Supporting Information

Panchromatic aza-Bodipy based π-conjugates

Thumuganti Gayathri,[a,c] Ravulakollu Srinivasa Rao,[a,c] Vinay Gupta,[b,c] and Surya Prakash Singh*[a,c]

[a]Polymers and Functional Materials Division, CSIR-Indian Institute of Chemical Technology (IICT), Uppal Road, Tarnaka, Hyderabad, 500007, India.

[b]CSIR-National Physical Laboratory, New Delhi-110012, India.

[c]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, Uttar Pradesh, India.

Contents **Page No.**

1. Cyclic voltammograms of Aza-Bodipy dyes

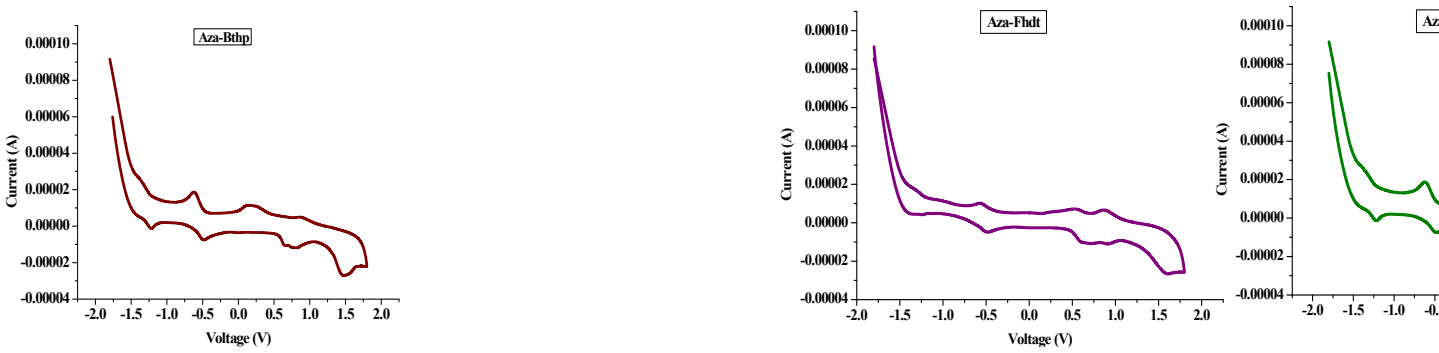


Figure S1 Cyclic voltammograms of Aza-Bthp, Aza-Fhdt and Aza-Sty dyes measured at a scan rate of 100 mV sec^{-1}.

2. Density functional theory - Calculations:

Table S1. Major allowed transitions for the dye Aza-Bthp; calculated by B3LYP/6-311g (d,p) level of theory in chloroform solvent.

Excited State	Wavelength (nm)	Osc.Strength (f)	Maj.contribution
S1	805	0.7752	HOMO->LUMO (99%)
S2	680	0.5776	H-2->LUMO (46%), H-1->LUMO (53%)
S3	679	0.7017	H-2->LUMO (52%), H-1->LUMO (47%)
S4	585	0.0255	H-3->LUMO (98%)
S5	501	0.157	H-4->LUMO (94%)
S6	433	0.6899	HOMO->L+1 (97%)
S7	418	0.0086	HOMO->L+2 (96%)
S8	388	0.0673	H-7->LUMO (57%), H-1->L+1 (22%)
S9	383	0.897	H-2->L+1 (59%), H-1->L+1 (16%)
S10	382	0.2057	H-7->LUMO (15%), H-2->L+1 (19%), H-1>L+1 (50%)

Table S2. Major allowed transitions for the dye Aza-Fhdt; calculated by B3LYP/6-311g (d,p) level of theory in chloroform solvent.

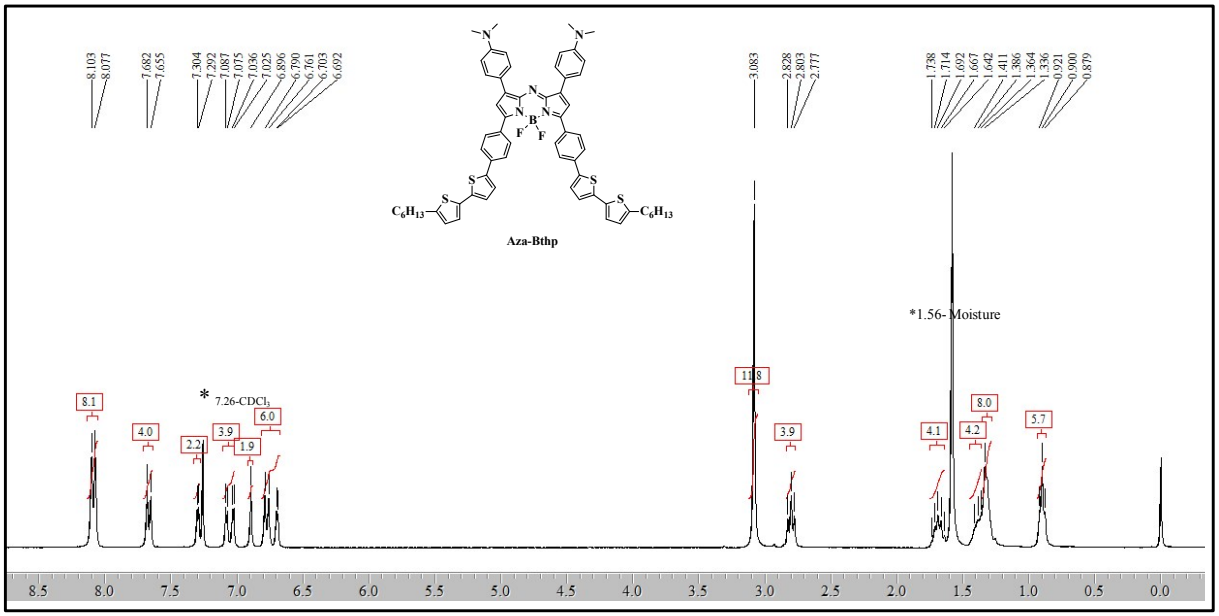
Excited State	Wavelength (nm)	Osc.Strength (f)	Maj.Contribution
S1	854	0.6597	HOMO->LUMO (100%)
S2	734	0.7902	H-2->LUMO (13%), H-1->LUMO (84%)
S3	707	0.3793	H-2->LUMO (84%), H-1->LUMO (13%)
S4	606	0.239	H-3->LUMO (95%), H-1->LUMO (3%)
S5	521	0.1882	H-4->LUMO (93%), H-2->LUMO (3%)
S6	421	0.3824	H-5->LUMO (50%), HOMO->L+1 (43%)
S7	417	1.2911	H-5->LUMO (45%), HOMO->L+1 (46%)
S8	402	0.0391	H-1->L+1 (17%), HOMO->L+2 (72%)
S9	384	0.1373	H-9->LUMO (13%), H-6->LUMO (66%)
S10	383	0.0102	H-2->L+3 (12%), H-1->L+1 (17%), H-1->L+3 (20%), HOMO->L+3 (29%)

Table S3. Major allowed transitions for the dye Aza-Sty; calculated by B3LYP/6-311g (d,p) level of theory in chloroform solvent.

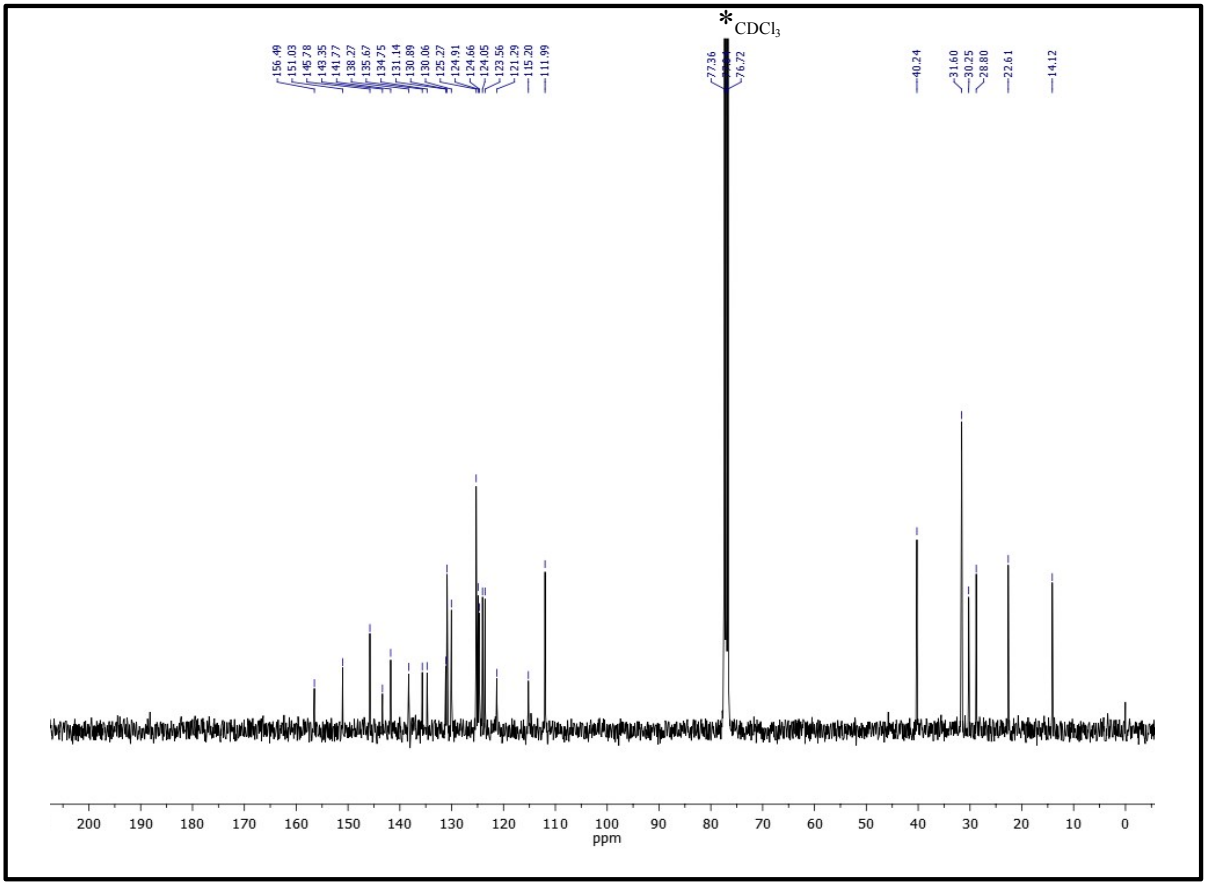
Excited State	Wavelength (nm)	Osc.Strength (f)	Wavelength (nm)
S1	796	0.7042	HOMO->LUMO (98%)
S2	664	0.9952	H-1->LUMO (99%)
S3	645	0.2658	H-2->LUMO (97%)
S4	522	0.1868	H-3->LUMO (96%)
S5	455	0.061	H-4->LUMO (91%)
S6	424	0.8032	HOMO->L+1 (96%)
S7	409	0.0013	HOMO->L+2 (95%)
S8	385	0.021	H-5->LUMO (84%)
S9	375	0.002	H-6->LUMO (94%)
S10	374	0.0043	H-8->LUMO (10%), H-7->LUMO (78%)

3. NMR Spectra

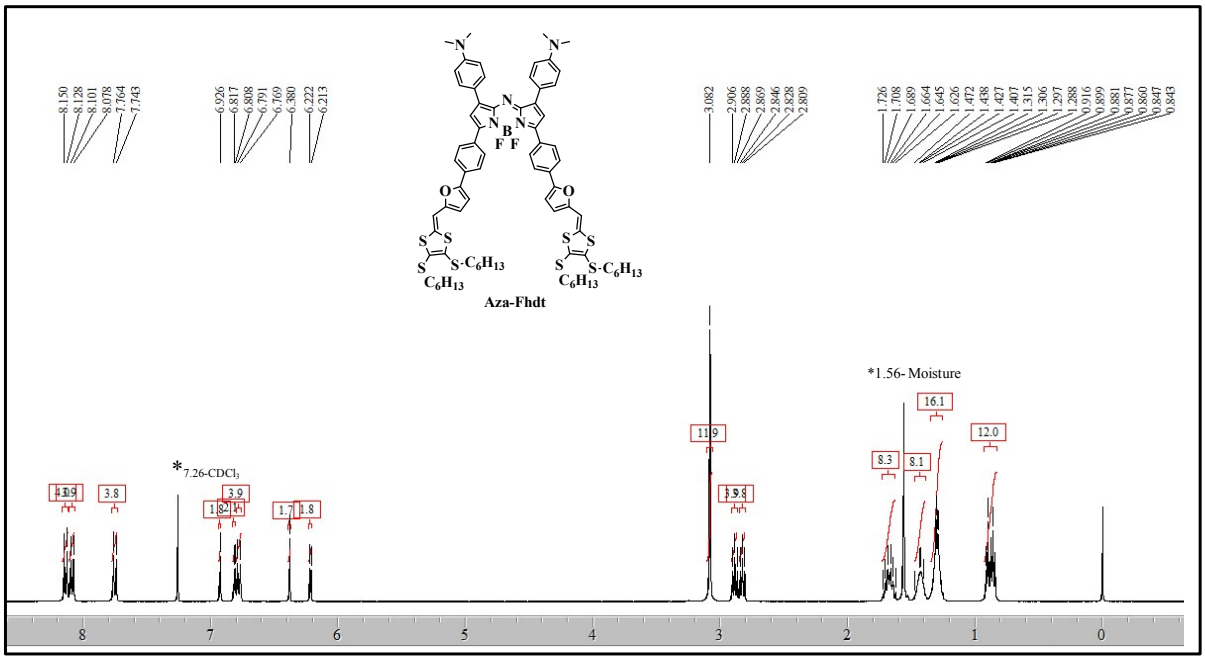
3.1a ^{1}H NMR Spectrum of Aza-Bthp in $CDCl_3$



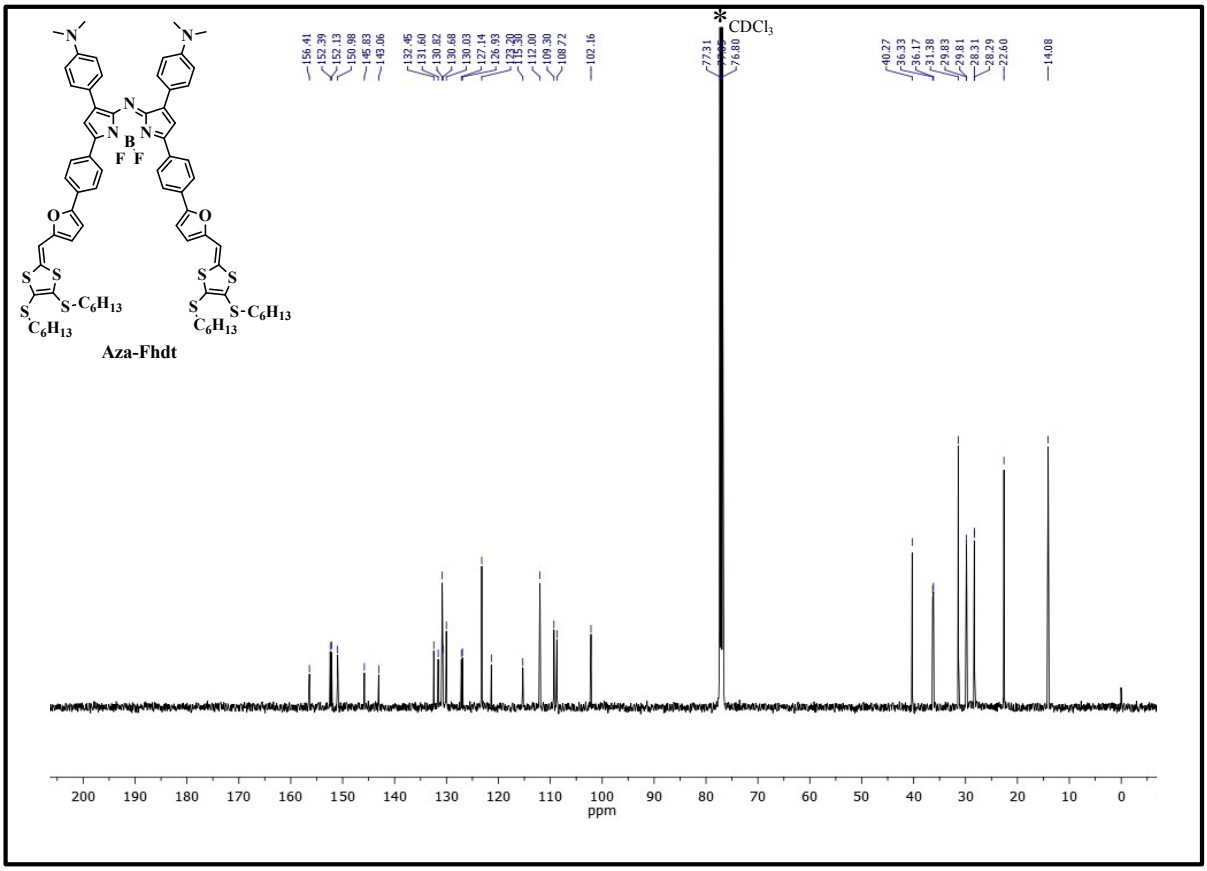
3.1b ^{13}C NMR Spectrum of Aza-Bthp in $CDCl_3$



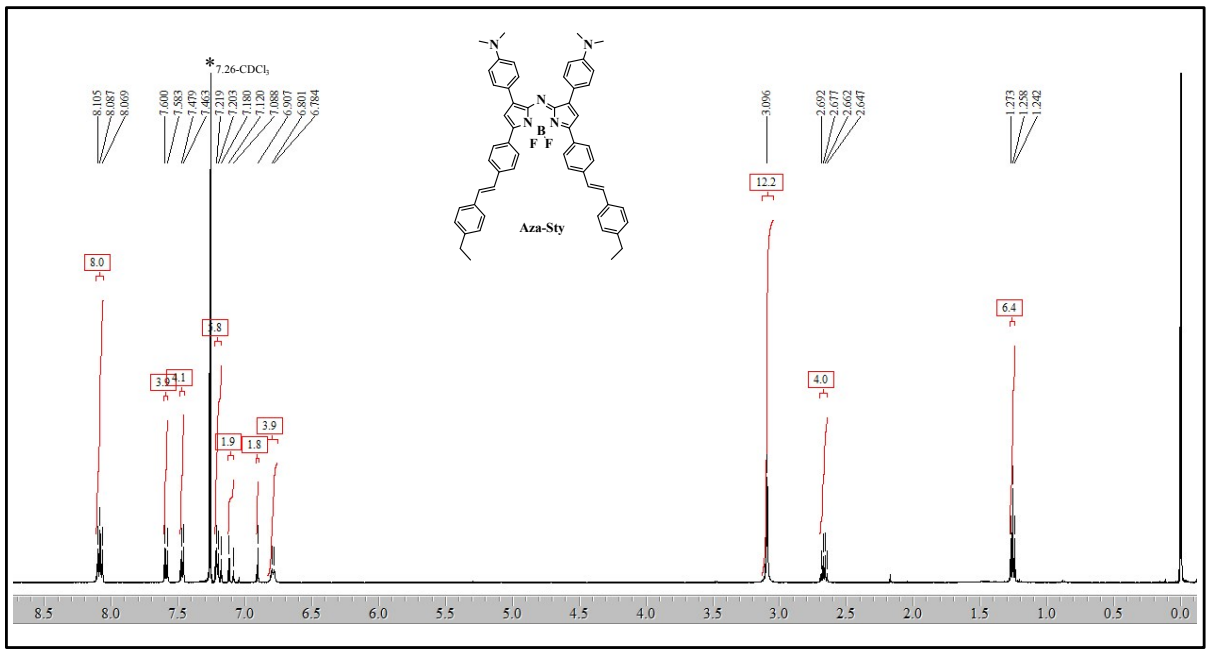
3.2a ^{1}H NMR Spectrum of Aza-Fhdt in $CDCl_3$



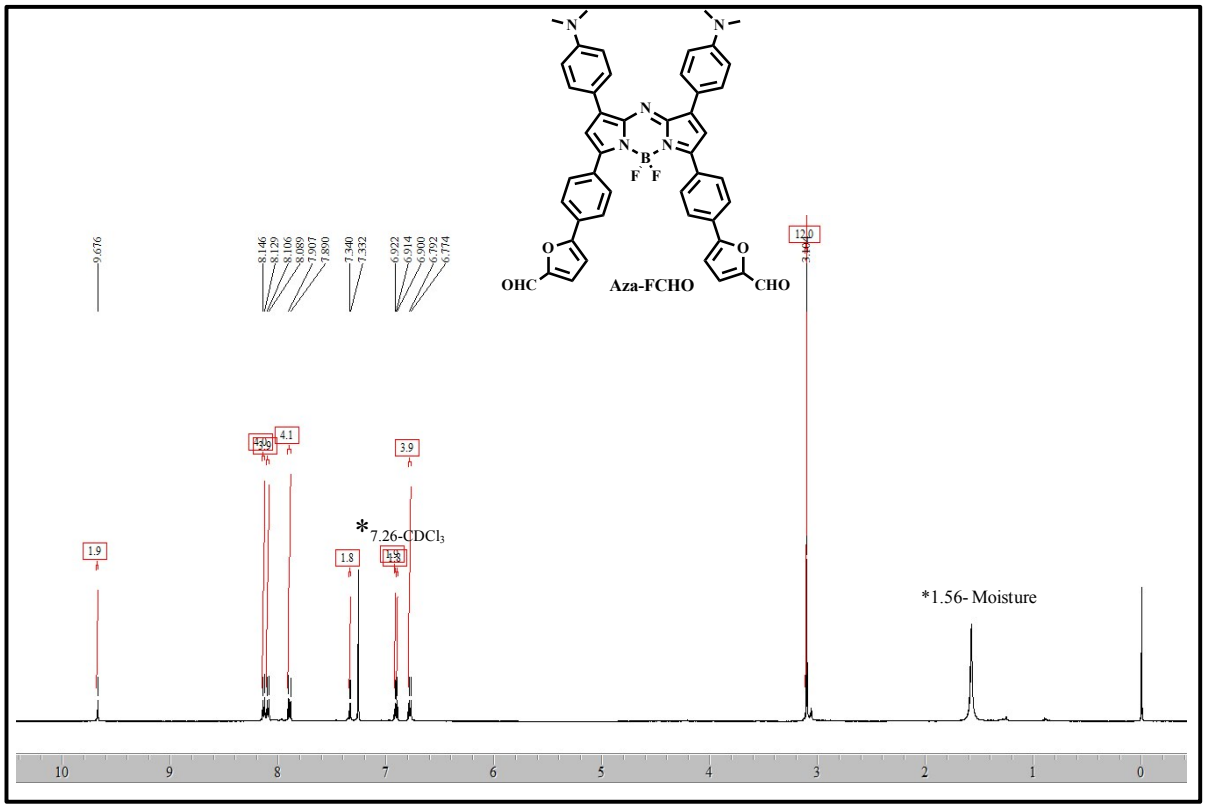
3.2b ^{13}C NMR Spectrum of Aza-Fhdt in $CDCl_3$



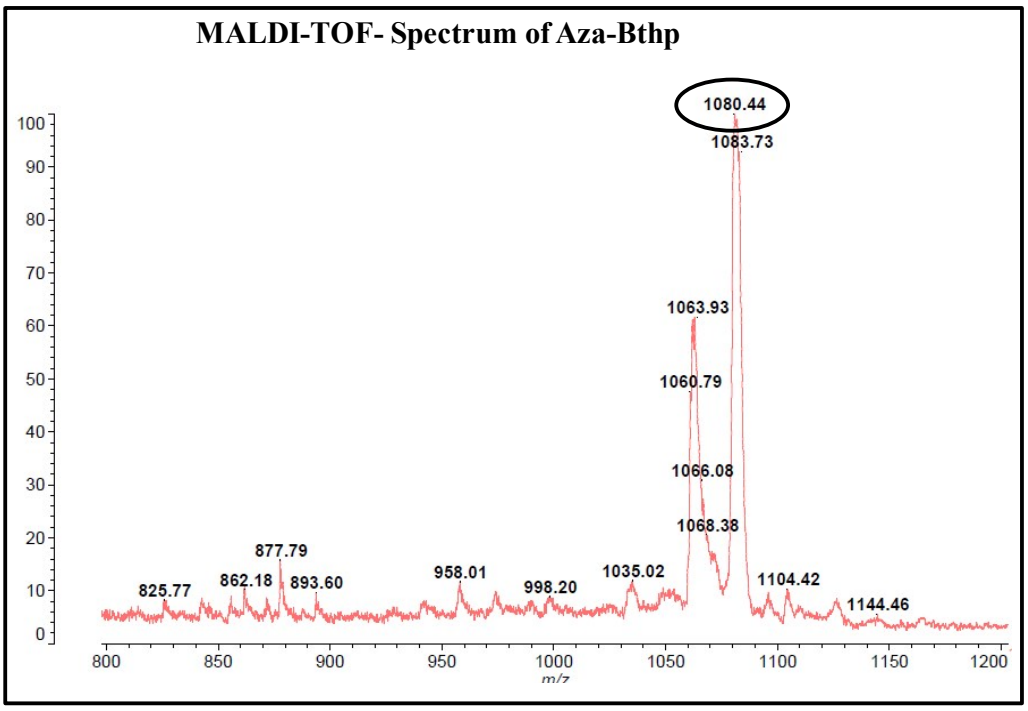
3.3a ^{1}H NMR Spectrum of Aza-Sty in $CDCl_3$

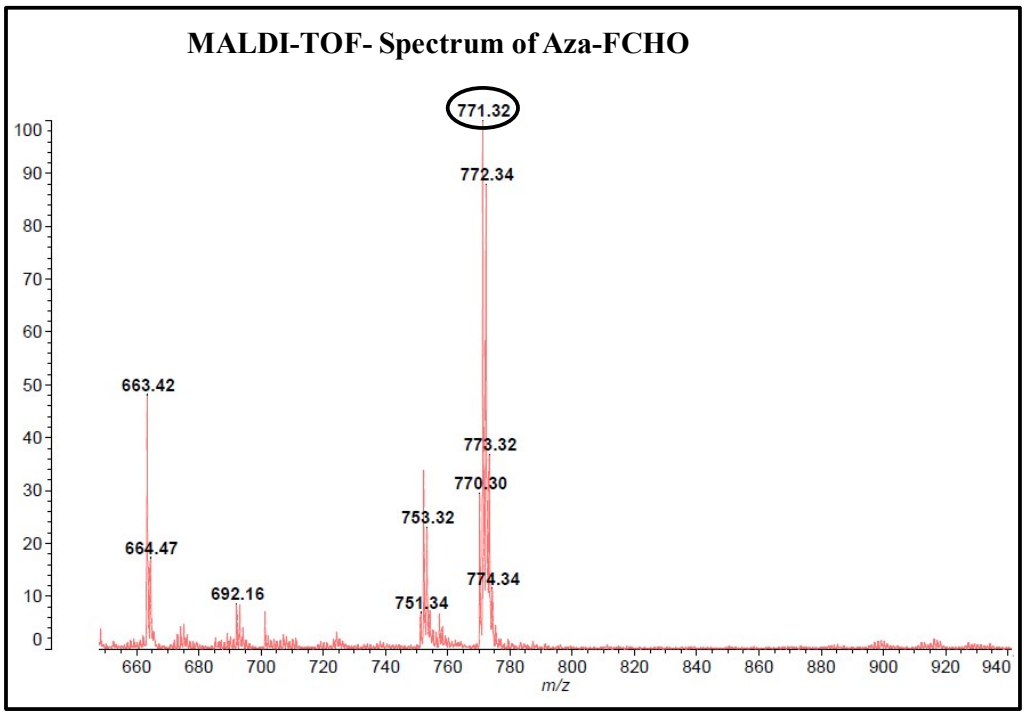


3.4a ^{1}H NMR Spectrum of Aza-FCHO in $CDCl_3$

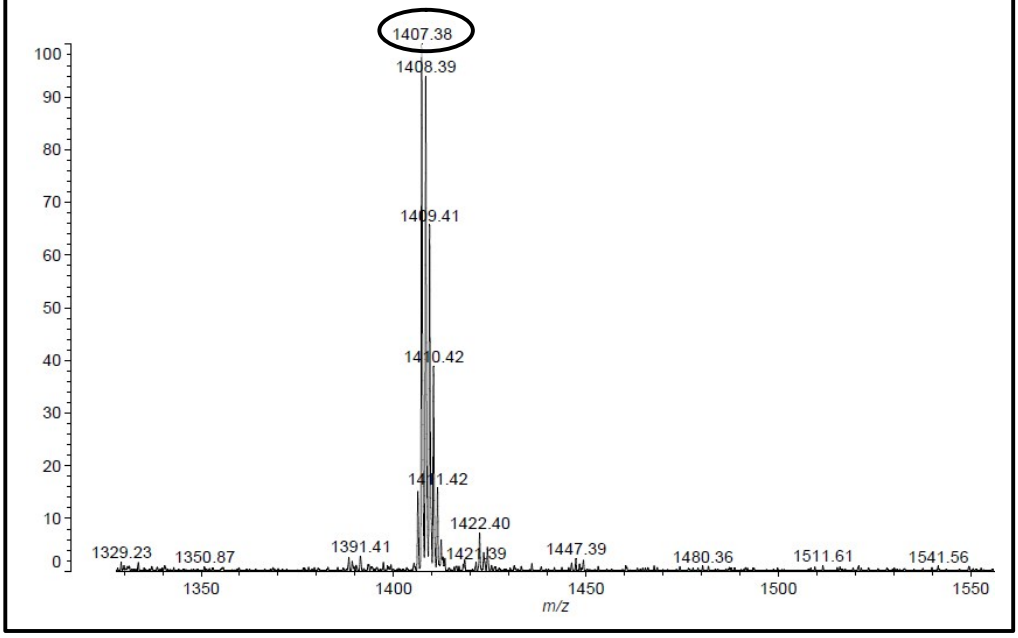


4. MALDI-TOF spectra





MALDI-TOF- Spectrum of Aza-FHDT



MALDI-TOF- Spectrum of Aza-Sty