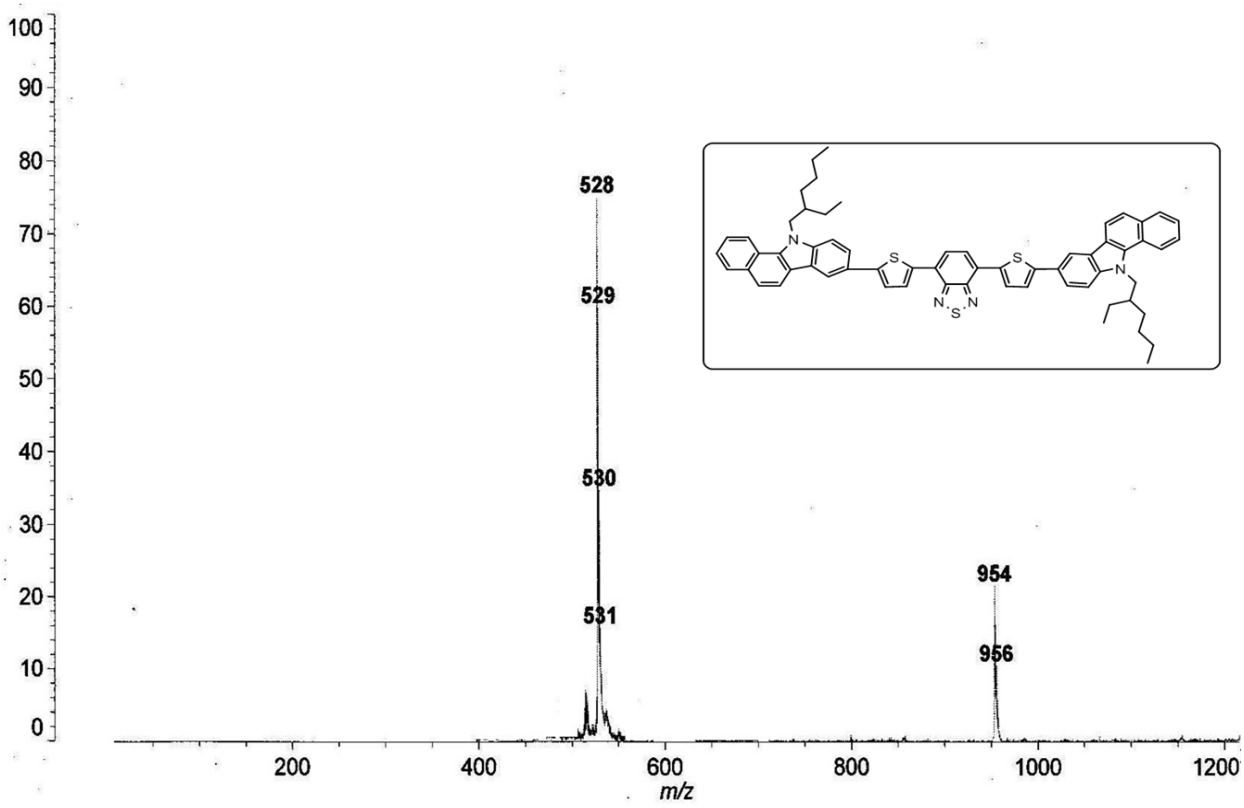
IR Spectrum of BFBFB



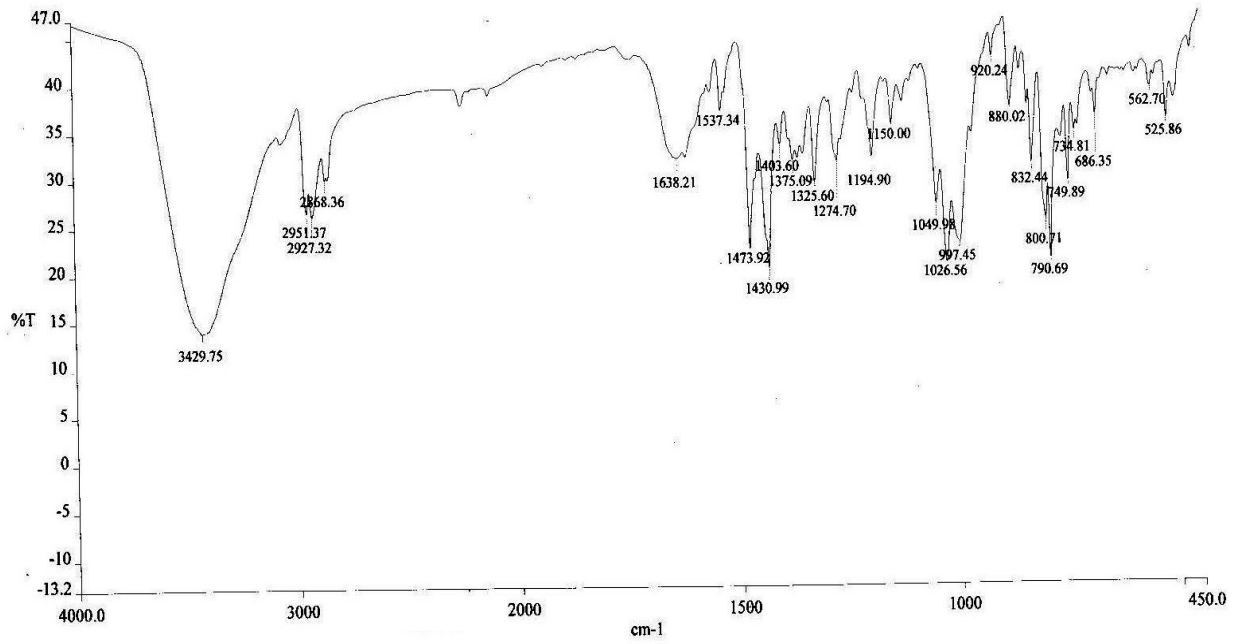
MALDI-TOF mass Spectrum of CFBFC



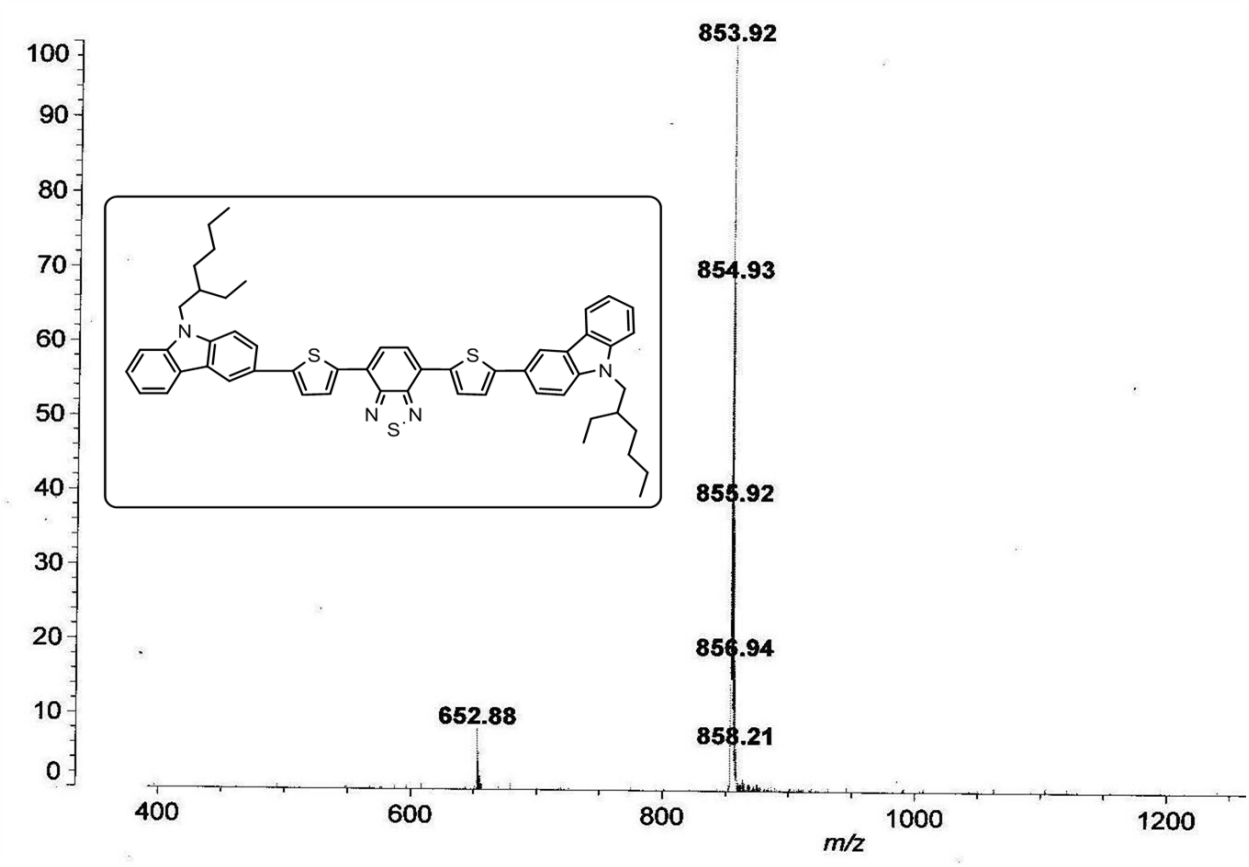
IR Spectrum of CFBFC



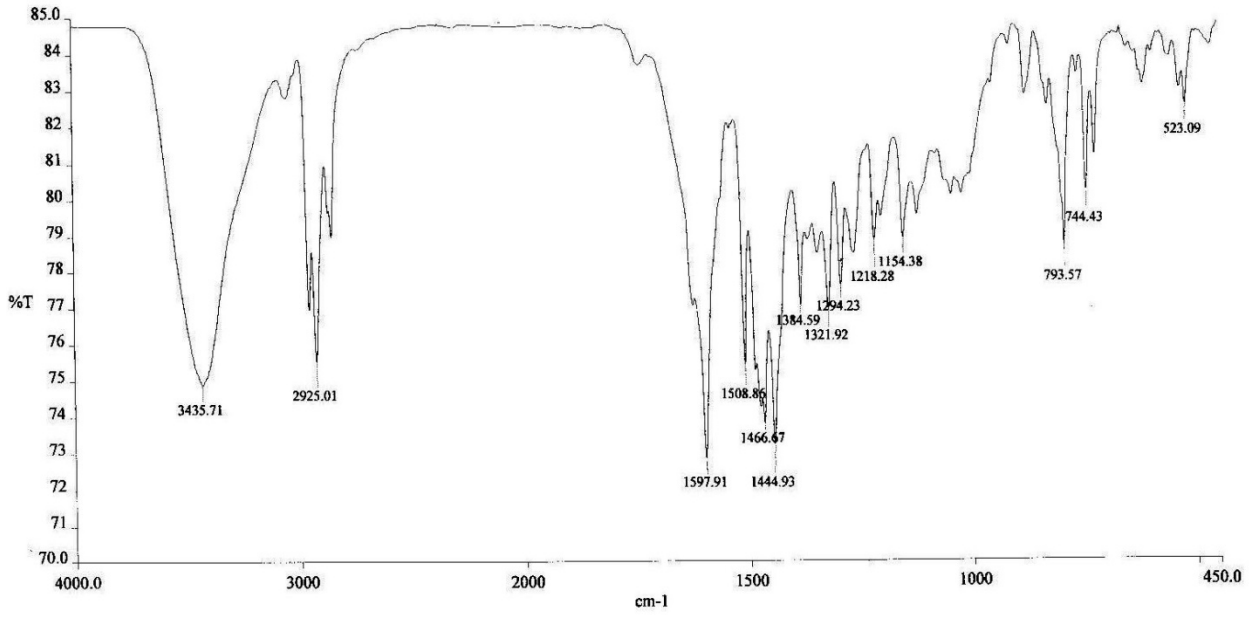
MALDI-TOF mass Spectrum of BTBTB



IR Spectrum of BTBTB



MALDI-TOF mass Spectrum of CTBTC



IR Spectrum of CTBTC