Electronic Supplementary information

for

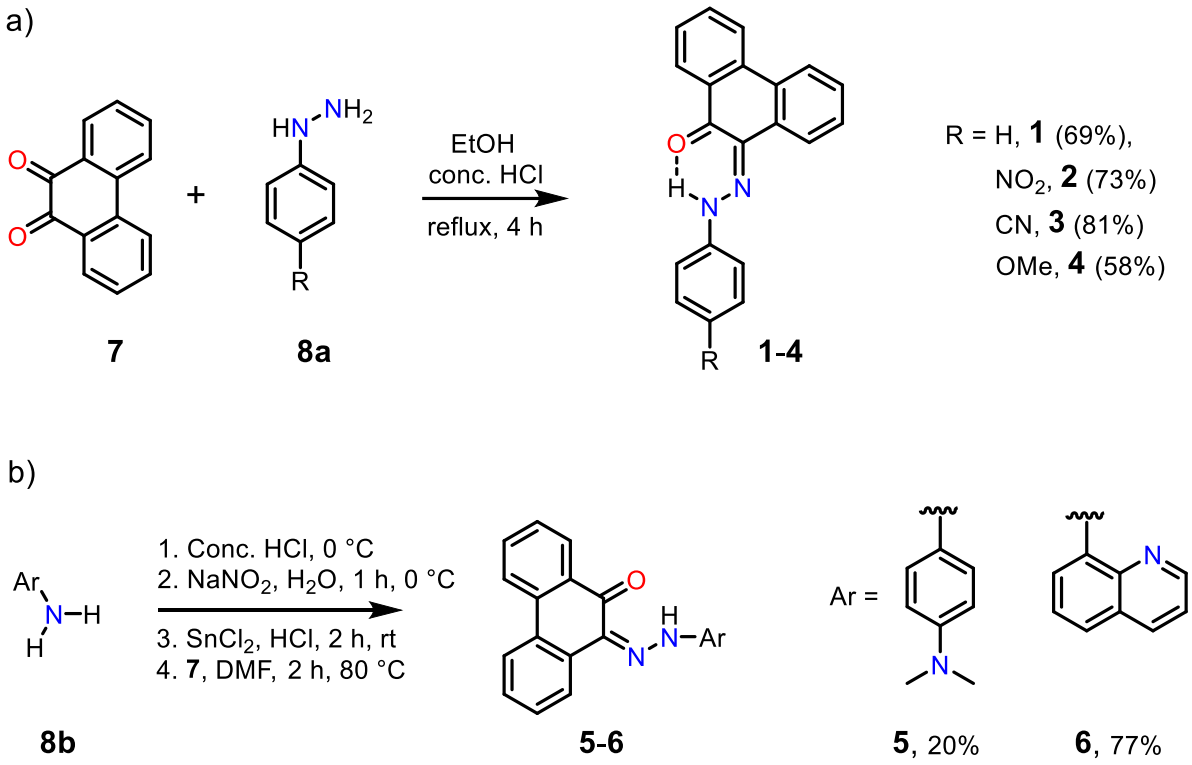
Effect of Substituents on the Aggregation-Induced Emission of 9,10-Phenanthraquinone-Hydrazones

Naveen Kumar M,[a] Deikrisha Lyngdoh Lyngkhoi,[b] Sudhakar Gaikwad,[c] Debabrata Samanta,[d] Snehadrinarayan Khatua*[b] and Susnata Pramanik*[a]

[a]Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, 603203 India. E-mail: susmatap@srmist.edu.in
[b]Centre for Advanced Studies, Department of Chemistry, North-Eastern Hill University Shillong, Meghalaya 793022, India. E-mail: snehadri@gmail.com; skhatua@nehu.ac.in
[c]Division of Organic Chemistry, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, 411 008, Pune, Maharashtra, India.
[d]Department of Chemistry, Dukhulal Nibaran Chandra College Aurangabad, Suti, West Bengal 742201, India.

Table of Content

1. Synthetic Scheme



Scheme 1. Synthesis of hydrazones **1-6.**

2. NMR Characterization

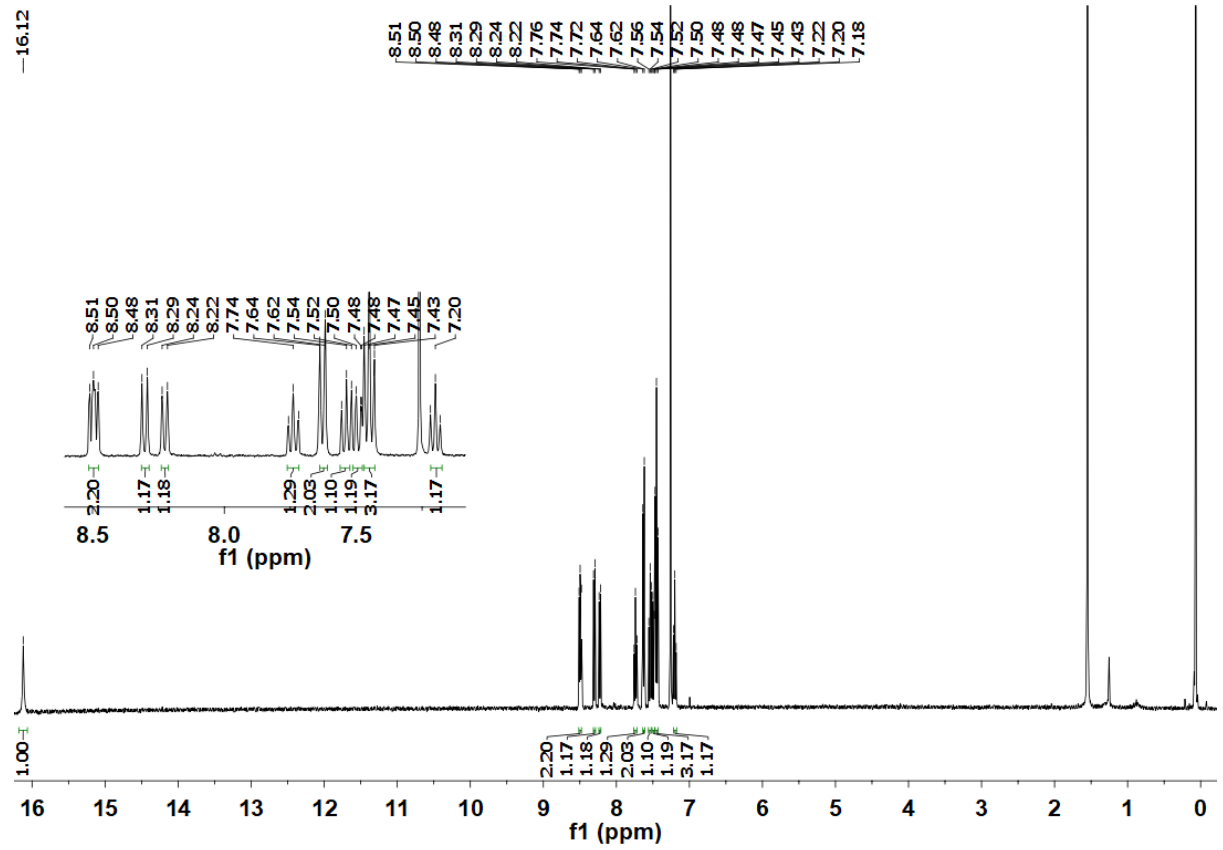


Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) spectrum of **1**.

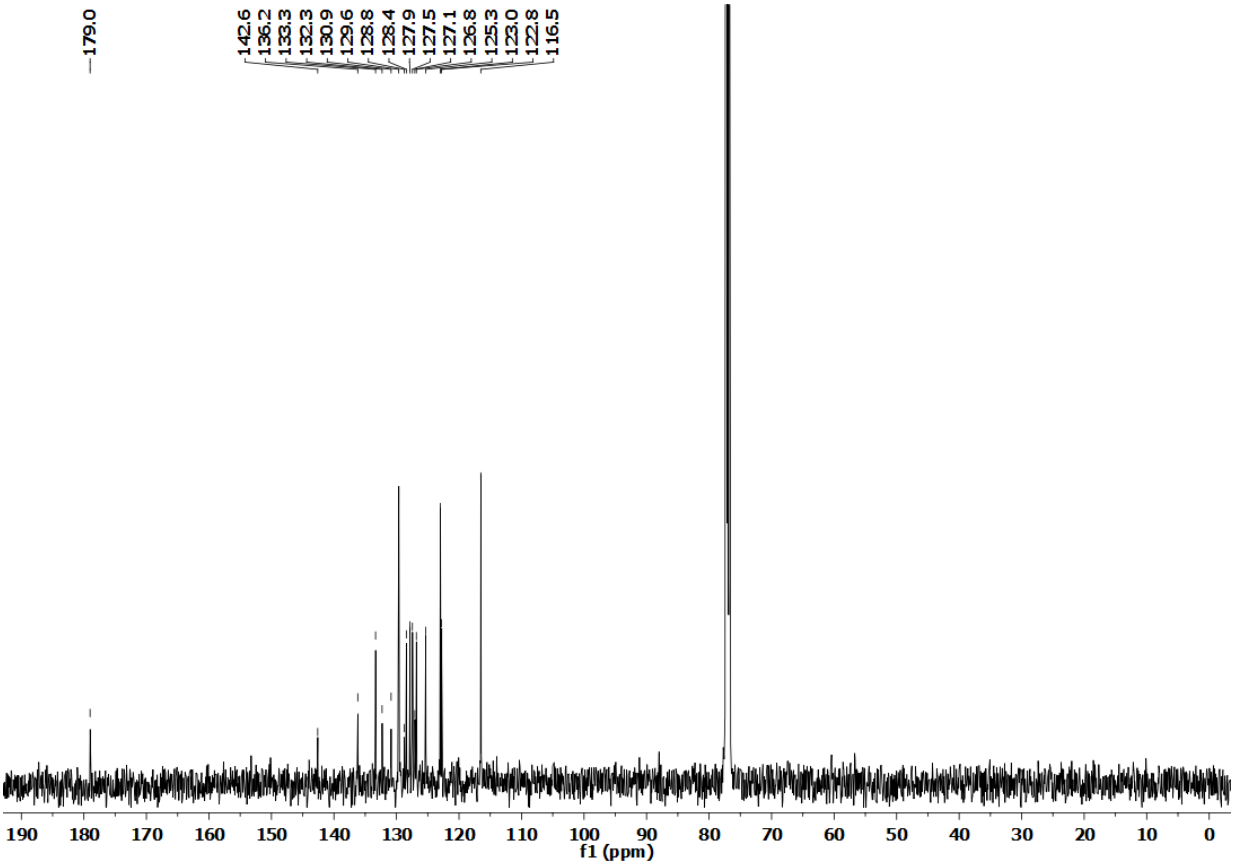


Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) spectrum of **1**.

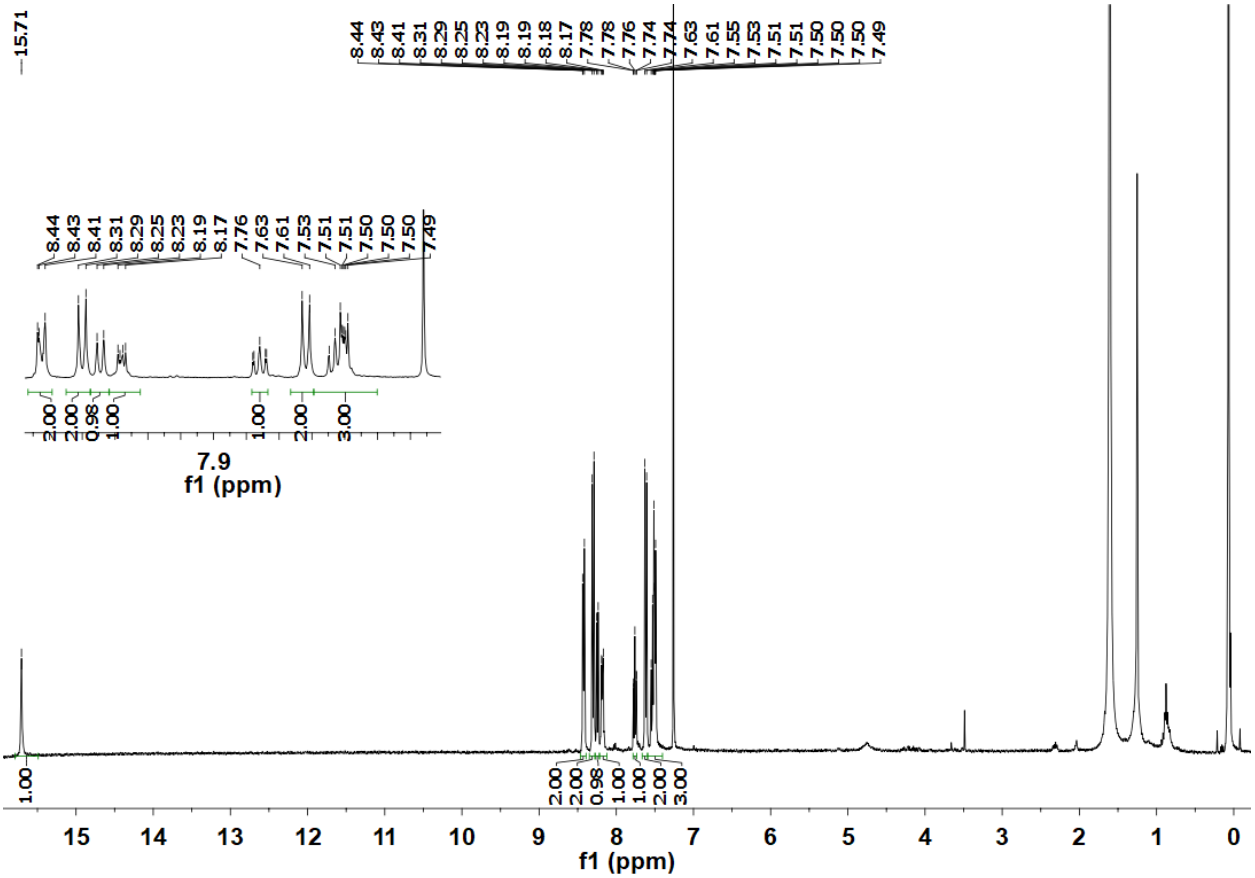


Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) spectrum of **2**.

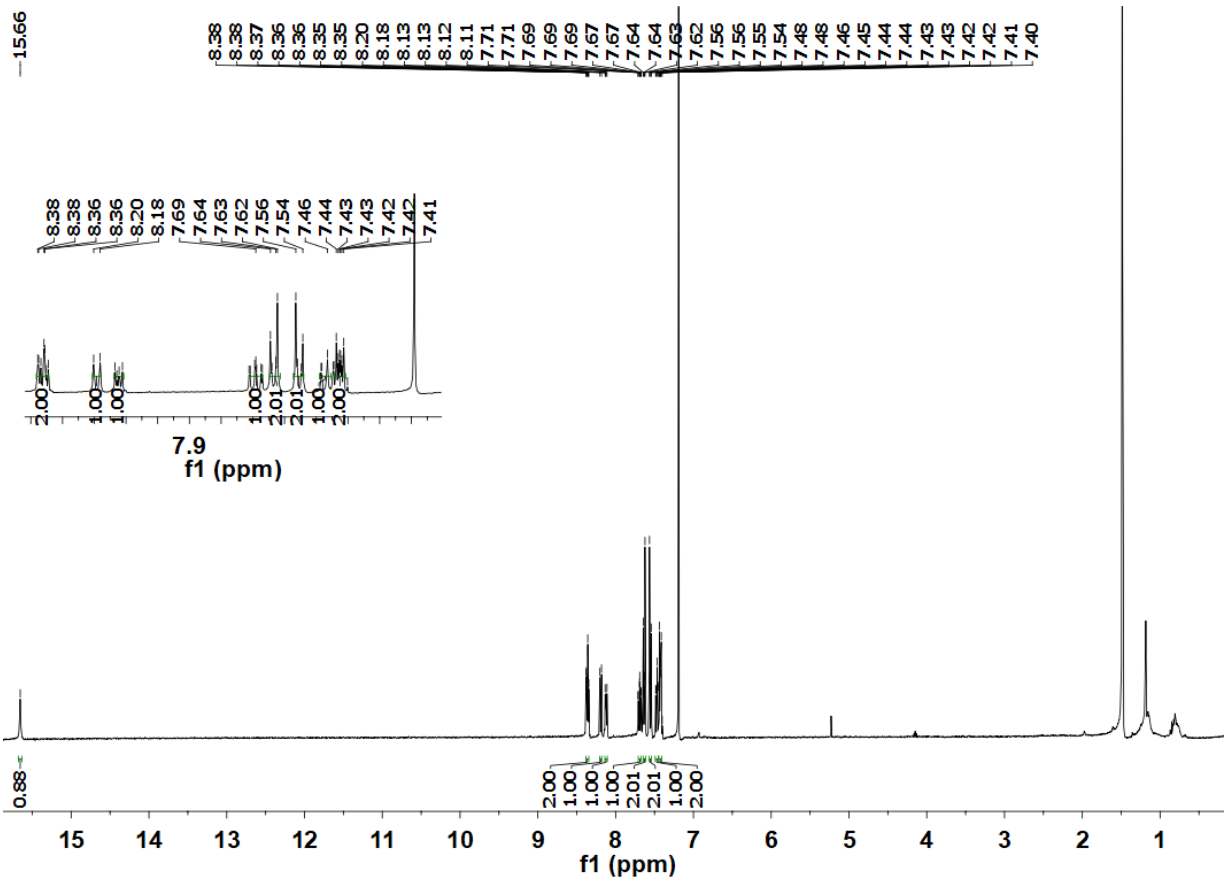


Figure S4. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) spectrum of **3**.

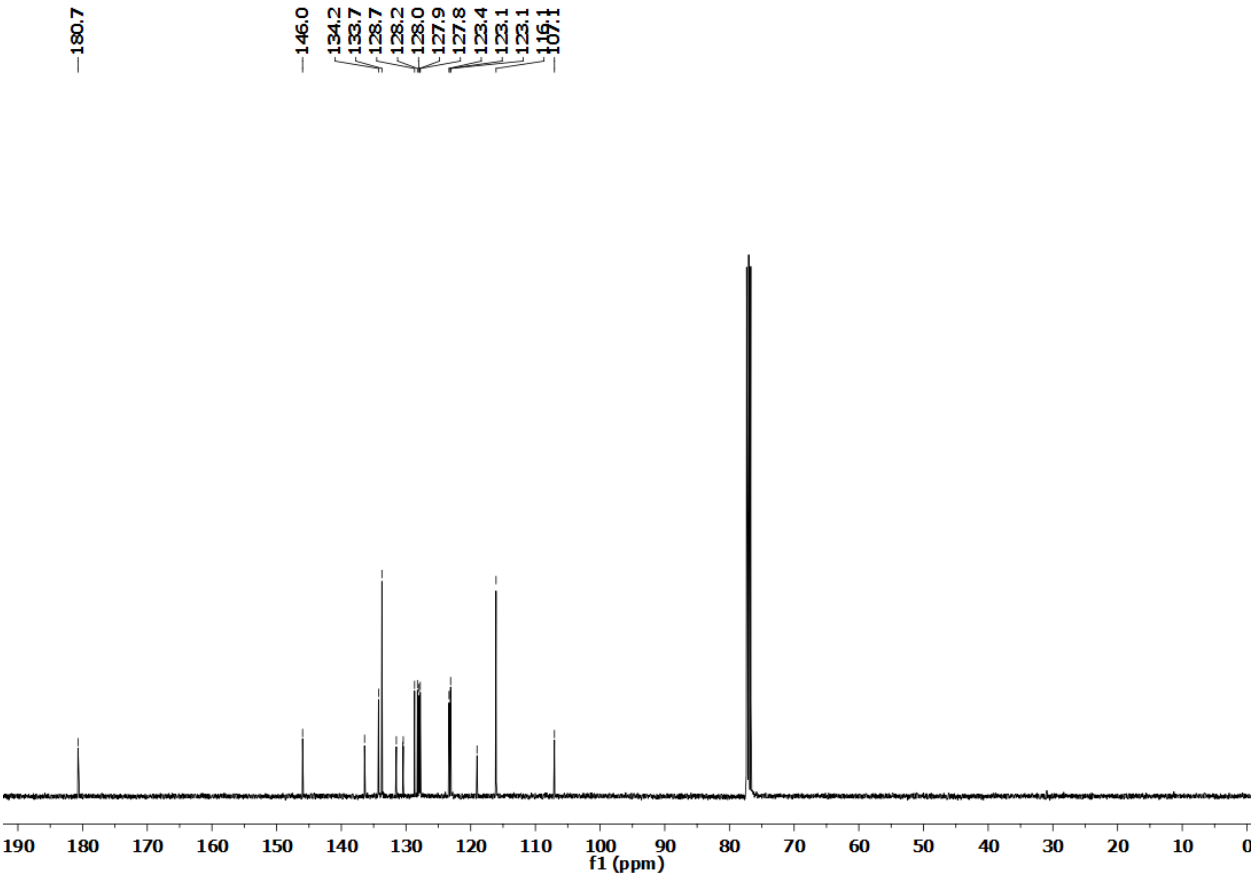


Figure S5. ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) spectrum of **3**.

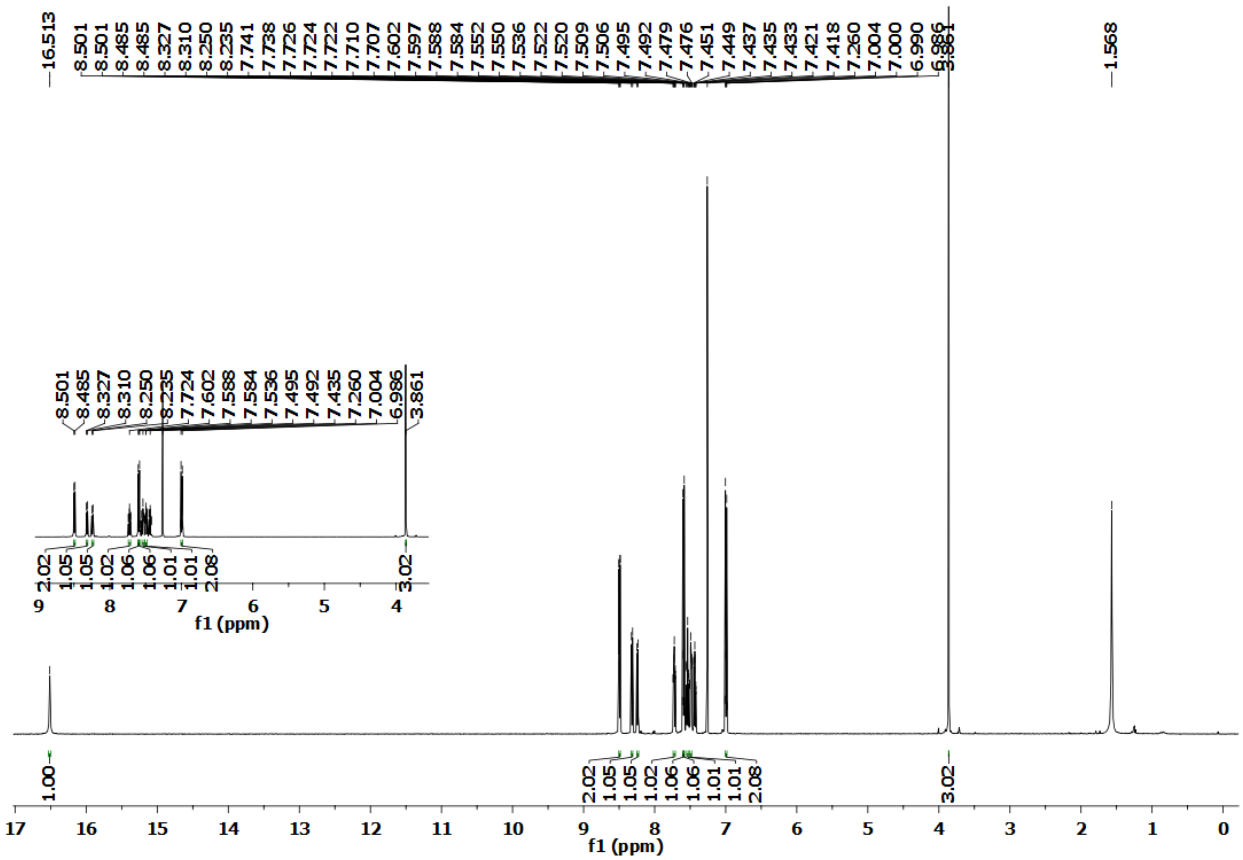


Figure S6. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) spectrum of **4**.

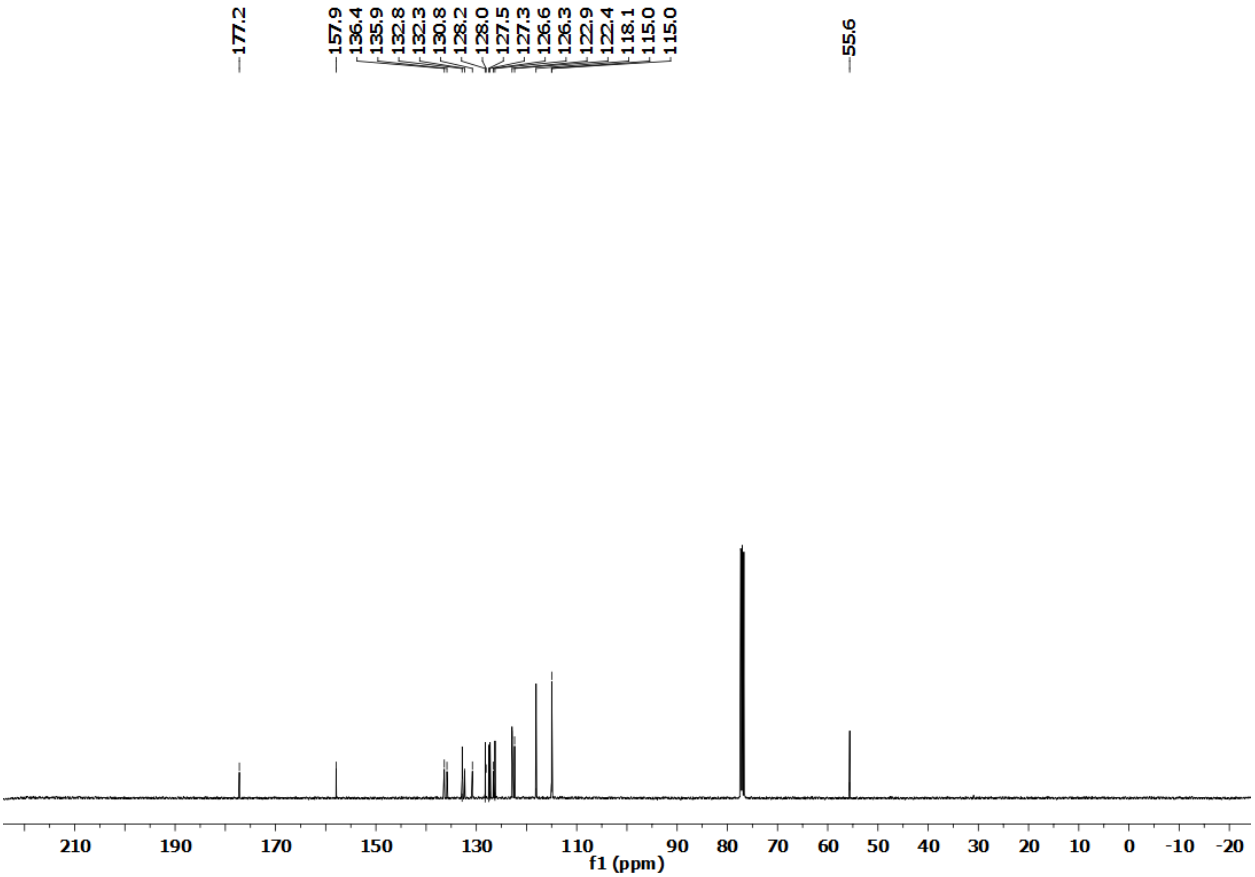


Figure S7. ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) spectrum of **4**.

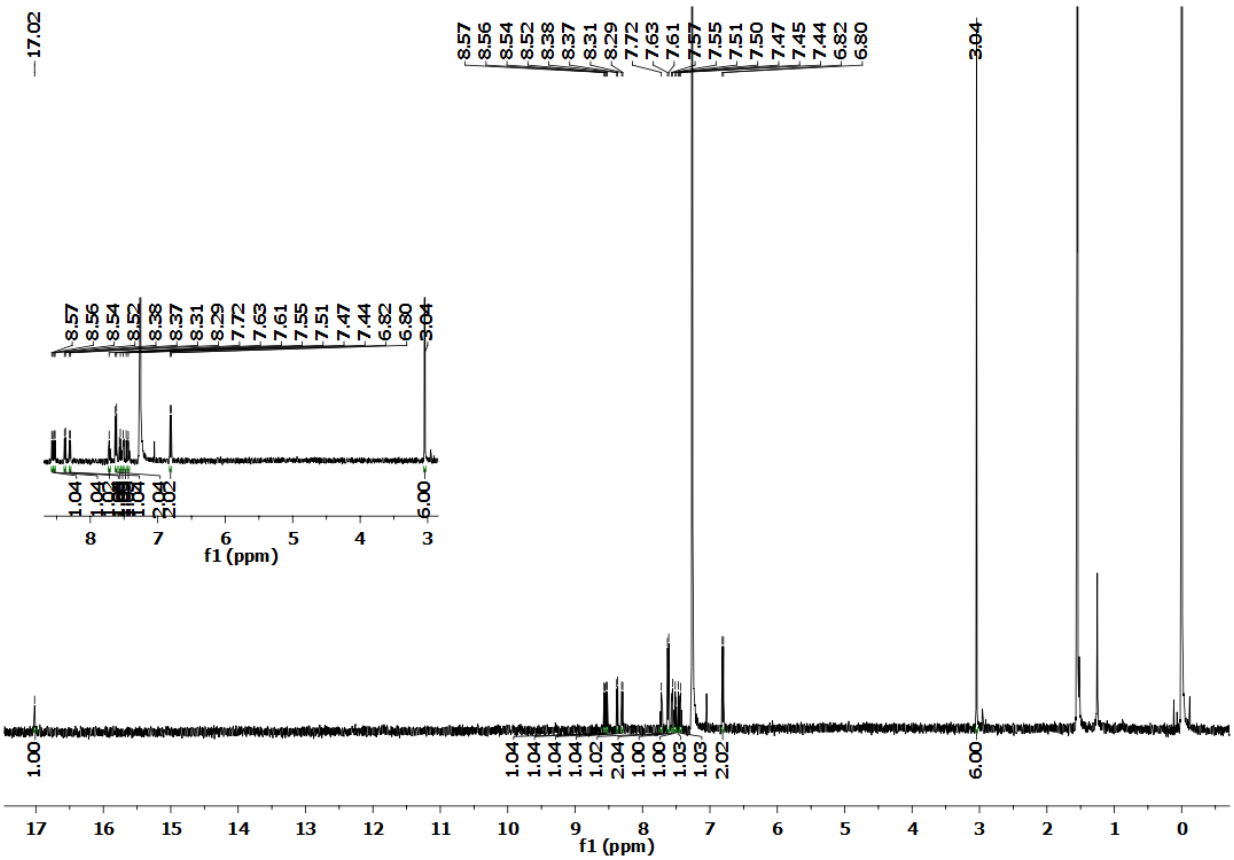


Figure S8. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) spectrum of **5**.

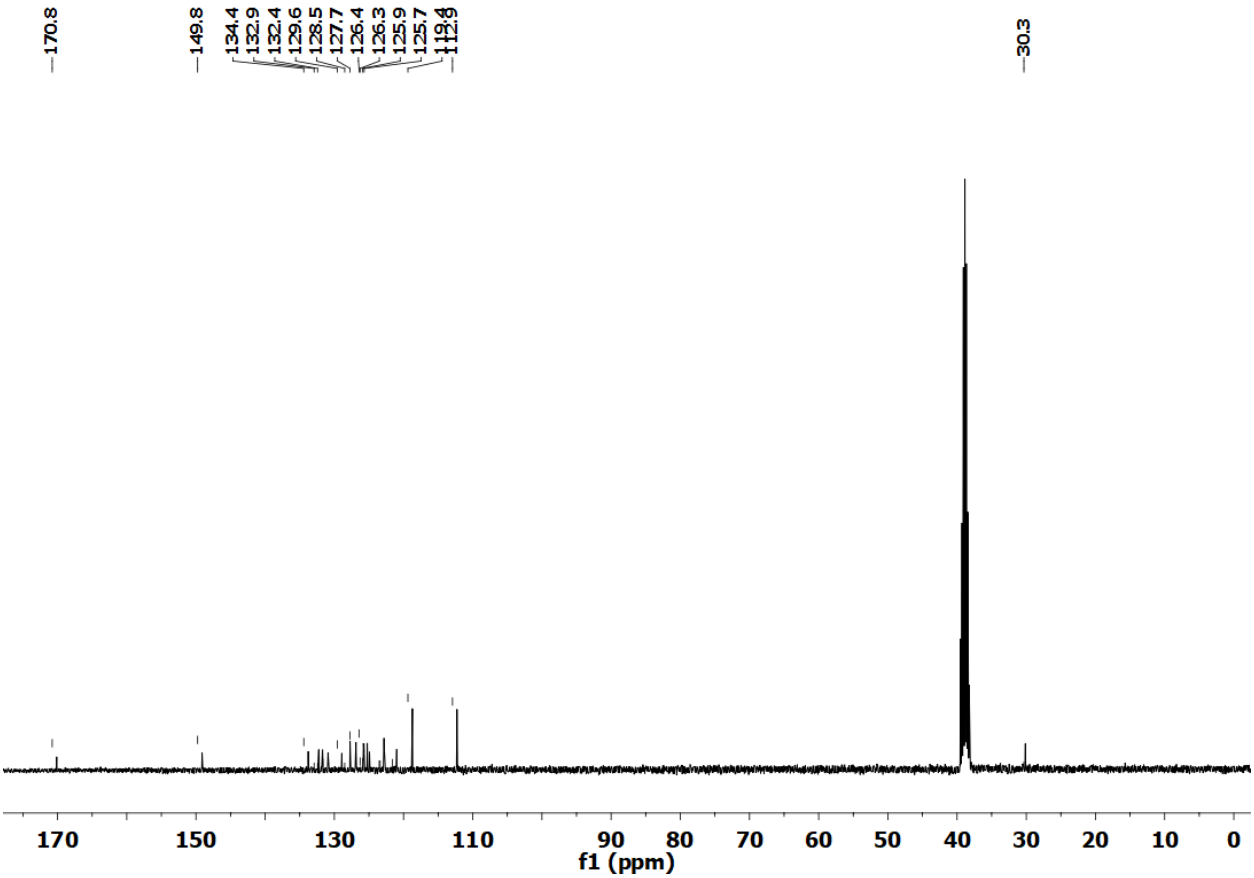


Figure S9. ^{13}C NMR (125 MHz, $CDCl_3$, 298 K) spectrum of **5**.

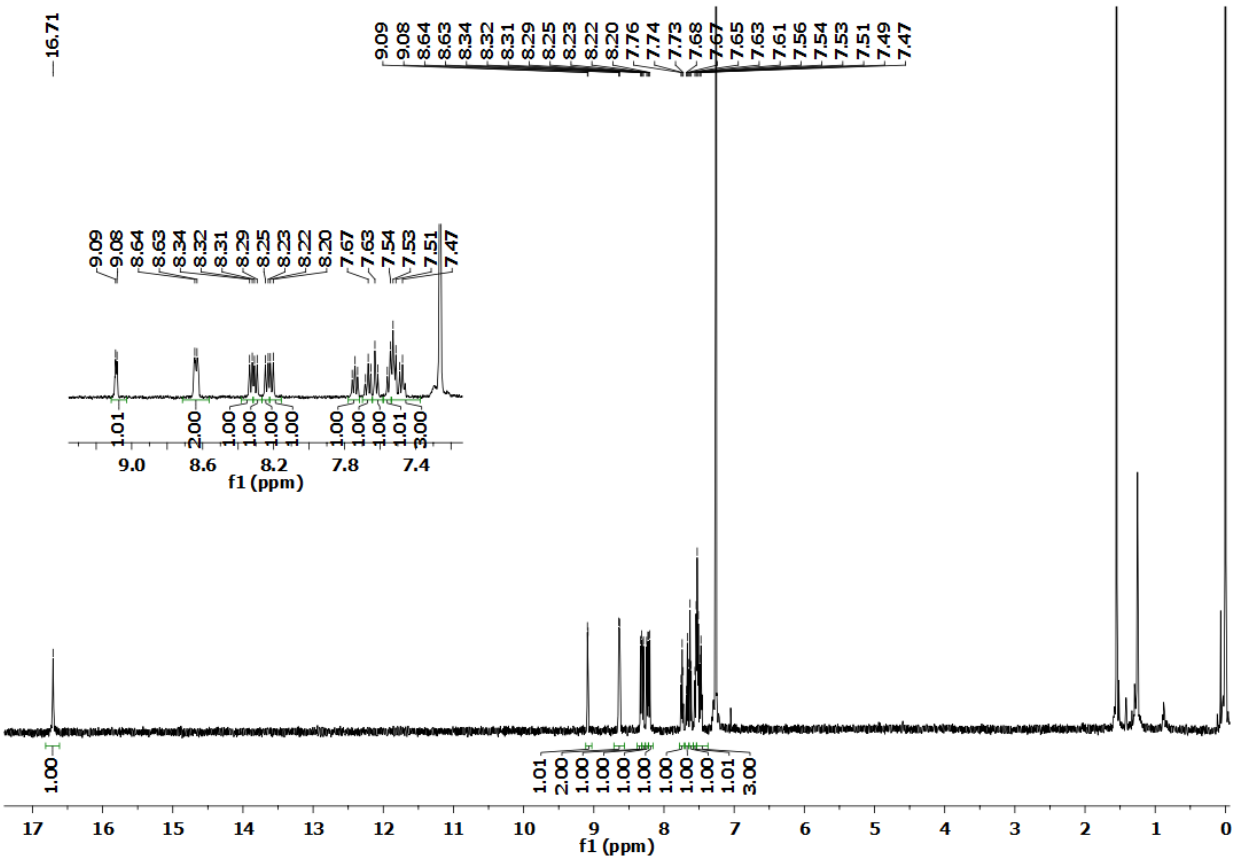


Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) spectrum of **6**.

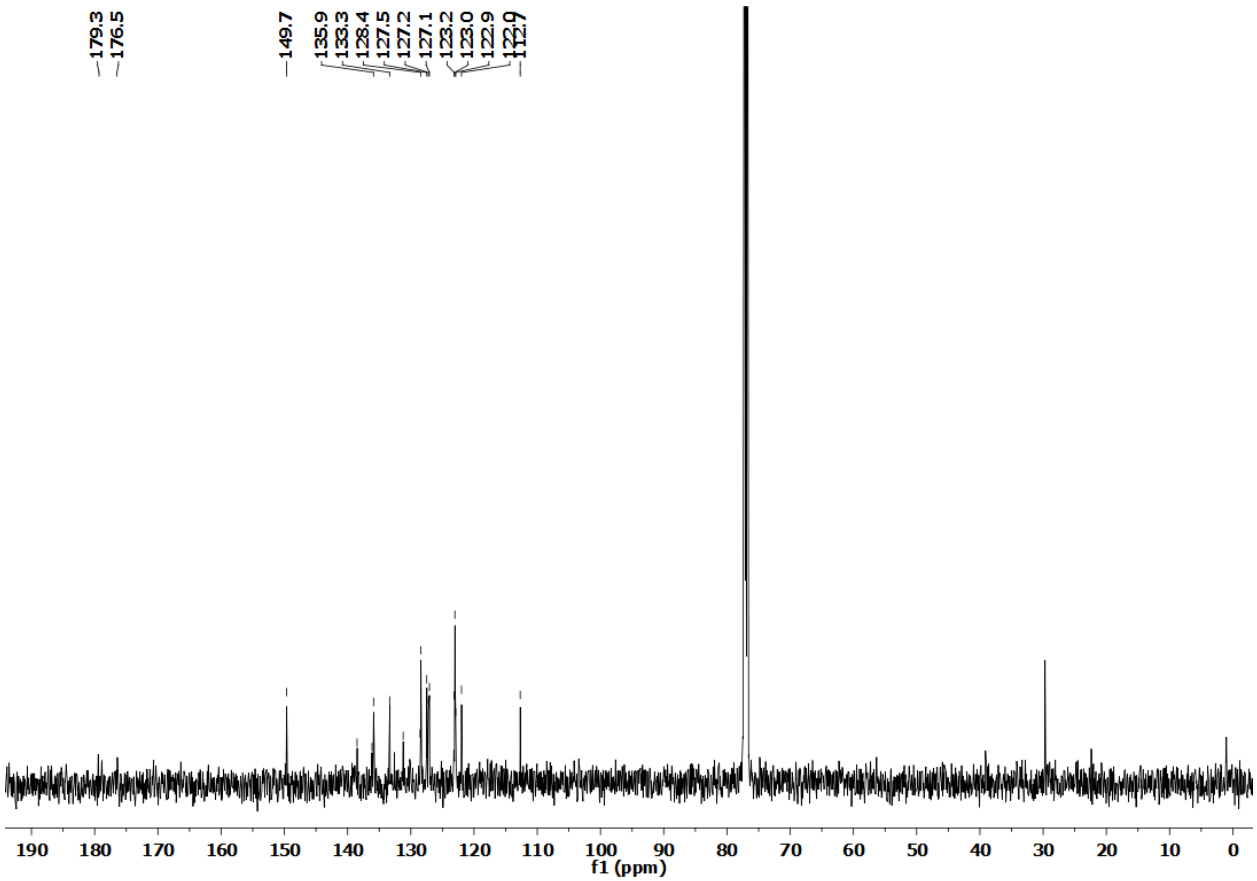
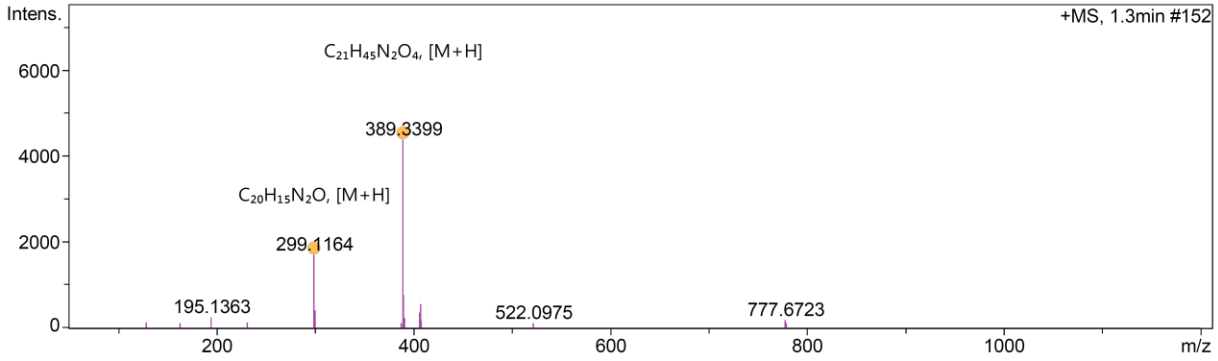


Figure S11. ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) spectrum of **6**. Compound has poor solubility in common organic solvent.

3. ESI-HRMS Characterization



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
299.1164	1	C20H15N2O	299.1179	4.9	17.7	1	100.00	15.0	even	ok
389.3399	1	C21H45N2O4	389.3374	-6.5	38.3	1	54.98	1.0	even	ok
	2	C22H41N6	389.3387	-3.1	51.7	2	100.00	6.0	even	ok
	3	C26H45O2	389.3414	3.8	63.6	3	56.45	5.0	even	ok

Figure S12. ESI-HRMS spectrum of compound **1**.

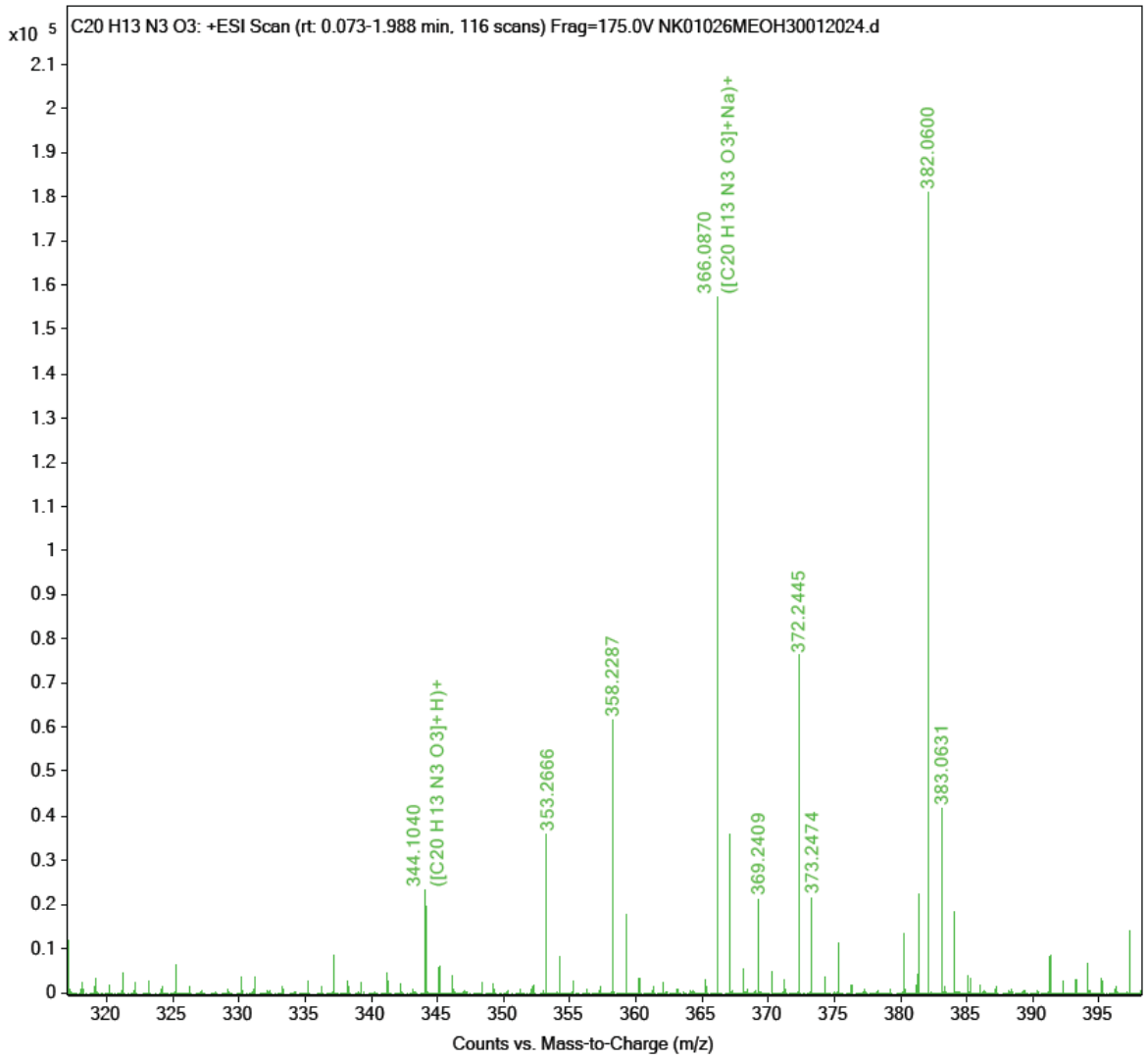


Figure S13. ESI-HRMS spectrum of compound **2**.

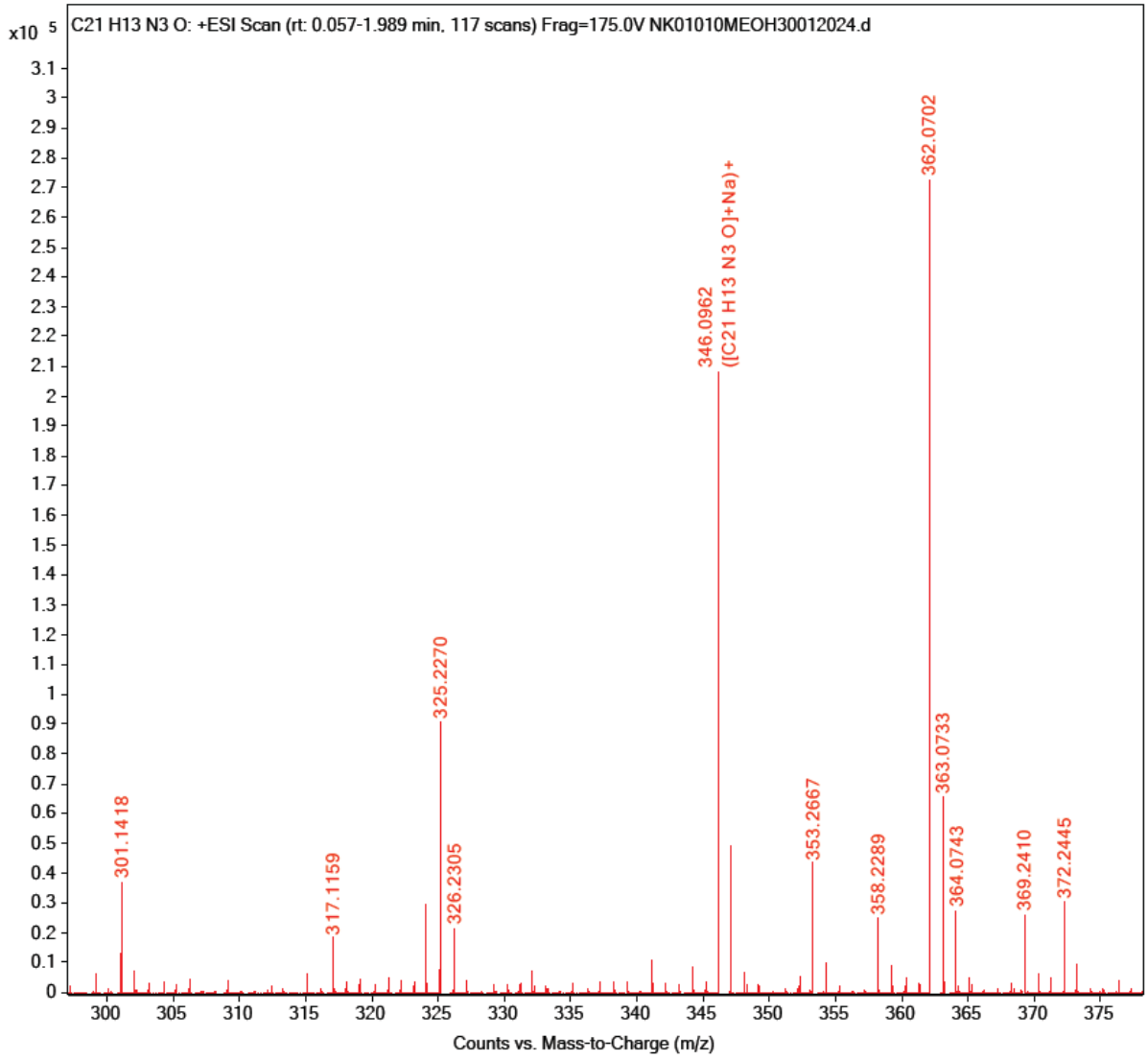


Figure S14. ESI-HRMS spectrum of compound **3**.

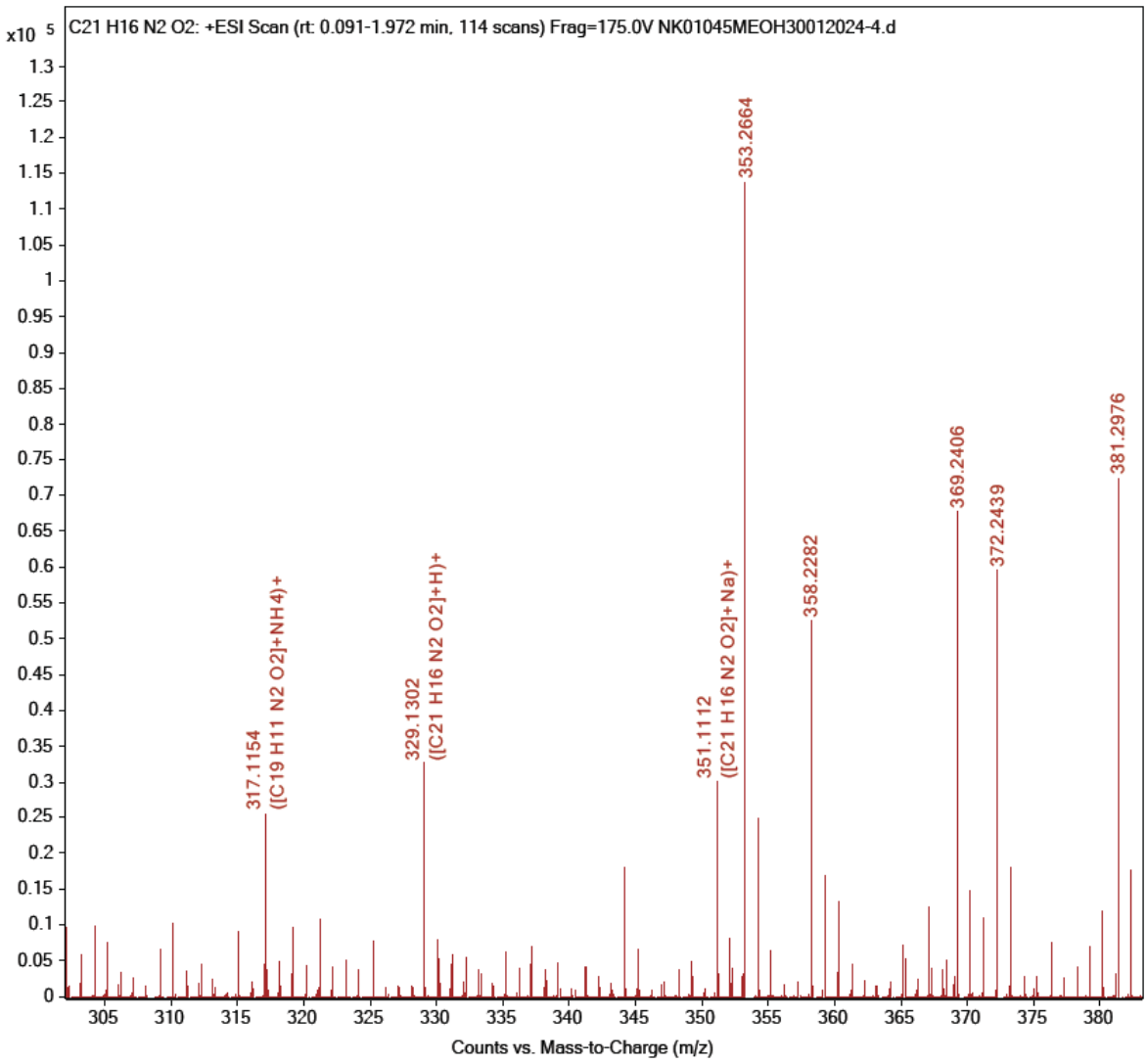
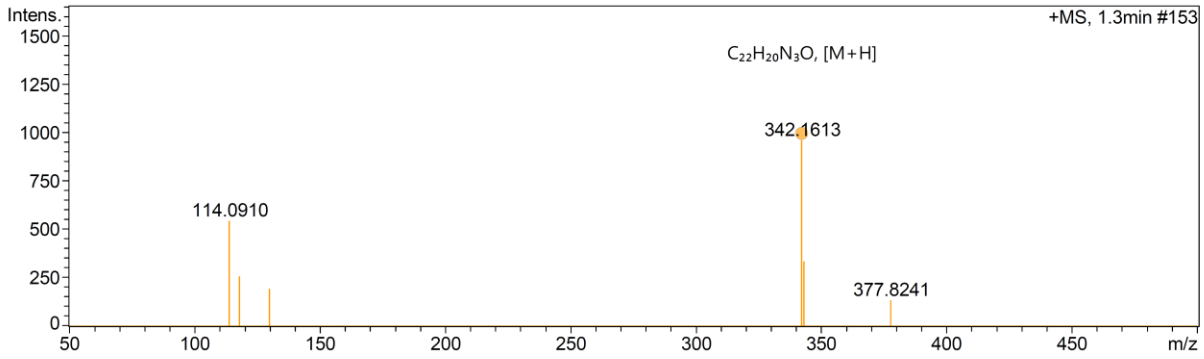
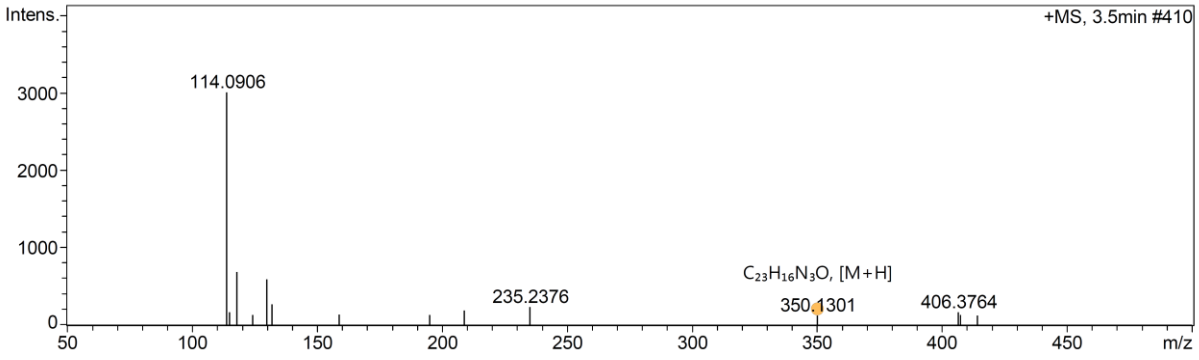


Figure S15. ESI-HRMS spectrum of compound **4**.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
342.1613	1	C22H20N3O	342.1601	-3.5	59.6	1	100.00	15.0	even	ok
	2	C12H16N13	342.1646	9.7	98.9	2	3.63	12.0	even	ok
	3	C11H20N9O4	342.1633	5.8	112.6	3	6.11	7.0	even	ok
	4	C7H16N15O2	342.1606	-2.0	125.2	4	6.97	8.0	even	ok
	5	C10H24N5O8	342.1619	1.9	126.3	5	6.72	2.0	even	ok

Figure S16. ESI-HRMS spectrum of compound **5**.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
350.1301	1	C23H16N3O	350.1288	-3.8	n.a.	1	100.00	18.0	even	ok

Figure S17. ESI-HRMS spectrum of compound **6**.

4. Linear Free Energy Relationship

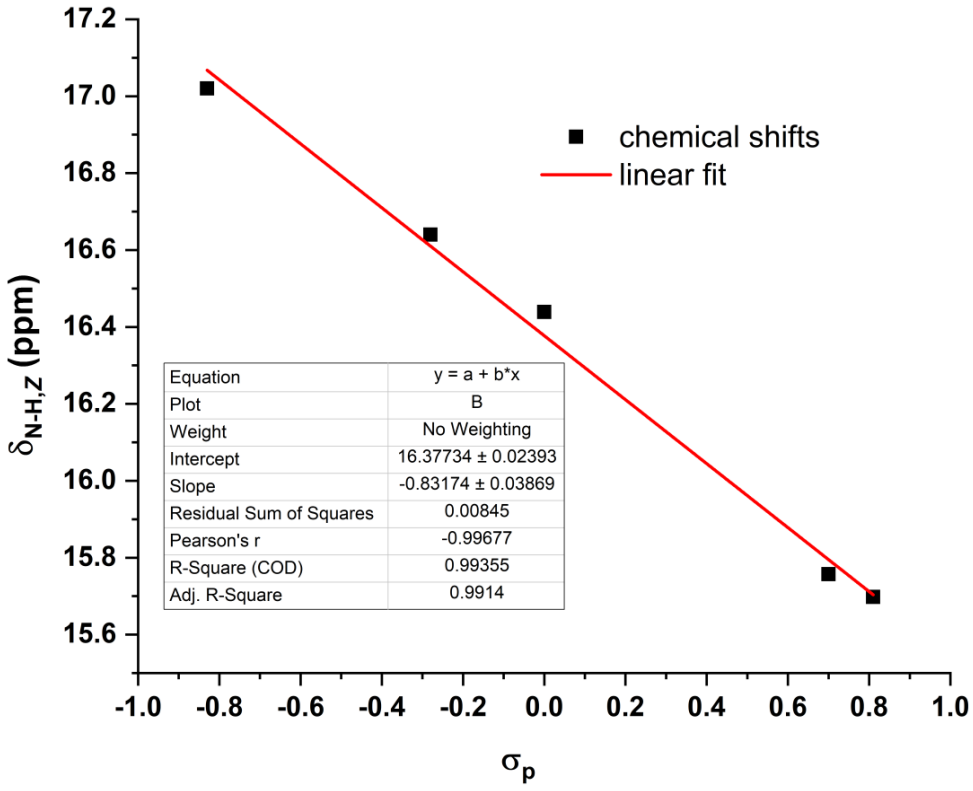


Figure S18. Hammett plot of δ_{N-H} of different hydrazones (in their *Z*-form) vs. substituent constants (σ_p).

5. Aggregation Studies of Hydrazones 1-6

Monitored by UV-Vis and Fluorescence Spectrometers

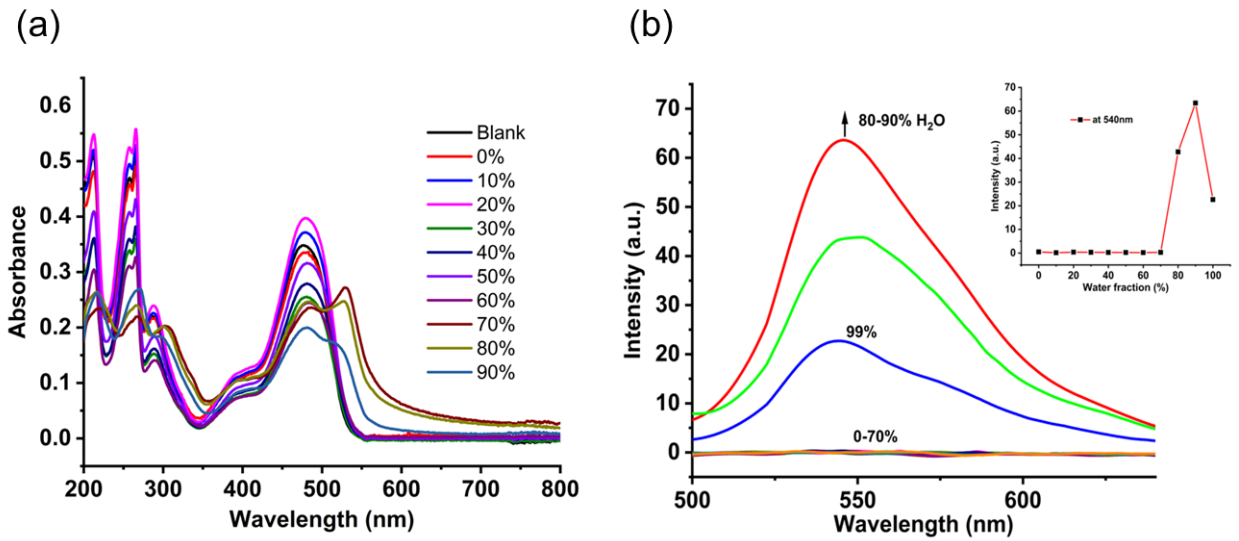


Figure S19. Change in (a) UV absorption and (b) emission spectra (λ_{ex} = 478 nm) of **1** upon changing the water −acetonitrile ratio (at 298 K, 10^{-5} M). Inset: showing change of emission at 540 nm.

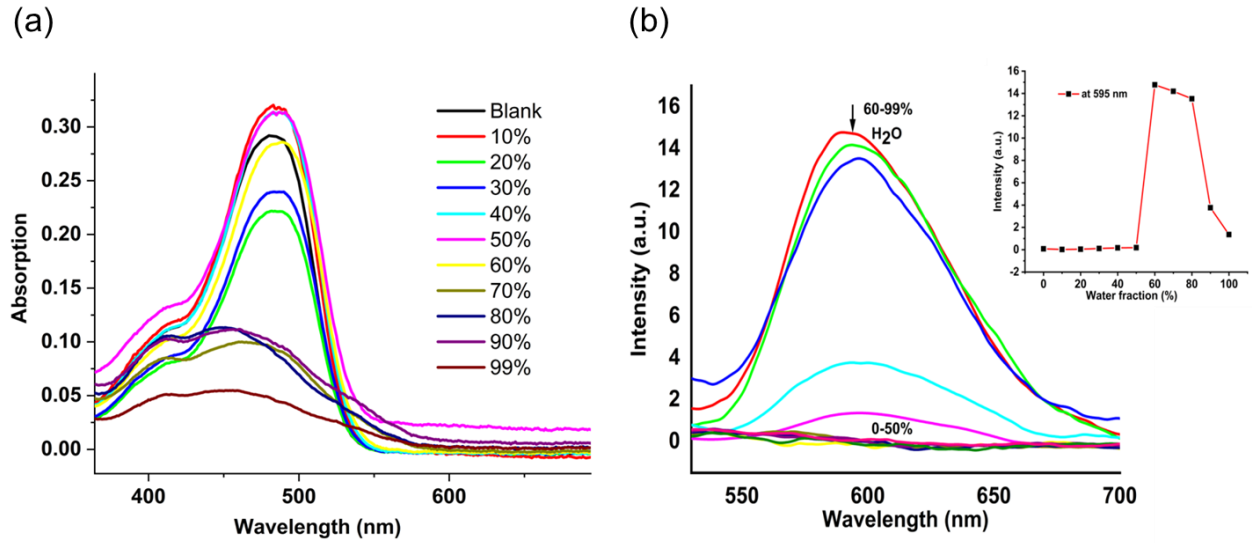


Figure S20. Change in (a) UV absorption and (b) emission spectra (λ_{ex} = 483 nm) of **2** upon changing the water −acetonitrile ratio (at 298 K, 10^{-5} M). Inset: showing change of emission at 595 nm.

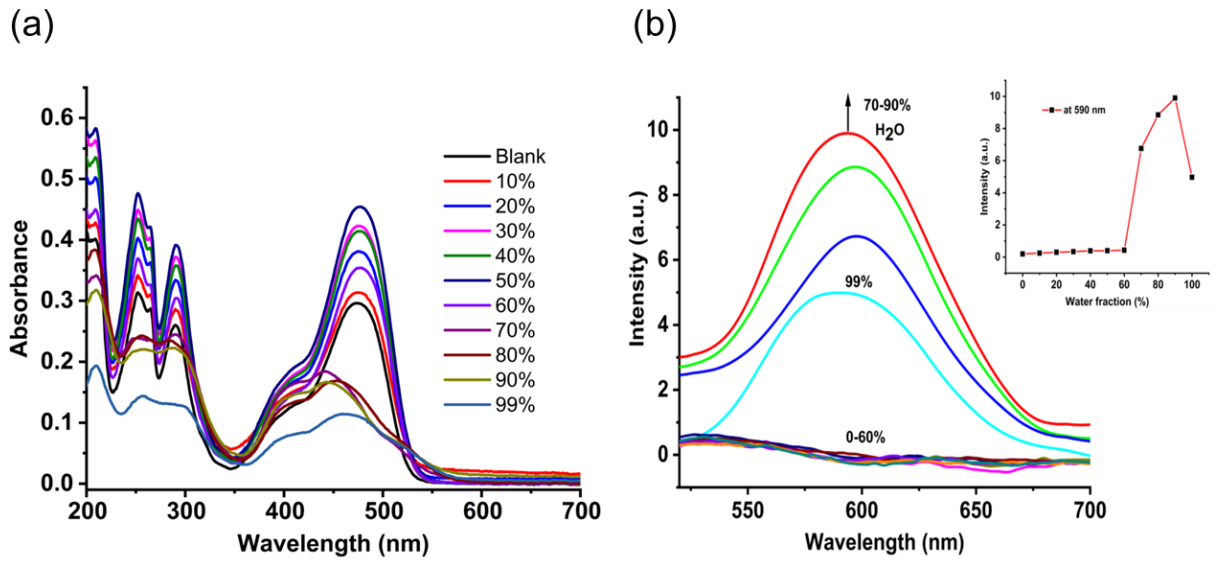


Figure S21. Change in (a) UV absorption and (b) emission spectra (λ_{ex} = 474 nm) of **3** upon changing the water −acetonitrile ratio (at 298 K, 10^{-5} M). Inset: showing change of emission at 590 nm.

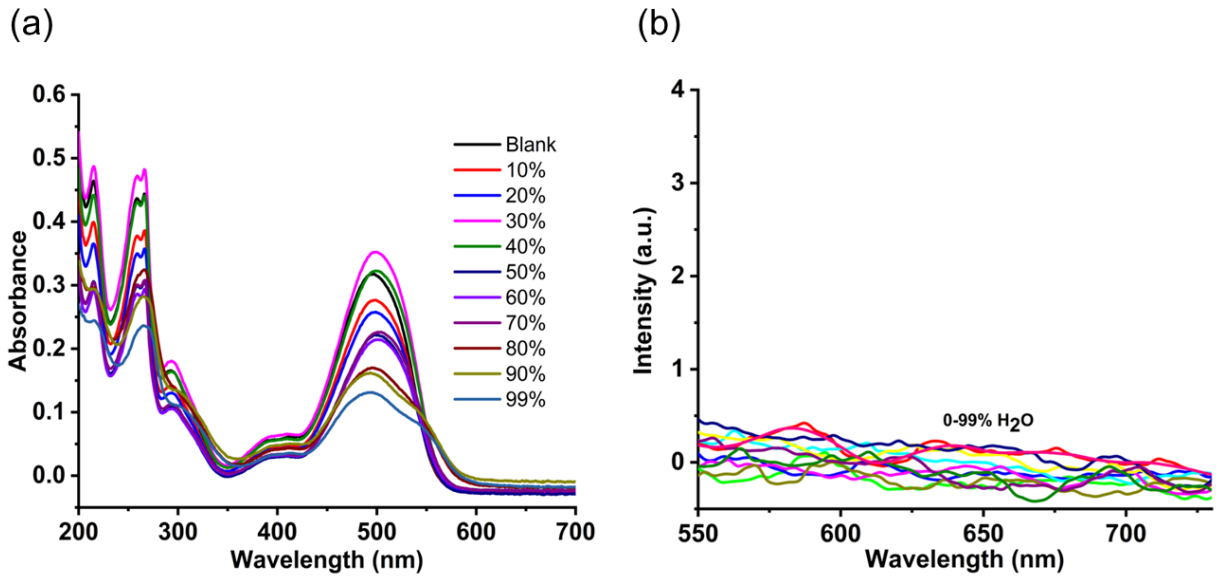


Figure S22. Change in (a) UV absorption and (b) emission spectra (λ_{ex} = 495 nm) of **4** upon changing the water −acetonitrile ratio (at 298 K, 10^{-5} M).

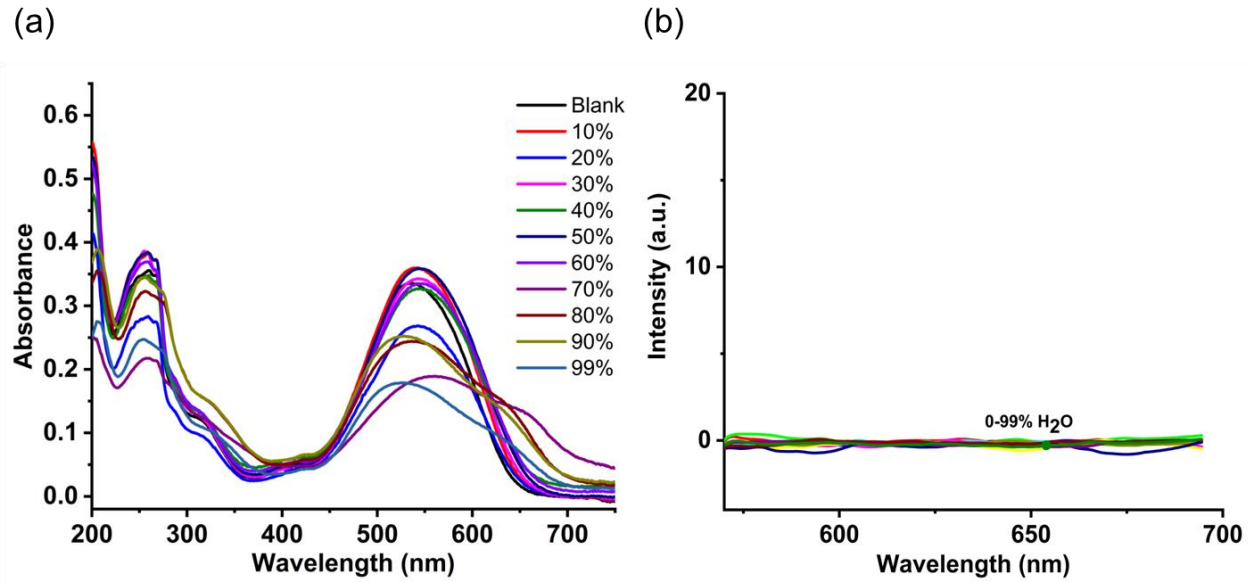


Figure S23. Change in (a) UV absorption and (b) emission spectra (λ_{ex} = 536 nm) of **5** upon changing the water −acetonitrile ratio (at 298 K, 10^{-5} M).

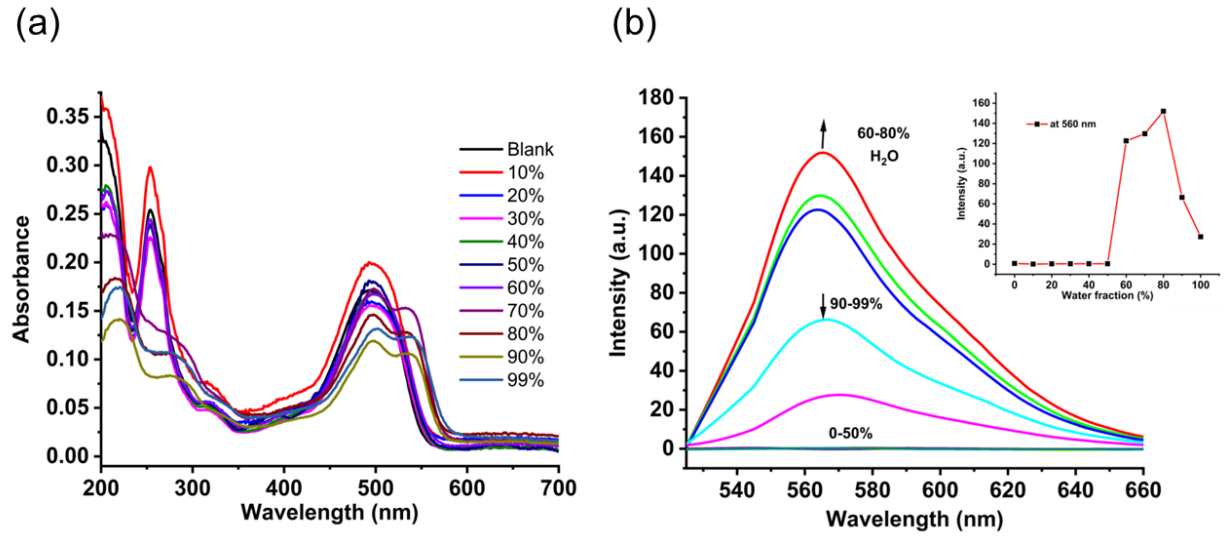


Figure S24. Change in (a) UV absorption and (b) emission spectra (λ_{ex} = 496 nm) of **6** upon changing the water −acetonitrile ratio (at 298 K, 10^{-5} M). Inset: showing change of emission at 560 nm.

6. Solid State Emission and Powder XRD

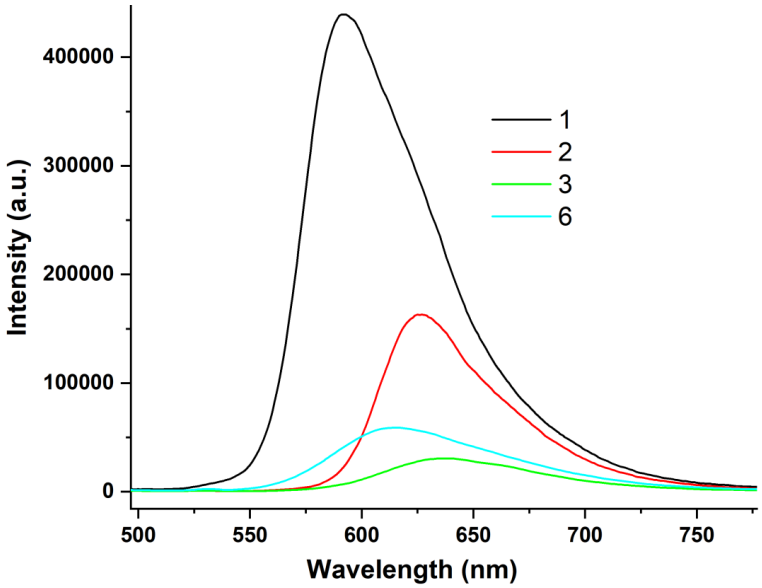


Figure S25. Emission spectra of compounds **1-3** and **6** recorded in their amorphous solid state. Excitation wavelengths are the λ_{max} obtained from their absorption spectra recorded in acetonitrile.

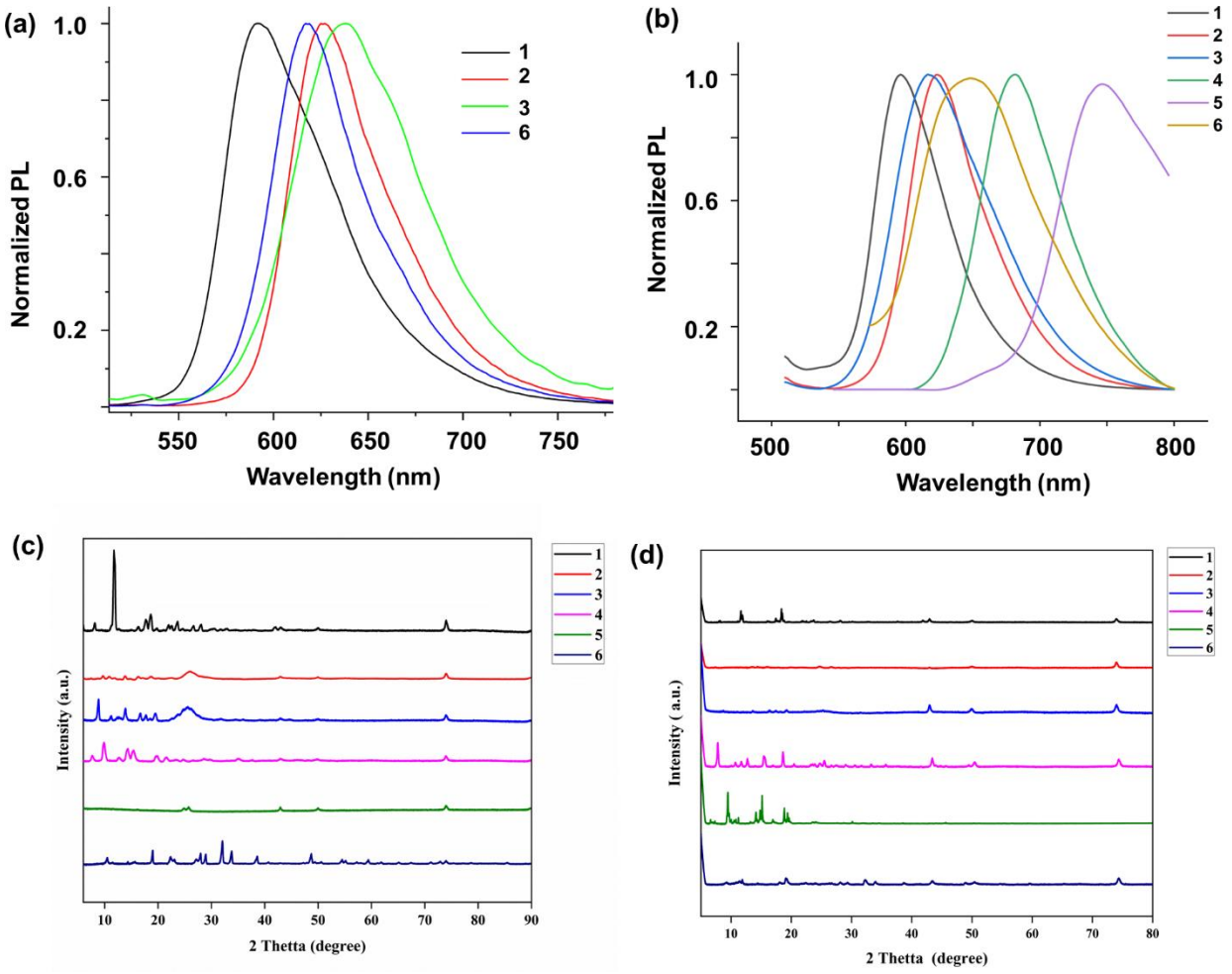


Figure S26. (a) Normalized emission spectra of compounds **1-3** and **6** recorded in their crystalline solid state. (b) Normalized emission of compounds **1-6** in their thin needle like crystals. The λ_{max} in acetonitrile were chosen for excitation. (c) and (d) X-Ray Difraction (XRD) analysis of compound **1-6** in their crystalline solid and thin needle like crystals, respectively.

7. Fluorescence lifetime measurements

Time-correlated single photon counting (TCSPC) was used to measure fluorescence lifetime using Horiba–Jobin–Yvon Fluorolog FL3-111 spectrometer. The samples are excited at their λ_{max} observed from their absorption spectra in acetonitrile.

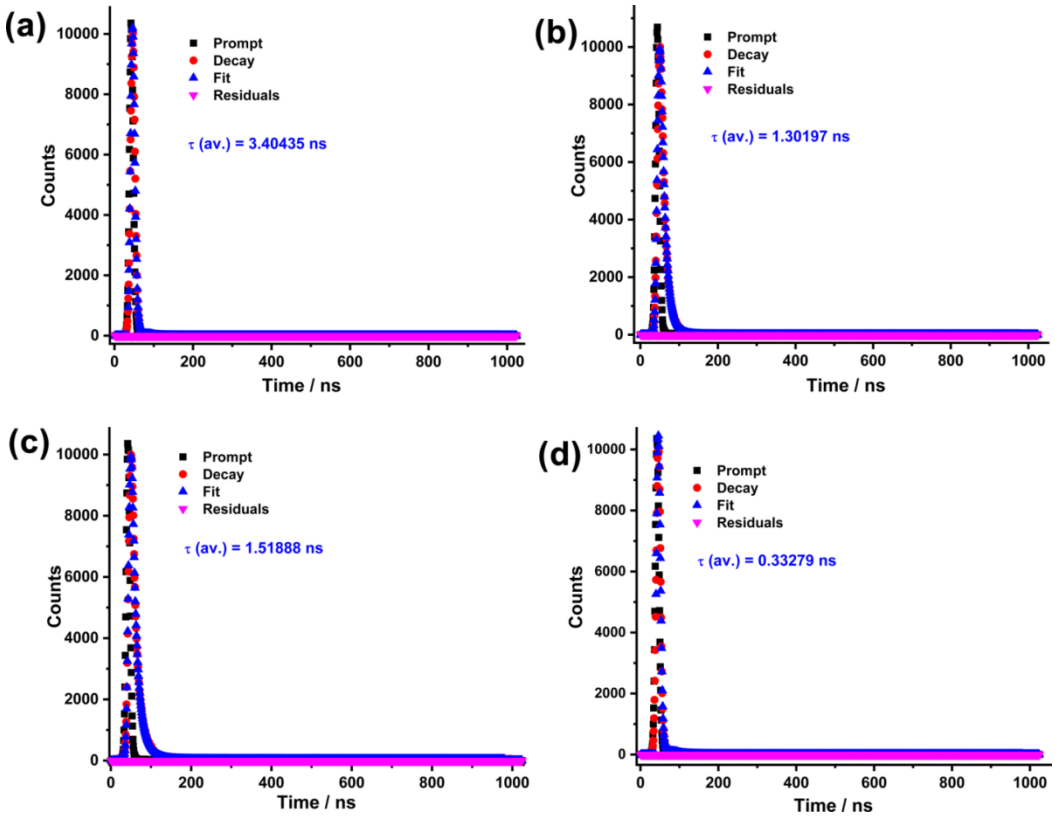


Figure S27. Fluorescence life-time profiles of the compound of (a) **1** (λ_{ex} = 478 nm); (b) **2** (λ_{ex} = 483 nm); (c) **3** (λ_{ex} = 474) and (d) **6** (λ_{ex} = 4896 nm) in their aggregated state monitored at maximum emission wavelengths (at 298 K, 10^{-5} M).

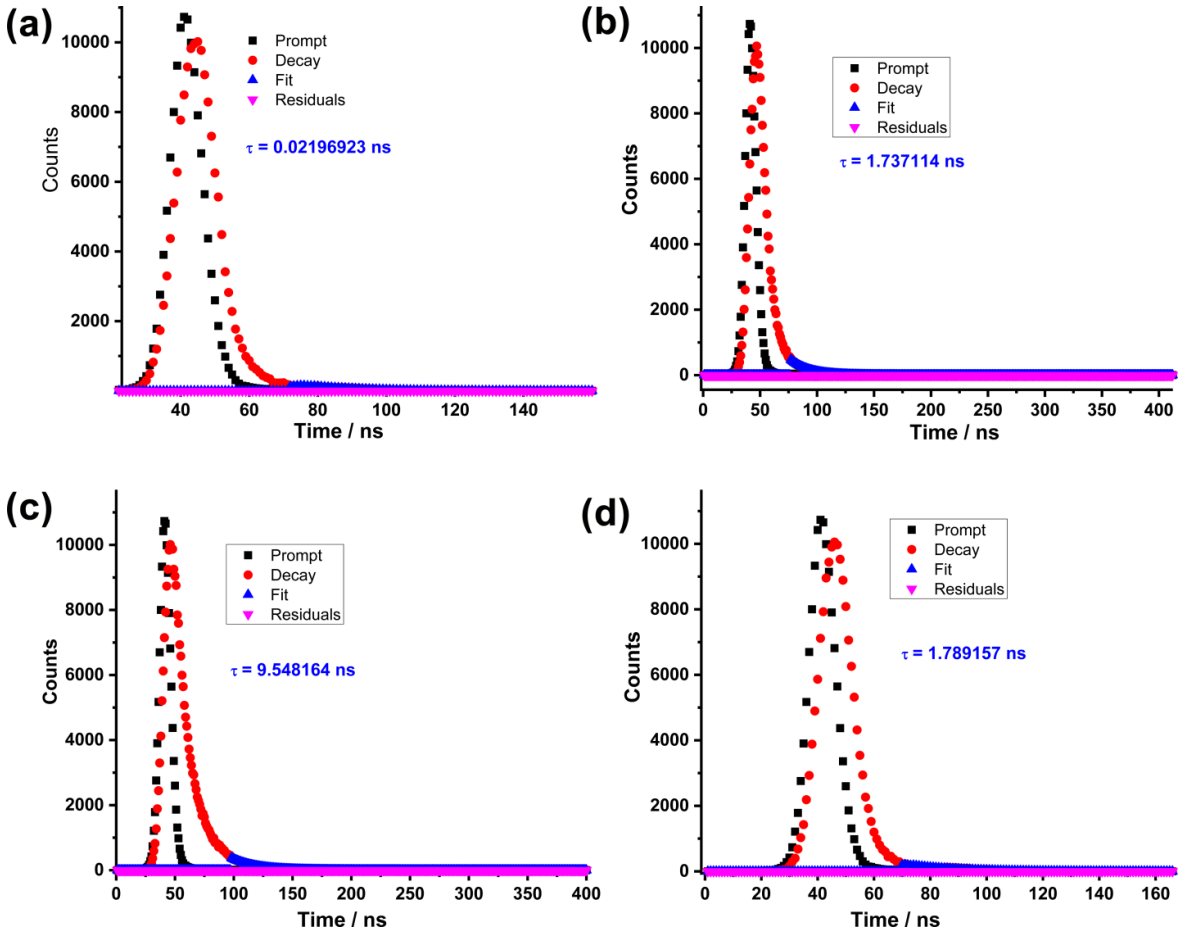


Figure S28. Fluorescence life-time profiles of the compound of (a) **1** (λ_{ex} = 478 nm); (b) **2** (λ_{ex} = 483 nm); (c) **3** (λ_{ex} = 474) and (d) **6** (λ_{ex} = 4896 nm) in their amorphous solids monitored at maximum emission wavelengths (at 298 K).

8. X-ray crystallography

Table S1. Crystal data and structure refinement for compound **1**.

Empirical formula	$C_{20}H_{14}N_2O$	
Formula weight	298.33	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.1687(11) Å	α= 90°.
	b = 15.6842(10) Å	β= 101.468(2)°.
	c = 6.4380(4) Å	γ = 90°.
Volume	1501.08(17) $Å^3$	
Z	4	
Density (calculated)	1.320 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	624	
Crystal size	0.250 x 0.190 x 0.140 mm^3	
Theta range for data collection	2.937 to 24.999°.	
Index ranges	-18<=h<=18, -18<=k<=18, -7<=l<=7	
Reflections collected	32645	
Independent reflections	2622 [*R(int)* = 0.0615]	
Completeness to theta = 24.999°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.989 and 0.980	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2622 / 0 / 208	
Goodness-of-fit on F^2	1.075	
Final *R* indices [*I>2sigma(I)*]	*R*1 = 0.0511, *wR*2 = 0.1119	
R indices (all data)	*R*1 = 0.0650, *wR*2 = 0.1188	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.130 and -0.139 e.$Å^{-3}$	

$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2\}^{1/2}$.

Table S2. Crystal data and structure refinement for Compound **4**.

Empirical formula	$C_{21}H_{16}N_2O_2$	
Formula weight	328.36	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*P*na2$_1$	
Unit cell dimensions	*a* = 24.6783(9) Å	α= 90°.
	b = 12.9905(4) Å	β= 90°.
	c = 5.0465(2) Å	γ = 90°.
Volume	1617.82(10) Å^3	
Z	4	
Density (calculated)	1.348 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	688	
Crystal size	0.200 x 0.040 x 0.030 mm^3	
Theta range for data collection	2.276 to 24.997°.	
Index ranges	-29<=h<=29, -15<=k<=14, -6<=l<=6	
Reflections collected	15092	
Independent reflections	2836 [R(*int*) = 0.0514]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.997 and 0.983	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2836 / 1 / 227	
Goodness-of-fit on F^2	1.107	
Final R indices [*I>2sigma(I)*]	*R*1 = 0.0485, *wR*2 = 0.1070	
R indices (all data)	*R*1 = 0.0620, *wR*2 = 0.1128	
Absolute structure parameter	-0.6(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.124 and -0.115 e.Å^{-3}	

$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2\}^{1/2}$.

Table S3. Crystal data and structure refinement for compound **5**.

Empirical formula	$C_{22}H_{21}N_3O_2$	
Formula weight	359.42	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	*I*-4	
Unit cell dimensions	a = 26.8526(11) Å	α = 90°.
	b = 26.8526(11) Å	β = 90°.
	c = 5.0570(3) Å	γ = 90°.
Volume	3646.4(4) $Å^3$	
Z	8	
Density (calculated)	1.309 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	1520	
Crystal size	0.604 x 0.047 x 0.039 mm^3	
Theta range for data collection	2.145 to 24.990°.	
Index ranges	-31<=h<=31, -31<=k<=30, -6<=l<=6	
Reflections collected	8663	
Independent reflections	3190 [*R(int)* = 0.0523]	
Completeness to theta = 24.990°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.997 and 0.954	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3190 / 0 / 237	
Goodness-of-fit on F^2	1.095	
Final *R* indices [*I>2sigma(I)*]	*R*1 = 0.0681, *wR*2 = 0.1363	
R indices (all data)	*R*1 = 0.0988, *wR*2 = 0.1502	
Absolute structure parameter	0.2(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.163 and -0.185 e.$Å^{-3}$	

$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2\}^{1/2}$.

9. DFT Calculations

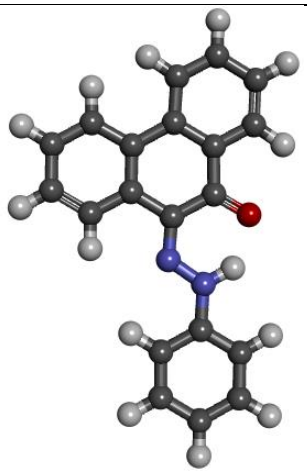
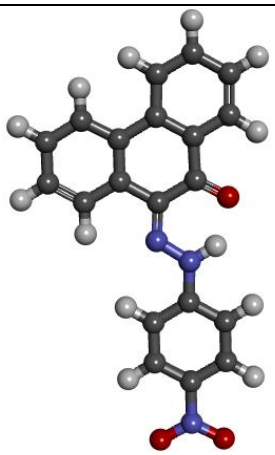
The geometry optimizations of compounds **1-4** and **6** were carried out using DFT method with the Gaussian 16 using the B3LYP/6-31+g(d,p) basis set. Time dependent density functional (TD-DFT) calculations were carried out using the B3LYP/6-31+g*. The comparison between the experimental and calculated data, and ground state optimized structures are summarized Table S4 and Table S5, respectively.

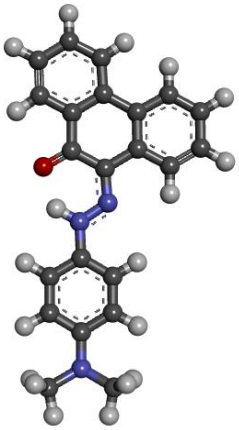
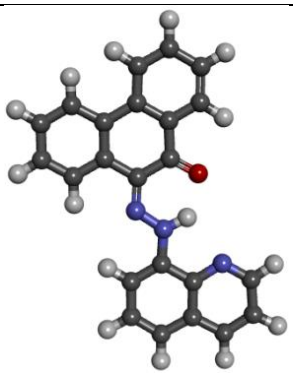
Table S4. Comparison of photophysical properties between the experimental and calculated data of the hydrazones.

Hydrazones	λ_{max}(nm)[a]	$\lambda_{max/keto}$ (nm)[b]	$\lambda_{max/enol.}$ (nm)[b]
1	478	449	452
2	483	473	500
3	474	461	476
4	495	467	457
5	536	502	503
6	496	470	574

[a] Experimental data in acetonitrile. [b] Theoretical data obtained from TD-DFT simulation.

Table S5. Summarizing optimized structures, H-bond distances and angles, and the dihedral angles between upper and lower part of the hydrazone compounds.

Hydrazones	Top view	Side view	N−H···O=C (Å/°)	$\Theta_{(top/bottom)}$ (°)
1			2.556/135.69	179.96
2			2.555/135.40	179.99
3			2.554/135.51	179.99

4			2.550/136.28	179.99
5			2.547/136.81	179.91
6			2.577/130.46	179.99

Keto-form

Hydrazone-1

Atom	X	Y	Z
C	-4.03205000	-2.88982300	0.00023200
C	-2.66336200	-2.67877900	-0.00029700
C	-2.13783700	-1.37504000	-0.00035500
C	-2.99456500	-0.24707400	0.00012400
C	-4.38276200	-0.49162600	0.00064500
C	-4.89168700	-1.78339500	0.00070600
H	-4.43421900	-3.89813700	0.00027200
H	-1.96093000	-3.50482600	-0.00068500
H	-5.08157600	0.33612800	0.00101400
H	-5.96781300	-1.93166100	0.00111900
C	-2.42915200	1.11400000	0.00002100
C	-3.25205300	2.25817100	0.00023100
C	-1.02224700	1.29725900	-0.00026700
C	-2.72056100	3.53864900	0.00016200
H	-4.32998200	2.14785000	0.00045100
C	-0.49929900	2.60466500	-0.00031900
C	-1.33155500	3.71226000	-0.00011200
H	-3.38261700	4.39919900	0.00032700
H	0.57663500	2.72861500	-0.00052700
H	-0.90395600	4.71057000	-0.00015700
C	-0.12259700	0.13442800	-0.00046900
C	-0.67254900	-1.22402800	-0.00097100
O	0.07223000	-2.23146100	-0.00102500
N	1.18030700	0.38425200	-0.00005900
N	2.04166900	-0.60193700	0.00014300
H	1.64684800	-1.55618000	0.00038400
C	3.42308500	-0.37067200	0.00017400
C	4.26987200	-1.48908300	0.00049900
C	3.96576600	0.92230200	-0.00009500
C	5.65076800	-1.31203600	0.00054800
H	3.84216100	-2.48788400	0.00071500
C	5.34814400	1.08180500	-0.00004200
H	3.30083100	1.77685600	-0.00033800
C	6.19834300	-0.02778100	0.00027800
H	6.29968100	-2.18260100	0.00080300
H	5.76586500	2.08434200	-0.00025200
H	7.27518800	0.10799700	0.00031900

Hydrazone-2

Atom	X	Y	Z
C	-3.69453200	-2.65900800	-0.00002500
C	-3.14988300	-1.36305100	0.00000400
C	-3.98852500	-0.22167400	-0.00006300
C	-5.37938100	-0.44441000	-0.00018300
C	-5.90804600	-1.72892700	-0.00021500
C	-5.06649500	-2.84861500	-0.00013000
H	-3.00607500	-3.49664000	0.00003300
H	-6.06586300	0.39337600	-0.00026300
H	-6.98623200	-1.86025000	-0.00031000
H	-5.48429600	-3.85034400	-0.00015100
C	-3.40255600	1.13209100	0.00000300
C	-4.20951100	2.28669200	0.00003400
C	-3.65986200	3.56012500	0.00009800
H	-5.28872600	2.19202600	0.00002100
C	-1.45243200	2.59685900	0.00012200
C	-2.26945500	3.71623900	0.00014100
H	-4.31051600	4.42918500	0.00012300
H	-0.37504500	2.70677700	0.00017200
H	-1.82872300	4.70855000	0.00019800
C	-1.68407200	-1.23439200	0.00008300
C	-1.99414200	1.29803700	0.00004700
C	-1.10820300	0.12266500	0.00002900
O	-0.95268800	-2.24793200	0.00018400
N	0.19203100	0.35220800	0.00002100
N	1.04385400	-0.65383500	0.00010200
H	0.63623500	-1.60175800	0.00016400
C	2.41693100	-0.43697100	0.00005100
C	3.25804800	-1.56541000	0.00021800
C	2.97173200	0.85565500	-0.00016400
C	4.63526100	-1.40749000	0.00017600
H	2.82417800	-2.56073800	0.00038400
C	4.34895800	1.01174900	-0.00020100
H	2.31441900	1.71516000	-0.00030300
C	5.16976100	-0.11836200	-0.00003100
H	5.30276600	-2.25960800	0.00030200
H	4.80397700	1.99413800	-0.00036500
O	7.31965100	-0.96420600	0.00005600
O	7.06520800	1.20270400	-0.00027700
N	6.62196600	0.05231300	-0.00007300

Hydrazone-3

Atom	X	Y	Z
C	3.29170300	-2.65817900	-0.00007300
C	2.74871600	-1.36152600	-0.00007900
C	3.58915300	-0.22143900	0.00003400
C	4.97987800	-0.44623100	0.00016900
C	5.50671600	-1.73135000	0.00017800
C	4.66335200	-2.84979700	0.00005200
H	2.60187500	-3.49469000	-0.00016700
H	5.66745700	0.39070100	0.00027800
H	6.58472200	-1.86430400	0.00028600
H	5.07968900	-3.85217500	0.00005500
C	3.00511500	1.13284100	0.00000000
C	3.81346700	2.28665900	0.00000600
C	3.26545600	3.56064700	-0.00001900
H	4.89259300	2.19054200	0.00002300
C	1.05677300	2.59966600	-0.00006900
C	1.87506000	3.71803300	-0.00005500
H	3.91701200	4.42905100	-0.00001500
H	-0.02051100	2.71074400	-0.00011400
H	1.43539700	4.71087400	-0.00008000
C	1.28285500	-1.23071200	-0.00020300
C	1.59674900	1.29997200	-0.00003900
C	0.71000700	0.12553700	-0.00005300
O	0.55034000	-2.24436400	-0.00029600
N	-0.59124100	0.35656700	0.00003800
N	-1.44275200	-0.64739700	0.00008400
H	-1.03519600	-1.59567900	0.00022700
C	-2.81793700	-0.42995200	0.00006100
C	-3.37303500	0.86074300	0.00004700
C	-3.65979000	-1.55552700	0.00006500
C	-4.75042500	1.01589400	0.00002600
H	-2.71595700	1.72066600	0.00005900
C	-5.03701800	-1.39522700	0.00005000
H	-3.22744500	-2.55166800	0.00007800
C	-5.59949000	-0.10663700	0.00002800
H	-5.18286000	2.01067000	0.00001600
H	-5.68588100	-2.26413500	0.00005200
C	-7.02063500	0.06207100	0.00001100
N	-8.17652800	0.19960100	-0.00000400

Hydrazone-4

Atom	X	Y	Z
C	3.51449500	-2.60333500	0.00010700
C	2.93609500	-1.32194900	0.00002000
C	3.74695600	-0.16036200	-0.00000900
C	5.14426600	-0.34857200	0.00007800
C	5.70509400	-1.61837800	0.00015200
C	4.89048700	-2.75868400	0.00016100
H	2.84596300	-3.45702500	0.00012500
H	5.80879000	0.50702100	0.00007800
H	6.78633800	-1.72320500	0.00020400
H	5.33316600	-3.74994400	0.00022900
C	3.12681300	1.17588500	-0.00005300
C	3.90180900	2.35330000	0.00000600
C	3.31828700	3.61070200	-0.00002100
H	4.98341200	2.28721900	0.00007600
C	1.13706200	2.58586800	-0.00011400
C	1.92296600	3.72654200	-0.00009000
H	3.94416300	4.49794000	0.00001300
H	0.05692000	2.66546600	-0.00014900
H	1.45461800	4.70648800	-0.00010300
C	1.46602900	-1.22989100	-0.00000500
C	1.71302200	1.30035800	-0.00008900
C	0.86358700	0.10199400	-0.00008500
O	0.76207800	-2.26884200	0.00006400
N	-0.45206100	0.29783900	-0.00014000
N	-1.26654100	-0.72408600	-0.00018400
H	-0.82480400	-1.65962000	-0.00031200
C	-2.65785600	-0.55816100	-0.00010500
C	-3.45822800	-1.71293800	-0.00030800
C	-3.26697300	0.70043500	0.00015100
C	-4.83986600	-1.60640700	-0.00024700
H	-2.99029800	-2.69342200	-0.00051700
C	-4.65642500	0.80829200	0.00020800
H	-2.64803300	1.58908000	0.00030700
C	-5.45335900	-0.34448500	0.00001100
H	-5.46880300	-2.48995000	-0.00039900
H	-5.10501500	1.79432000	0.00041200
O	-6.81760000	-0.34823100	0.00004800
C	-7.49340900	0.89993500	0.00029000
H	-7.25430000	1.49015600	-0.89353000
H	-8.55857100	0.66508500	0.00026200
H	-7.25427400	1.48982300	0.89432400

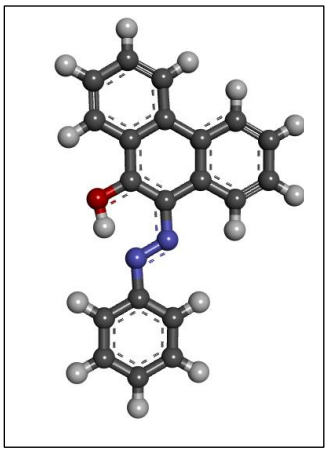
Hydrazone-6

Atom	X	Y	Z
C	-4.18741300	-3.37055900	-0.00092800
C	-2.89051100	-2.88393700	-0.00057100
C	-2.64288000	-1.50106900	-0.00025900
C	-3.71125200	-0.57233000	-0.00031800
C	-5.02024600	-1.09475100	-0.00068200
C	-5.25480600	-2.46362300	-0.00097700
H	-4.37477200	-4.43976400	-0.00116300
H	-2.03337400	-3.54810500	-0.00051100
H	-5.87352400	-0.42749000	-0.00074600
H	-6.27794200	-2.82842900	-0.00125700
C	-3.43445400	0.87686300	-0.00004700
C	-4.47359200	1.82855400	-0.00000500
C	-2.09481800	1.34435600	0.00012800
C	-4.21564900	3.19118400	0.00021600
H	-5.50603200	1.50018400	-0.00015000
C	-1.85114000	2.73100300	0.00034600
C	-2.89200800	3.64538100	0.00039300
H	-5.03996200	3.89776000	0.00024500
H	-0.82327300	3.07203300	0.00047900
H	-2.67749400	4.70994000	0.00056400
C	-0.97373500	0.39117400	0.00009100
C	-1.23564200	-1.05554900	0.00013900
O	-0.30427600	-1.88409100	-0.00103600
N	0.24497600	0.90426100	0.00009900
N	1.30439500	0.12866700	0.00024800
H	1.18234600	-0.89418800	0.00046000
C	2.58498400	0.67360500	0.00019800
C	3.67678400	-0.25647500	0.00036100
C	2.83813300	2.03569200	0.00000600
C	5.01424500	0.24555500	0.00032400
C	4.16541300	2.51128400	-0.00002700
H	2.00433400	2.72627000	-0.00011400
C	5.23889800	1.64580100	0.00012800
H	4.33521800	3.58368300	-0.00017700
H	6.25805200	2.02079400	0.00010200
C	4.38591300	-2.44167600	0.00069100
H	4.12007100	-3.49716200	0.00083400
C	6.05710000	-0.71616900	0.00049100
C	5.74839300	-2.05621700	0.00067500
H	7.09021300	-0.37891600	0.00047000
H	6.52437300	-2.81463100	0.00080500
N	3.38429700	-1.58404700	0.00054000

Enol-form

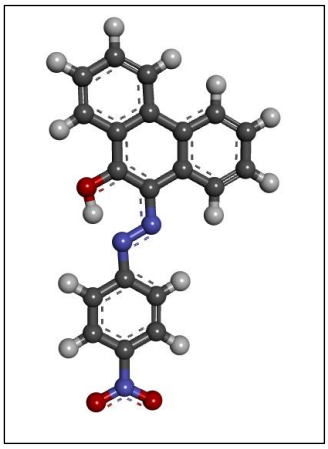
Hydrazone-1

Atom	X	Y	Z
C	-3.97940000	-2.89840000	0.00010000
C	-2.61630000	-2.67780000	0.00010000
C	-2.10190000	-1.36200000	0.00000000
C	-2.97800000	-0.24120000	0.00000000
C	-4.36570000	-0.50560000	0.00010000
C	-4.85650000	-1.80010000	0.00020000
H	-4.37090000	-3.91090000	0.00020000
H	-1.91570000	-3.50450000	0.00010000
H	-5.07230000	0.31560000	0.00010000
H	-5.93010000	-1.96460000	0.00020000
C	-2.42720000	1.11320000	0.00000000
C	-3.25160000	2.26070000	-0.00010000
C	-1.01610000	1.29540000	-0.00010000
C	-2.71790000	3.53660000	-0.00010000
H	-4.32970000	2.14980000	0.00000000
C	-0.49120000	2.60620000	-0.00020000
C	-1.32490000	3.70910000	-0.00020000
H	-3.37700000	4.39940000	-0.00020000
H	0.58440000	2.72970000	-0.00020000
H	-0.89920000	4.70830000	-0.00030000
C	-0.13170000	0.13790000	0.00000000
C	-0.67460000	-1.15700000	-0.00010000
N	1.22550000	0.38950000	0.00000000
N	2.00500000	-0.62570000	0.00000000
C	3.39000000	-0.35850000	0.00000000
C	4.23530000	-1.47810000	-0.00040000
C	3.94450000	0.93320000	0.00050000
C	5.61820000	-1.31250000	-0.00040000
H	3.79170000	-2.46900000	-0.00080000
C	5.32570000	1.08810000	0.00050000
H	3.28230000	1.79030000	0.00090000
C	6.16840000	-0.02970000	0.00010000
H	6.26550000	-2.18430000	-0.00080000
H	5.75270000	2.08690000	0.00090000
H	7.24620000	0.10160000	0.00010000
O	0.10060000	-2.23410000	0.00000000
H	1.05860000	-1.87940000	-0.00010000



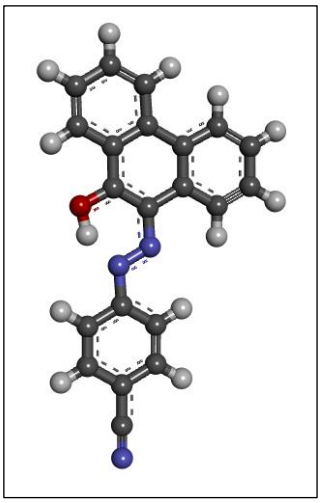
Hydrazone-2

Atom	X	Y	Z
C	-5.00654400	-2.86018300	0.00031900
C	-3.64051000	-2.65953100	0.00013400
C	-3.10806800	-1.35075400	0.00004400
C	-3.96673300	-0.21614600	0.00012600
C	-5.35721800	-0.46044200	0.00034000
C	-5.86623800	-1.74855100	0.00043200
H	-5.41320700	-3.86644700	0.00037600
H	-2.95222400	-3.49651700	0.00006700
H	-6.05260700	0.36999400	0.00046600
H	-6.94208400	-1.89700100	0.00060600
C	-3.39726900	1.13194500	-0.00003700
C	-4.20722800	2.28898700	-0.00009400
C	-1.98510100	1.29723300	-0.00018500
C	-3.65697600	3.55826700	-0.00025700
H	-5.28652000	2.19236600	-0.00003800
C	-1.44286400	2.59952200	-0.00036400
C	-2.26262800	3.71352200	-0.00039200
H	-4.30517000	4.42914000	-0.00029400
H	-0.36591900	2.71070000	-0.00052200
H	-1.82428800	4.70704400	-0.00053600
C	-1.11489500	0.12605400	-0.00015400
C	-1.67916500	-1.16679500	-0.00009500
N	0.23702400	0.35171800	-0.00012200
N	1.00574600	-0.67923200	-0.00017500
C	2.38725300	-0.42353100	-0.00008100
C	3.22687600	-1.55117200	-0.00068100
C	2.95131400	0.86720800	0.00064100
C	4.60715400	-1.40301600	-0.00061700
H	2.77889900	-2.53932500	-0.00121700
C	4.32854600	1.02120200	0.00071200
H	2.29614100	1.72884900	0.00115900
C	5.14200900	-0.11536900	0.00007500
H	5.27290300	-2.25645200	-0.00108900
H	4.79002100	2.00063900	0.00127200
O	-0.91813800	-2.24816700	-0.00015800
H	0.04824300	-1.90587100	-0.00018400
O	7.29225900	-0.96772600	-0.00040700
N	6.59916000	0.05087800	0.00015700
O	7.04488100	1.19947300	0.00078100



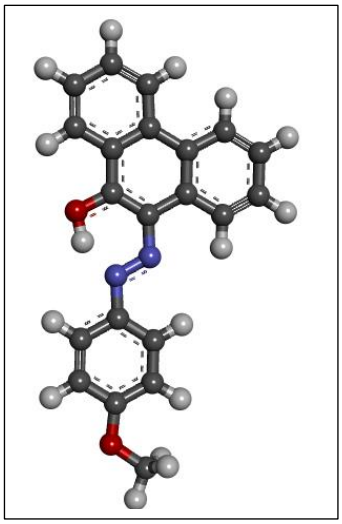
Hydrazone-3

Atom	X	Y	Z
C	-4.60809600	-2.85881300	0.00001600
C	-3.24212900	-2.65760900	0.00000000
C	-2.70994500	-1.34872900	-0.00000400
C	-3.56935800	-0.21475000	0.00000700
C	-4.95993600	-0.45958000	0.00002400
C	-5.46855500	-1.74770100	0.00002800
H	-5.01422900	-3.86533600	0.00001900
H	-2.55355600	-3.49435200	-0.00000900
H	-5.65551300	0.37075100	0.00003500
H	-6.54434100	-1.89669700	0.00004200
C	-3.00022700	1.13312400	0.00000000
C	-3.81019000	2.29033200	0.00000000
C	-1.58784300	1.29821800	-0.00001000
C	-3.26013400	3.55957100	-0.00001000
H	-4.88949500	2.19352800	0.00000600
C	-1.04589400	2.60090100	-0.00002300
C	-1.86563300	3.71476400	-0.00002200
H	-3.90835000	4.43045900	-0.00001000
H	0.03105800	2.71195000	-0.00003600
H	-1.42734000	4.70835500	-0.00003200
C	-0.71764700	0.12750500	-0.00001300
C	-1.28096800	-1.16401500	-0.00001500
N	0.63596600	0.35528900	-0.00001600
N	1.40494500	-0.67390700	-0.00006400
C	2.78721000	-0.41750300	-0.00002900
C	3.62808900	-1.54256500	-0.00017400
C	3.35164100	0.87181800	0.00015000
C	5.00777600	-1.39200700	-0.00015100
H	3.18133300	-2.53145100	-0.00030900
C	4.72845100	1.02481700	0.00017600
H	2.69635600	1.73363000	0.00027000
C	5.57081100	-0.10453300	0.00002400
H	5.65574600	-2.26161800	-0.00026600
H	5.16838500	2.01647900	0.00031500
O	-0.52008900	-2.24717200	-0.00001600
H	0.44478200	-1.90639900	-0.00000900
C	6.99328300	0.05993400	0.00005200
N	8.14932300	0.19418900	0.00007500

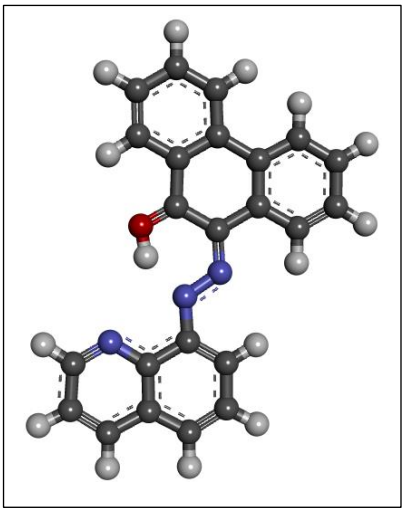


Hydrazone-4

Atom	X	Y	Z
C	-4.84667300	-2.76007400	0.00027400
C	-3.47518500	-2.59965800	0.00013200
C	-2.90274600	-1.30791000	0.00008800
C	-3.72954300	-0.15019600	0.00015000
C	-5.12766800	-0.35318800	0.00034300
C	-5.67523300	-1.62464500	0.00040200
H	-5.28201300	-3.75458700	0.00028000
H	-2.81175700	-3.45648700	0.00006800
H	-5.79730200	0.49851200	0.00049600
H	-6.75504300	-1.74196700	0.00055300
C	-3.11919600	1.17779300	-0.00002300
C	-3.89135900	2.36122200	-0.00008500
C	-1.70096600	1.29640400	-0.00015400
C	-3.30163700	3.61204700	-0.00023400
H	-4.97336400	2.29825500	-0.00006000
C	-1.11858100	2.58318900	-0.00032800
C	-1.90207200	3.72207200	-0.00035300
H	-3.92167800	4.50342500	-0.00026600
H	-0.03854400	2.65817200	-0.00047400
H	-1.43228200	4.70143500	-0.00048800
C	-0.86846200	0.10166900	-0.00009800
C	-1.46784100	-1.16574400	-0.00001500
N	0.50100800	0.29691300	-0.00011400
N	1.23591400	-0.75082500	-0.00025300
C	2.62756600	-0.54921500	-0.00018200
C	3.43007100	-1.70403000	-0.00077100
C	3.24807300	0.70922500	0.00050000
C	4.81171800	-1.60680300	-0.00074800
H	2.94812100	-2.67685000	-0.00130500
C	4.63444900	0.81495900	0.00054800
H	2.63003700	1.59900100	0.00103300
C	5.42678700	-0.34495400	-0.00008600
H	5.44046800	-2.49051900	-0.00123200
H	5.09023300	1.79785400	0.00108700
O	-0.74201600	-2.27965500	-0.00003000
H	0.22825400	-1.97032100	-0.00016700
O	6.78775600	-0.35105300	-0.00001300
C	7.47220200	0.89403900	0.00073800
H	7.23635800	1.48389000	0.89516300
H	8.53542200	0.65115900	0.00070500
H	7.23648900	1.48486800	-0.89306800



Hydrazone-6



Atom	X	Y	Z
C	4.18440800	-3.36699100	0.00092300
C	2.88742800	-2.88057800	0.00056600
C	2.63957300	-1.49775000	0.00025400
C	3.70779500	-0.56883900	0.00031300
C	5.01687300	-1.09104800	0.00067700
C	5.25165500	-2.45988200	0.00097200
H	4.37194000	-4.43616500	0.00115800
H	2.03039800	-3.54488500	0.00050600
H	5.87004300	-0.42364900	0.00074100
H	6.27484900	-2.82452300	0.00125200
C	3.43076300	0.88031000	0.00004200
C	4.46974700	1.83216900	0.00000000
C	2.09105100	1.34758600	-0.00013300
C	4.21158300	3.19475700	-0.00022100
H	5.50224000	1.50396600	0.00014500
C	1.84714900	2.73419400	-0.00035100
C	2.88786900	3.64874000	-0.00039800
H	5.03578200	3.90146600	-0.00025000
H	0.81922700	3.07505800	-0.00048400
H	2.67318300	4.71326400	-0.00056900
C	0.97012200	0.39422300	-0.00009600
C	1.23226300	-1.05245800	-0.00014400
O	0.30103100	-1.88115000	0.00103100
N	-0.24867200	0.90711300	-0.00010400
N	-1.30796500	0.13134800	-0.00025300
C	-2.58864200	0.67607900	-0.00020300
C	-3.68029200	-0.25417800	-0.00036600
C	-2.84201200	2.03812500	-0.00001100
C	-5.01783400	0.24763600	-0.00032900
C	-4.16936900	2.51350200	0.00002200
H	-2.00832400	2.72883700	0.00010900
C	-5.24271400	1.64784600	-0.00013300
H	-4.33934700	3.58587400	0.00017200
H	-6.26192800	2.02267400	-0.00010700
C	-4.38906800	-2.43949300	-0.00069600
H	-4.12305500	-3.49493600	-0.00083900
C	-6.06053400	-0.71425700	-0.00049600
C	-5.75161000	-2.05425500	-0.00068000
H	-7.09370100	-0.37717100	-0.00047500
H	-6.52746800	-2.81279400	-0.00081000
N	-3.38759100	-1.58170300	-0.00054500
H	-0.53971300	-1.41773900	0.00037400