Supporting Information

Synthesis and Photophysics of Extended π-conjugated systems of substituted 10-aryl-pyrenoimidazoles

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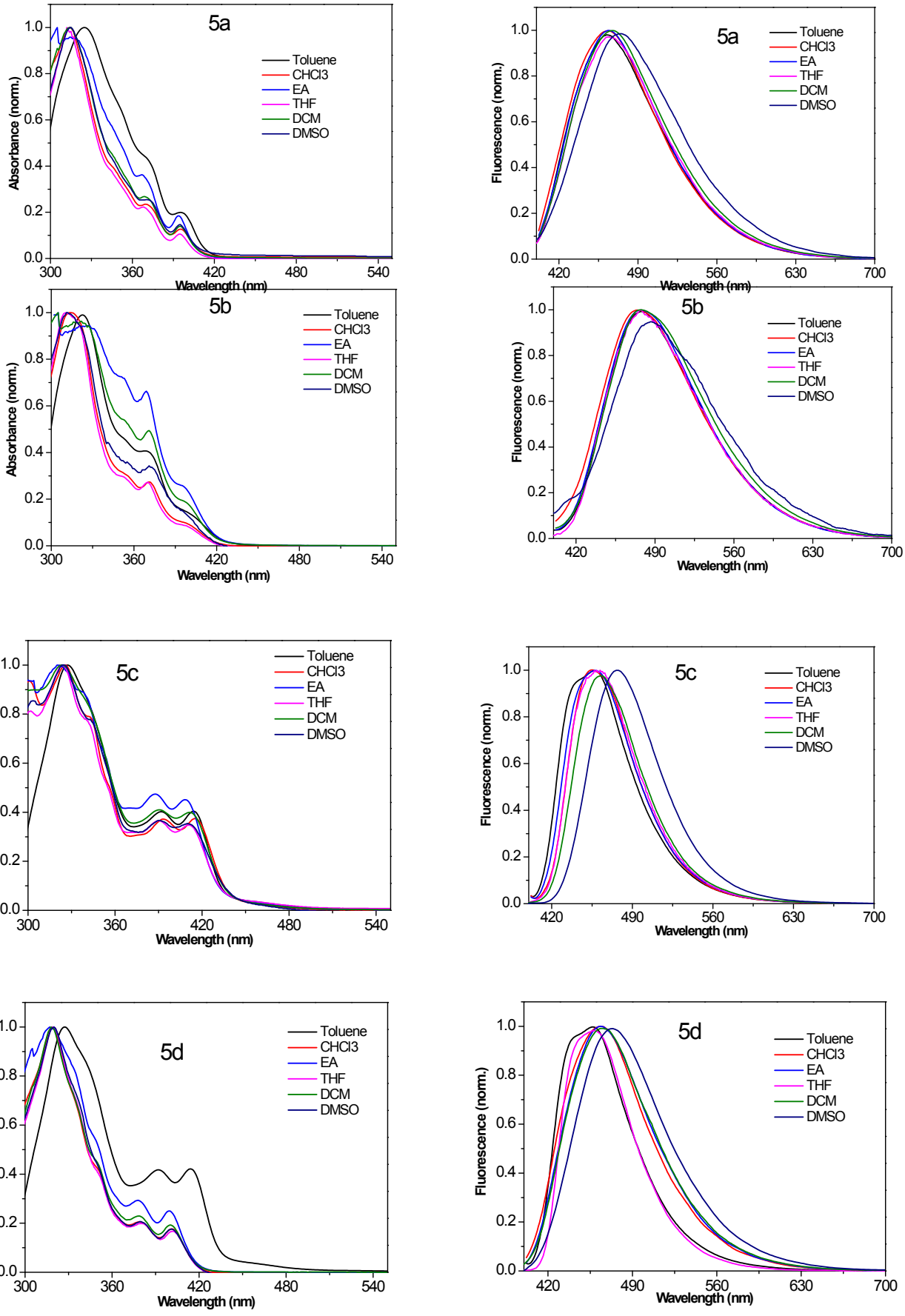
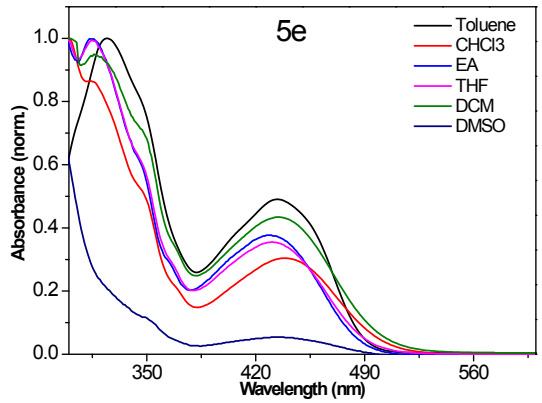
Table S1 Photophysical properties of the compounds **5a-5h** in different solvents

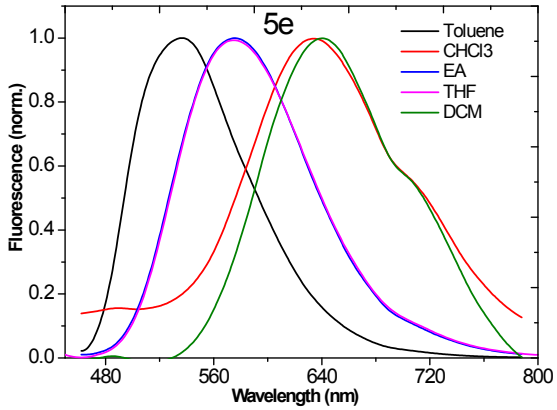
Compounds	λ_{abs}(nm) (ε 10^5 $M^{-1}cm^{-1}$)	Medium	λ_F (nm)	Stokes Shift [cm^{-1}]	Φ_F
5a	395	Toluene	463	3718	0.16
	395	THF	464	3764	…..
	396	DCM	467	3839	0.15
	395	EA	464	3765	0.17
	396	DMSO	475	4199	…..
5b	399	Toluene	478	4142	0.18
	386	THF	476	4244	…..
	400	DCM	479	4123	0.17
	399	EA	476	4054	0.14
	396	DMSO	487	4718	…..
5c	414	Toluene	452	2031	0.26
	411	THF	459	2545	…..
	411	DCM	463	2733	0.38
	408	EA	458	2676	0.24
	410	DMSO	476	3382	…..
5d	414	Toluene	456	2224	0.21
	401	THF	457	3055	…..
	399	DCM	467	3649	0.22
	400	EA	462	3354	0.17
	400	DMSO	475	3947	…..
5e	435	Toluene	535	4296	0.59

	435	DCM	640	7363	0.05
	430	EA	576	5894	0.19
	432	DMSO	707	9003	…..
5f	409	Toluene	446	2028	0.45
	408	THF	456	2579	…..
	409	DCM	462	2804	0.66
	407	EA	455	2592	0.43
	408	DMSO	478	3589	…..
5g	418	Toluene	475	2870	0.33
	415	THF	476	3087	…..
	416	DCM	475	2985	0.39
	414	EA	473	3012	0.29
	415	DMSO	483	3392	…..
5h	408	Toluene	462	2864	0.12
	406	THF	460	2891	…..
	405	DCM	462	3046	0.09
	404	EA	458	2918	0.08
	406	DMSO	467	3217	…..

Fig. S1 UV-Visible absorption and emission spectra of **5a-5h** in different solvents




5e
Toluene
CHCl3
EA
THF
DCM
DMSO
Absorbance (norm.)
Wavelength (nm)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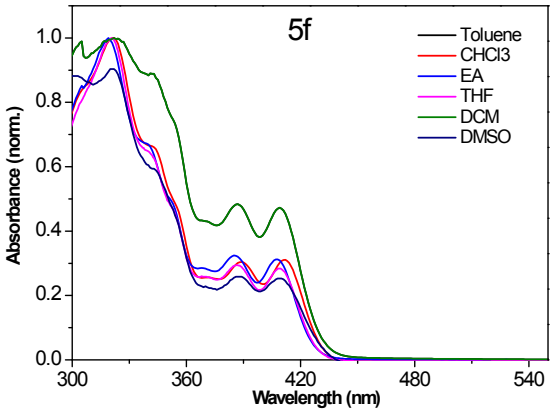
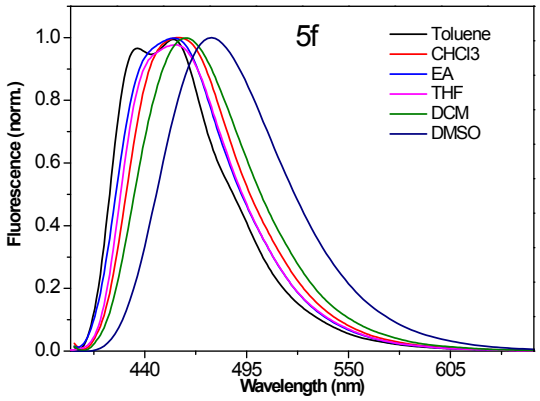
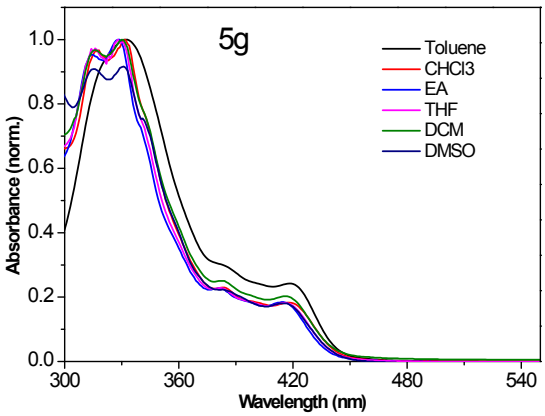
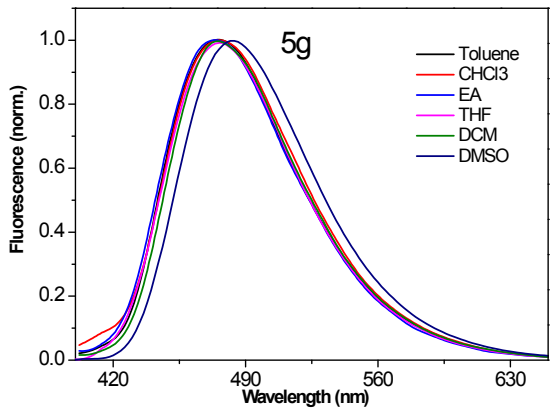
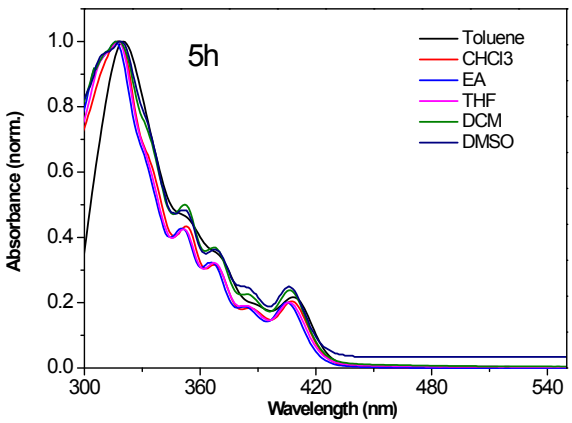
Toluene
CHCl3
EA
THF
DCM
Fluorescence (norm.)
Wavelength (nm)


5f
Toluene
CHCl3
EA
THF
DCM
DMSO
Absorbance (norm.)
Wavelength (nm)


5f
Toluene
CHCl3
EA
THF
DCM
DMSO
Fluorescence (norm.)
Wavelength (nm)


5g
Toluene
CHCl3
EA
THF
DCM
DMSO
Absorbance (norm.)
Wavelength (nm)


5g
Toluene
CHCl3
EA
THF
DCM
DMSO
Fluorescence (norm.)
Wavelength (nm)


5h
Toluene
CHCl3
EA
THF
DCM
DMSO
Absorbance (norm.)
Wavelength (nm)

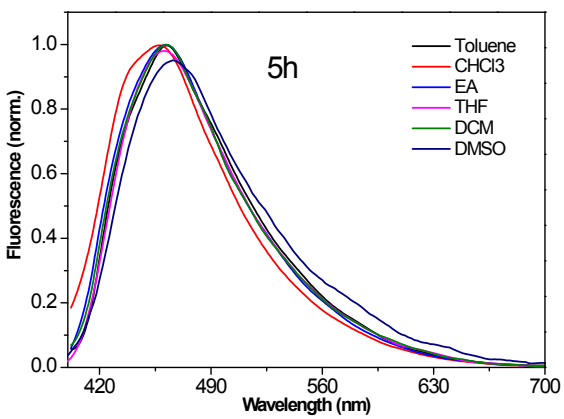
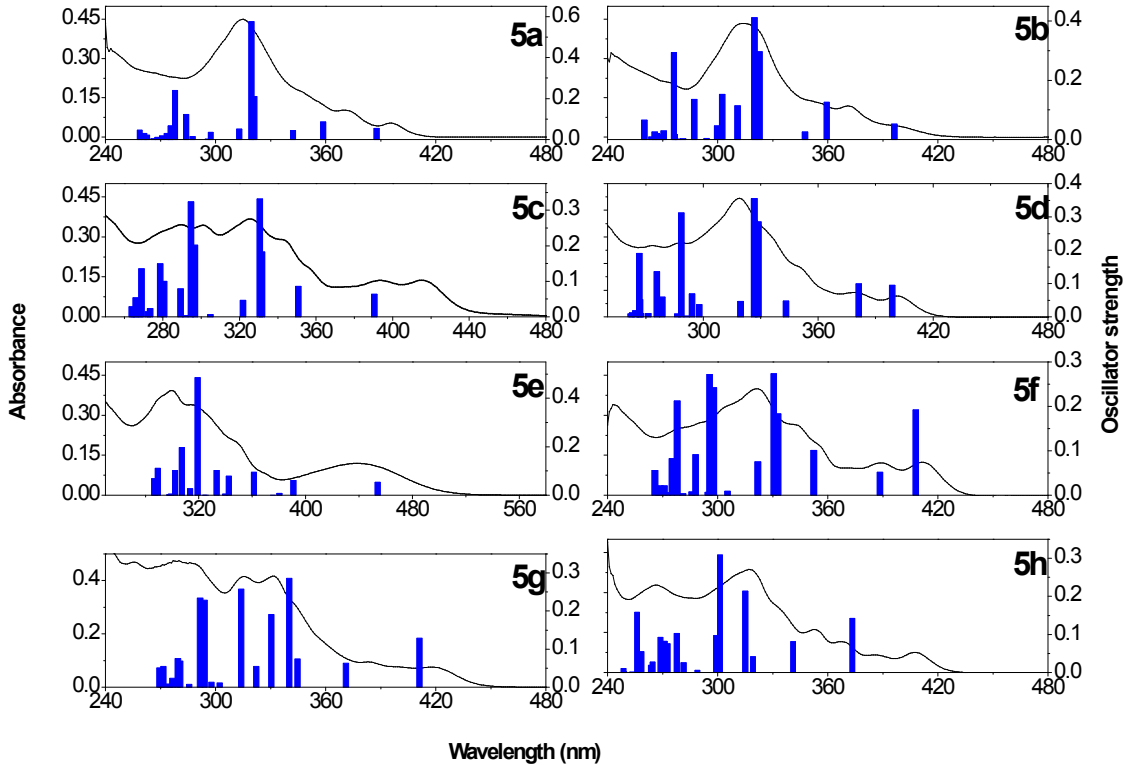

5h
Toluene
CHCl3
EA
THF
DCM
DMSO
Fluorescence (norm.)
Wavelength (nm)

Fig. S2 Absorption spectra of pyrene derivatives **5a-5h** in chloroform.



Calculated (blue) and experimental (black) absorption spectra of pyrene derivatives **5a-5h** in chloroform. The calculations were carried at B3LYP/6-31G*level of theory

Fig. S3 Cyclic voltammograms of pyrene derivatives **5a-5h (**10^{-3}M solutions, scan rate of 100 mVs^{-1} vs Ag/Ag^{+}) in 0.1 M solution of tetrabutylammonium hexafluorophosphate in chloroform solvent.

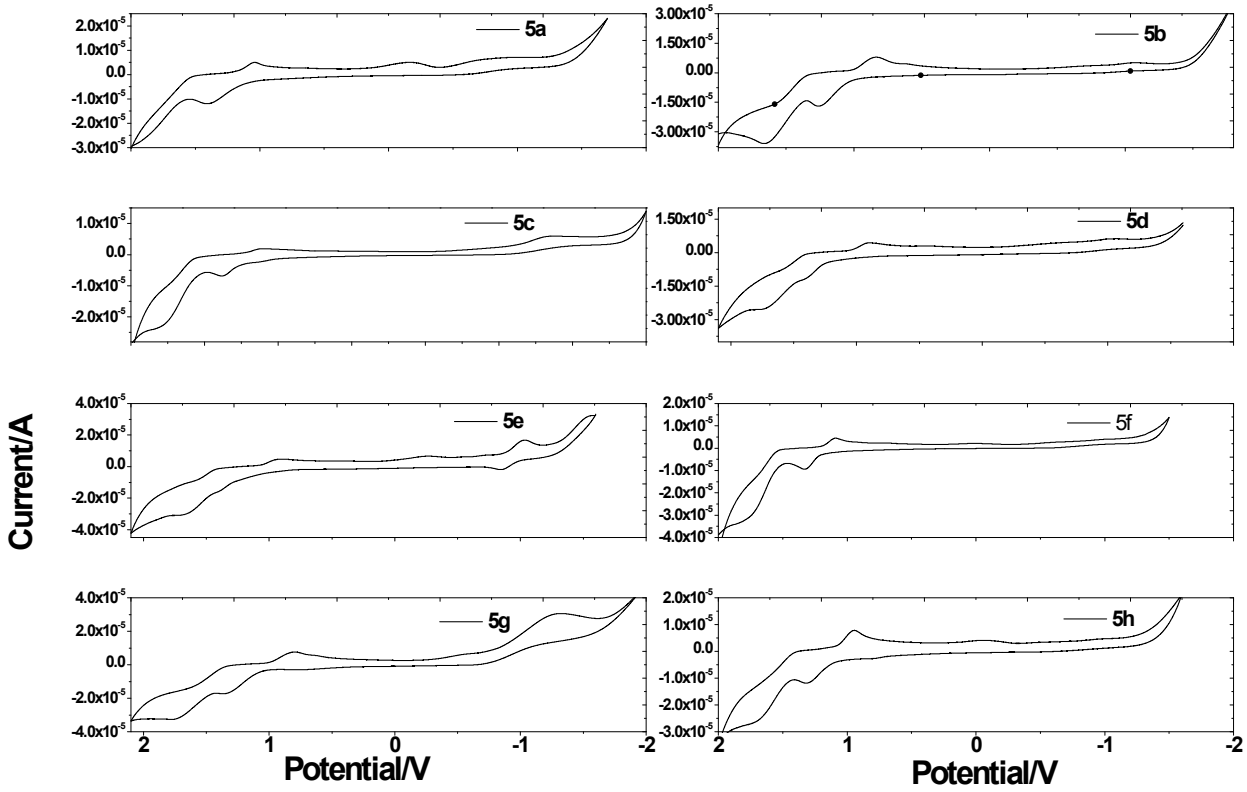
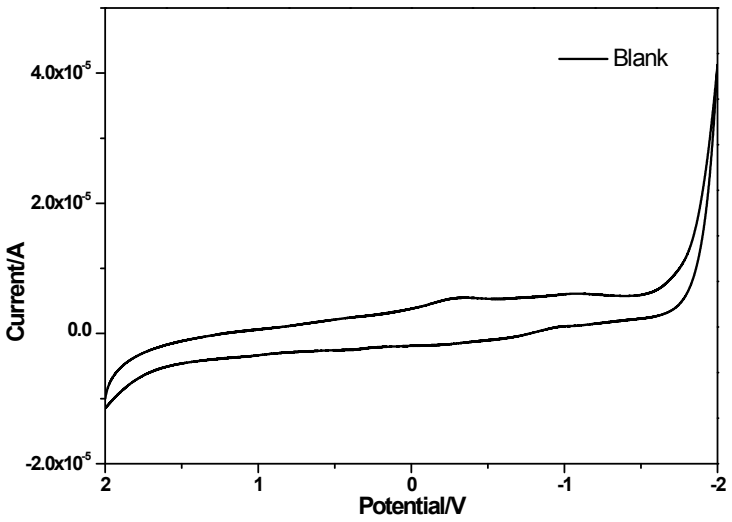


Fig. S4 Cyclic voltammetry background (potential window of chloroform)



CV background was taken in chloroform solvent. Glassy carbon as working electrode, in the presence of 0.1 M tetrabutylammonium hexafluorophosphate as supporting electrolyte.

Fig. S5 Solid state emission spectra of **5b, 5d, 5g** and **5h.**

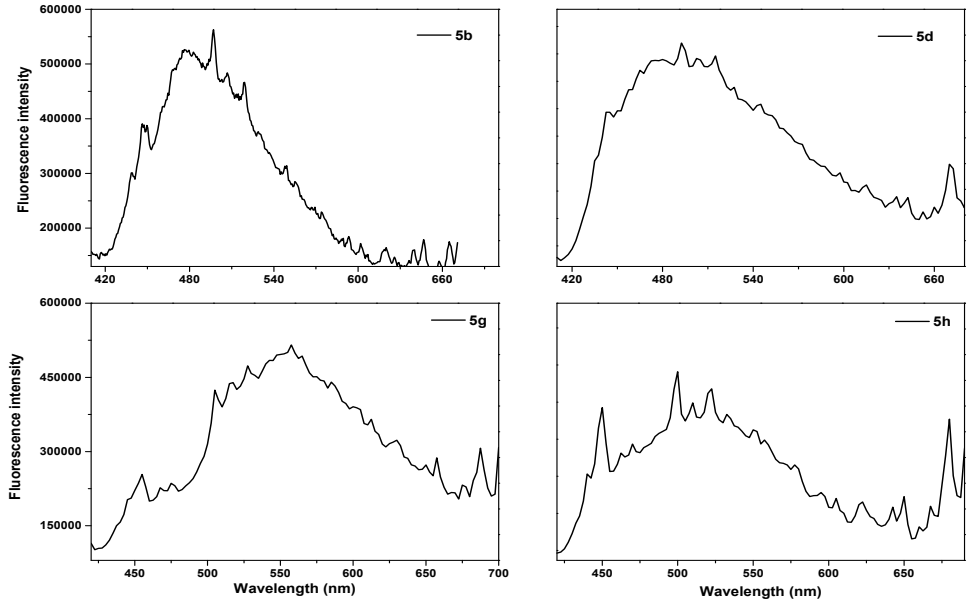
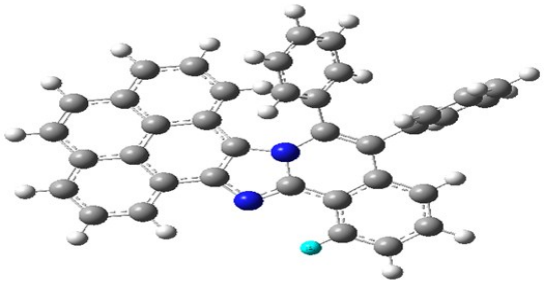
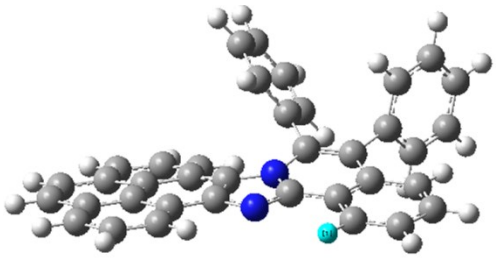
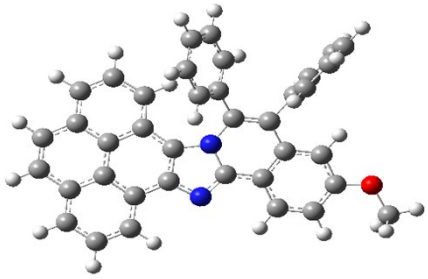
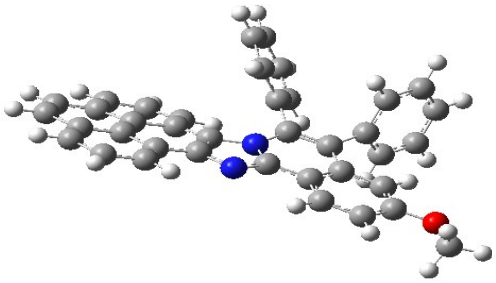
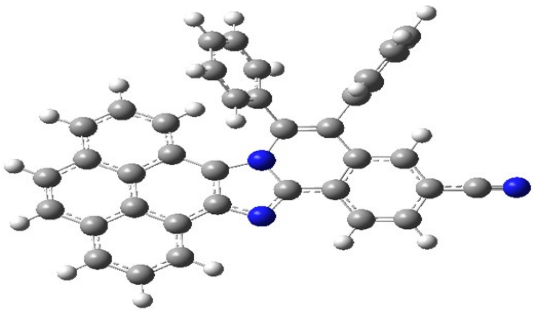
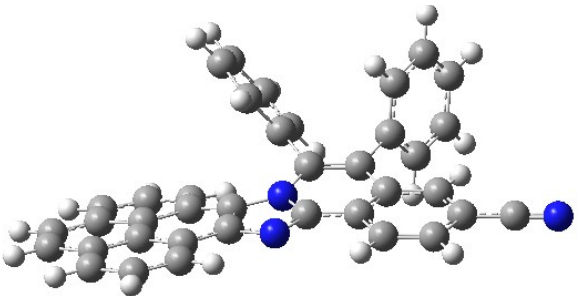
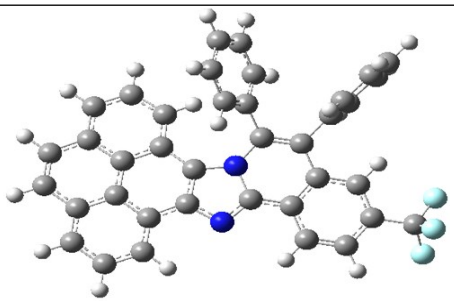
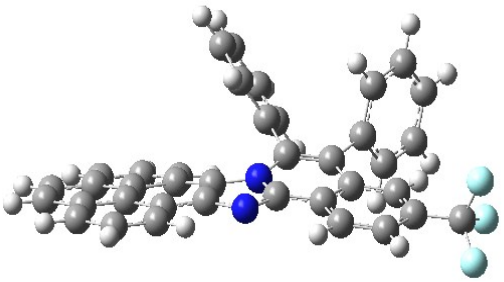
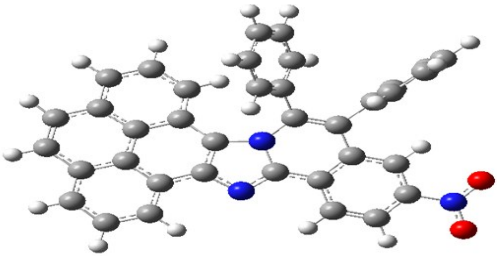
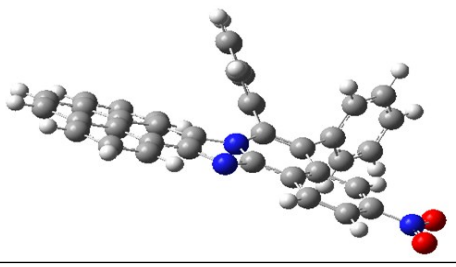


Table S2 Optimized geometries of **5a-5h** calculated at B3LYP/6-31G*

Vertical View	Horizontal view
5a 	
5b 	
5c 	
5d 	
5e 	

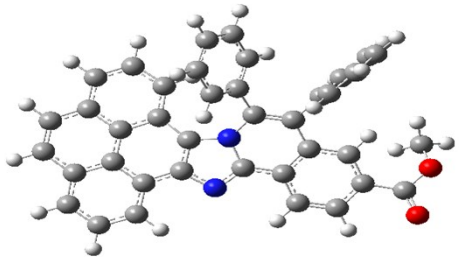
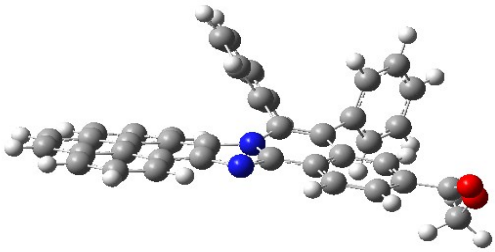
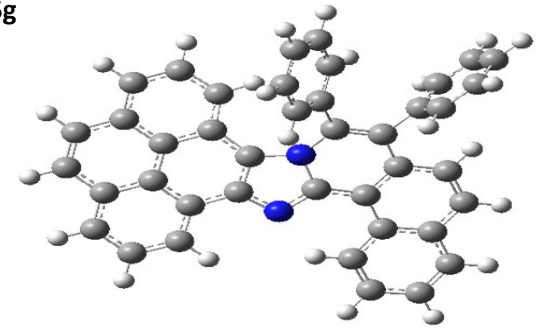
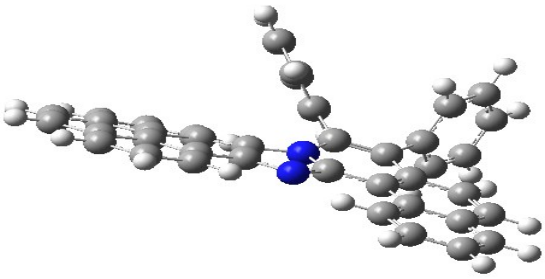
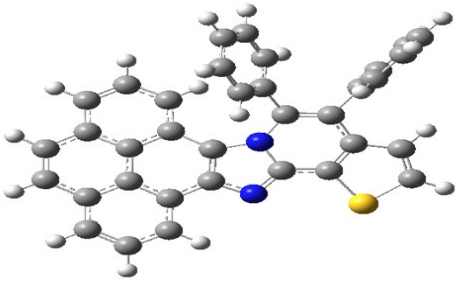
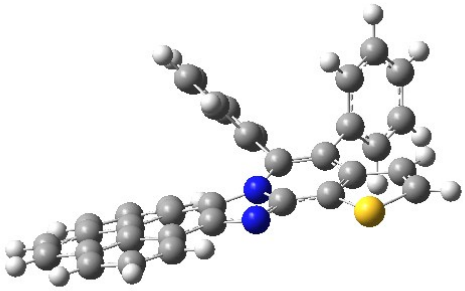
5f 	
5g 	
5h 	

Table S3 Selected transitions obtained from TD-DFT calculations

Compounds	Wavelength (nm)	Osc. Strength	Major Contributions
5a	387.82	0.0542	HOMO->LUMO (58%), HOMO->L+1 (31%)
	358.56	0.0852	H-1->LUMO (13%), HOMO->LUMO (21%), HOMO->L+1 (37%), HOMO->L+2 (15%)
	321.08	0.2102	H-1->L+1 (48%), HOMO->L+2 (13%)
	319.58	0.5742	H-1->LUMO (55%), HOMO->L+2 (18%)
	283.90	0.123	H-3->LUMO (22%), H-3->L+1 (16%), H-2->LUMO (28%)
	277.95	0.2396	H-2->L+1 (48%), HOMO->L+7 (25%)

Compounds	Wavelength (nm)	Osc. Strength	Major Contributions
5b	396.29	0.0526	HOMO->LUMO (69%), HOMO->L+1 (22%)
	359.40	0.126	H-1->LUMO (12%), HOMO->LUMO (15%), HOMO->L+1 (46%), HOMO->L+2 (12%)
	322.78	0.2964	H-1->LUMO (38%), H-1->L+1 (19%), HOMO->L+3 (11%)
	320.08	0.4113	H-1->LUMO (14%), H-1->L+1 (23%), HOMO->L+2 (27%), HOMO->L+3 (10%)
	310.82	0.1133	H-3->LUMO (14%), H-2->LUMO (12%), H-1->L+1 (29%), HOMO->L+3 (21%)
	302.45	0.1522	H-2->LUMO (52%), HOMO->L+3 (18%)
	287.25	0.1349	H-3->LUMO (45%), H-2->L+1 (12%), H-1->L+2 (19%)
	276.14	0.2939	H-3->LUMO (10%), H-3->L+1 (39%), HOMO->L+5 (11%)

Compounds	Wavelength (nm)	Osc. Strength	Major Contributions
5c	407.4245	0.181	HOMO->LUMO (70%), HOMO->L+1 (17%)
	331.6836	0.1821	H-1->LUMO (11%), HOMO->L+2 (41%)
	330.7016	0.3312	H-1->L+1 (61%)
	296.8026	0.2018	H-2->L+1 (22%), H-1->L+2 (37%), HOMO->L+3 (14%)
	294.6722	0.3231	H-3->LUMO (55%), H-2->L+1 (18%)
	280.7022	0.1001	H-2->L+1 (11%), HOMO->L+5 (39%), HOMO->L+6 (11%)
	278.4766	0.1494	H-4->L+1 (10%), H-2->L+1 (12%), HOMO->L+5 (26%)

Compounds	Wavelength (nm)	Osc. Strength	Major Contributions
5d	398.5962	0.0942	HOMO->LUMO (54%), HOMO->L+1 (34%)
	381.1705	0.099	HOMO->LUMO (30%), HOMO->L+1 (48%)
	328.6329	0.2852	H-1->LUMO (16%), H-1->L+1 (53%)
	326.6071	0.355	H-1->LUMO (17%), H-1->L+1 (11%), HOMO->L+2 (39%)
	288.5346	0.312	H-3->LUMO (29%), H-2->L+1 (22%), HOMO->L+3 (11%), HOMO->L+4 (11%)
	275.7514	0.1356	H-4->L+1 (18%), H-2->L+1 (11%), H-2->L+2 (11%), HOMO->L+5 (17%)
	266.5277	0.1902	H-4->LUMO (14%), H-4->L+1 (25%), H-1->L+3 (10%), HOMO->L+6 (13%)

Compounds	Wavelength (nm)	Osc. Strength	Major Contributions
5e	533.927637	0.19	HOMO->LUMO (92%)
	333.324381	0.1027	H-1->L+2 (18%), HOMO->L+2 (34%), HOMO->L+3 (17%)
	318.985635	0.4847	H-1->L+1 (42%), H-1->L+2 (16%), HOMO->L+3 (10%)
	307.155547	0.1963	H-1->L+2 (17%), HOMO->L+3 (42%), HOMO->L+4 (20%)
	302.059486	0.1023	H-2->L+1 (25%), H-1->L+2 (34%), HOMO->L+4 (17%)
	289.335924	0.1108	H-9->LUMO (10%), H-3->L+1 (63%)

Compounds	Wavelength (nm)	Osc. Strength	Major Contributions
5f	408.001	0.1923	HOMO->LUMO (76%), HOMO->L+1 (12%)
	352.3655	0.1005	H-1->LUMO (71%), HOMO->L+2 (16%)
	332.8859	0.1833	HOMO->L+2 (48%)
	330.6046	0.2731	H-1->L+1 (62%), HOMO->L+3 (12%)
	297.9438	0.2423	H-2->LUMO (10%), H-2->L+1 (14%), H-1->L+2 (29%), HOMO->L+3 (20%)
	295.5855	0.2721	H-3->LUMO (55%), H-2->L+1 (15%)

Compounds	Wavelength (nm)	Osc. Strength	Major Contributions
5g	373.4213	0.1424	HOMO->LUMO (87%)
	315.0864	0.2132	H-1->LUMO (61%), HOMO->L+1 (20%)
	301.2156	0.3084	H-1->L+1 (24%), HOMO->L+2 (51%)
	277.7031	0.103	H-3->LUMO (40%), H-2->LUMO (18%), H-1->L+2 (17%)

	256.1375	0.1585	H-2->L+1 (15%), H-1->L+3 (10%), H-1->L+4 (47%)
	373.4213	0.1424	HOMO->LUMO (87%)

Compounds	Wavelength (nm)	Osc. Strength	Major Contributions
5h	411.1671	0.129	HOMO->LUMO (88%)
	340.165	0.2859	H-1->LUMO (47%), HOMO->L+1 (17%), HOMO->L+2 (13%)
	330.4284	0.1913	H-2->LUMO (10%), H-1->L+1 (38%), HOMO->L+2 (14%)
	313.9057	0.2577	H-2->LUMO (31%), H-1->L+1 (17%), HOMO->L+3 (27%)
	293.9805	0.2282	H-2->L+1 (41%), H-1->L+2 (25%), HOMO->L+4 (14%)
	291.6226	0.2347	H-3->LUMO (21%), H-3->L+1 (12%), H-2->L+1 (17%), H-1->L+2 (26%)

Selected transitions obtained from TD-DFT calculation at B3LYP/6-31G* level

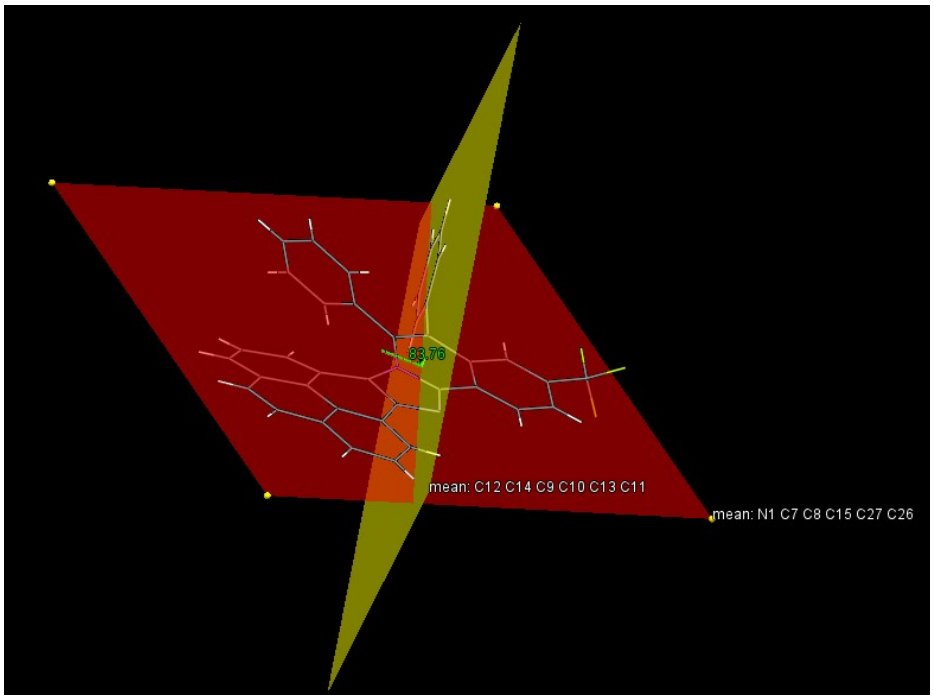
Table S4 Crystallographic data and structure refinement details for **5d** and **5f**

Identification code	**5d**	**5f**
CCDC No.	CCDC1497027	CCDC1059272
Empirical formula	C_{38} H_{21} F_3 N_2	C_{39} H_{24} N_2 O_2
Formula weight	562.57	552.60
Temperature	295 K	293 K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Mono clinic	triclinic
Space group	*P*21/n	*P*-1
a	9.5058(10) Å	10.877(5) Å
b	16.1683(16) Å	11.117(5) Å
c	17.7882(17) Å	11.854(5) Å
α	90°	97.983(5)°
β	93.270(3)°	103.313(5)°
γ	90°	94.203(5)°
Volume	2729.5(5) Å	1373.1(11) Å
Z, calculated density	4, 1.369 mg m^{-3}	2, 1.337 mg m^{-3}
Absorption coefficient	0.094 mm^{-1}	0.083 mm^{-1}

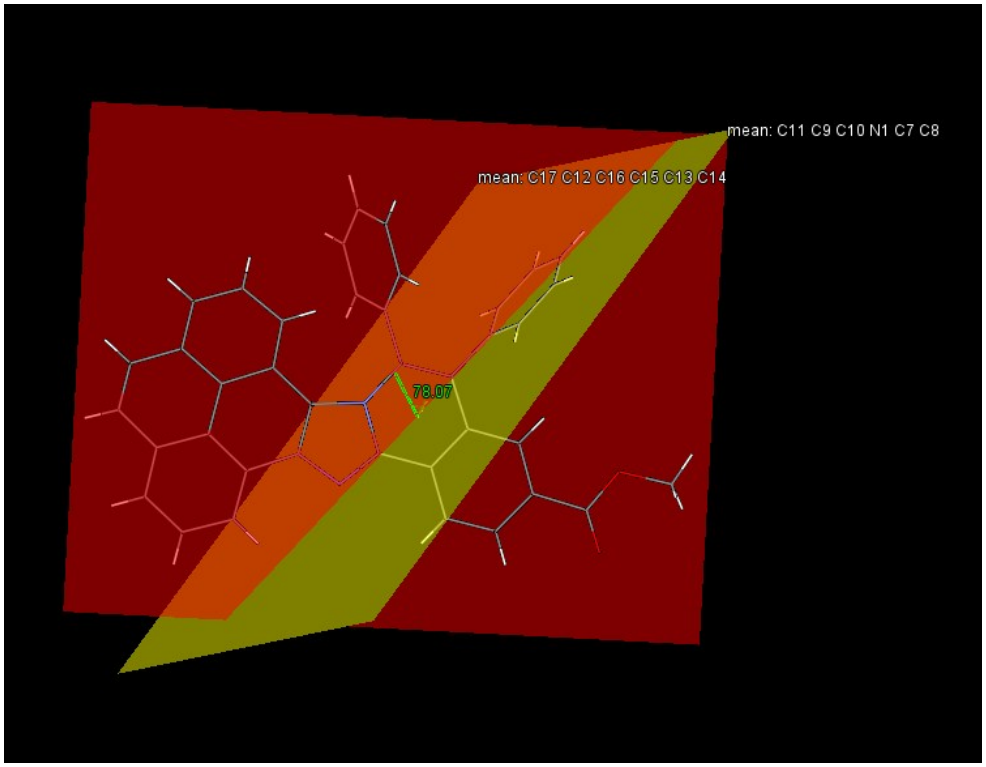
F(000)	1160	576
Limiting indices	$-12 \leq h \leq 12$ $-21 \leq k \leq 21$ $-23 \leq l \leq 23$	$-14 \leq h \leq 14$ $-14 \leq k \leq 14$ $-15 \leq l \leq 15$
Reflections collected /unique	91714/6824 $[R_{(int)} = 0.0547]$	65484/6810 $[R_{(int)} = 0.0359]$
Data/restraint/parameters	6824/0/388	6810/0/388
Goodness- of-fit on F^2	1.289	1.019
Final R indices [I> 2 sigma(I)]	$R_1 = 0.0621$ $wR_2 = 0.1757$	$R_1 = 0.0516$ $wR_2 =$ 0.1264
R indices (all data)	$R_1 = 0.0990$ $wR_2 = 0.1944$	$R_1 = 0.0747$ $wR_2 = 0.1413$

Fig. S6 Calculation of dihedral angles in **5d** and **5f**

5d

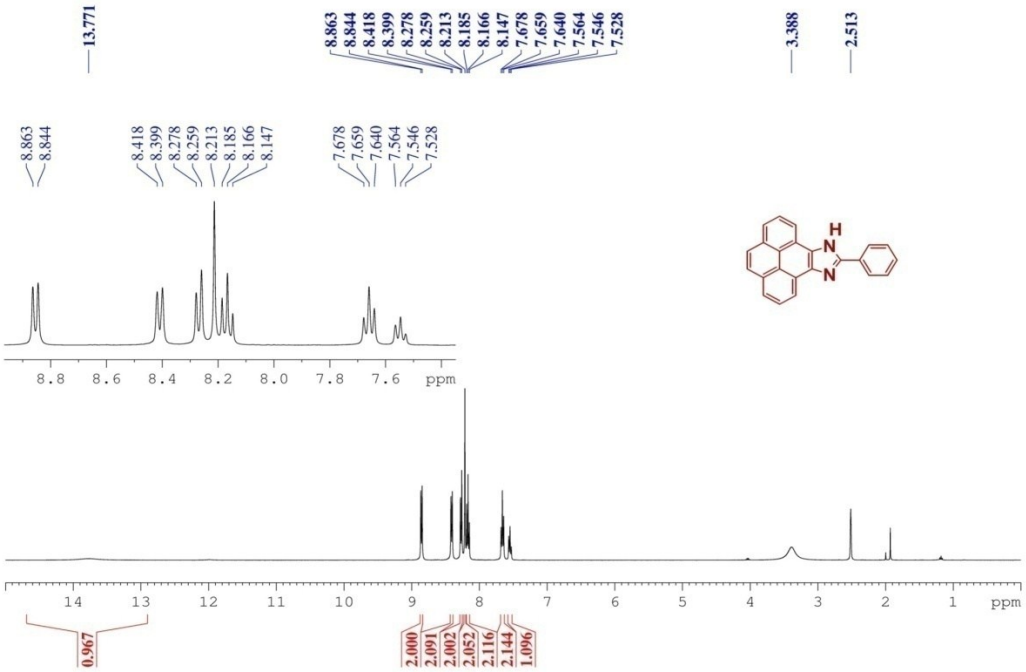


5f

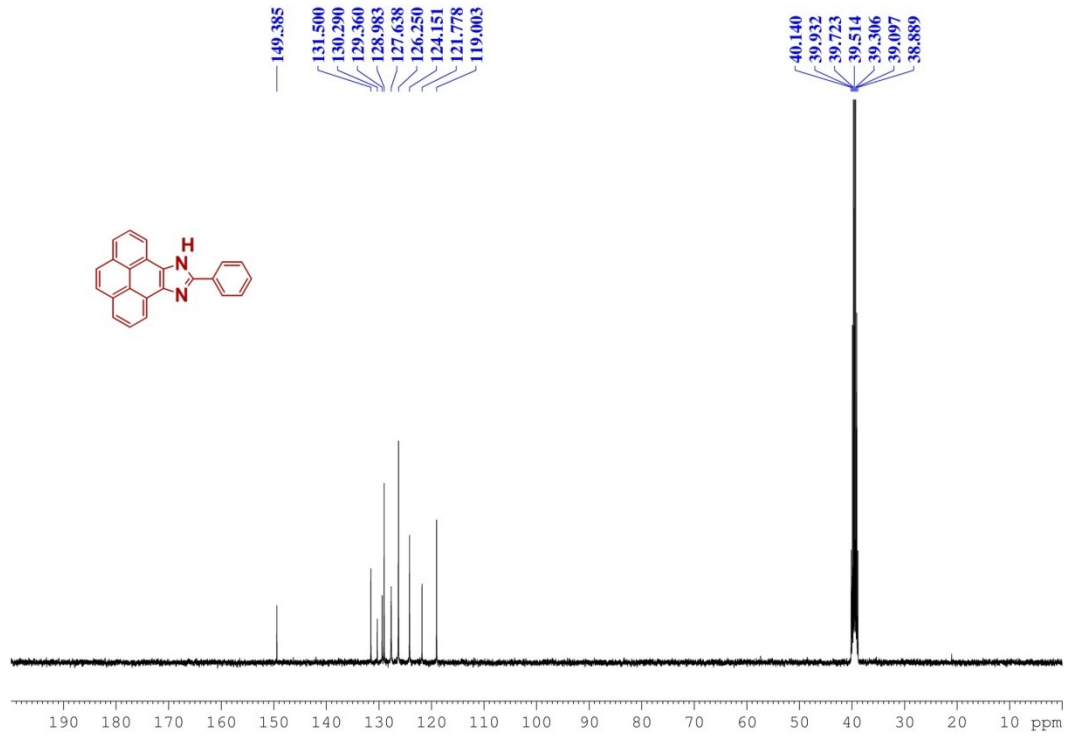


Copies of ^{1}H NMR, ^{13}C NMR and Mass spectra of **3a-3h** and **5a-5h**

^{1}H NMR spectrum of **3a** (400 MHz, DMSO-d^{6})



^{13}C NMR spectrum of 3**a** (100 MHz, DMSO-d^{6})



ESI mass spectrum of **3a**

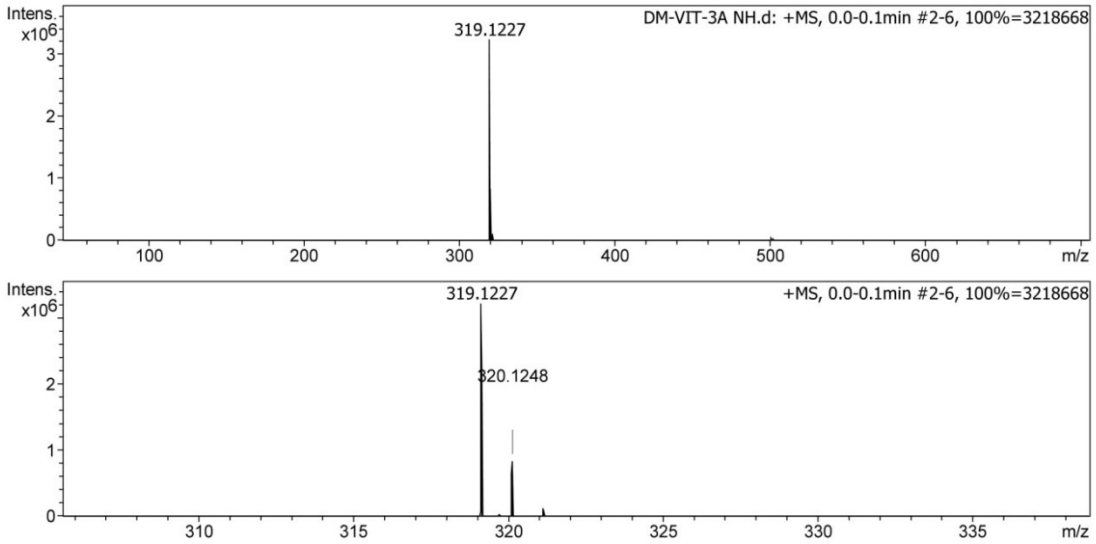
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-3A NH.d	Acquisition Date	9/29/2016 7:38:37 PM
Method	Tune_pos_NAICSI-500A.m	Operator	CPR_OUT
Sample Name	DM-VIT-3A NH	Instrument	maXis impact 282001.00081
Comment	C23H14N2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
319.1227	1	C23H15N2	319.1230	0.8	0.9	1	100.00	17.5	even	ok

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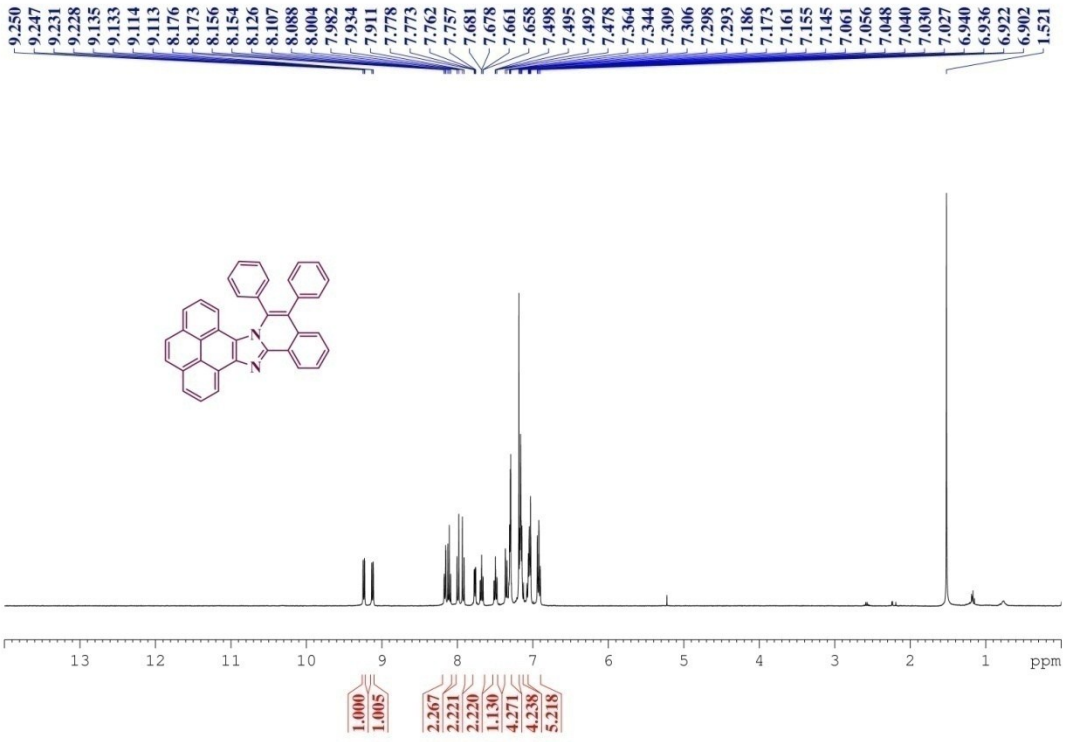
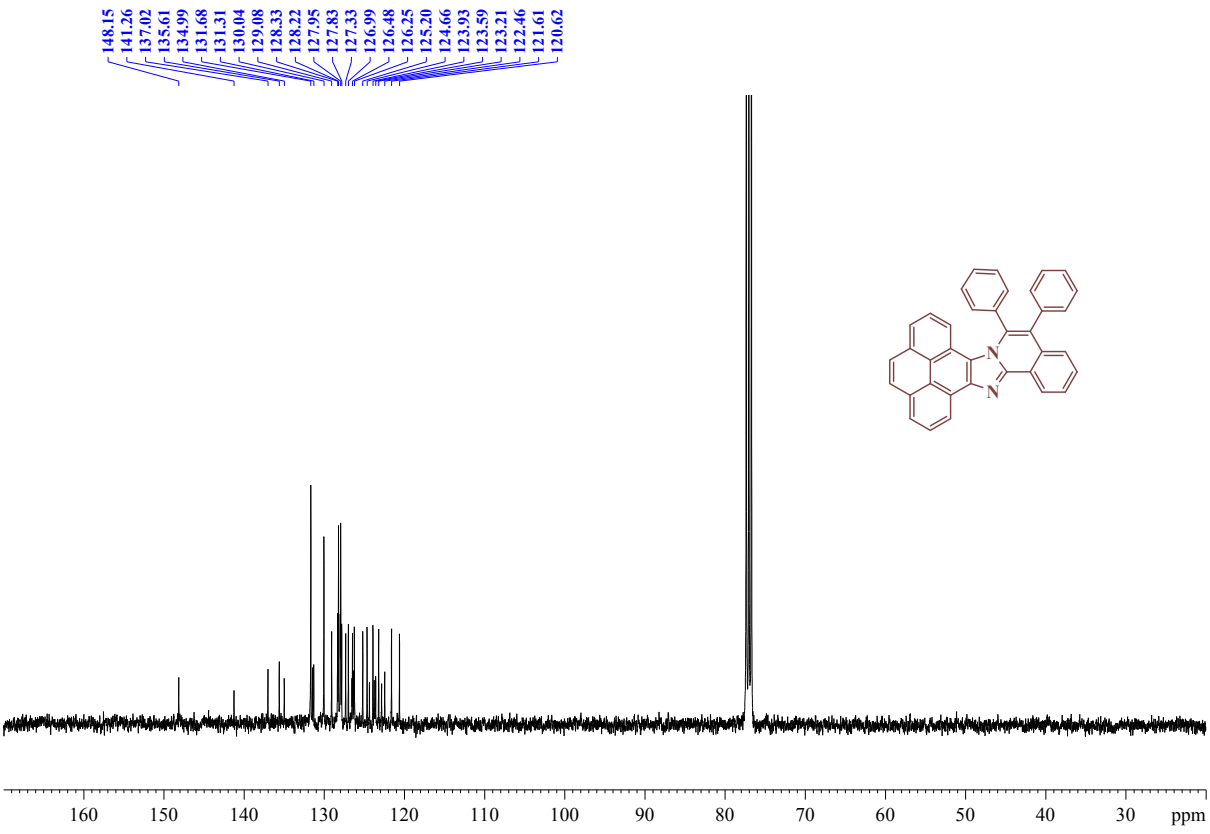
^{1}H NMR spectrum of **5a** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **5a** (100 MHz, $CDCl_3$)



ESI mass spectrum of **5a**

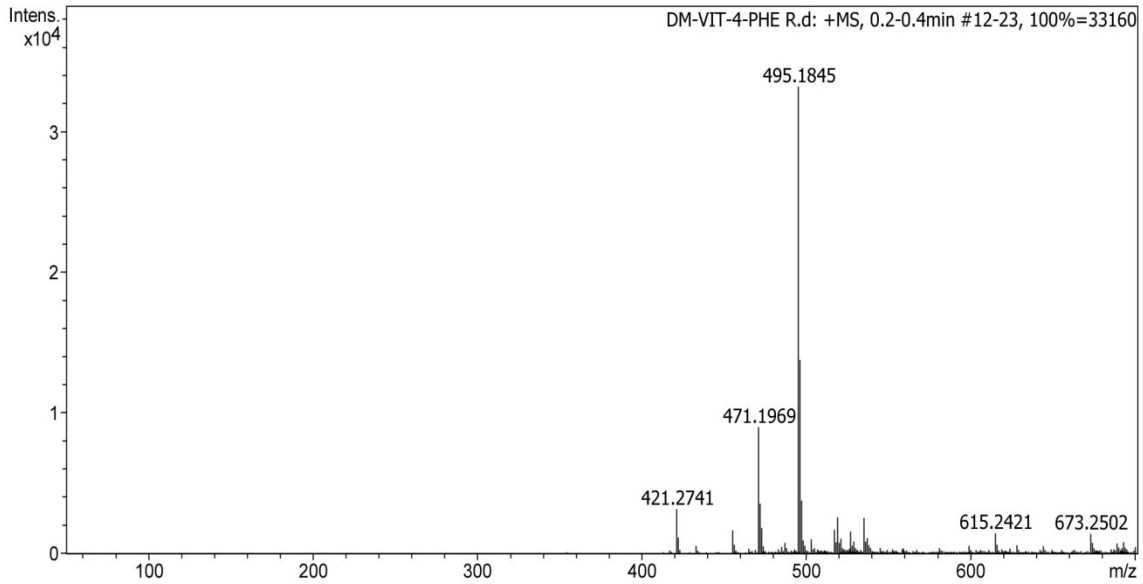
DEPARTMENT OF CHEMISTRY,I.I.T.(B)

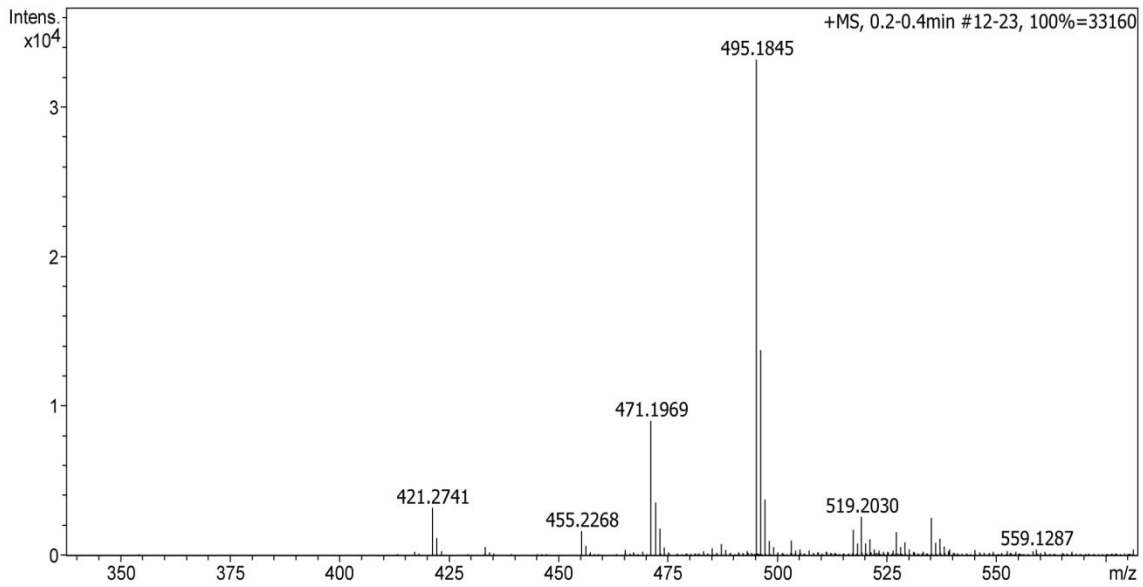
Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-4-PHE R.d	Acquisition Date	9/22/2016 3:32:49 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-4-PHE R	Instrument	maXis impact 282001.00081
Comment	C37H22N2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





DM-VIT-4-PHE R.d

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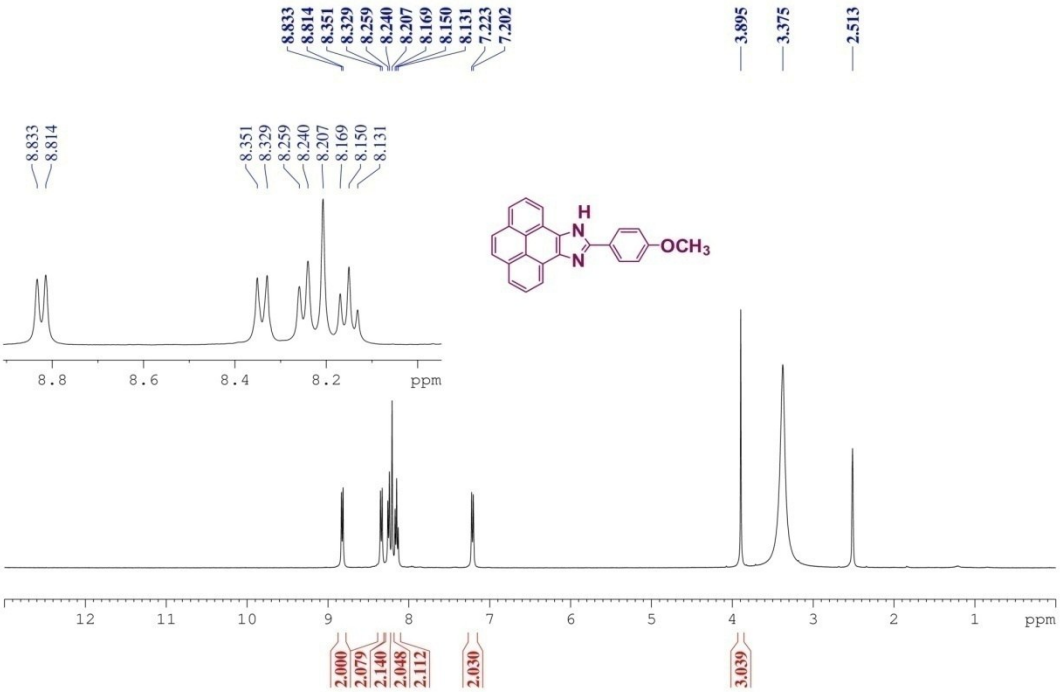
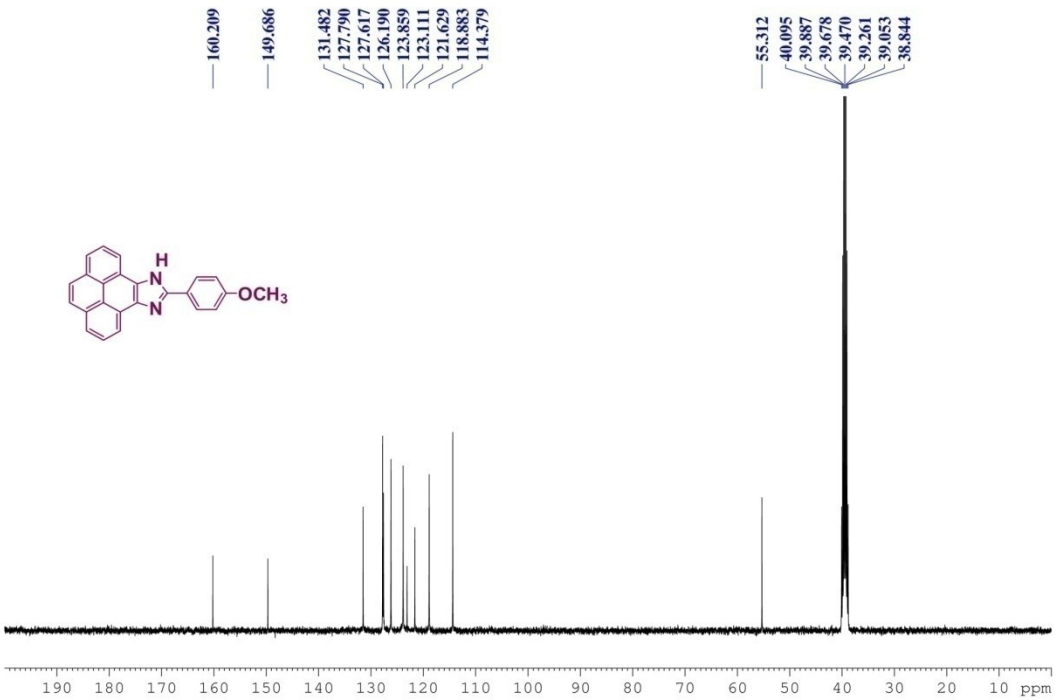
^{1}H NMR spectrum of **3b** (400 MHz,DMSO-d^{6})



^{13}C NMR spectrum of **3b** (100 MHz, DMSO-d^{6})



ESI mass spectrum of **3b**

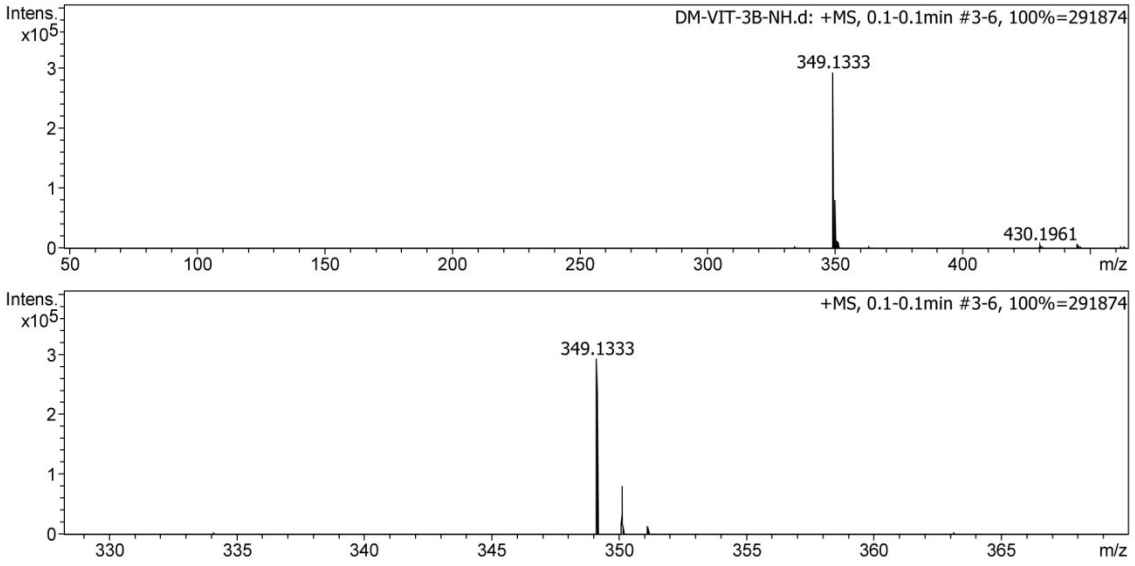
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-3B-NH.d	Acquisition Date	9/29/2016 7:45:21 PM
Method	Tune_pos_NAICSI-500A.m	Operator	CPR_OUT
Sample Name	DM-VIT-3B-NH	Instrument	maXis impact 282001.00081
Comment	C23H14N2		

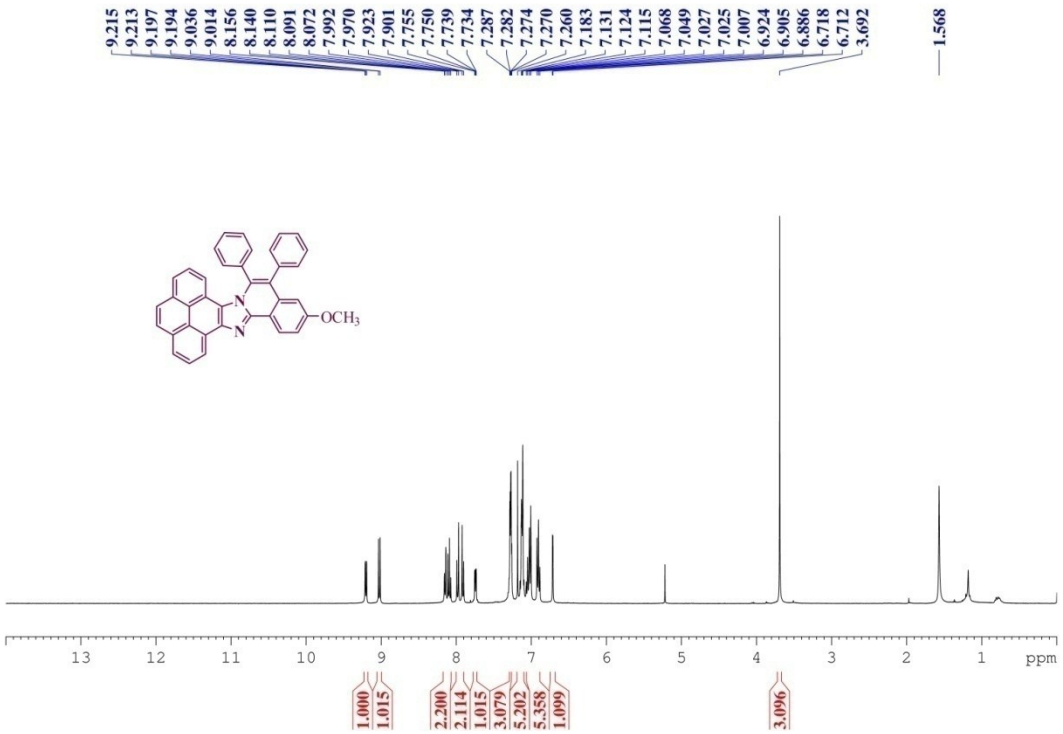
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

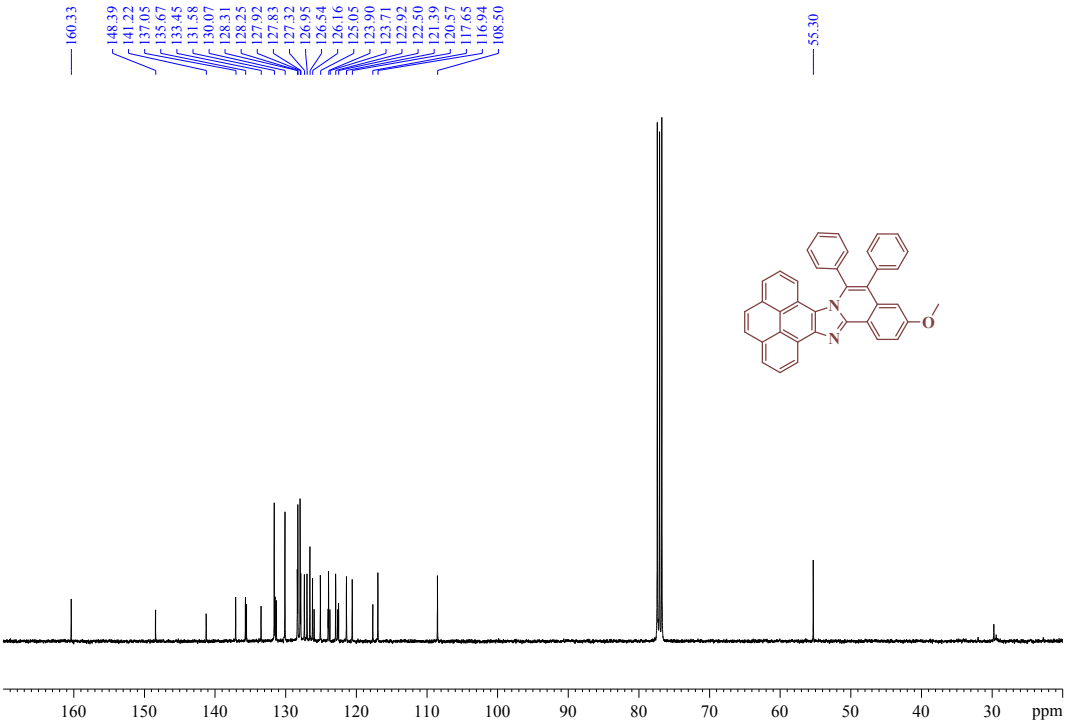


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
349.1333	1	C24H17N2O	349.1335	0.7	4.8	1	100.00	17.5	even	ok

^{1}H NMR spectrum of **5b** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **5b** (100 MHz, $CDCl_3$)



ESI mass spectrum of **5b**

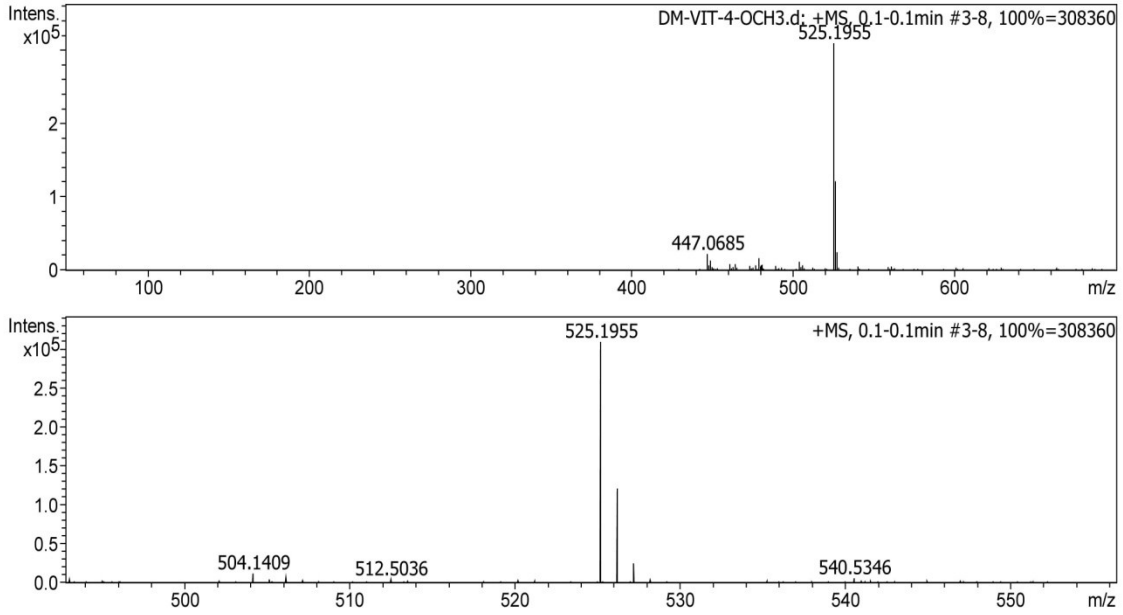
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-4-OCH3.d	Acquisition Date	9/27/2016 4:50:35 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-4-OCH3	Instrument	maXis impact 282001.00081
Comment	C38H24N2O		

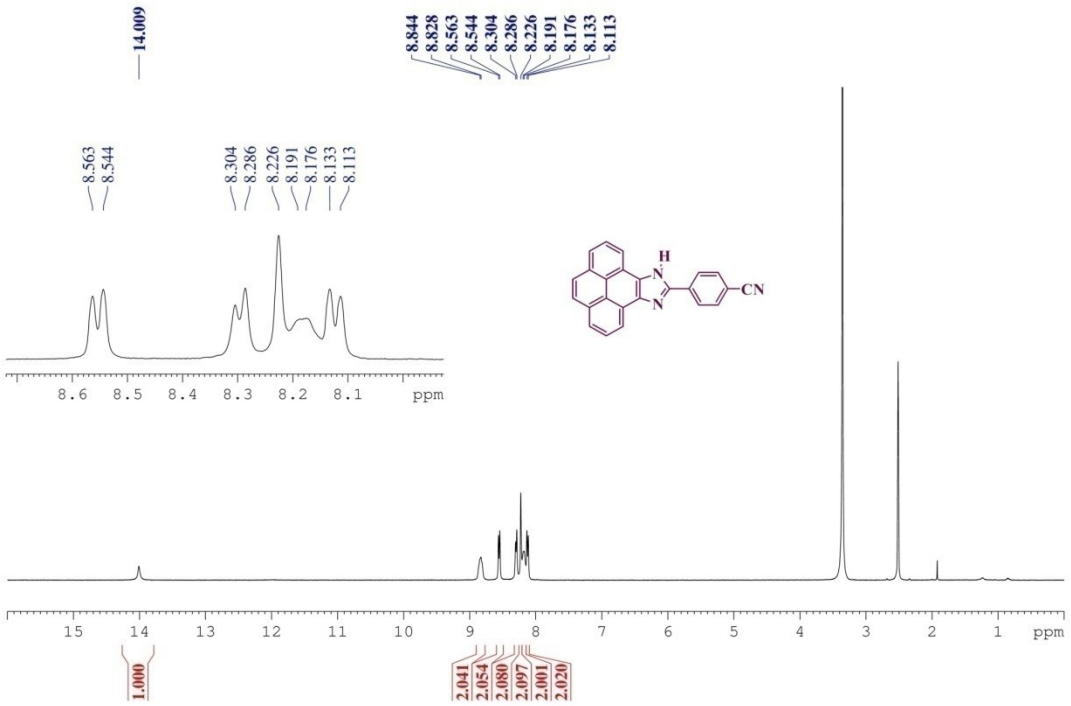
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

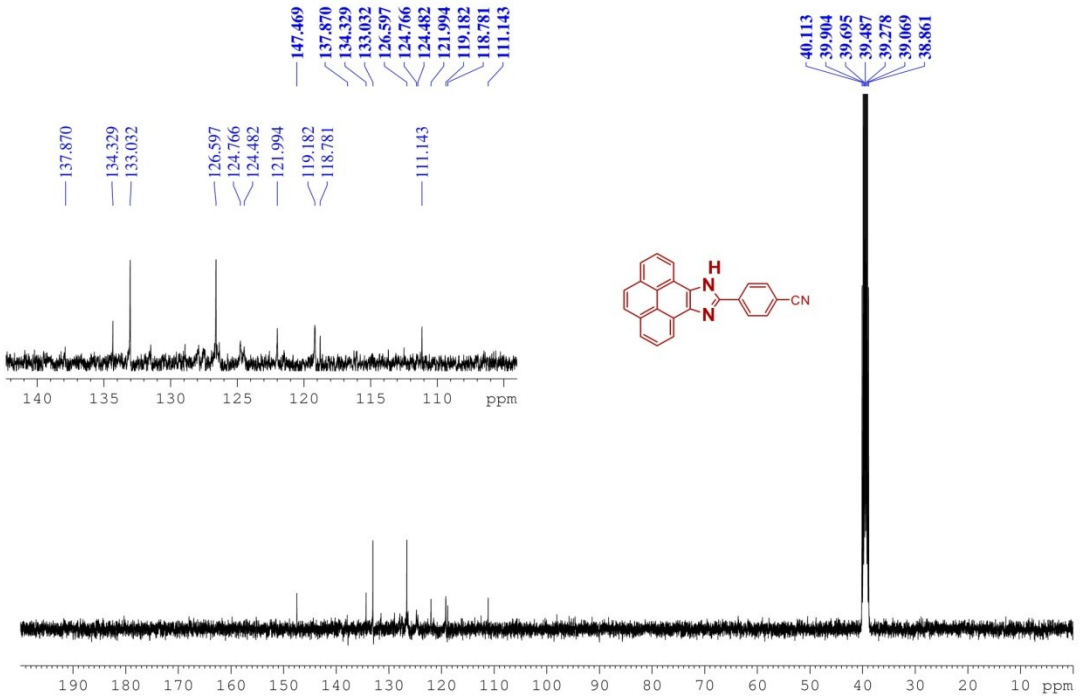


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
525.1955	1	C38H25N2O	525.1961	1.2	16.4	1	100.00	27.5	even	ok

^{1}H NMR spectrum of **3c** (400 MHz, DMSO-d^{6})



^{13}C NMR spectrum of **3c** (100 MHz, DMSO-d^{6})



ESI mass spectrum of **3c**

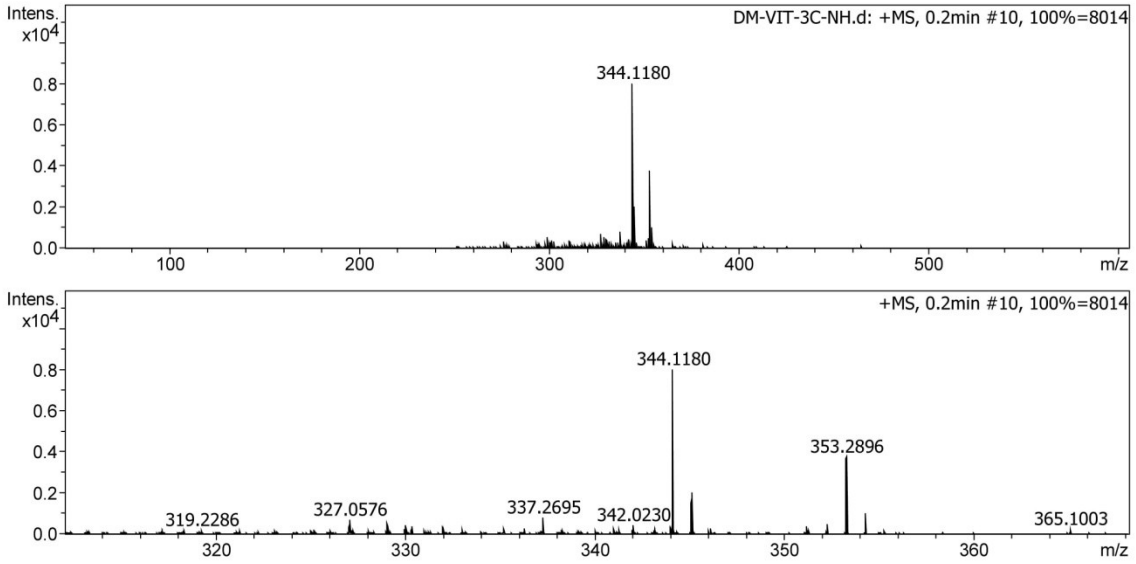
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\OCT-2016\DM-VIT-3C-NH.d	Acquisition Date	10/4/2016 4:40:41 PM
Method	Tune_pos_NAICSI-500.m	Operator	DM IN
Sample Name	DM-VIT-3C-NH	Instrument	maXis impact 282001.00081
Comment	C24H13N3		

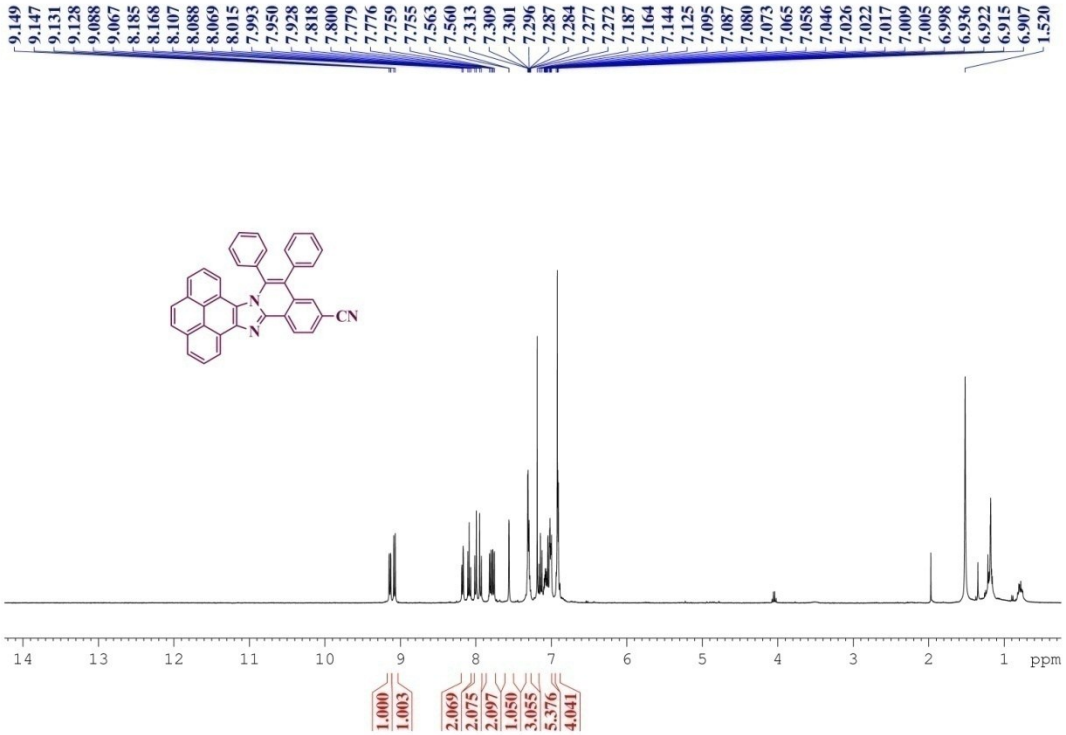
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

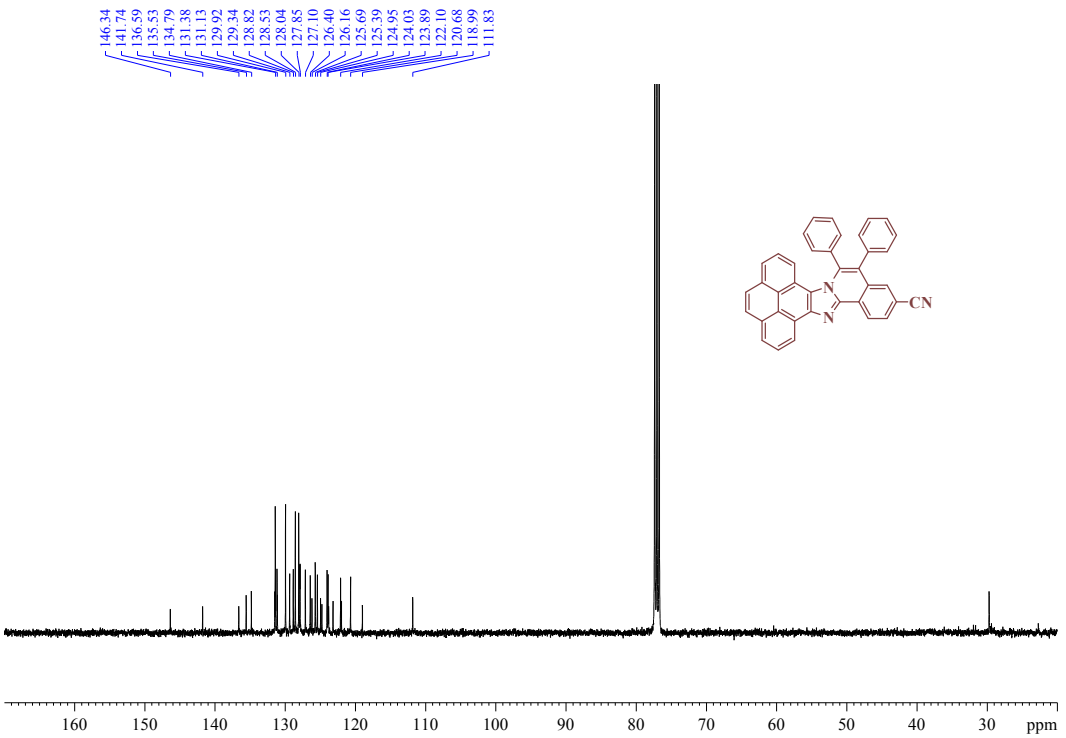


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
344.1180	1	C24H14N3	344.1182	0.5	10.4	1	100.00	19.5	even	ok

^{1}H NMR spectrum of **5c** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **5c** (100 MHz, $CDCl_3$)



ESI mass spectrum of **5c**

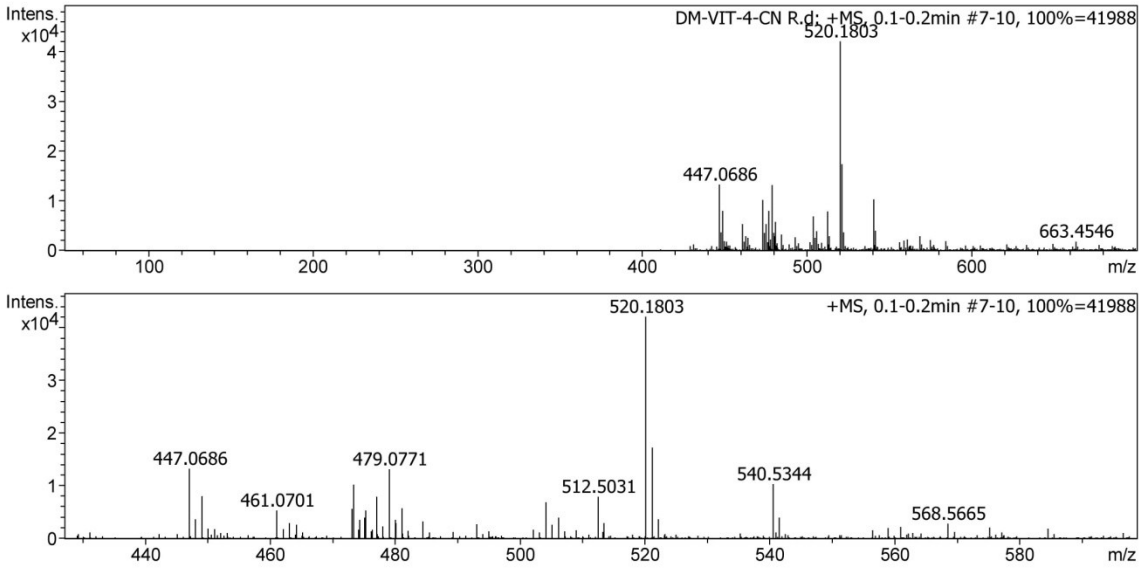
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-4-CN R.d	Acquisition Date	9/27/2016 4:46:18 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-4-CN R	Instrument	maXis impact 282001.00081
Comment	C38H21N3		

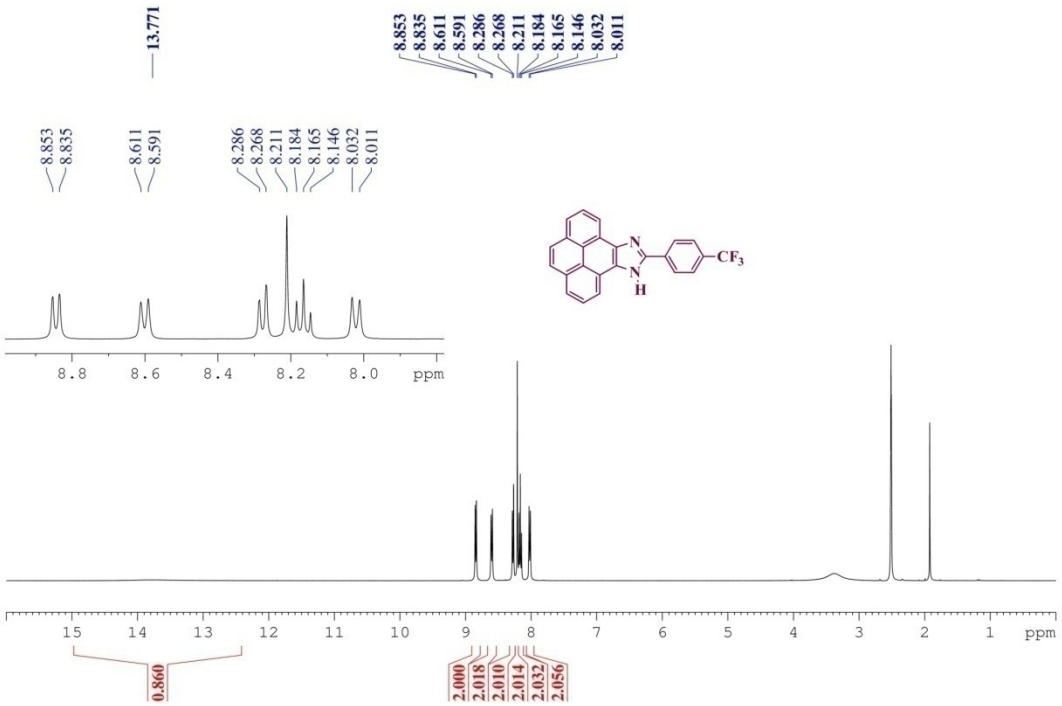
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

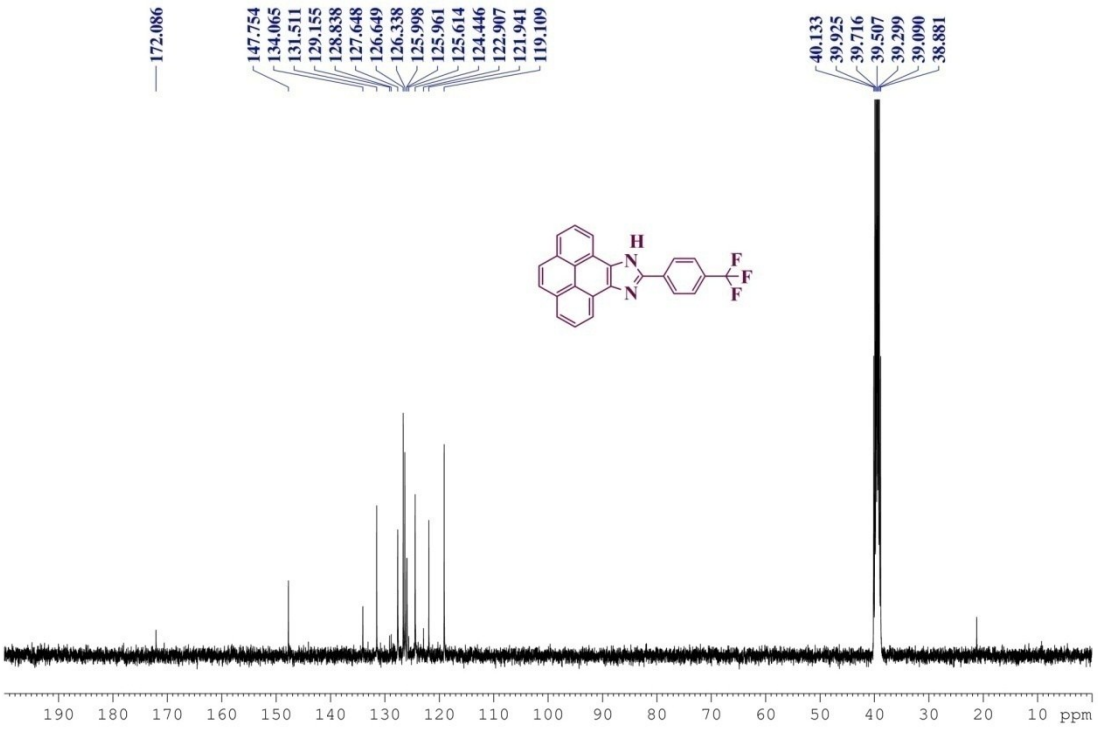


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
520.1803	1	C38H22N3	520.1808	-1.1	6.9	1	100.00	29.5	even	ok

[1]H NMR spectrum of **3d** (400 MHz, DMSO-d[6])



[13]C NMR spectrum of **3d** (100 MHz, DMSO-d[6])



ESI mass spectrum of **3d**

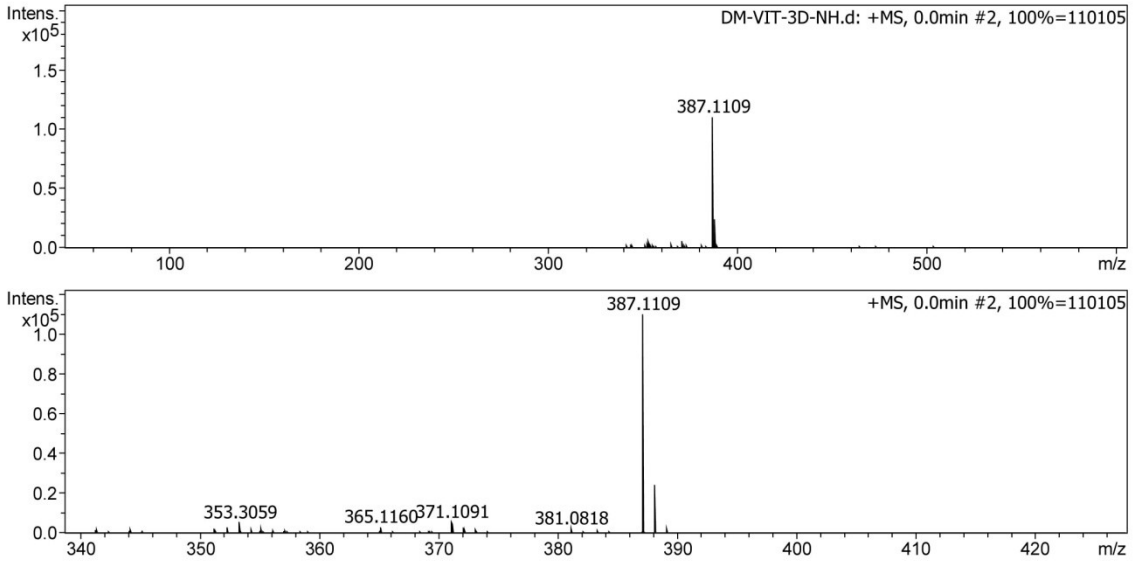
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\OCT-2016\DM-VIT-3D-NH.d	Acquisition Date	10/4/2016 4:48:50 PM
Method	Tune_pos_NAICSI-500.m	Operator	DM IN
Sample Name	DM-VIT-3D-NH	Instrument	maXis impact 282001.00081
Comment	C24H13N2F3		

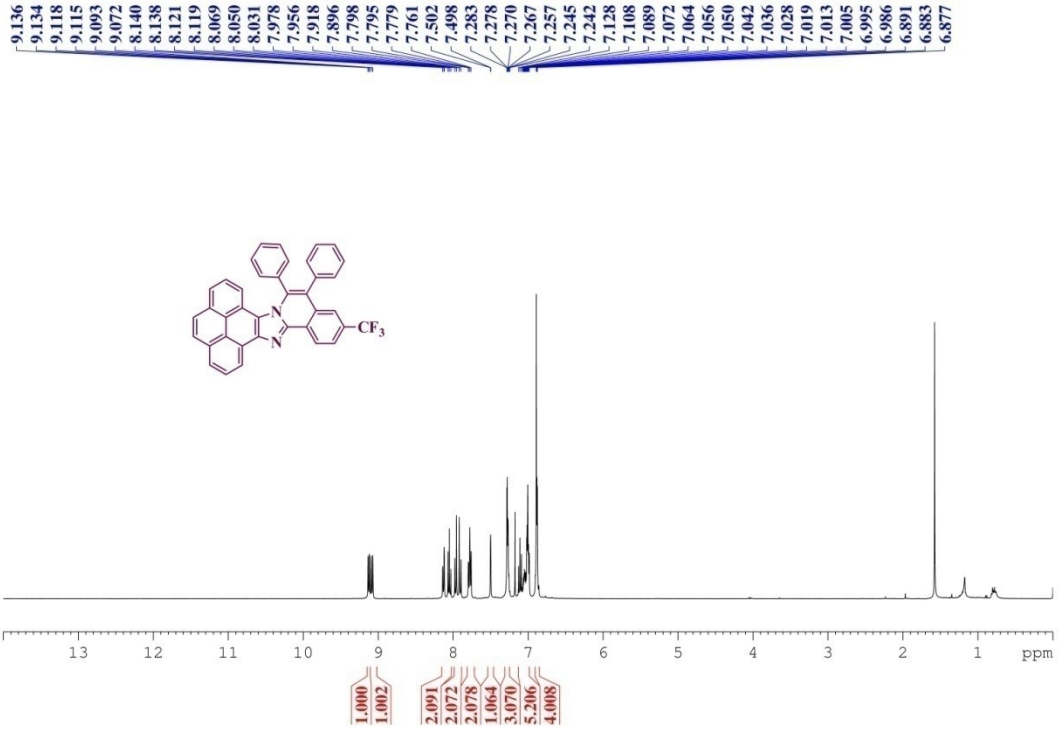
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

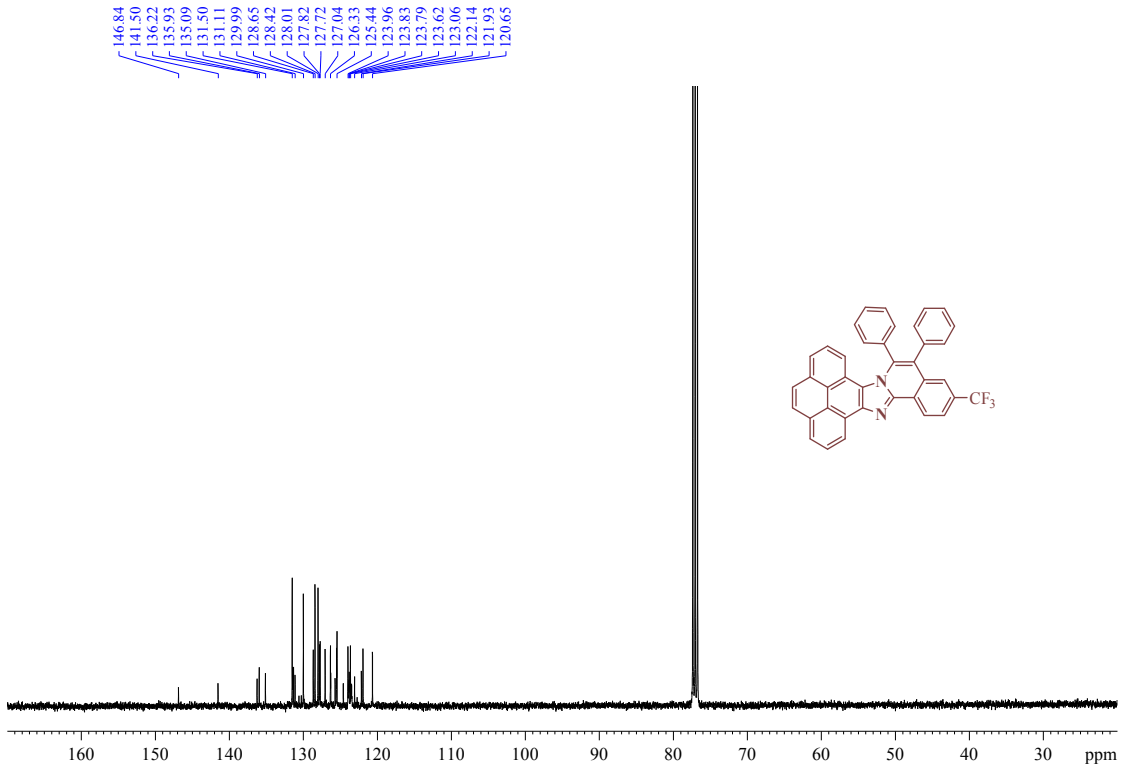


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
387.1109	1	C24H14F3N2	387.1104	-1.3	30.2	1	100.00	17.5	even	ok

^{1}H NMR spectrum of **5d** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **5d** (100 MHz, $CDCl_3$)



ESI mass spectrum of **5d**

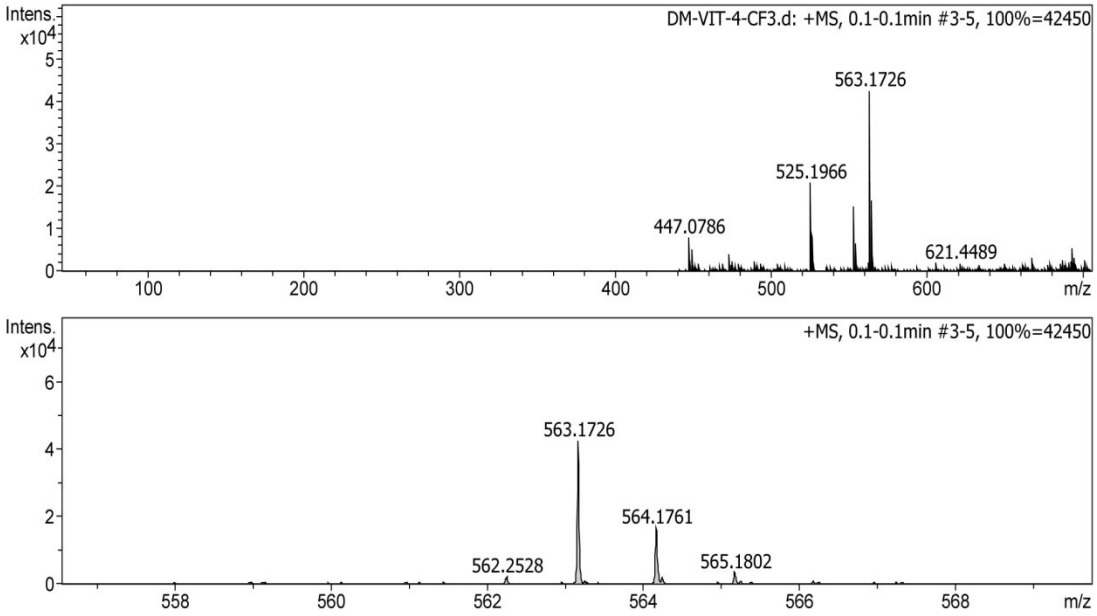
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-4-CF3.d	Acquisition Date	9/27/2016 5:24:48 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-4-CF3	Instrument	maXis impact 282001.00081
Comment	C38H21F3N2		

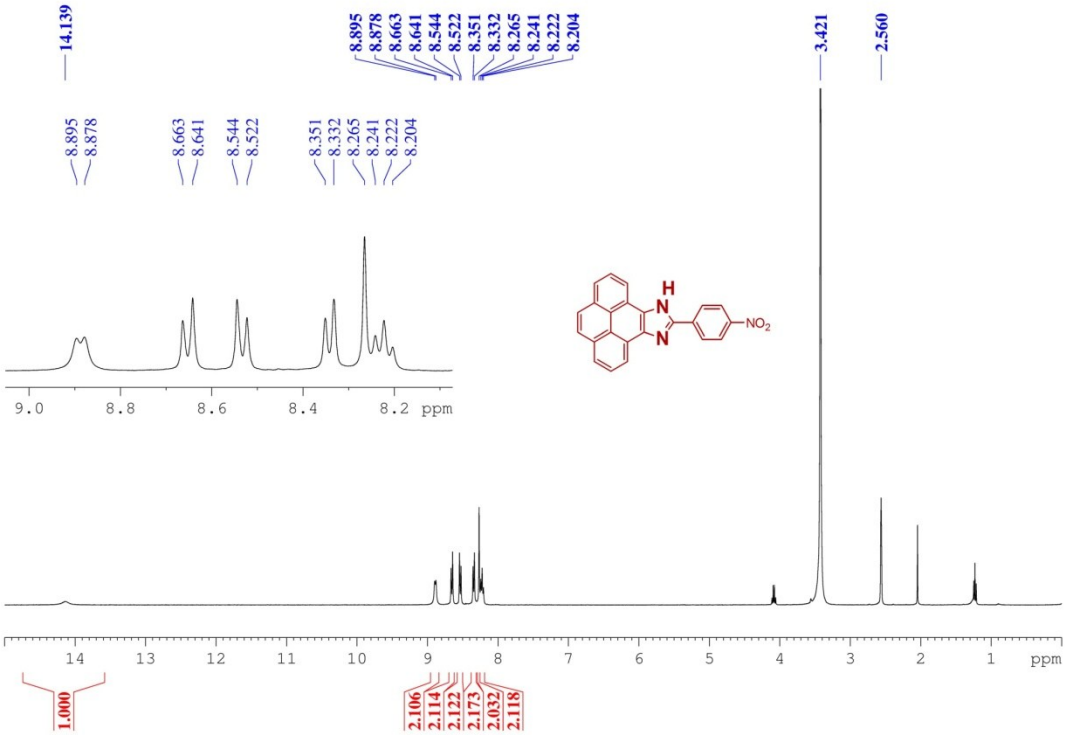
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

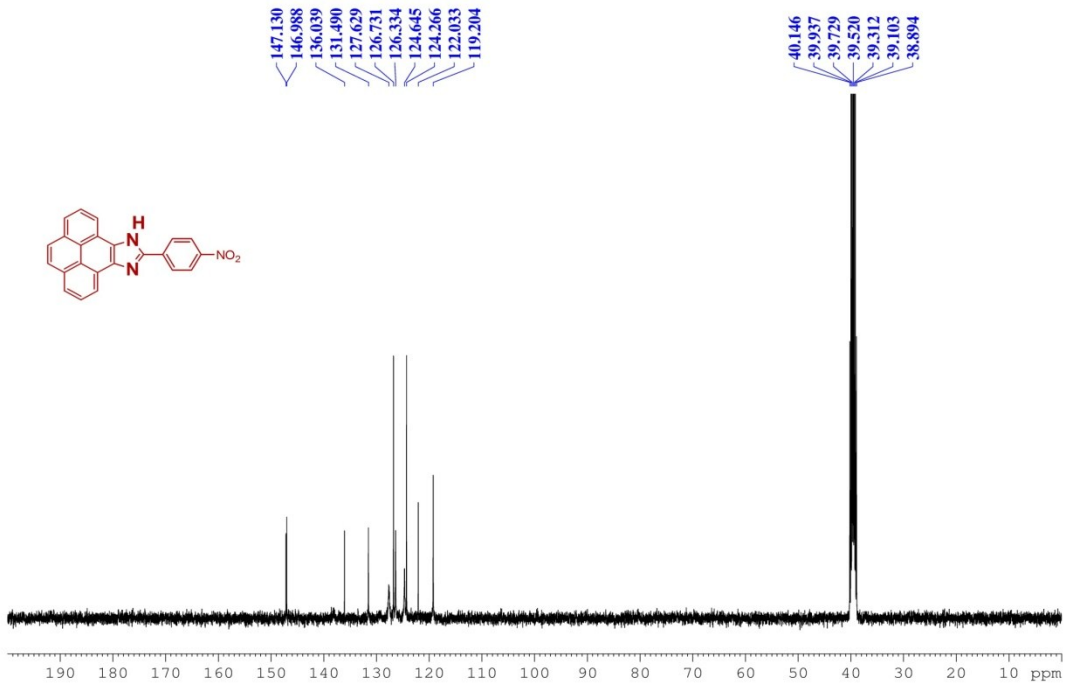


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
563.1726	1	C38H22F3N2	563.1730	0.7	15.6	1	100.00	27.5	even	ok

^{1}H NMR spectrum of **3e** (400 MHz, DMSO-d^{6})



^{13}C NMR spectrum of **3e** (100 MHz, DMSO-d^{6})



ESI mass spectrum of **3e**

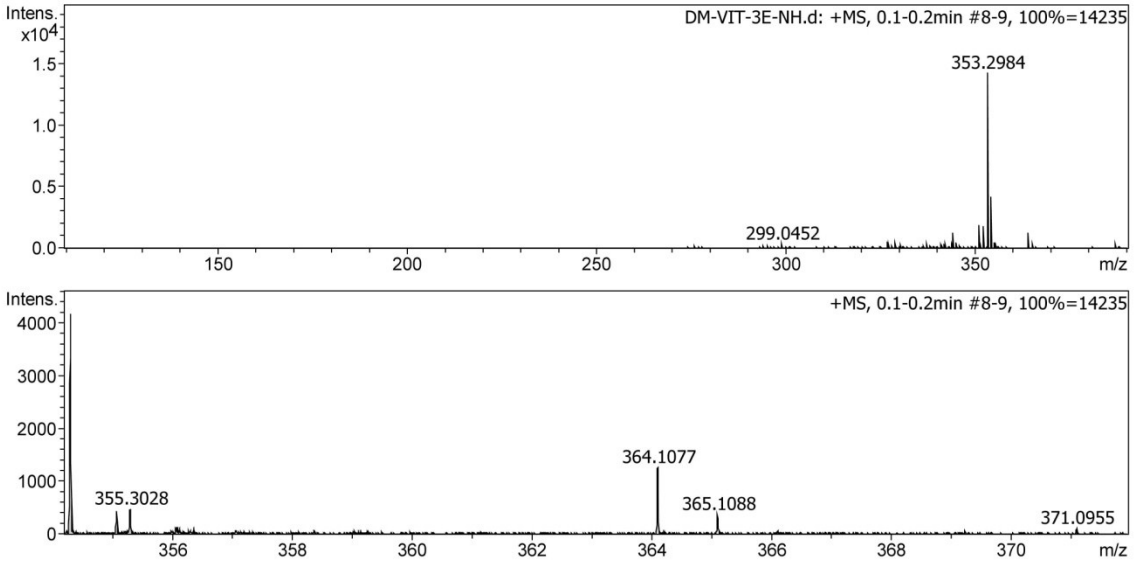
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\OCT-2016\DM-VIT-3E-NH.d	Acquisition Date	10/4/2016 5:09:19 PM
Method	Tune_pos_NAICSI-500.m	Operator	DM IN
Sample Name	DM-VIT-3E-NH	Instrument	maXis impact 282001.00081
Comment	C23H13N3O2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
364.1077	1	C23H14N3O2	364.1081	0.9	25.8	1	100.00	18.5	even	ok

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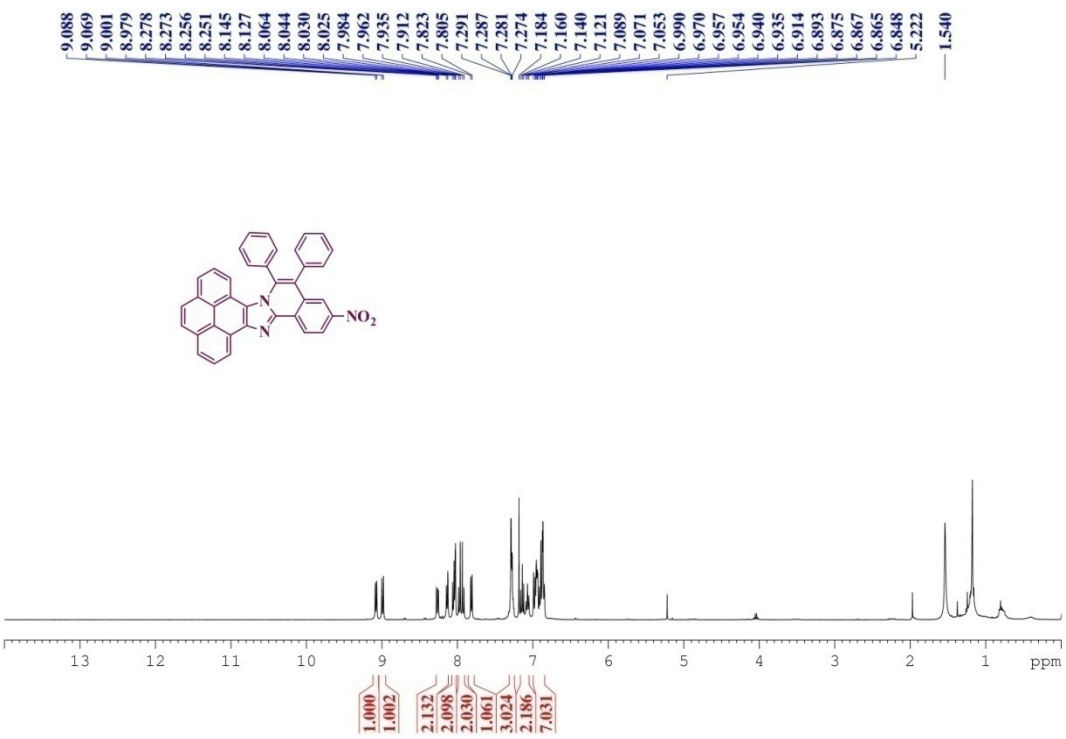
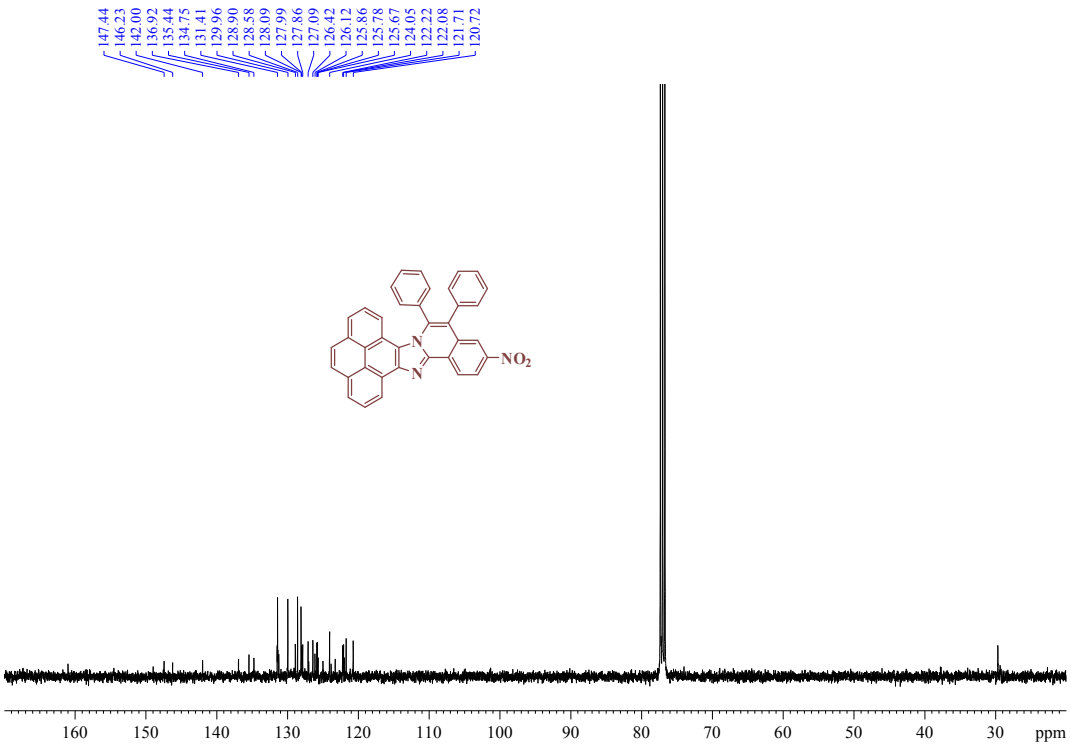
^{1}H NMR spectrum of **5e** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **5e** (100 MHz, $CDCl_3$)



ESI mass spectrum of **5e**

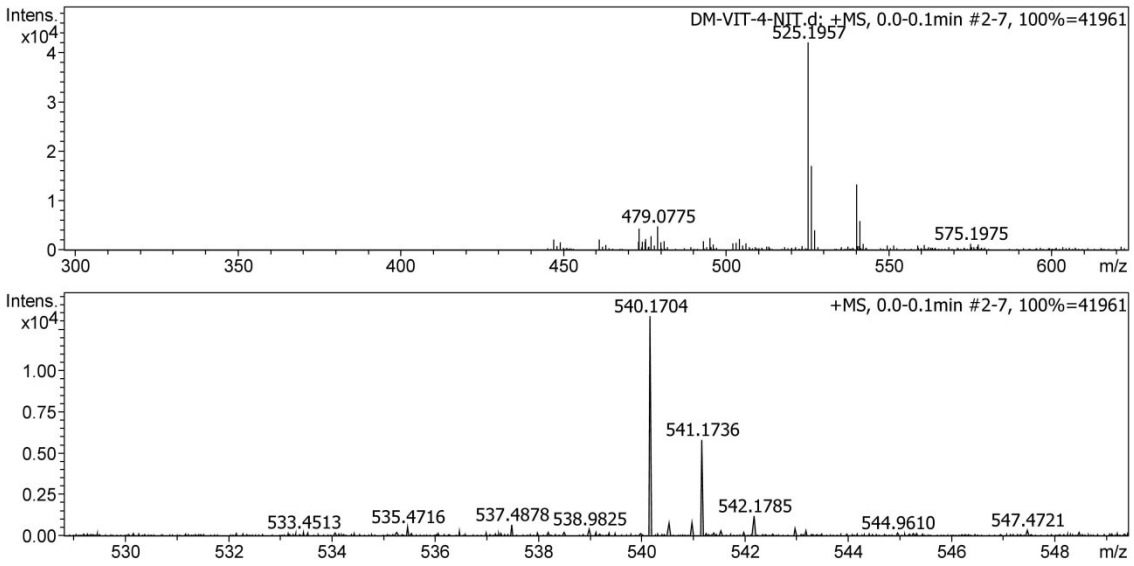
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-4-NIT.d	Acquisition Date	9/27/2016 5:07:11 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-4-NIT	Instrument	maXis impact 282001.00081
Comment	C37H21N3O2		

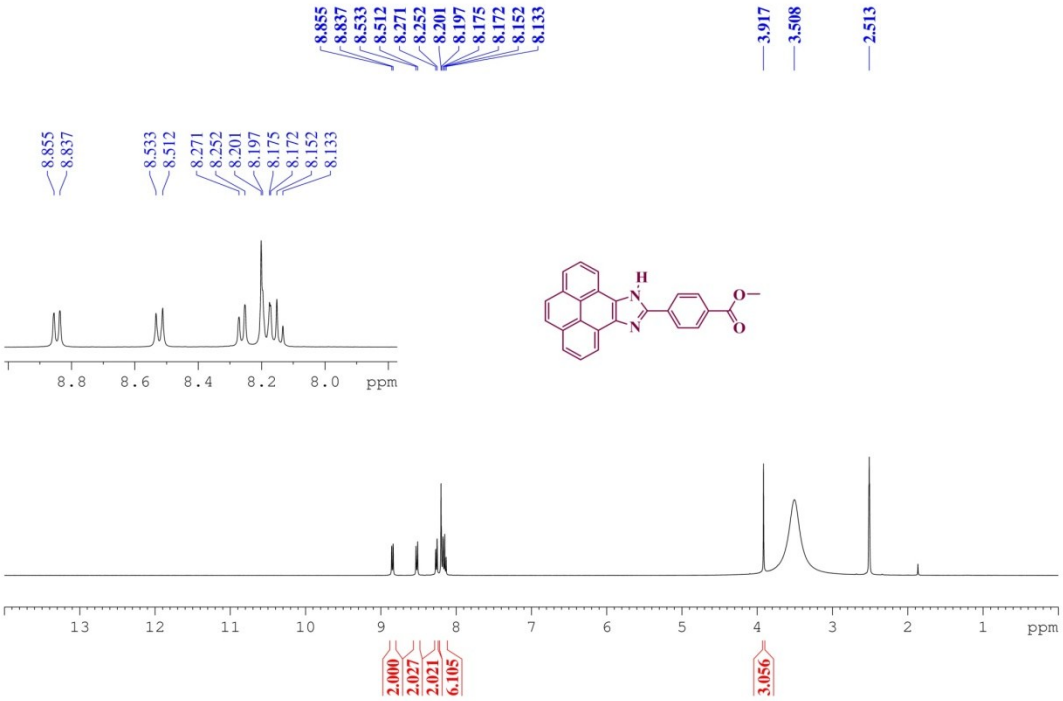
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

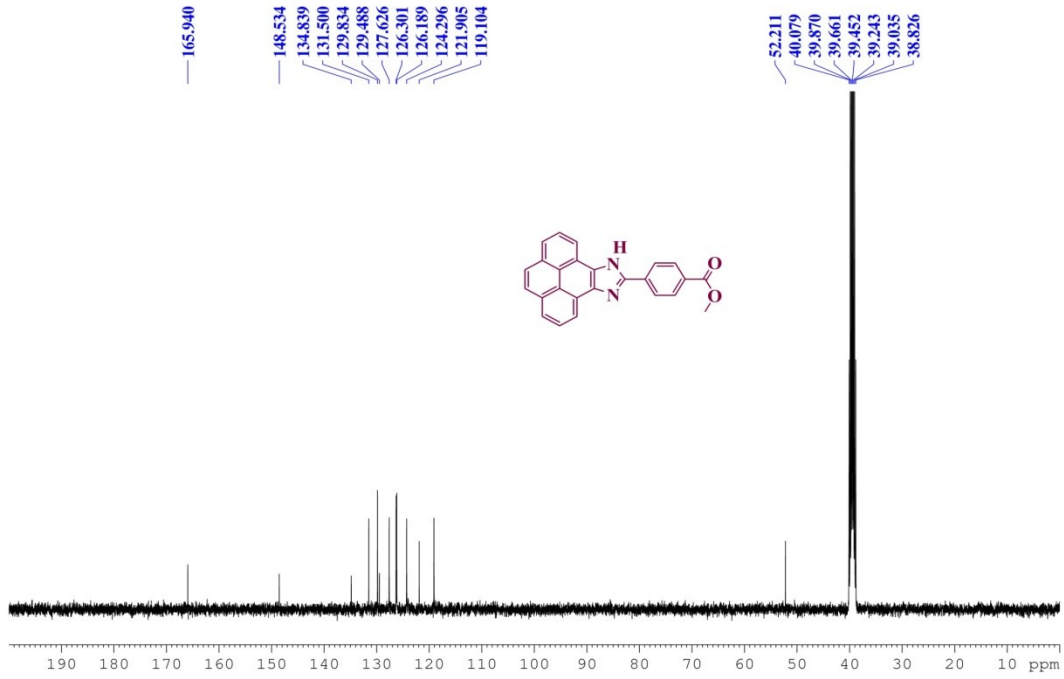


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
540.1704	1	C37H22N3O2	540.1707	0.5	12.3	1	100.00	28.5	even	ok

[1]H NMR spectrum of **3f** (400 MHz, DMSO-d[6])



[13]C NMR spectrum of **3f** (100 MHz, DMSO-d[6])



ESI mass spectrum of **3f**

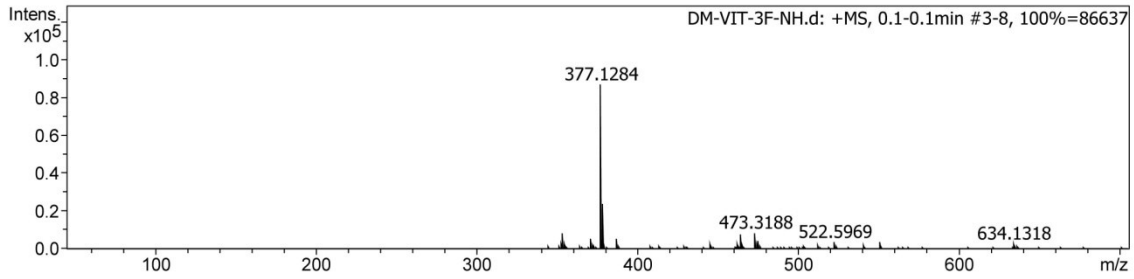
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

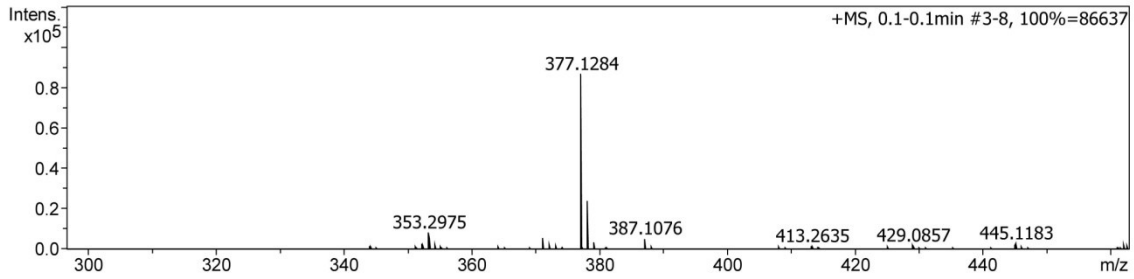
Analysis Info

Analysis Name	D:\Data\OCT-2016\DM-VIT-3F-NH.d	Acquisition Date	10/4/2016 5:20:35 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-3F-NH	Instrument	maXis impact 282001.00081
Comment	C25H16N2O2		

Acquisition Parameter

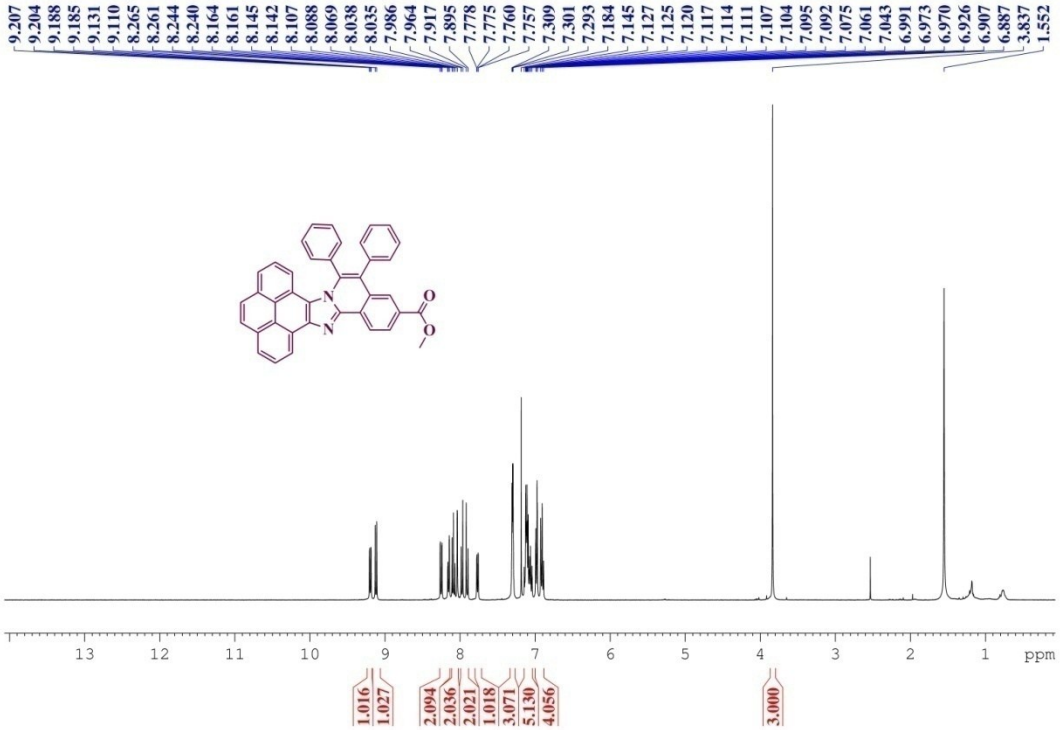
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



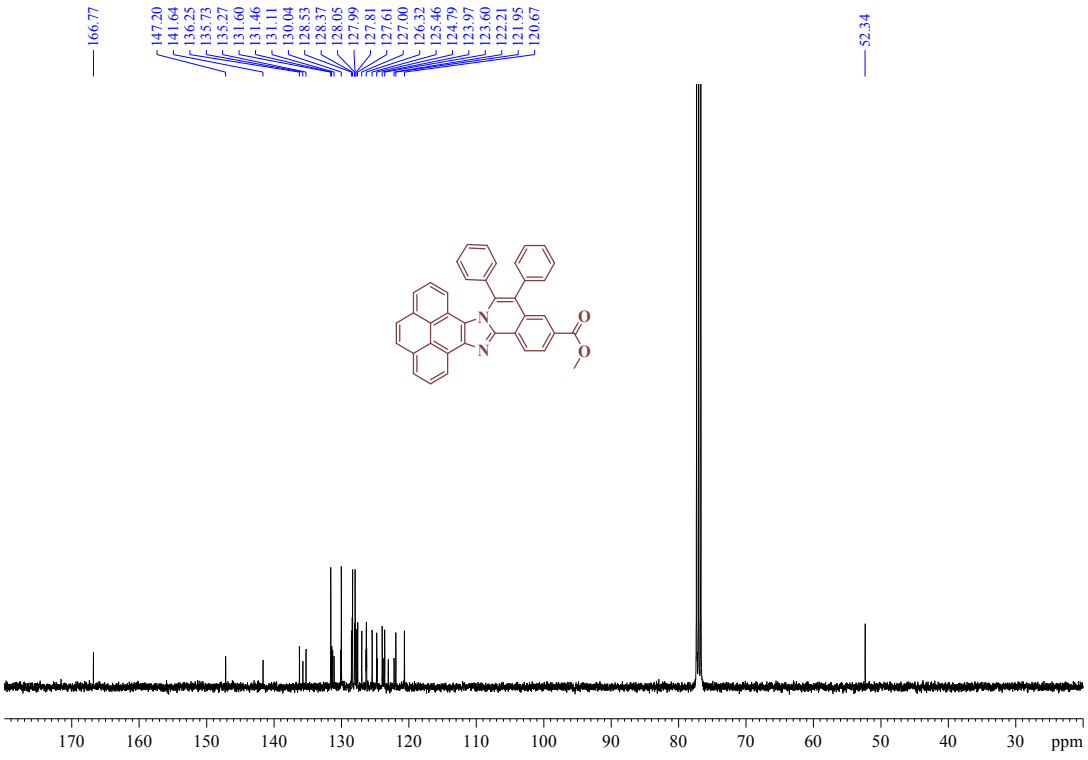


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
377.1284	1	C25H17N2O2	377.1285	0.0	4.5	1	100.00	18.5	even	ok

^{1}H NMR spectrum of **5f** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **5f** (100 MHz, $CDCl_3$)



ESI mass spectrum of **5f**

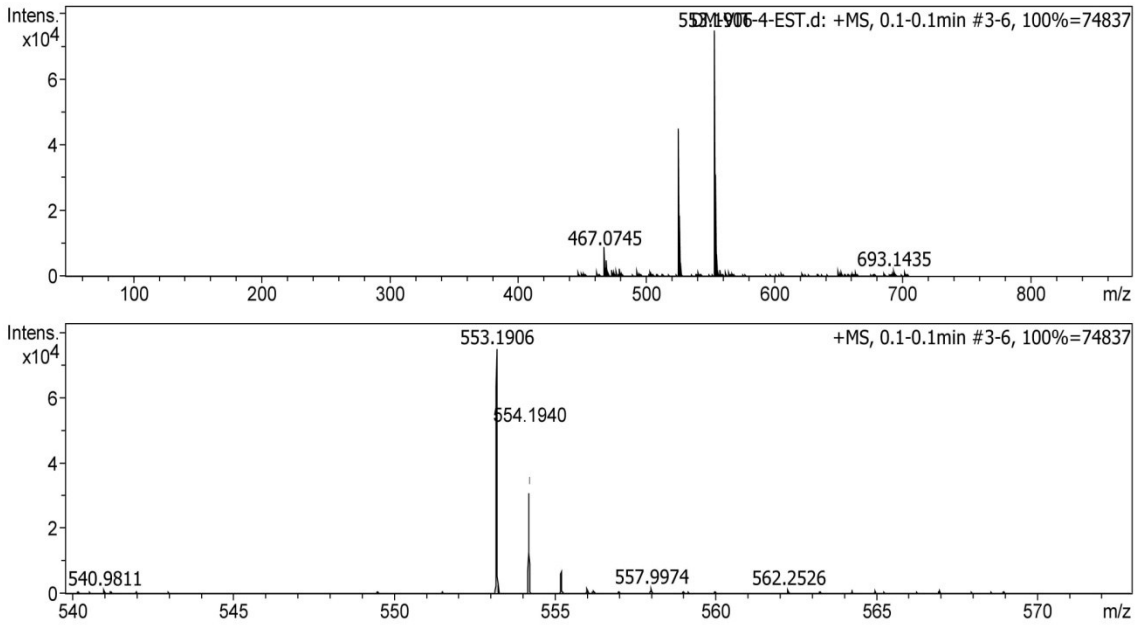
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-4-EST.d	Acquisition Date	9/27/2016 5:16:56 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-4-EST	Instrument	maXis impact 282001.00081
Comment	C39H24N2O2		

Acquisition Parameter

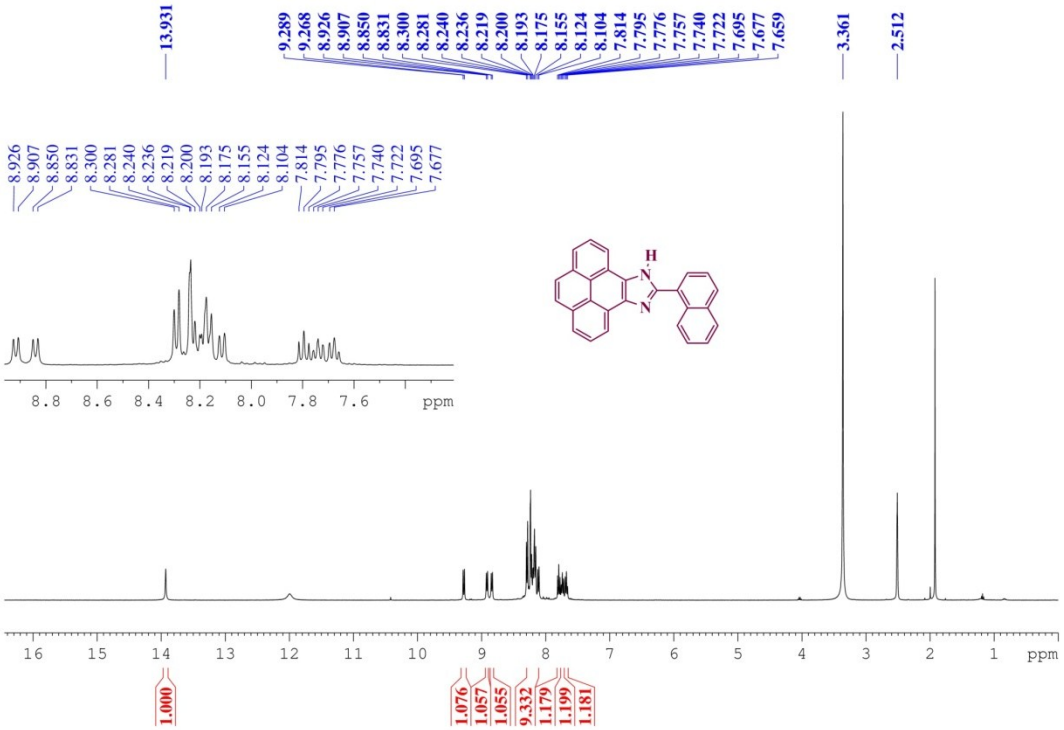
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



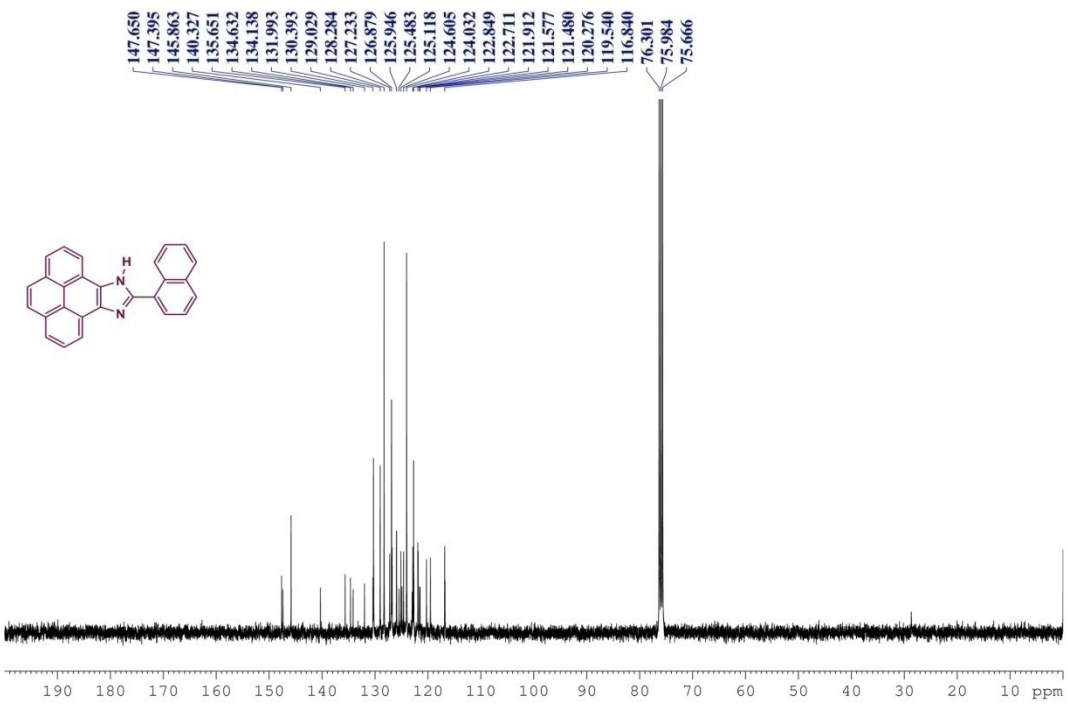
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
553.1906	1	C39H25N2O2	553.1911	-0.8	10.7	1	100.00	28.5	even	ok

Bruker Compass DataAnalysis 4.1 printed: 9/27/2016 5:19:41 PM by: DM IN Page 1 of 1

^{1}H NMR spectrum of **3g** (400 MHz, DMSO-d^{6})



^{13}C NMR spectrum of **3g** (100 MHz, DMSO-d^{6})



ESI mass spectrum of **3g**

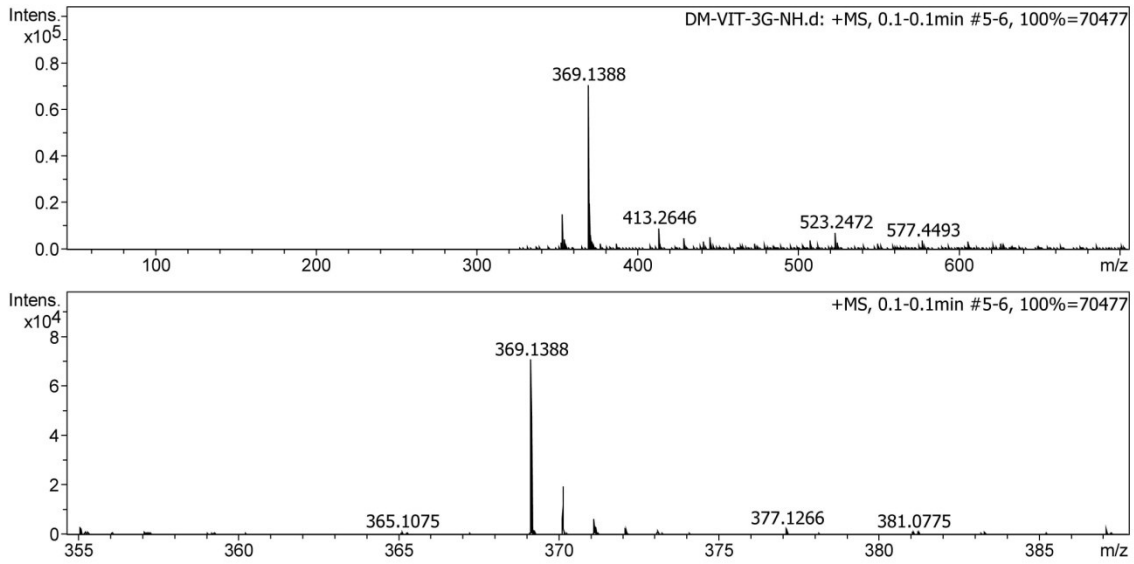
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\OCT-2016\DM-VIT-3G-NH.d	Acquisition Date	10/4/2016 5:33:00 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-3G-NH	Instrument	maXis impact 282001.00081
Comment	C27H16N2		

Acquisition Parameter

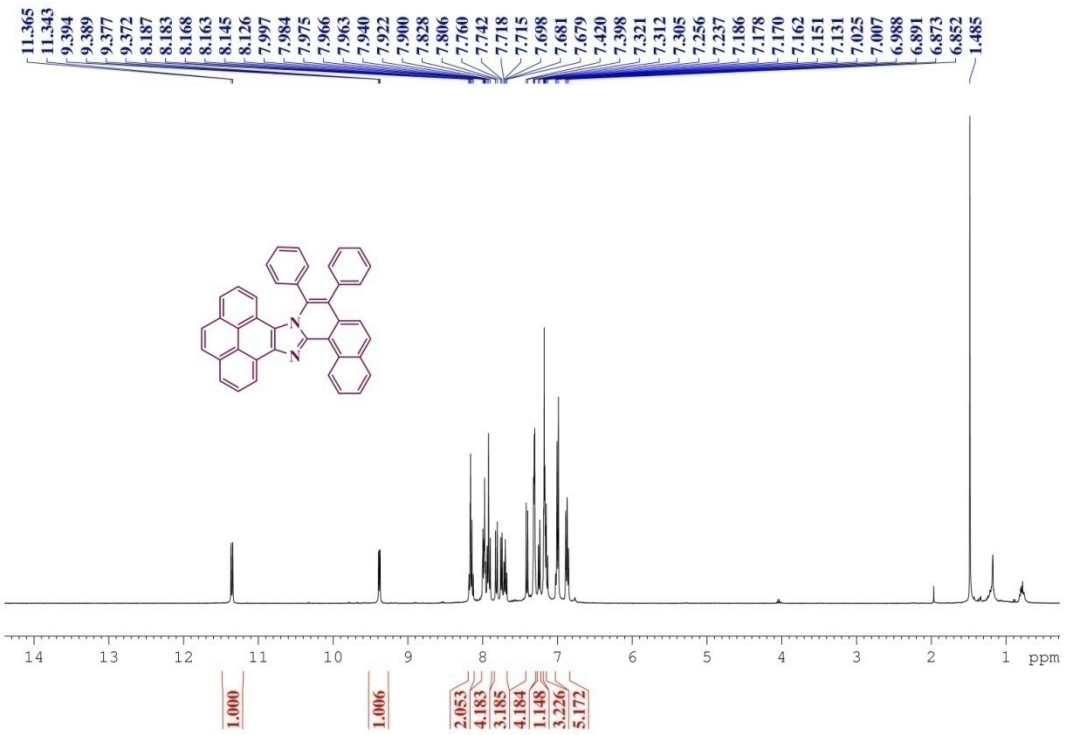
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



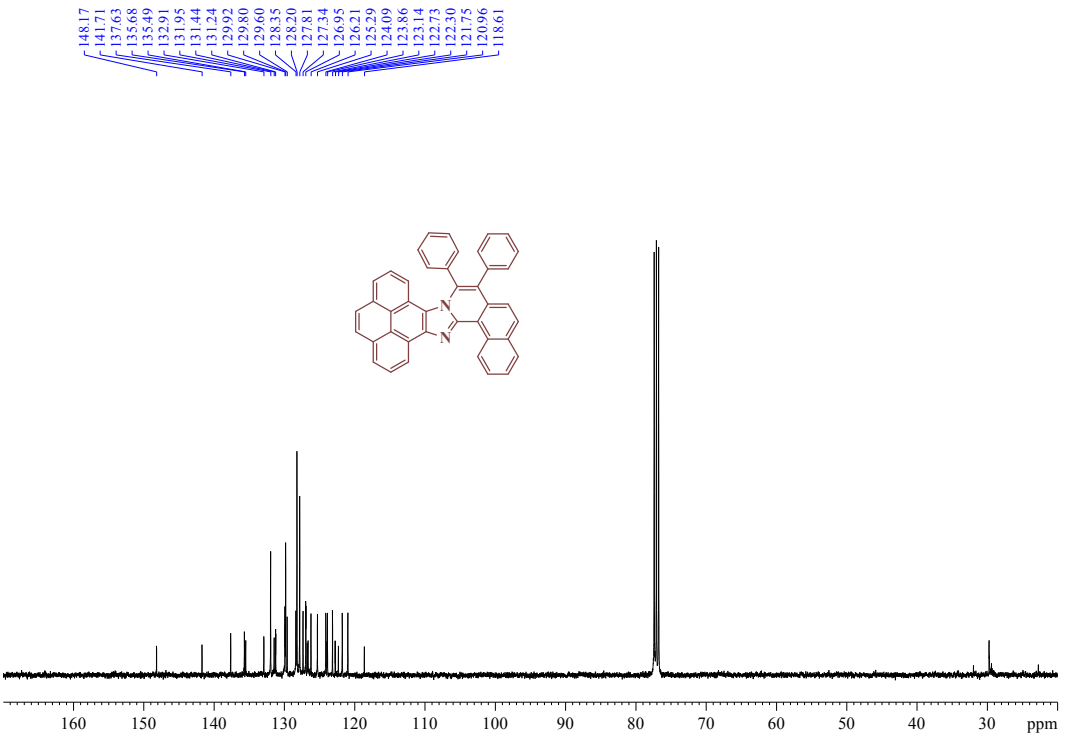
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
369.1388	1	C27H17N2	369.1386	0.6	12.5	1	100.00	20.5	even	ok

Bruker Compass DataAnalysis 4.1 printed: 10/4/2016 5:34:21 PM by: DM IN Page 1 of 1

^{1}H NMR spectrum of **5g** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **5g** (100 MHz, $CDCl_3$)



ESI mass spectrum of **5g**

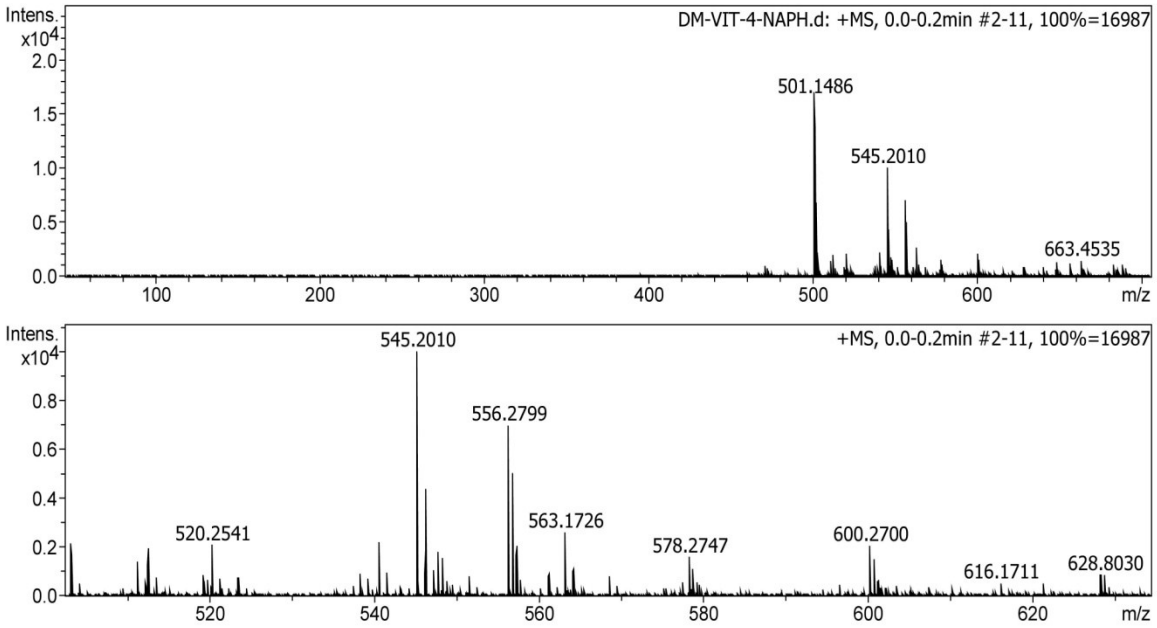
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-4-NAPH.d	Acquisition Date	9/29/2016 7:32:13 PM
Method	Tune_pos_NAICSI-500A.m	Operator	CPR_OUT
Sample Name	DM-VIT-4-NAPH	Instrument	maXis impact 282001.00081
Comment	C41H24N2		

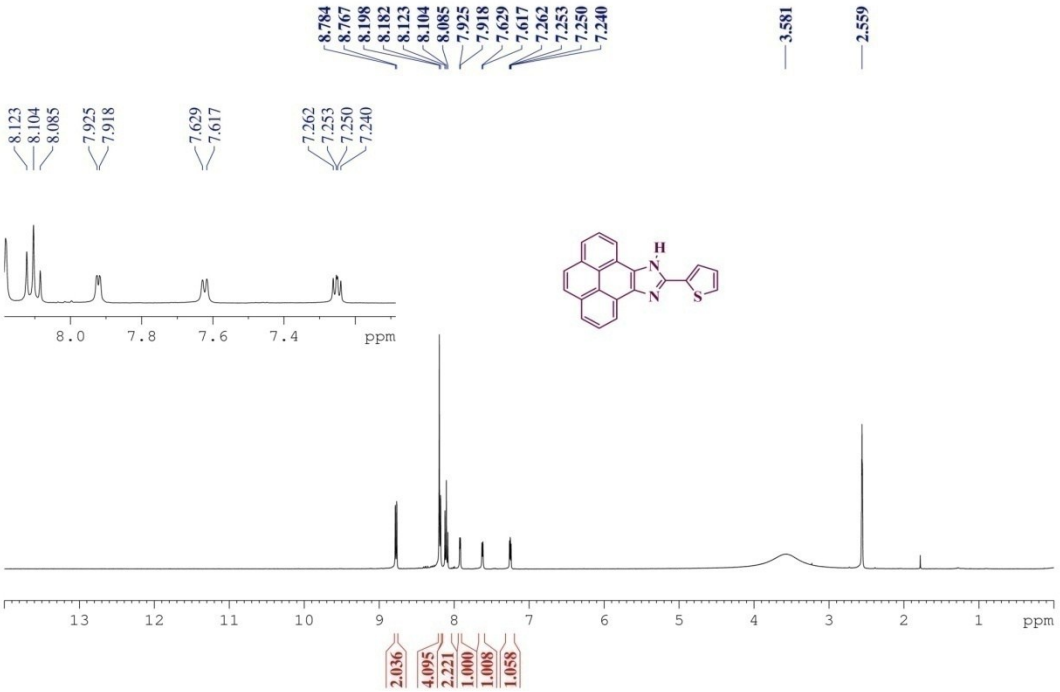
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

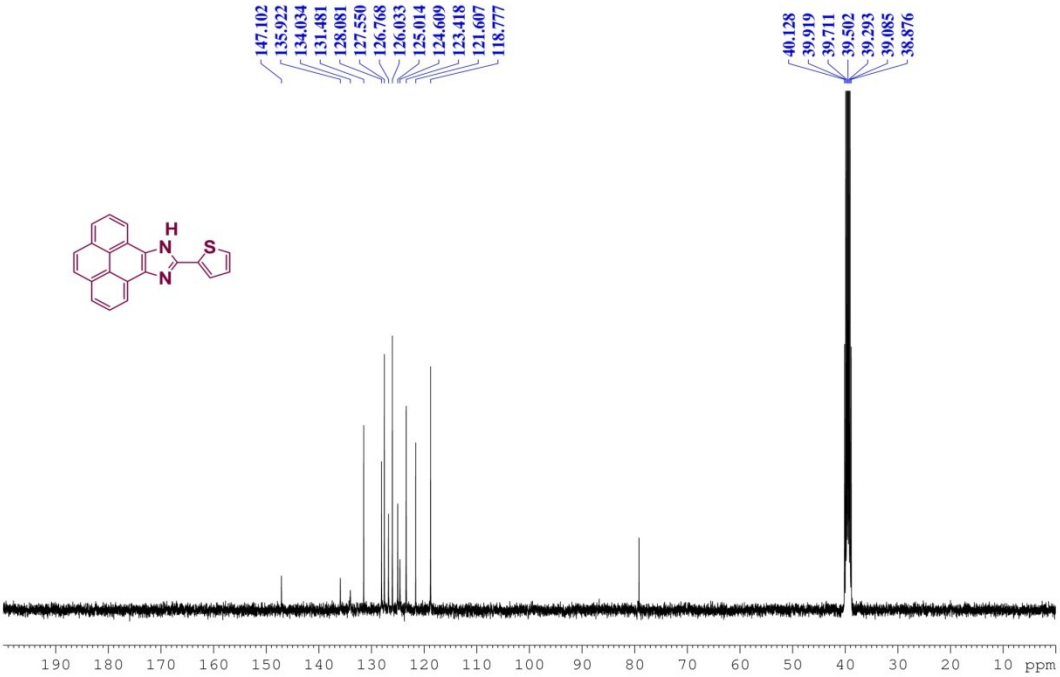


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
545.2010	1	C41H25N2	545.2012	-0.4	9.9	1	100.00	30.5	even	ok

^{1}H NMR spectrum of **3h** (400 MHz, DMSO-d^{6})



^{13}C NMR spectrum of **3h** (100 MHz, DMSO-d^{6})



ESI mass spectrum of **3h**

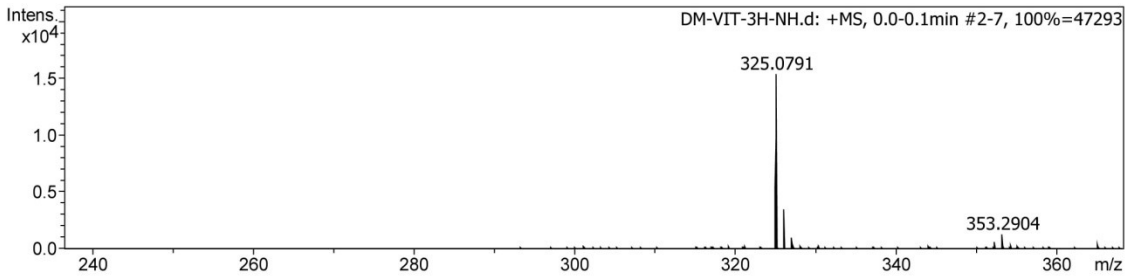
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

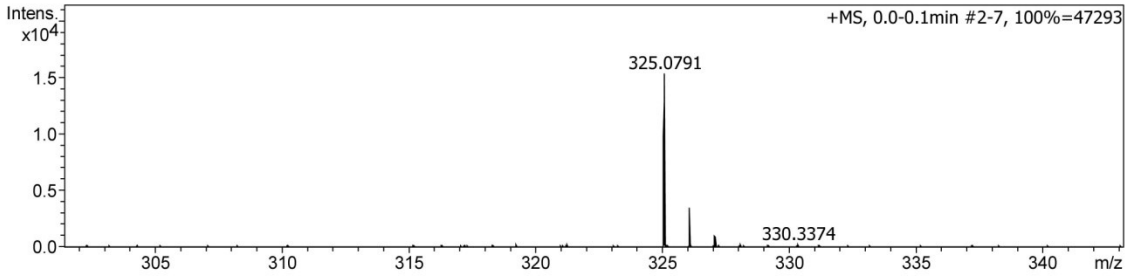
Analysis Info

Analysis Name	D:\Data\OCT-2016\DM-VIT-3H-NH.d	Acquisition Date	10/4/2016 5:43:29 PM
Method	Tune_pos_NAICSI-500A.m	Operator	DM IN
Sample Name	DM-VIT-3H-NH	Instrument	maXis impact 282001.00081
Comment	C21H12N2S		

Acquisition Parameter

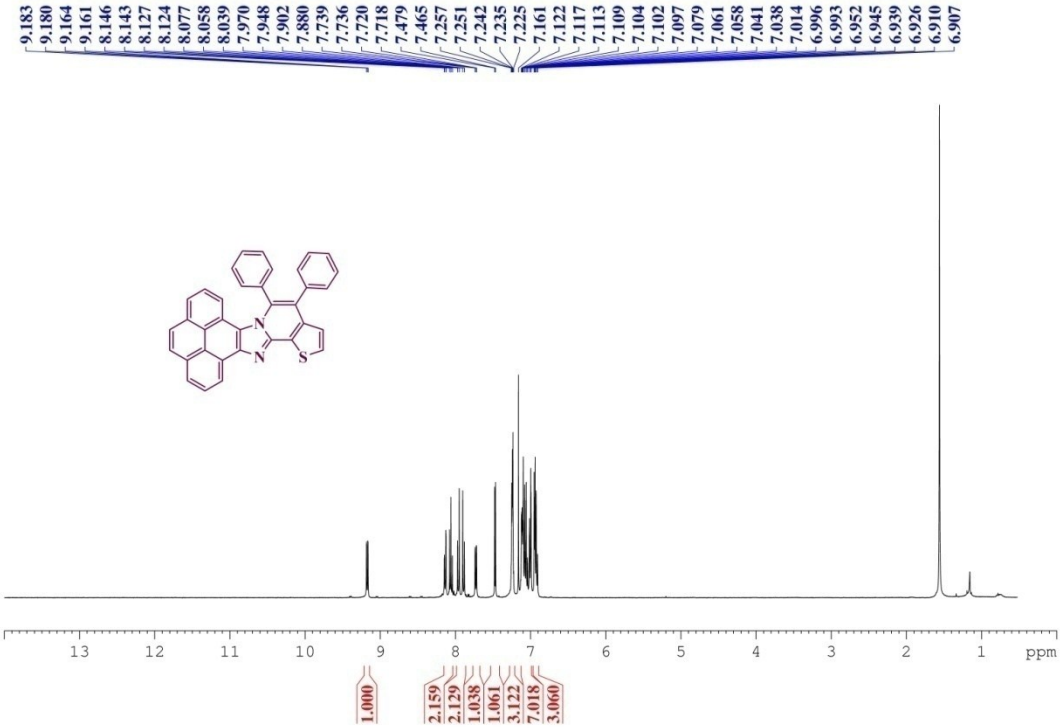
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



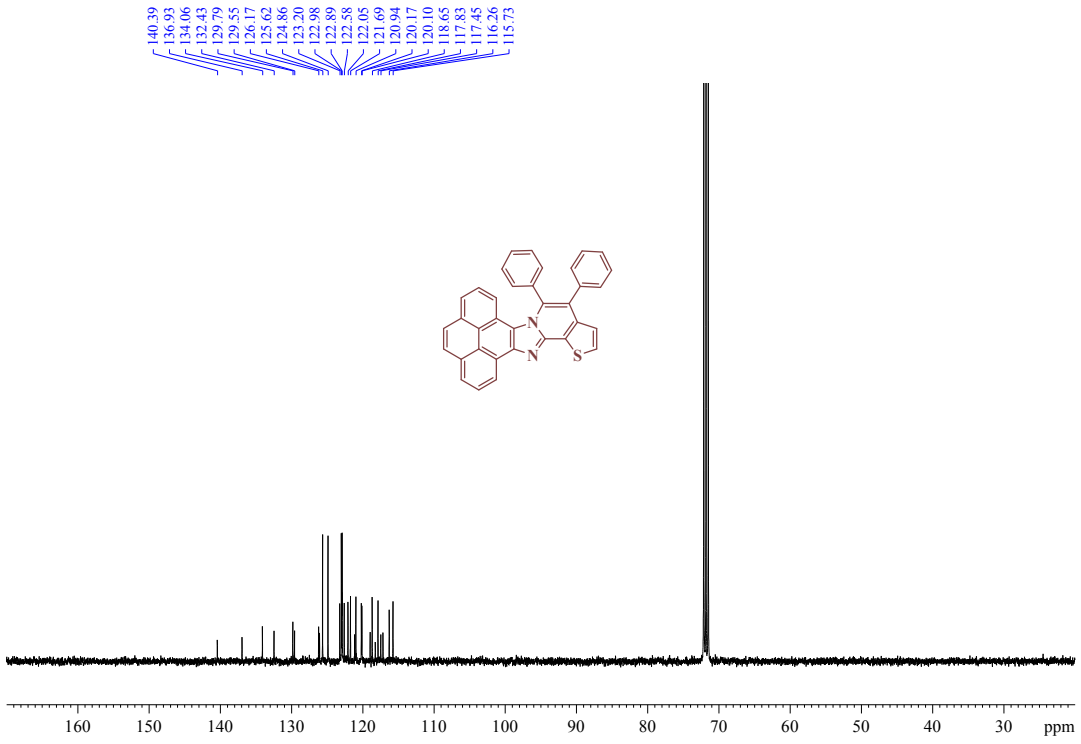


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
325.0791	1	C21H13N2S	325.0794	-0.9	11.2	1	100.00	16.5	even	ok

^{1}H NMR spectrum of **5h** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **5h** (100 MHz, $CDCl_3$)



ESI mass spectrum of **5h**

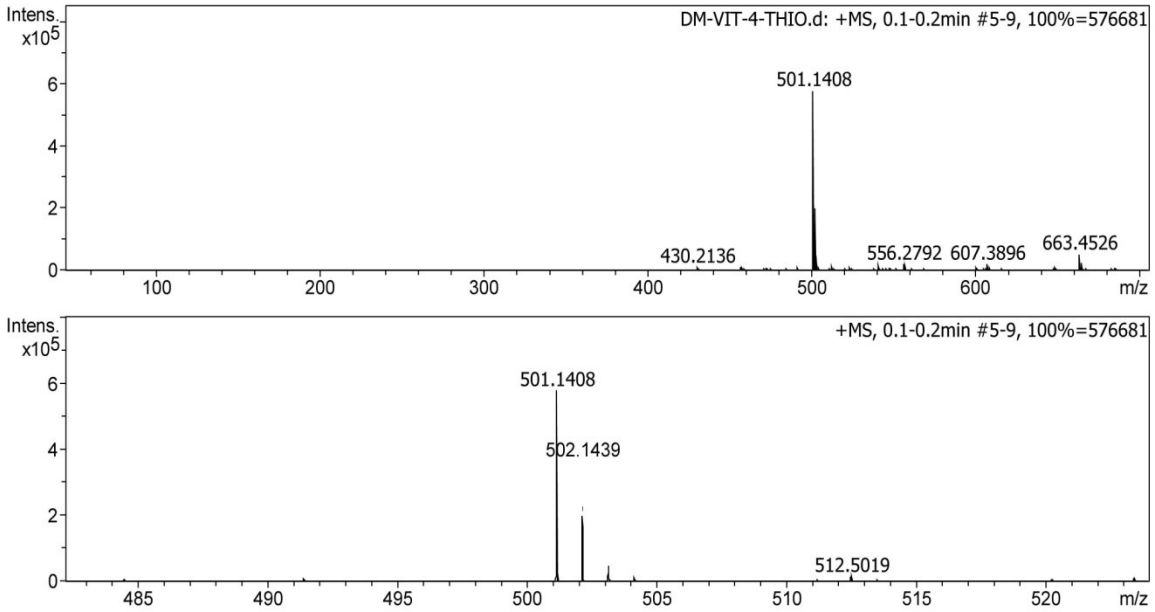
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\SEPT-2016\DM-VIT-4-THIO.d	Acquisition Date	9/29/2016 7:24:46 PM
Method	Tune_pos_NAICSI-500A.m	Operator	CPR_OUT
Sample Name	DM-VIT-4-THIO	Instrument	maXis impact 282001.00081
Comment	C35H20N2S		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
501.1408	1	C35H21N2S	501.1420	2.3	29.1	1	100.00	26.5	even	ok