

Supplementary Information

Red-Shifting Squaraine Dyes in the Near-Infrared Region using the Perimidine Heterocycle: Synthesis and Optical Properties

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Table S1: Physicochemical properties of **SQ1 - 9** calculated using MarvinSketch (ChemAxon). The measured Log D at pH 7.4, rotatable bonds, molecular surface area, molecular volume, hydrogen bond donor (HBD) and acceptor (HBA) ratio, and total polar surface area (TPSA), polarizability.

Dye	Log D pH 7.4	Rotatable Bond	Surface Area (Å ²)	TPSA (Å ²)	Volume (Å ³)	HBD/HBA	Polarizability
SQ1	0.65	1	628.34	90.19	418.24	4/8	54.40
SQ2	2.91	5	745.28	90.19	483.6	4/8	61.79
SQ3	2.59	3	744.36	90.19	483.88	4/8	61.79
SQ4	1.98	1	687.18	90.19	460.09	4/8	60.31
SQ5	2.87	1	748.51	90.19	496.41	4/8	64.00
SQ6	3.77	3	776.03	90.19	524.27	4/8	69.95
SQ7	3.14	3	790.76	130.65	541.84	6/12	71.09
SQ8	3.16	3	796.91	130.65	541.73	6/12	71.09
SQ9	4.98	3	804.00	90.19	552.04	4/8	73.59

Table S2: Absorbance maxima in wavelength (nm) and wavenumber (cm⁻¹) of **SQ1-9** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer.

Dye	λAbs (nm)				λAbs (cm ⁻¹)			
	ACN	EtOH	DMSO	HEPES	ACN	EtOH	DMSO	HEPES
SQ1	800	812	825	820, 756	12,500	12,315	12,121	12,195, 13,228
SQ2	801	815	830	830, 764	12,484	12,270	12,048	12,048, 13,089
SQ3	807	816	833	826, 754	12,392	12,255	12,005	12,107, 13,263
SQ4	806	819	830	820, 752	12,407	12,210	12,048	12,195, 13,298
SQ5	807	818	830	818, 756	12,392	12,225	12,048	12,225, 13,228
SQ6	806	818	834	820, 752	12,407	12,225	11,990	12,195, 13,298
SQ7	808	815	825	832, 756	12,376	12,270	12,121	12,019, 13,228
SQ8	812	820	839	836, 766	12,315	12,195	11,919	11,962, 13,055
SQ9	809	819	835	820, 756	12,361	12,210	11,976	12,195, 13,228

Table S3: Emission maxima and Stokes shift of **SQ1 - 9** in ethanol in wavelength (nm) and wavenumber (cm⁻¹).

Dye	λEm (nm)	Stokes Shift (nm)	λEm (cm ⁻¹)	Stokes Shift (cm ⁻¹)
SQ1	821	9	12,180	1,111,111
SQ2	823	8	12,151	1,250,000
SQ3	823	7	12,151	1,428,571
SQ4	825	6	12,121	1,666,667
SQ5	823	5	12,151	2,000,000
SQ6	827	9	12,092	1,111,111
SQ7	822	7	12,165	1,428,571
SQ8	825	5	12,121	2,000,000
SQ9	824	5	12,136	2,000,000

Table S4: Molar extinction coefficient ($M^{-1} cm^{-1}$) of **SQ1 - 9** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer.

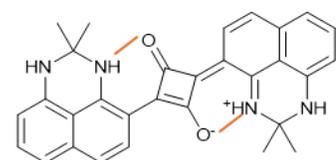
Dye	Molar Extinction Coefficient ($M^{-1} cm^{-1}$)			
	ACN	EtOH	DMSO	HEPES
SQ1	114,709	214,843	209,986	43,122
SQ2	99,724	110,095	92,440	62,527
SQ3	182,766	204,364	182,766	45,465
SQ4	97,439	90,964	95,387	25,363
SQ5	211,828	188,962	191,342	38,316
SQ6	140,987	148,485	122,404	35,789
SQ7	96,518	118,613	117,127	28,185
SQ8	95,201	95,310	83,796	32,869
SQ9	100,179	110,606	98,058	29,449

Table S5: Fluorescence Quantum Yield of **SQ1-9** in ethanol

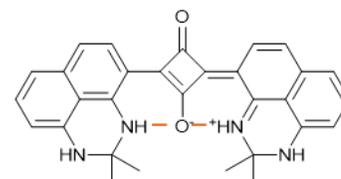
Dye	Quantum Yield (%)
SQ1	0.99
SQ2	1.07
SQ3	1.16
SQ4	1.41
SQ5	1.53
SQ6	1.11
SQ7	1.18
SQ8	1.12
SQ9	1.03

Table S6: Hydrogen bond distance in Å for **SQ1-9** for E and Z configuration with the average and standard deviation (St. Dev.) A depiction of the hydrogen bonds measured are shown on the right

DYE	E-Configuration		Z-Configuration	
	N ⁺ --H--O ⁻	N--H--O ⁻	N ⁺ --H--O ⁻	N--H--O ⁻
SQ1	2.620	2.742	2.632	2.999
SQ2	2.626	2.737	2.621	2.927
SQ3	2.610	2.741	2.633	3.017
SQ4	2.622	2.680	2.636	2.99
SQ5	2.624	2.759	2.634	3.006
SQ6	2.622	2.693	2.615	2.885
SQ7	2.620	2.738	2.709	3.052
SQ8	2.620	2.738	2.631	3.008
SQ9	2.621	2.749	2.634	3.007
Average	2.620	2.731	2.638	2.988
St. Dev.	0.004	0.025	0.027	0.051



E form



Z form

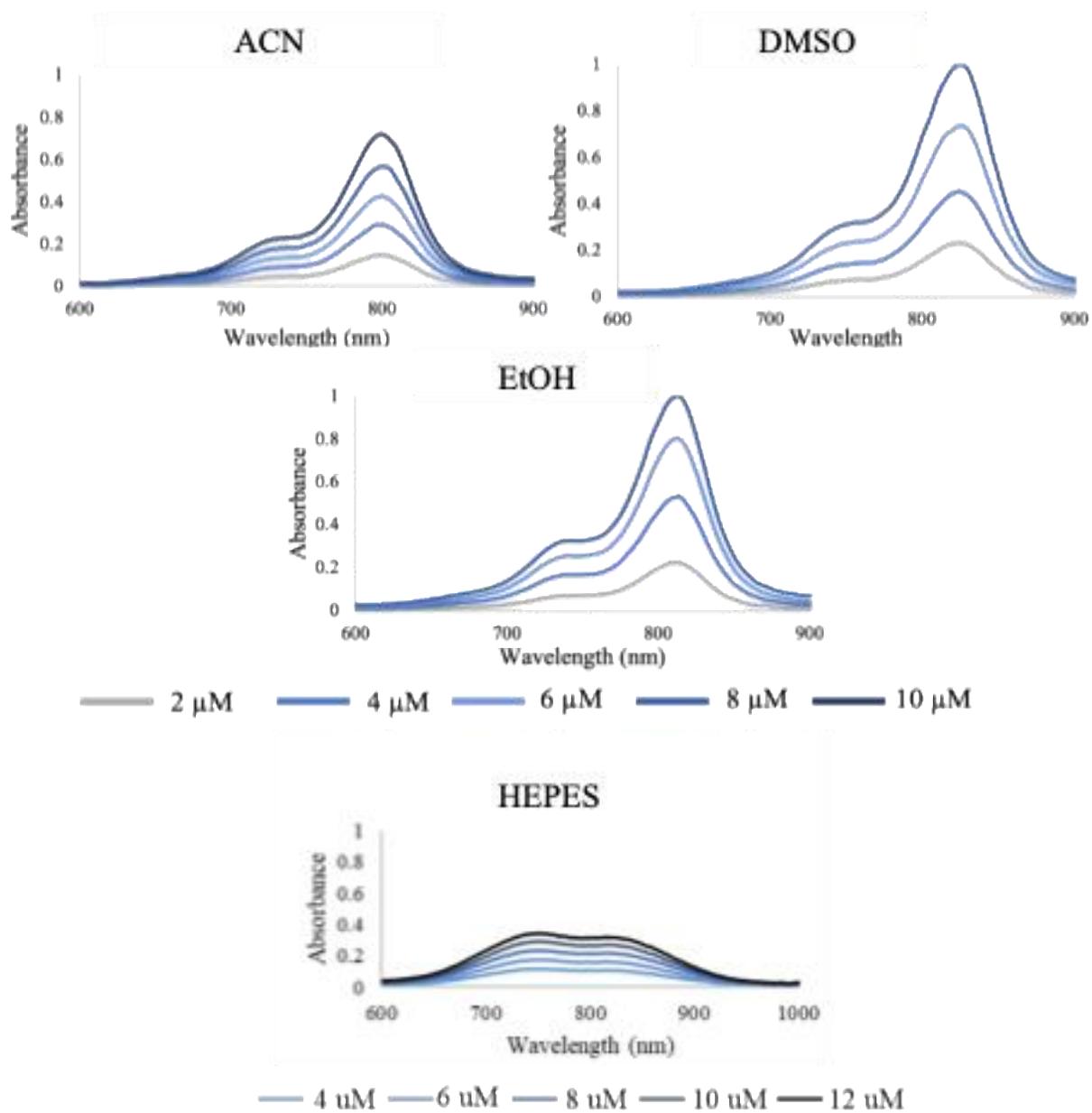


Figure S1: Absorbance Spectrum of **SQ1** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer (HEPES).

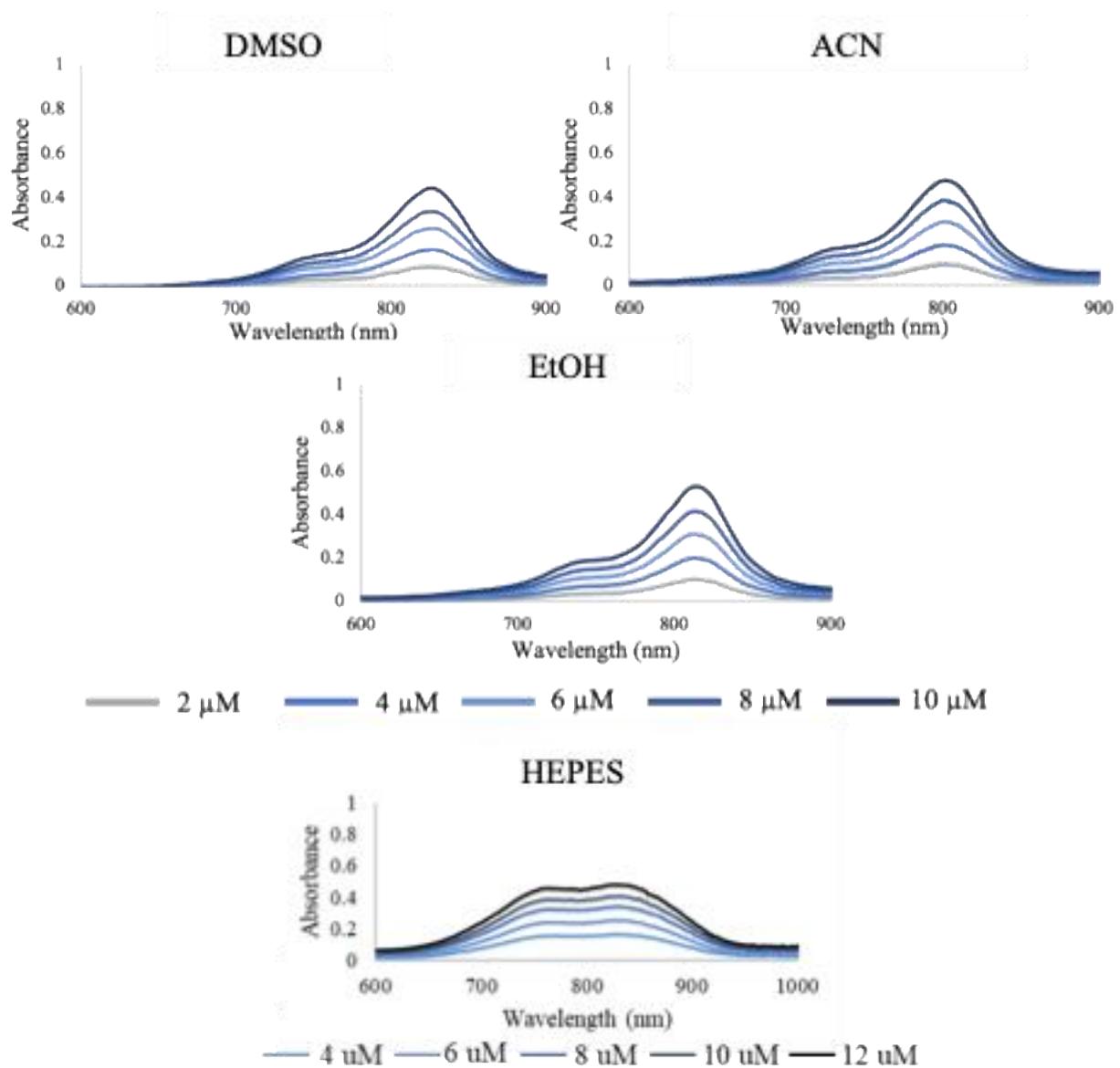


Figure S2: Absorbance Spectrum of **SQ2** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer (HEPES).

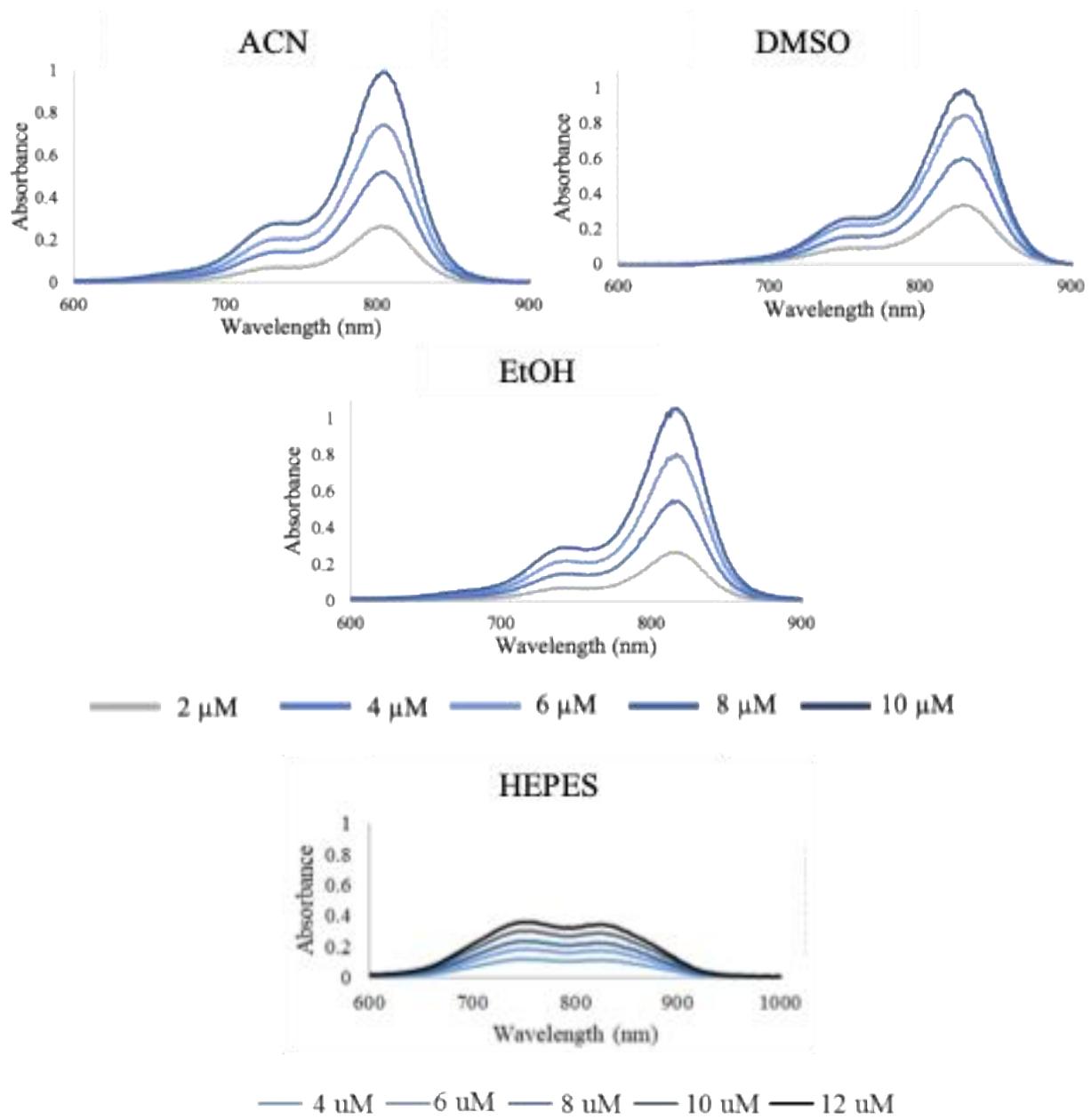


Figure S3: Absorbance Spectrum of **SQ3** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer (HEPES).

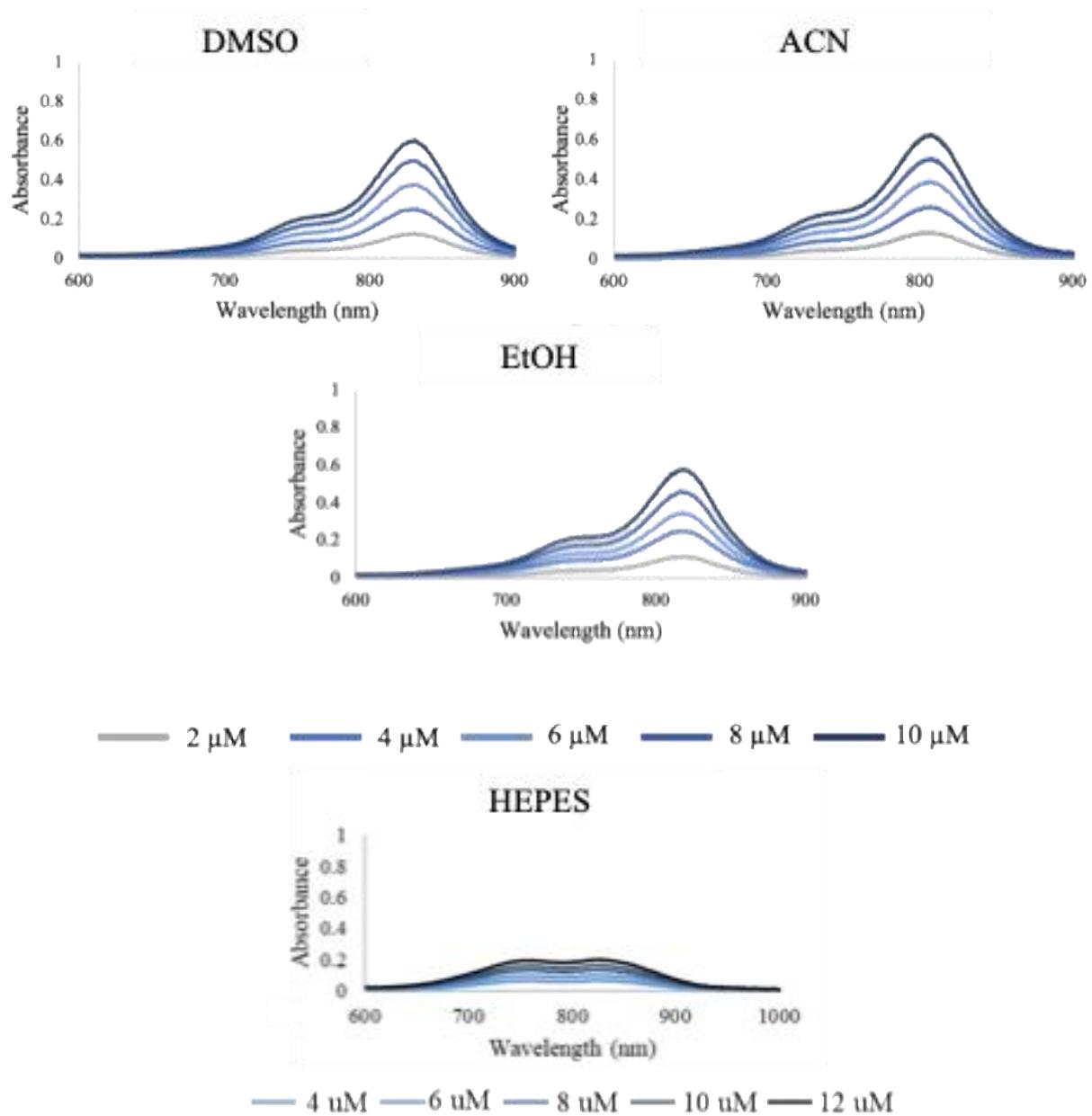


Figure S4: Absorbance Spectrum of **SQ4** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer(HEPES).

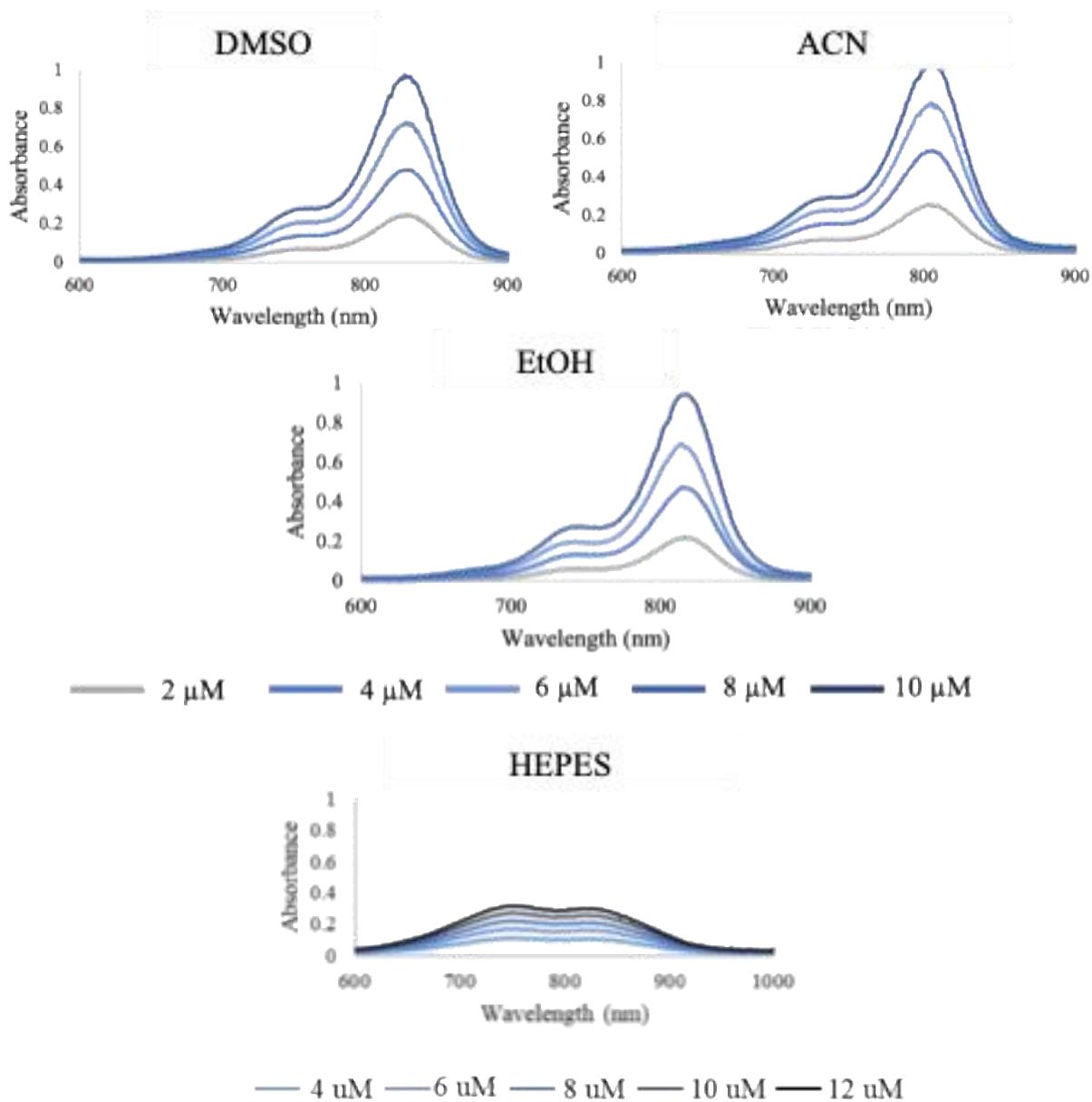


Figure S5: Absorbance Spectrum of **SQ5** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer (HEPES).

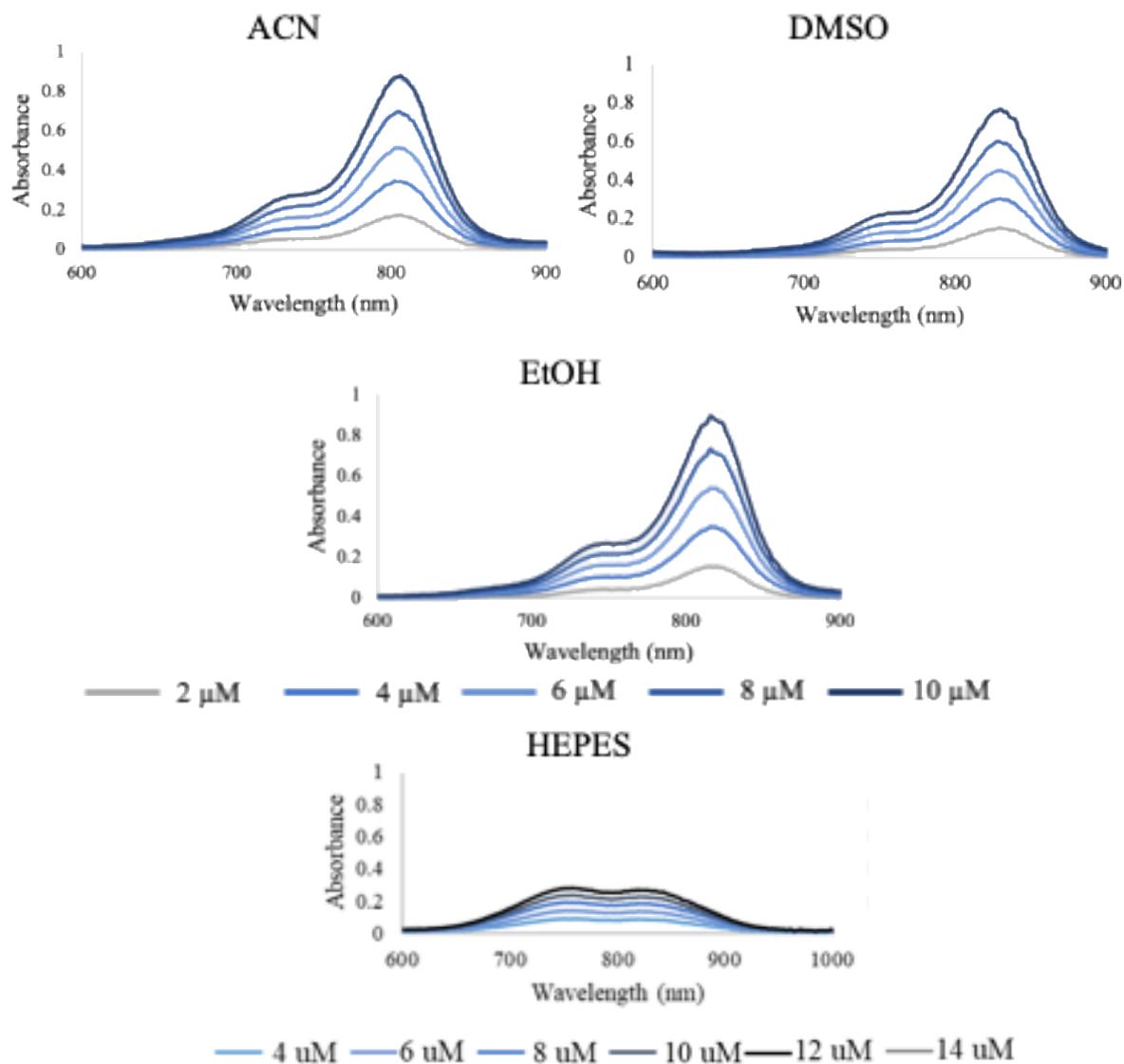


Figure S6: Absorbance Spectrum of **SQ6** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer (HEPES).

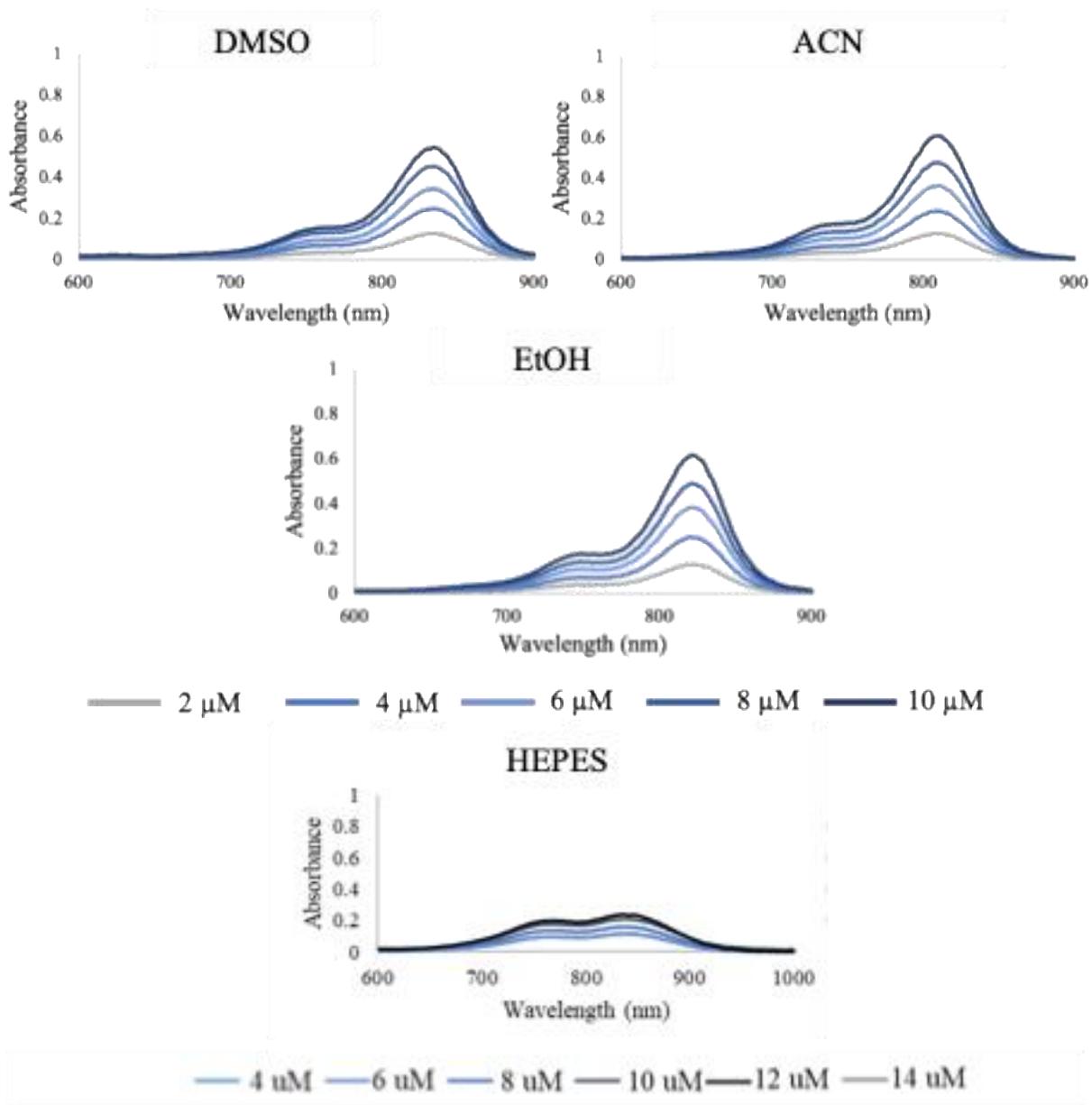


Figure S7: Absorbance Spectrum of **SQ7** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer(HEPES).

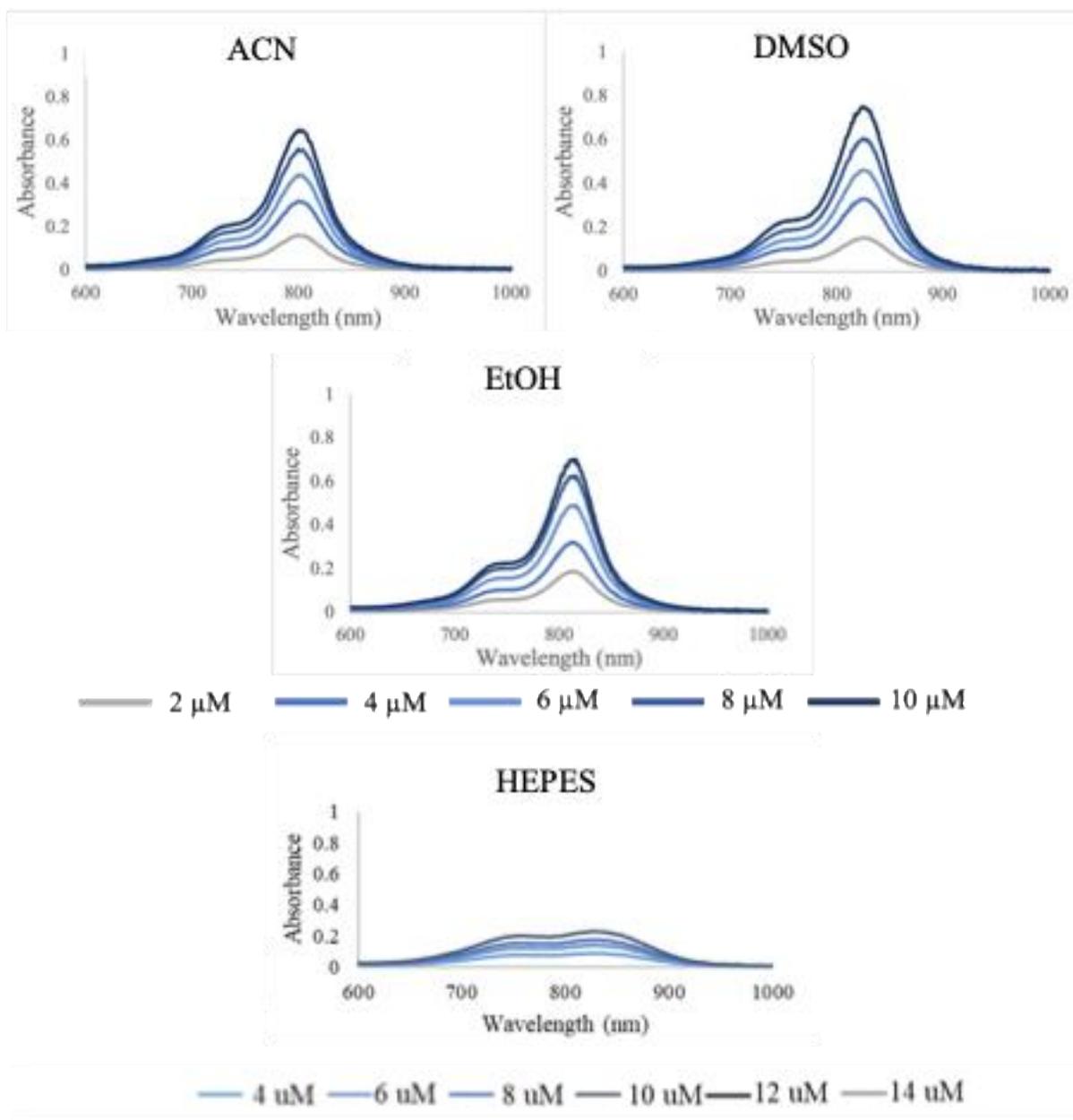


Figure S8: Absorbance Spectrum of **SQ8** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer (HEPES).

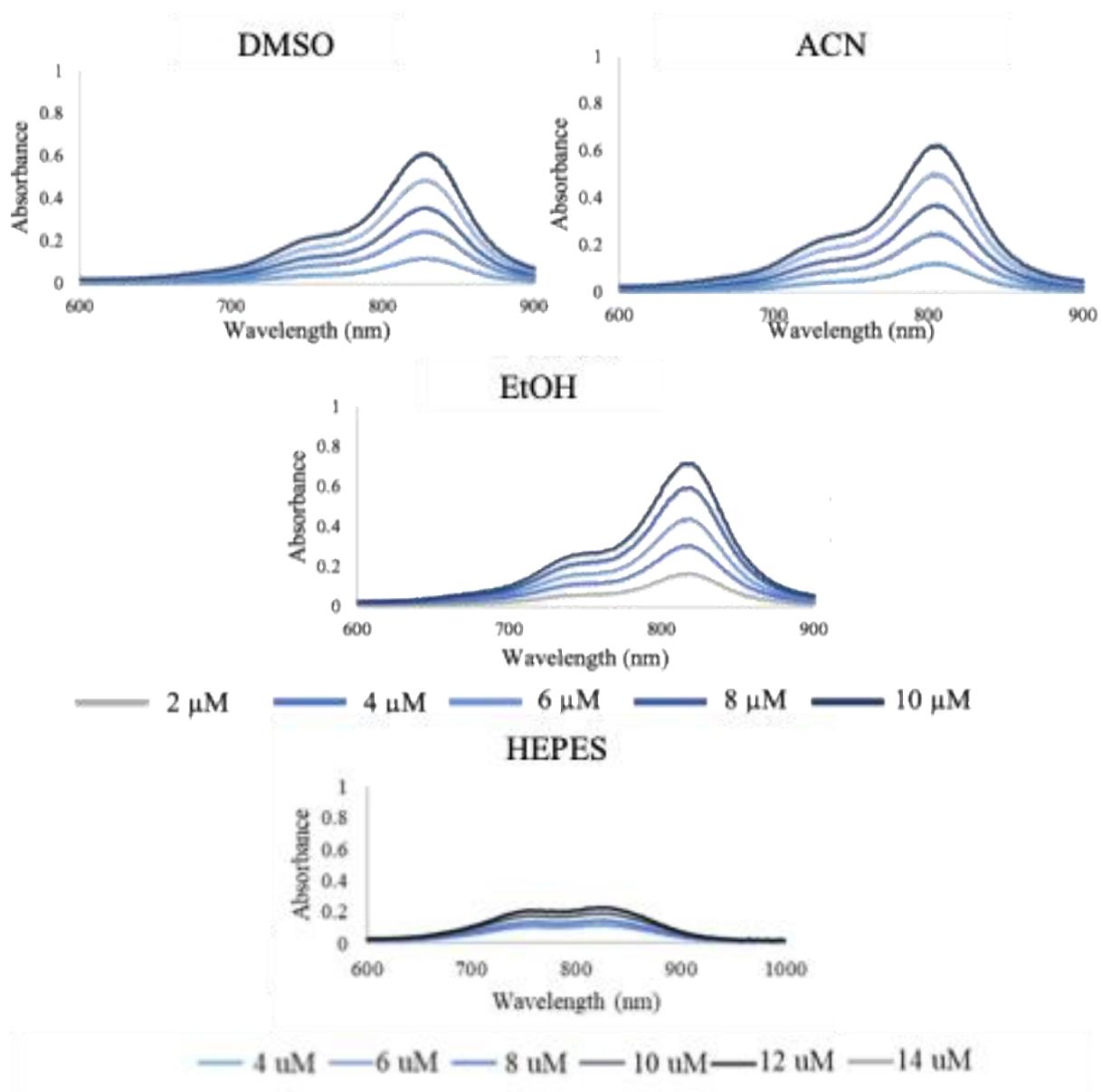


Figure S9: Absorbance Spectrum of **SQ9** in ethanol (EtOH), dimethyl sulfoxide (DMSO), Acetonitrile (ACN) and 50 mM HEPES buffer (HEPES).

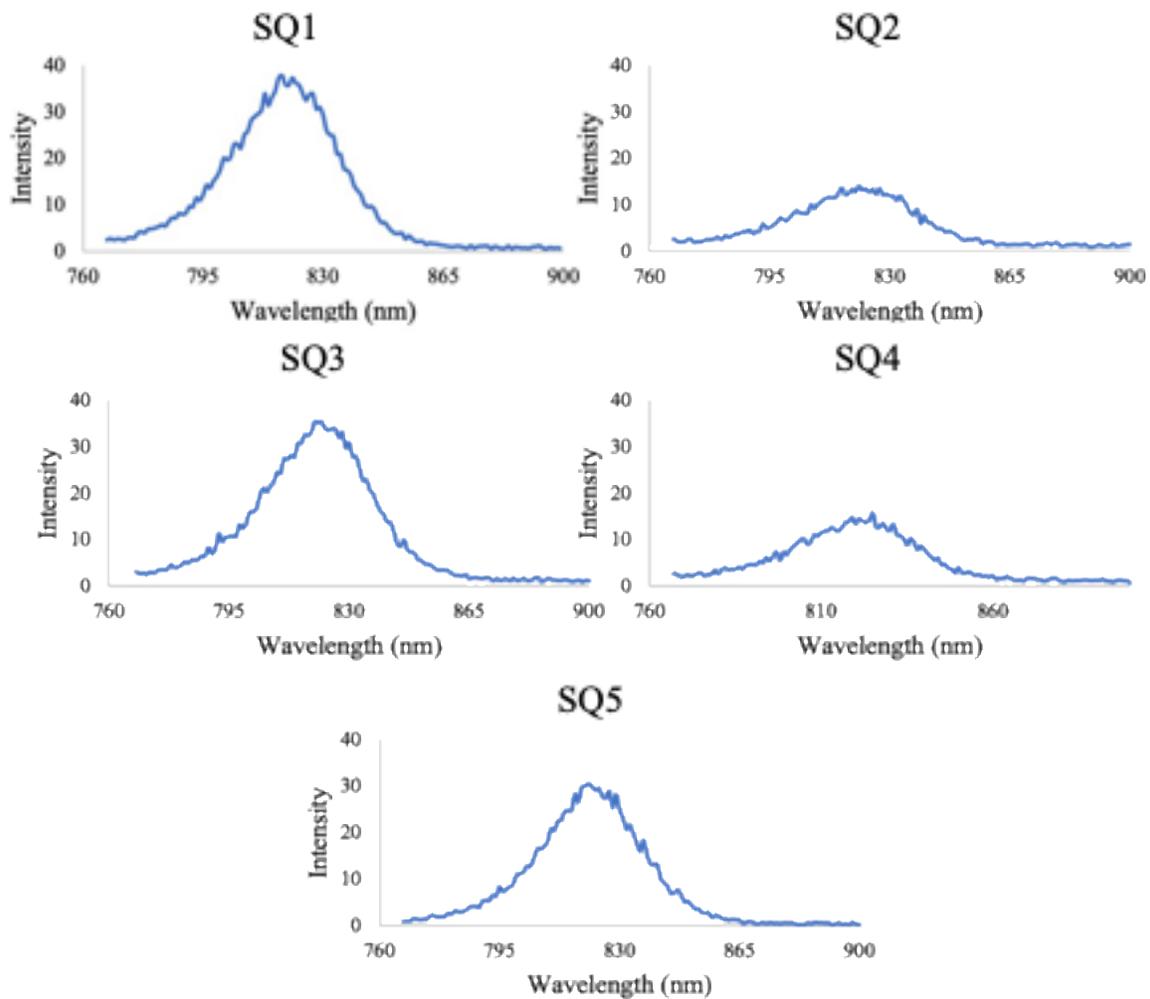


Figure S10: Fluorescence Spectrum of **SQ1** - 5 in ethanol.

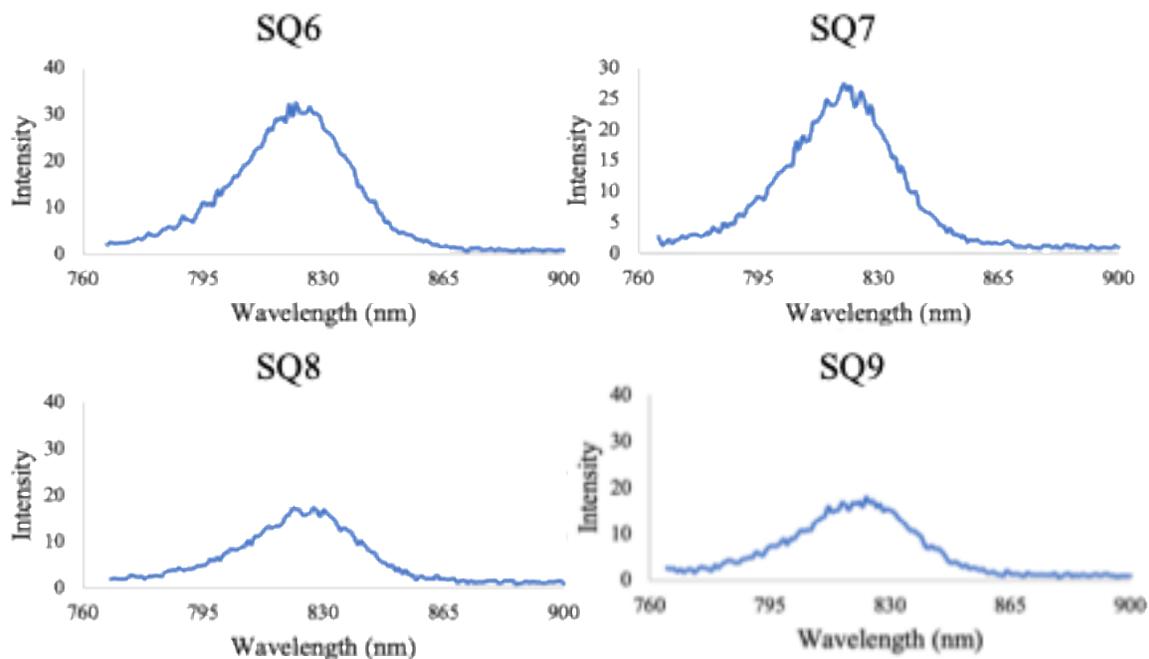


Figure S11: Fluorescence Spectrum of **SQ6 - 9** in Ethanol.

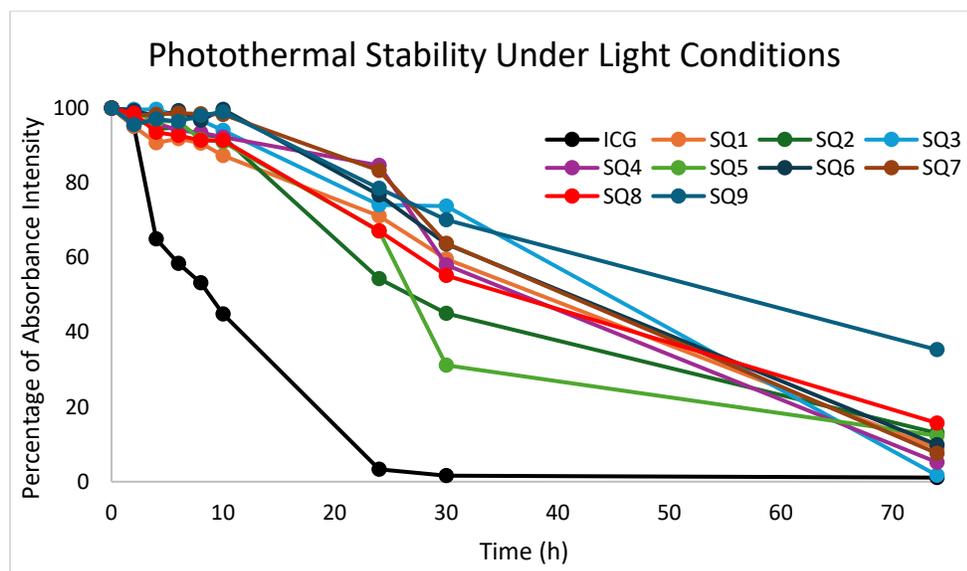


Figure S12: Photothermal stability of SQ1 - 9. Normalized absorbance over time under light using a 6000 mW 254 nm UV lamp. The dye solution is in ethanol.

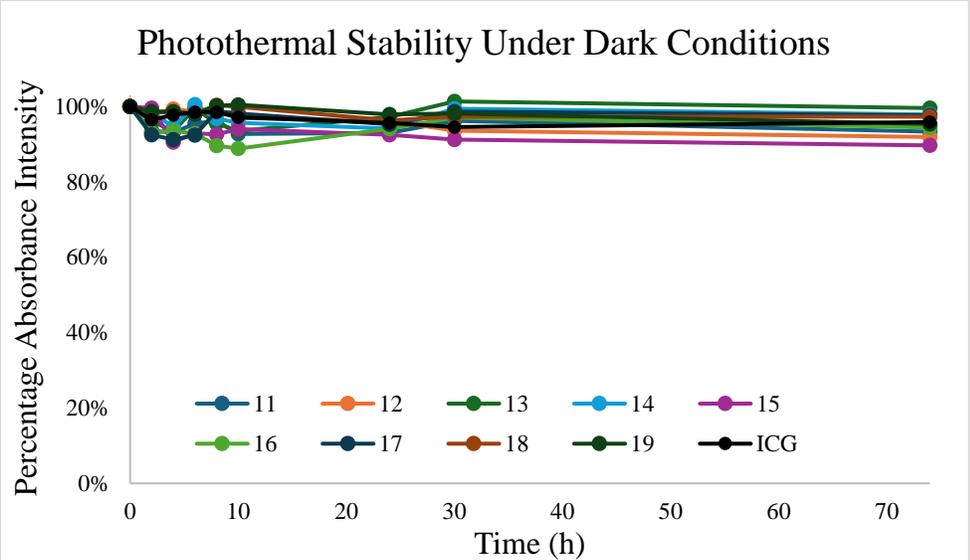


Figure S13: Photothermal stability of **SQ1 - 9** and ICG. Normalized absorbance over time under dark conditions. The dye solution is in ethanol at 25 °C covered with aluminum foil in the drawer.

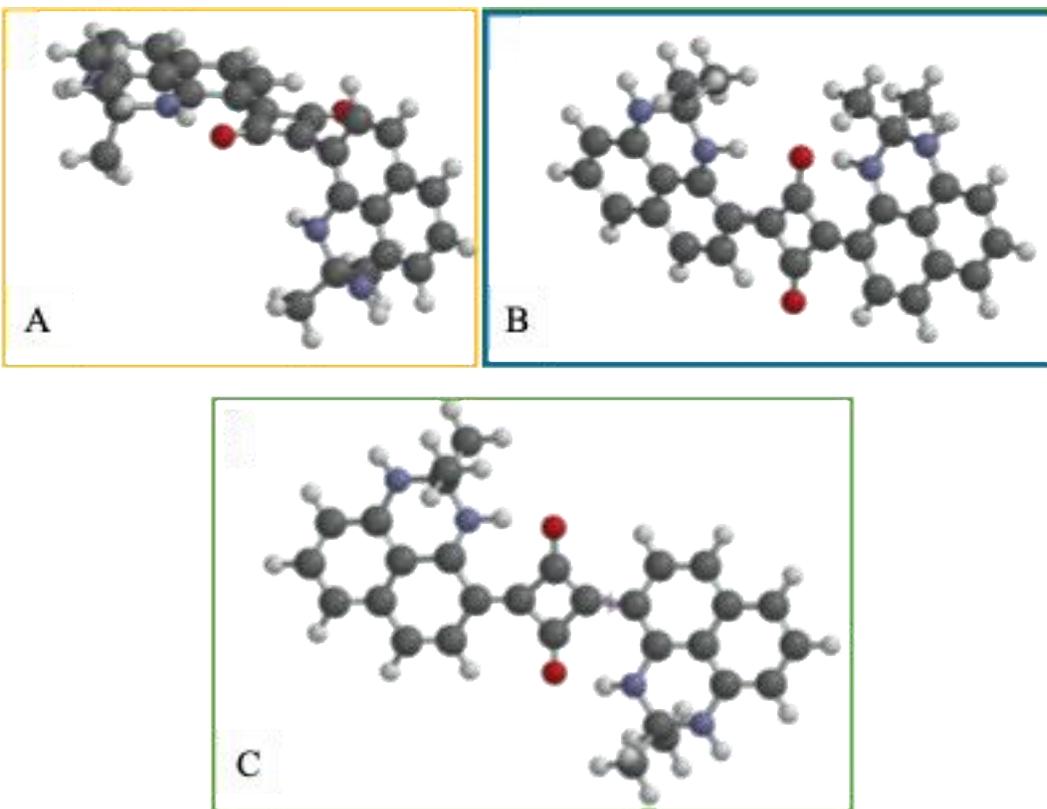


Figure S14: Structural orientation of **SQ1** in the highest energy, local and global minimum energy states. A. The configuration of the molecule at highest energy state. B. The orientation of the molecule in the lowest energy, Z form. C. The arrangement in local minimum energy state, E form.

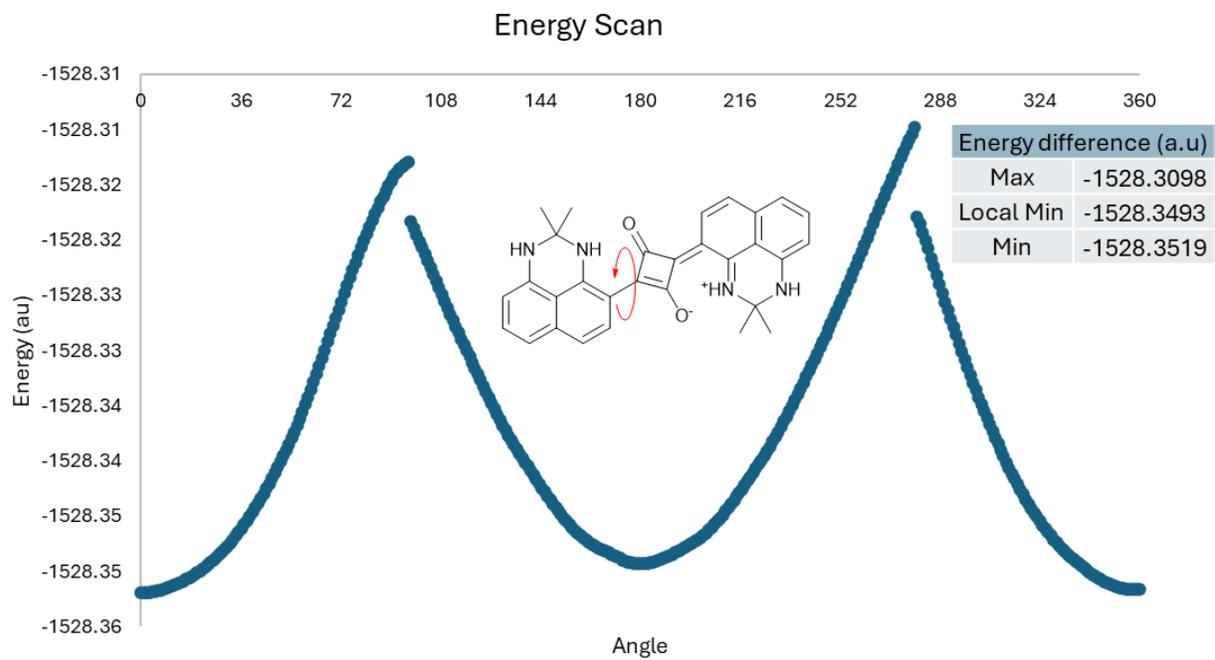
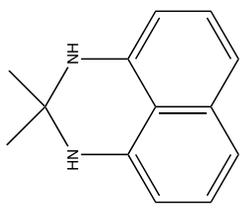
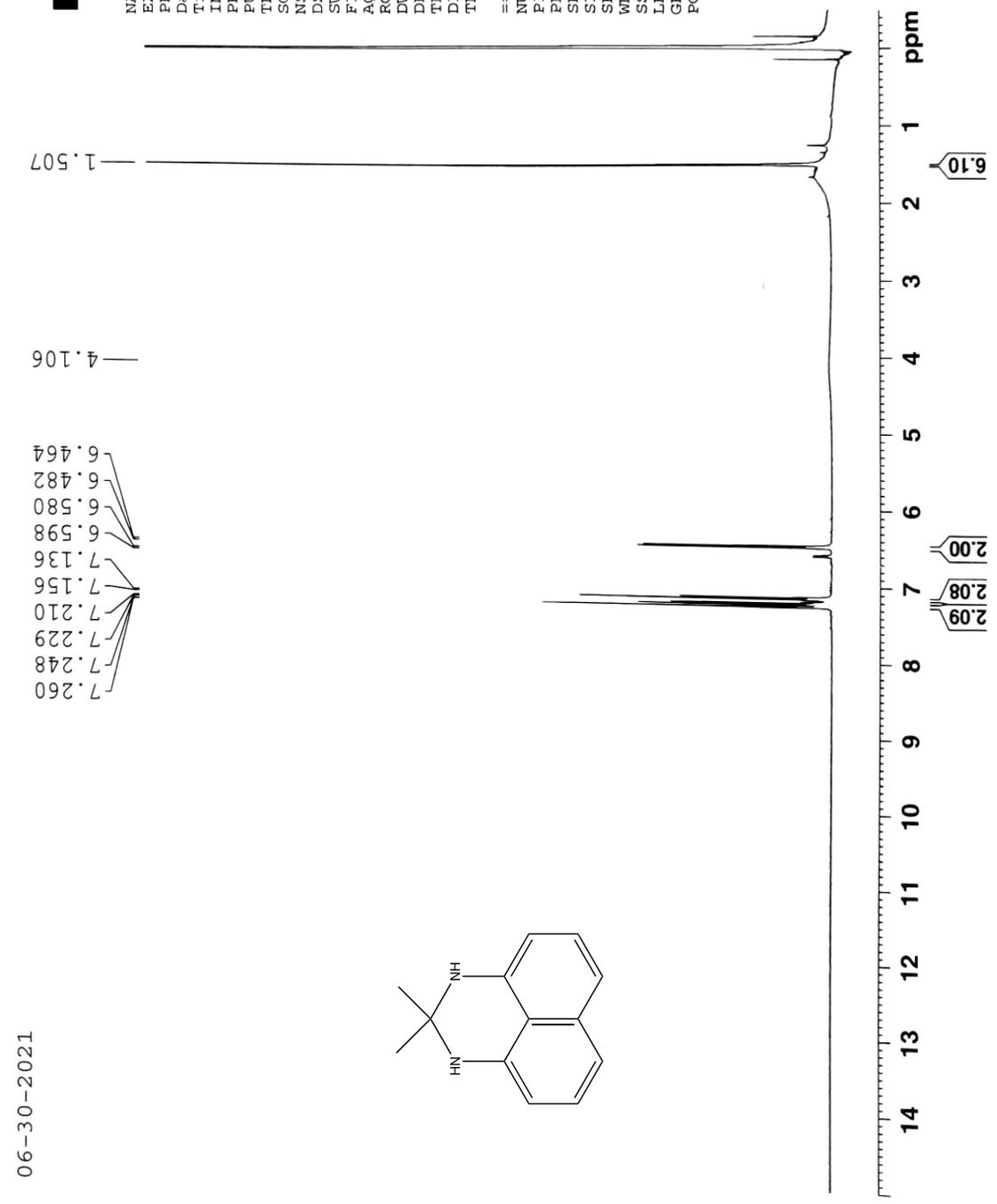


Figure S15: Energy profile analysis of **SQ1** with the dihedral angle of rotation depicted.



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FIDRES 0.126314 Hz
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RG 181
DW 60.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
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P1 11.00 usec
PL1 0.00 dB
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SI 32768
SF 400.1300098 MHz
EM
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0.30 Hz
0
1.00
PC



06-30-2021

Shahir06-07-2022



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PROCNO 1

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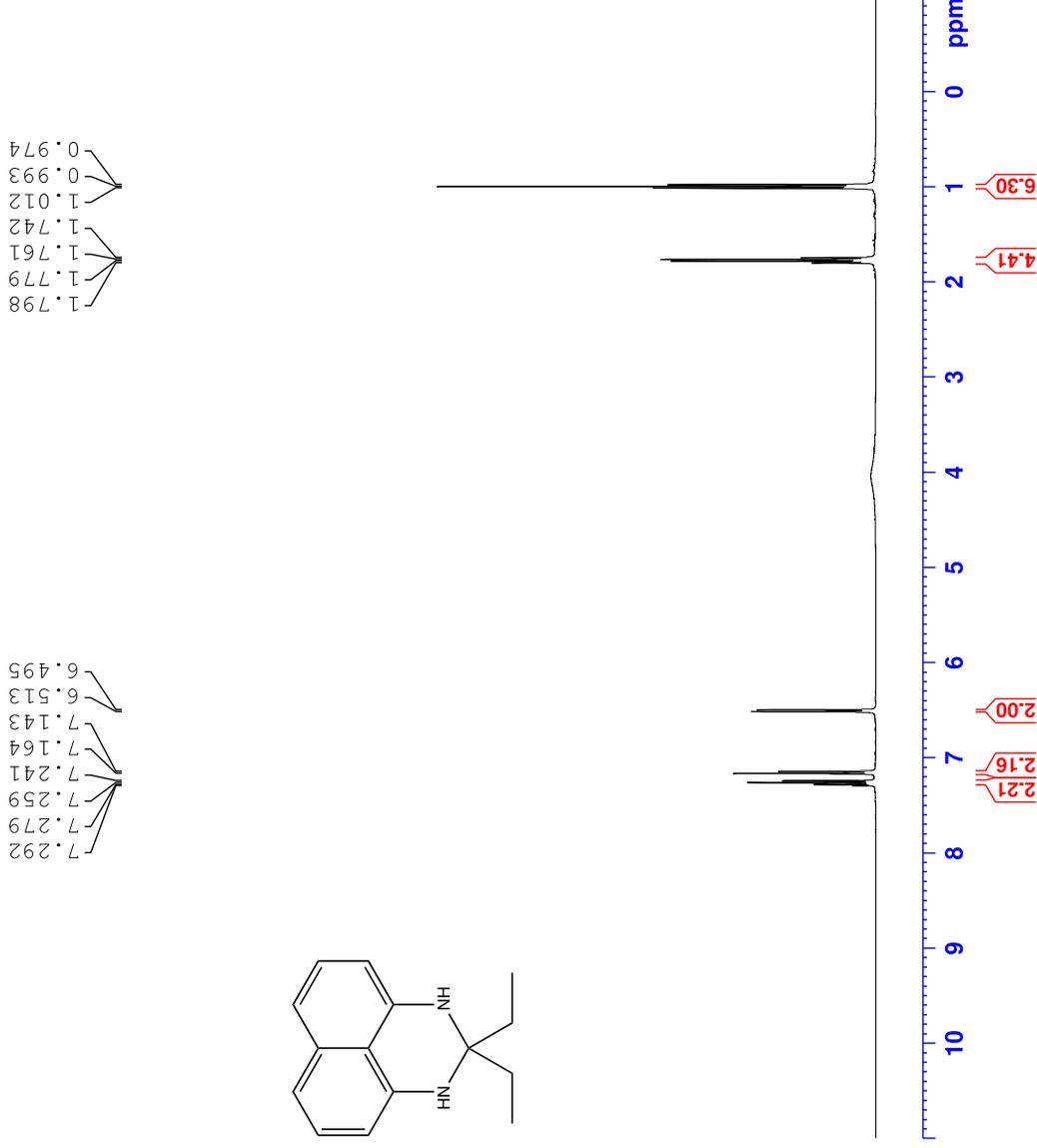
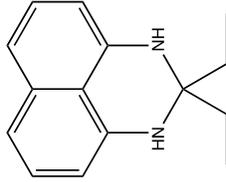
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FIDRES 0.122266 Hz
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RG 80.6
DM 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

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NUC1 1H
P1 13.55 usec
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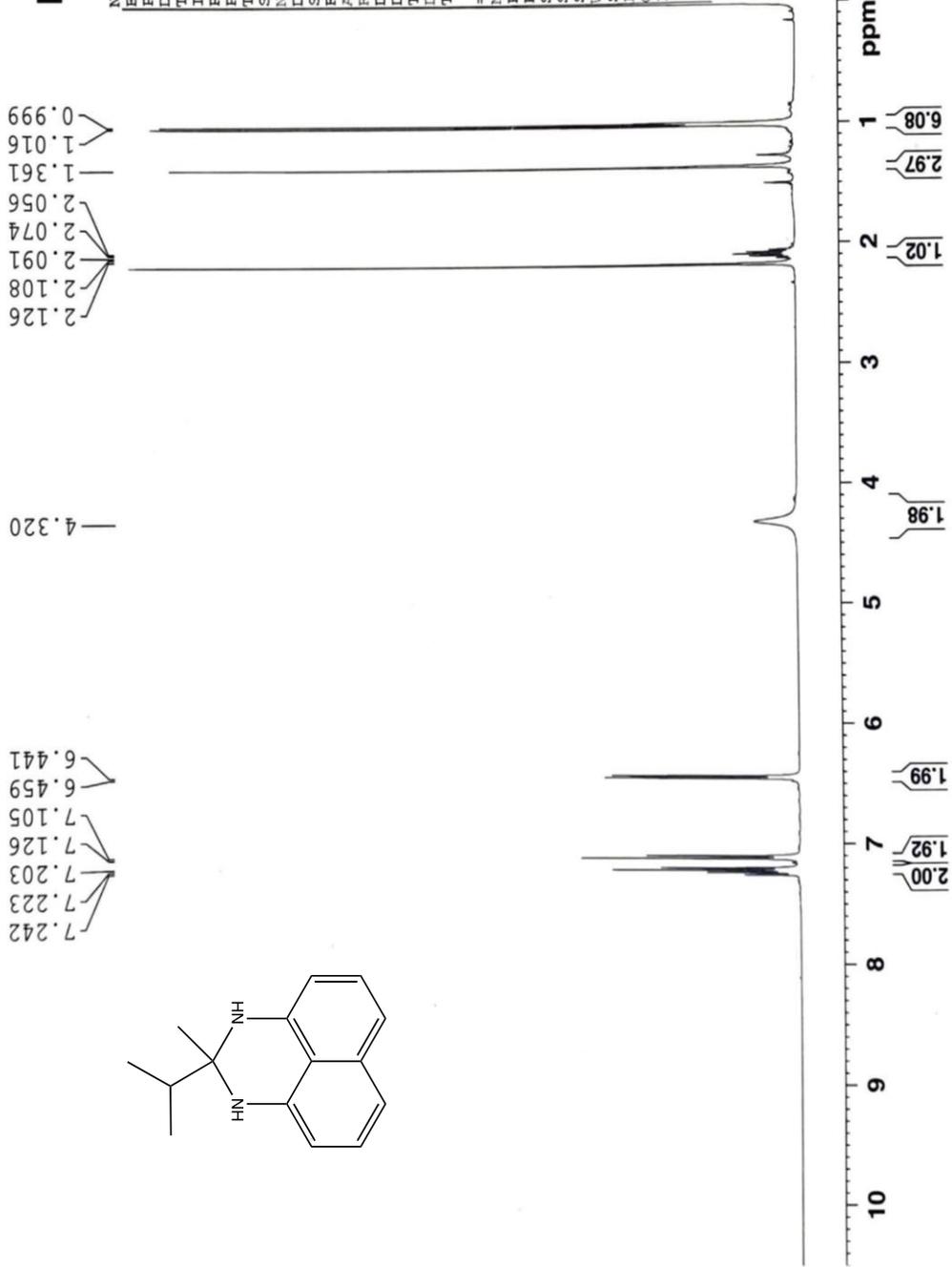
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6.513
6.495





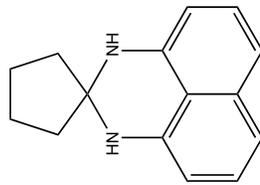
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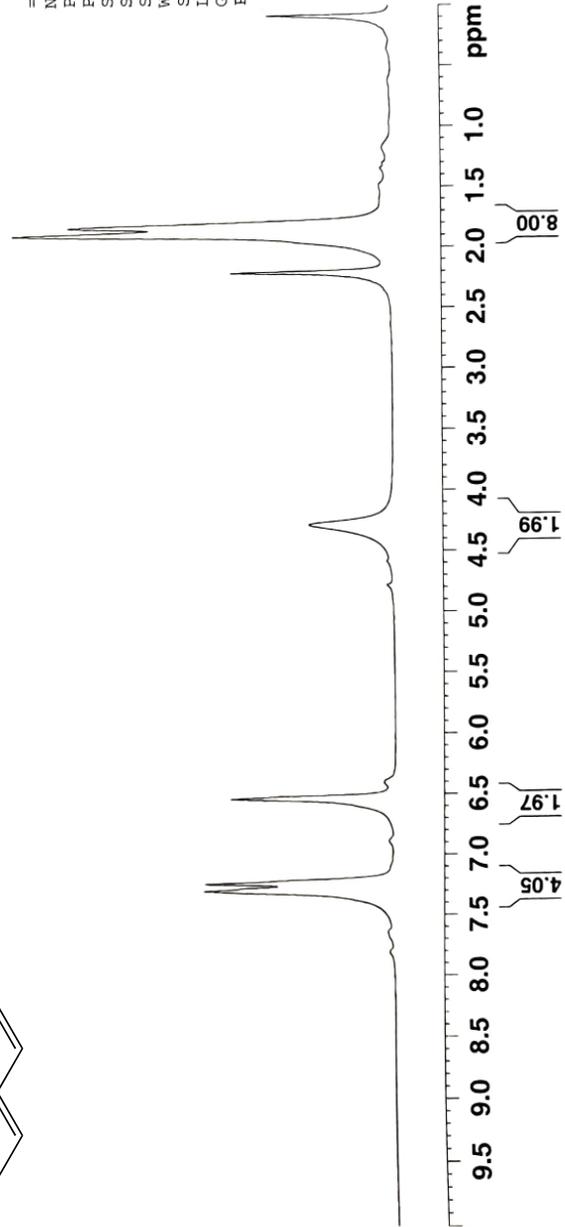
01/10/2021

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SOLVENT CDCl3
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DE 6.50 usec
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TD0 1

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03/01/2022



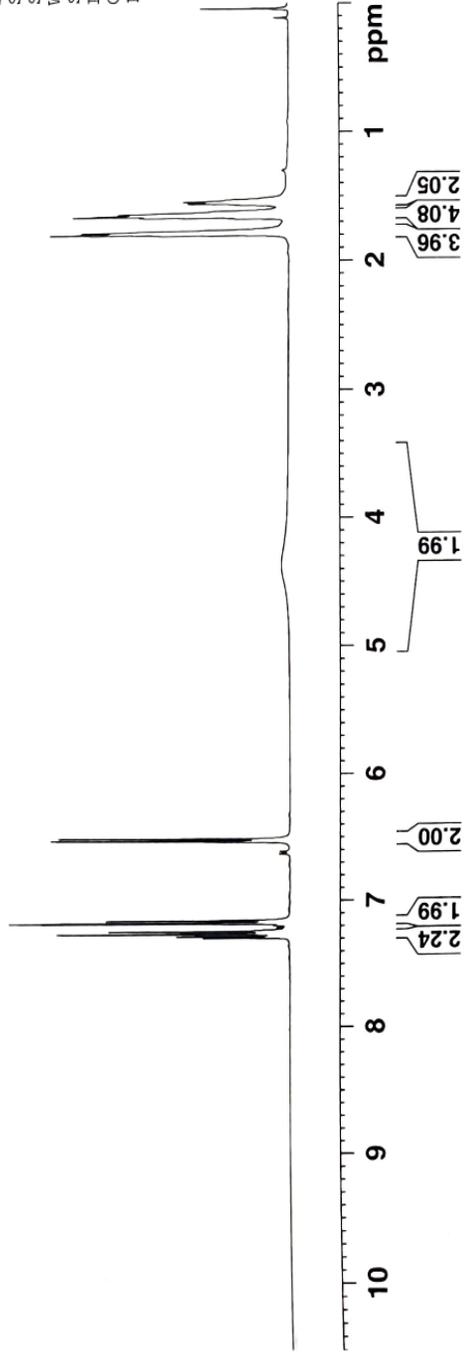
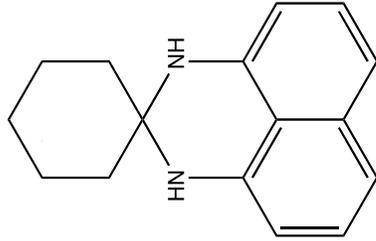
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RG 161.3
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TE 296.5 K
D1 1.00000000 se
TD0 1

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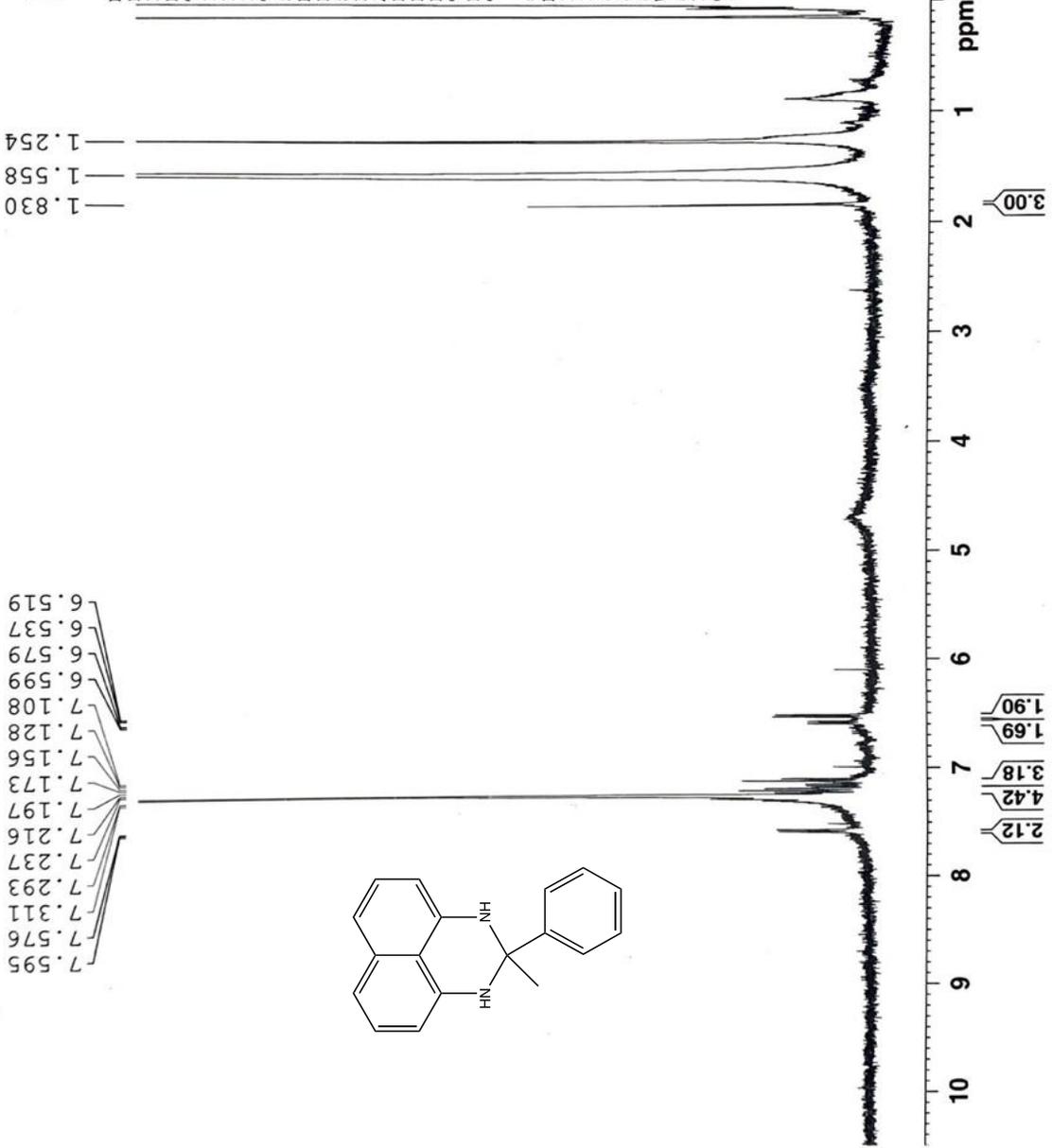
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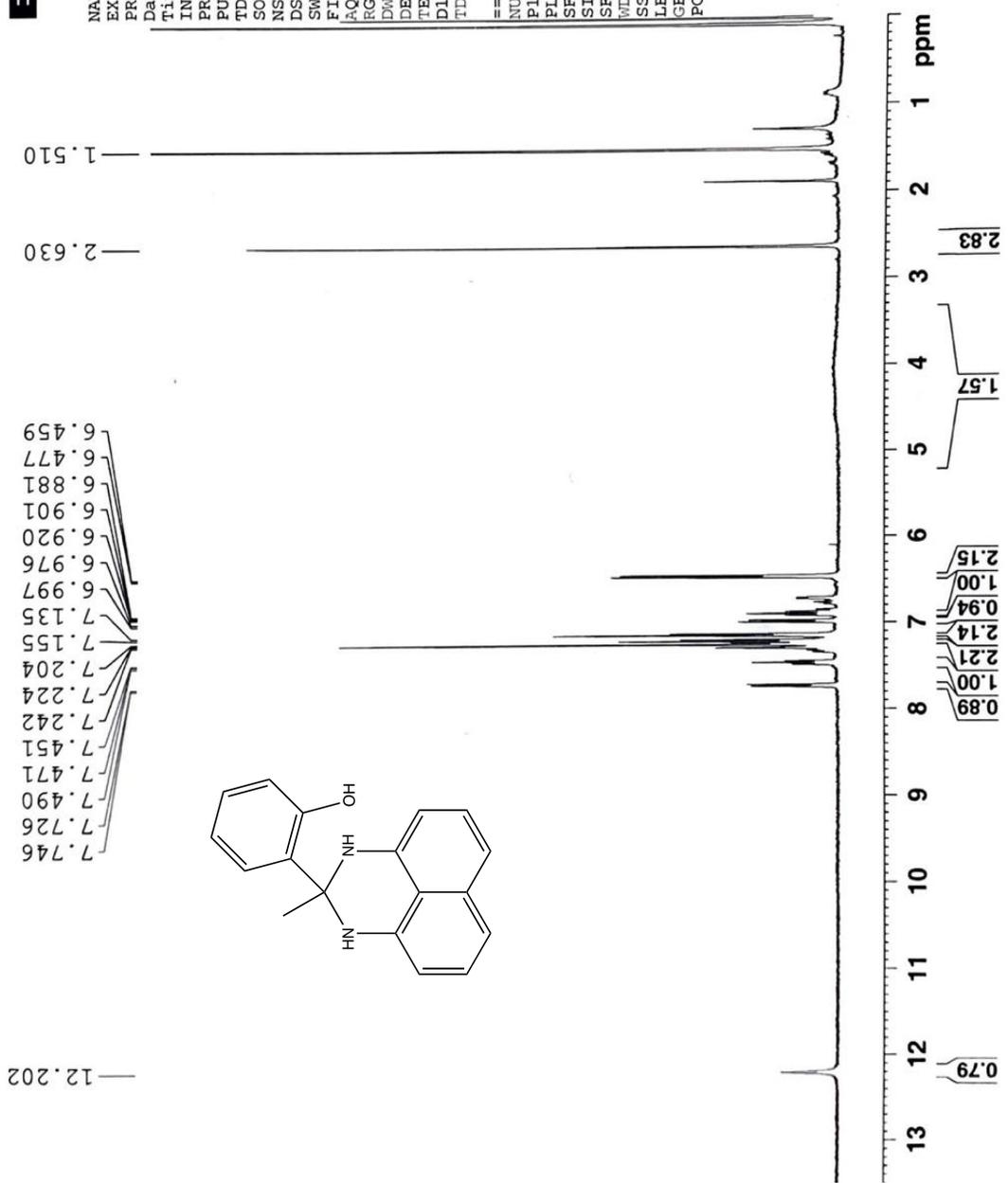
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DE 6.50 usec
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D1 1.00000000 sec
TD0 1
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PL1 0.00 dB
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01/20/2022



Shahir06-01-2022



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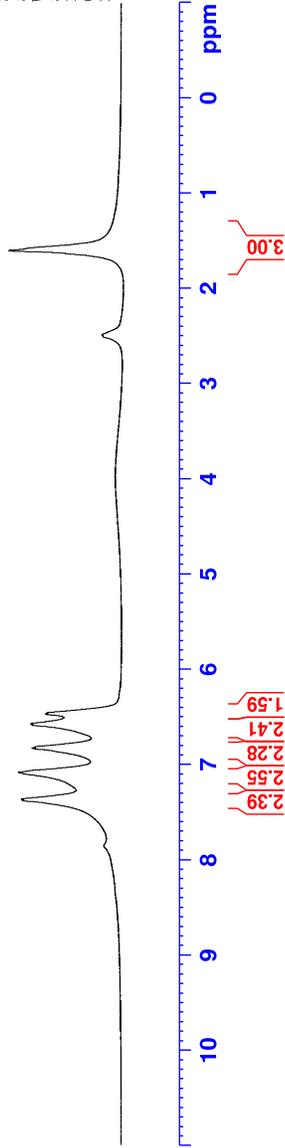
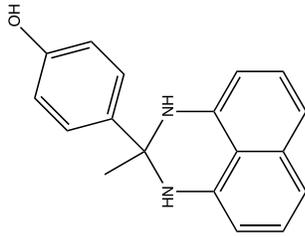
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TE 293.2 K
D1 1.00000000 sec
TDO 1

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test tube sample ... 03/01/2022



NAME Shahir

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FIDRES 0.126314 Hz

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DW 60.400 usec

DE 6.50 usec

TE 296.6 K

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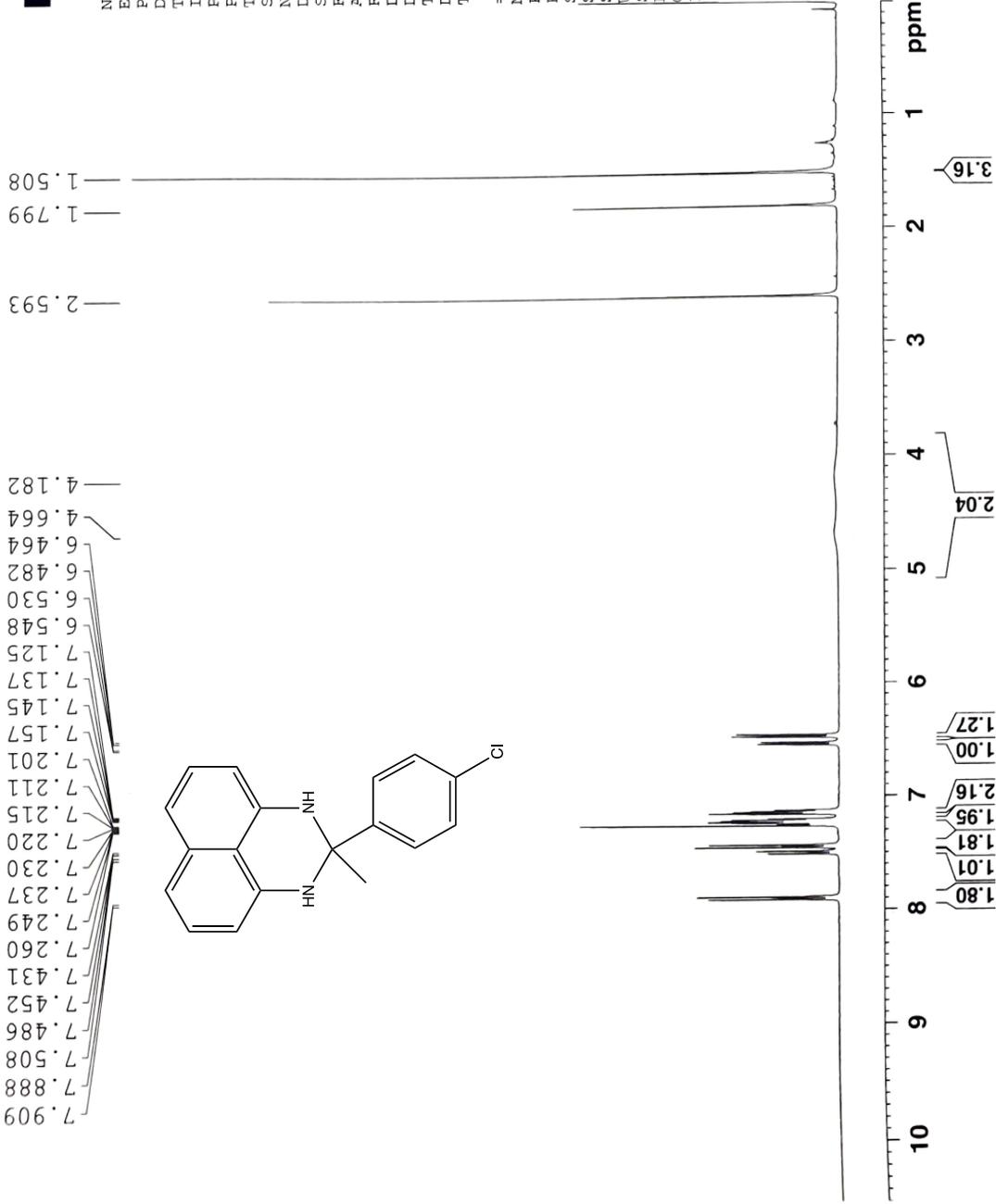
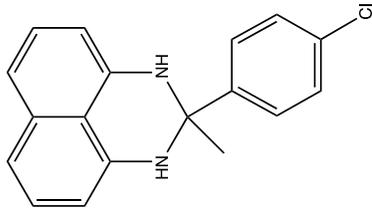
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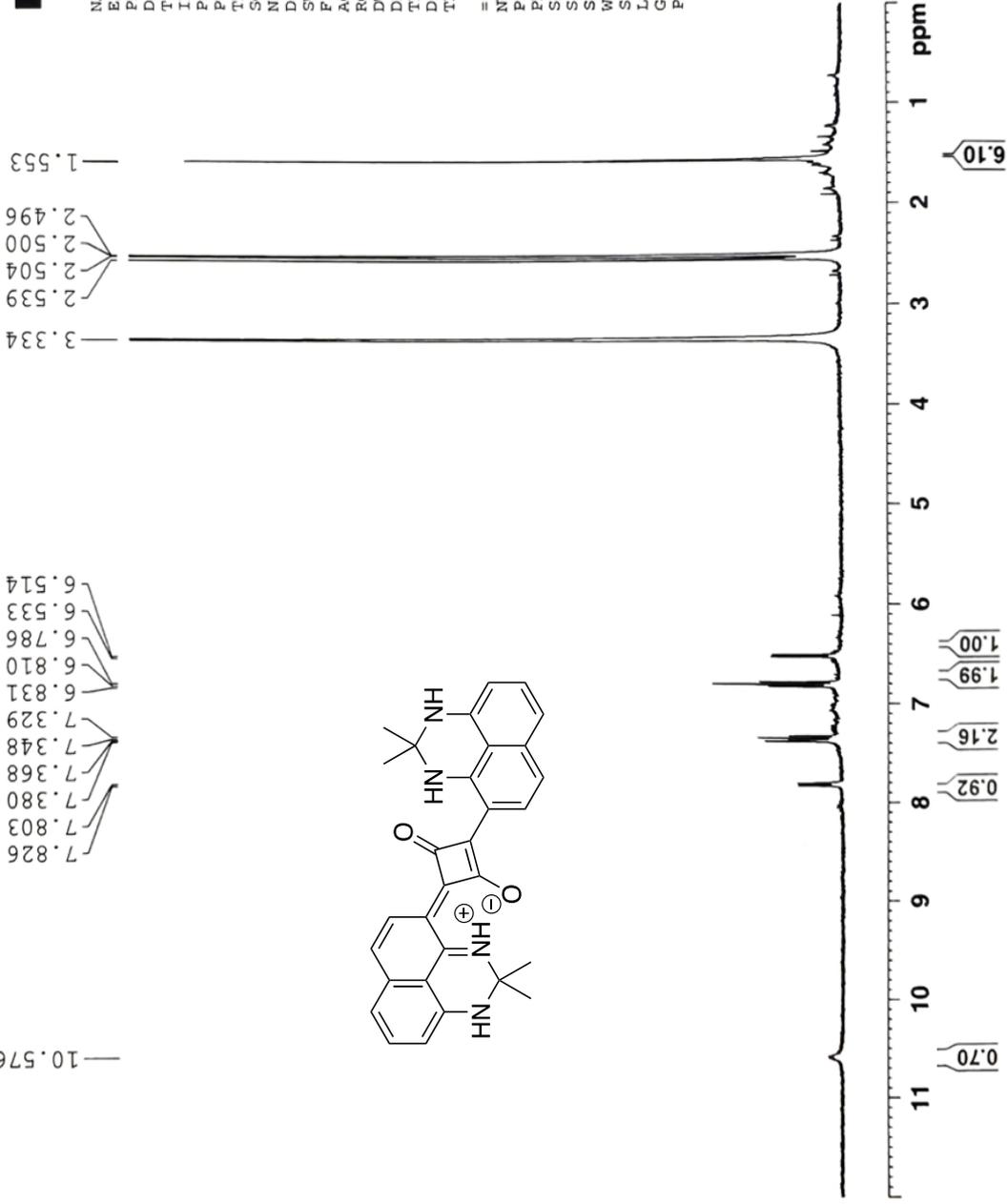
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4.664
4.182





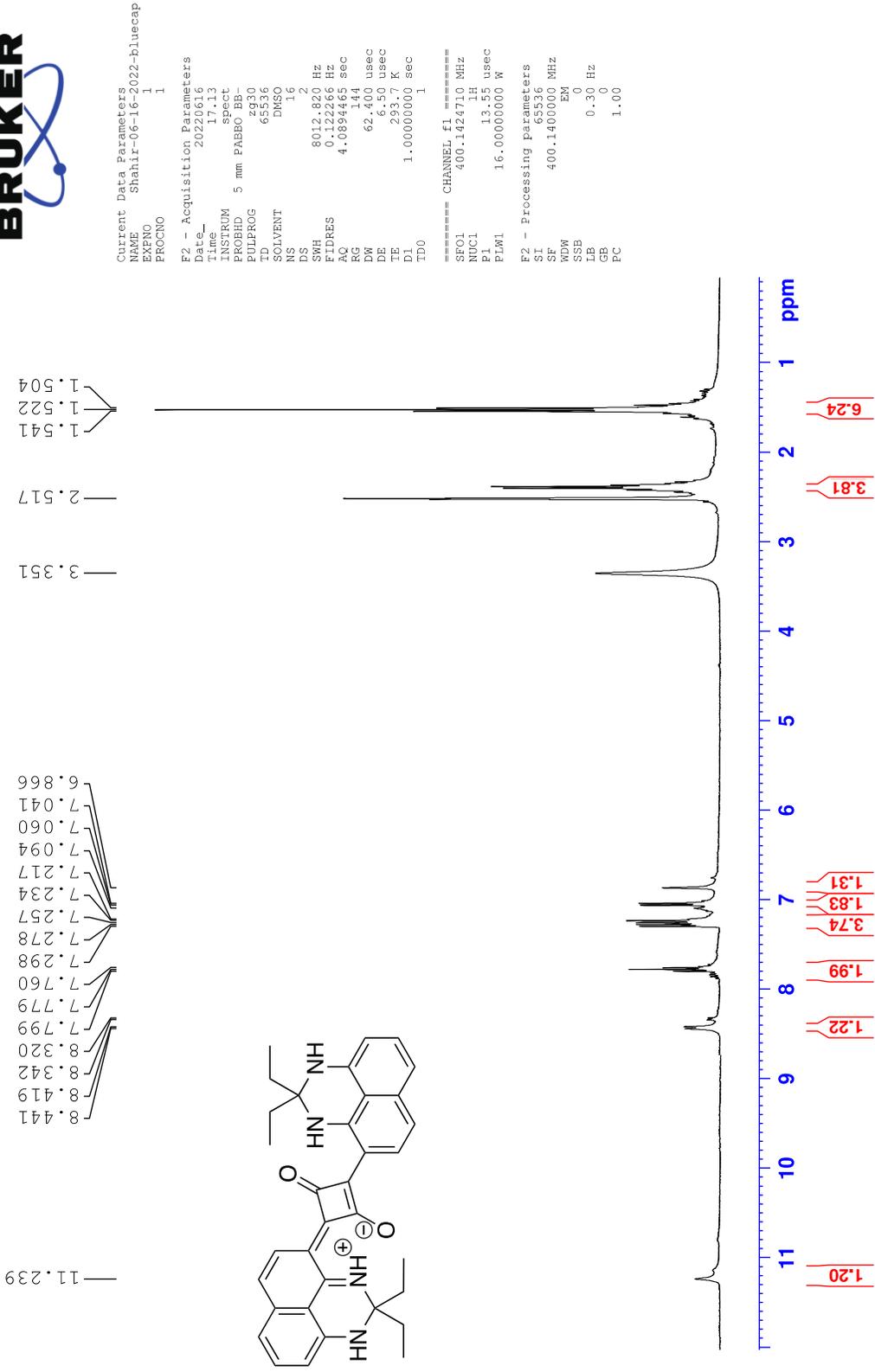
NAME Ken
EXPNO 17
PROCNO 1
Date_ 20210812
Time 18.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 456.1
DW 60.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SF01 400.1324710 MHz
SI 32768
SF 400.1300033 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

08-12-2021





Shahir-06-16-2022-bluecap

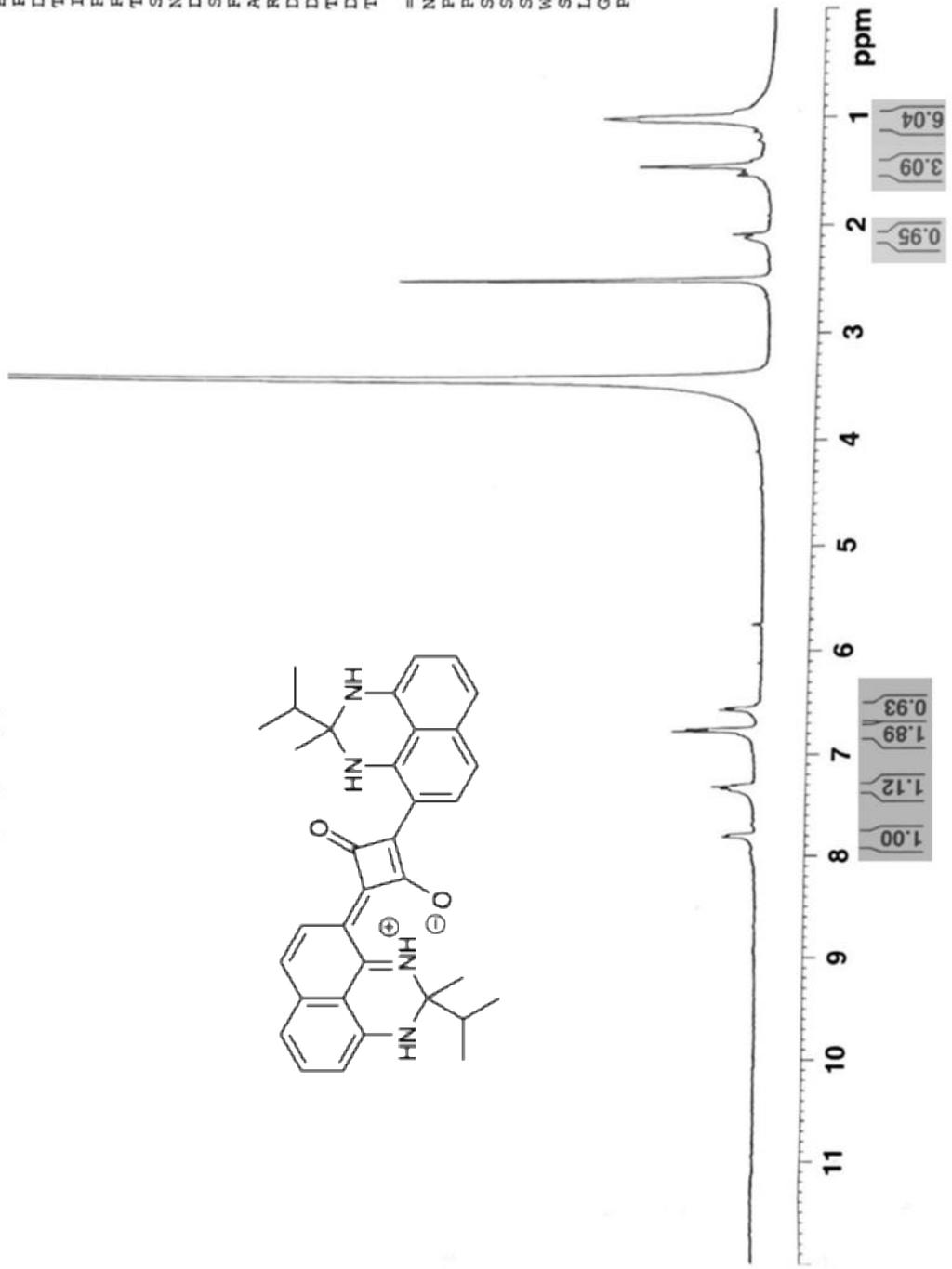
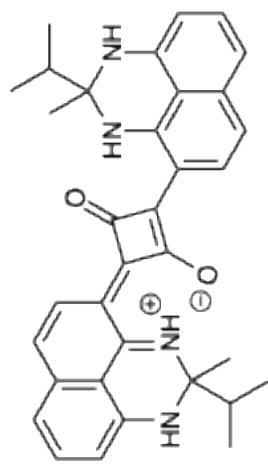




NAME Shahir
EXPNO 11
PROCNO 1
Date_ 20211022
Time_ 12.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TDO 1
===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz
SI 32768
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

0.990
1.008
1.454
2.113

6.549
6.569
6.754
6.774
7.302
7.321
7.340
7.353
7.795
7.811



red cap... 04/05/2022

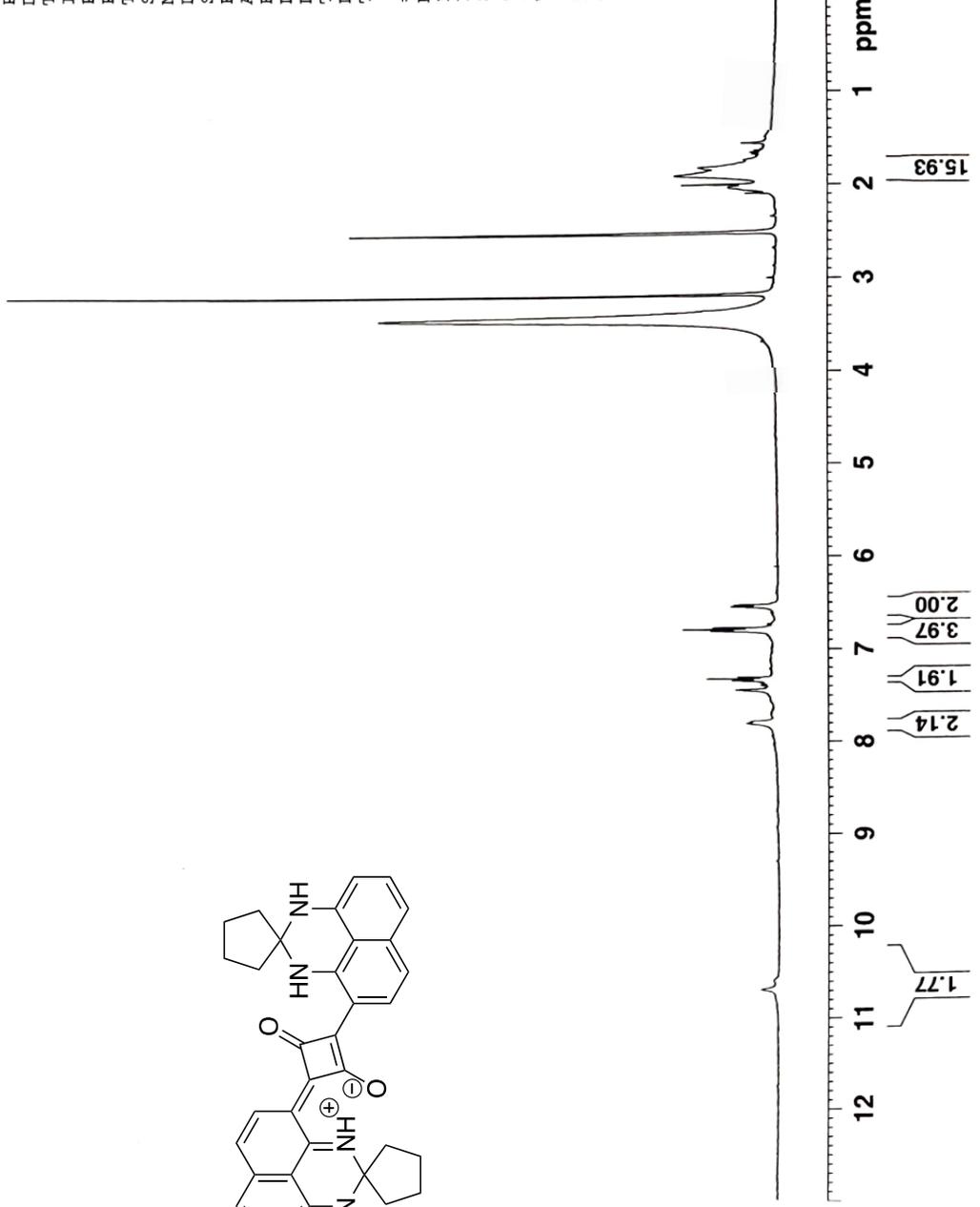
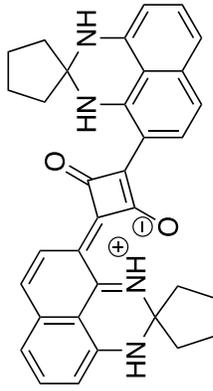


NAME Shahir
EXPNO 61
PROCNO 1
Date_ 20220405
Time_ 15.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.50 usec
TE 295.8 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SF01 400.1324710 MHz
SI 32768
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

2.021
1.886
1.802

7.811
7.795
7.350
7.330
7.311
6.815
6.800
6.778
6.553
6.533

10.686

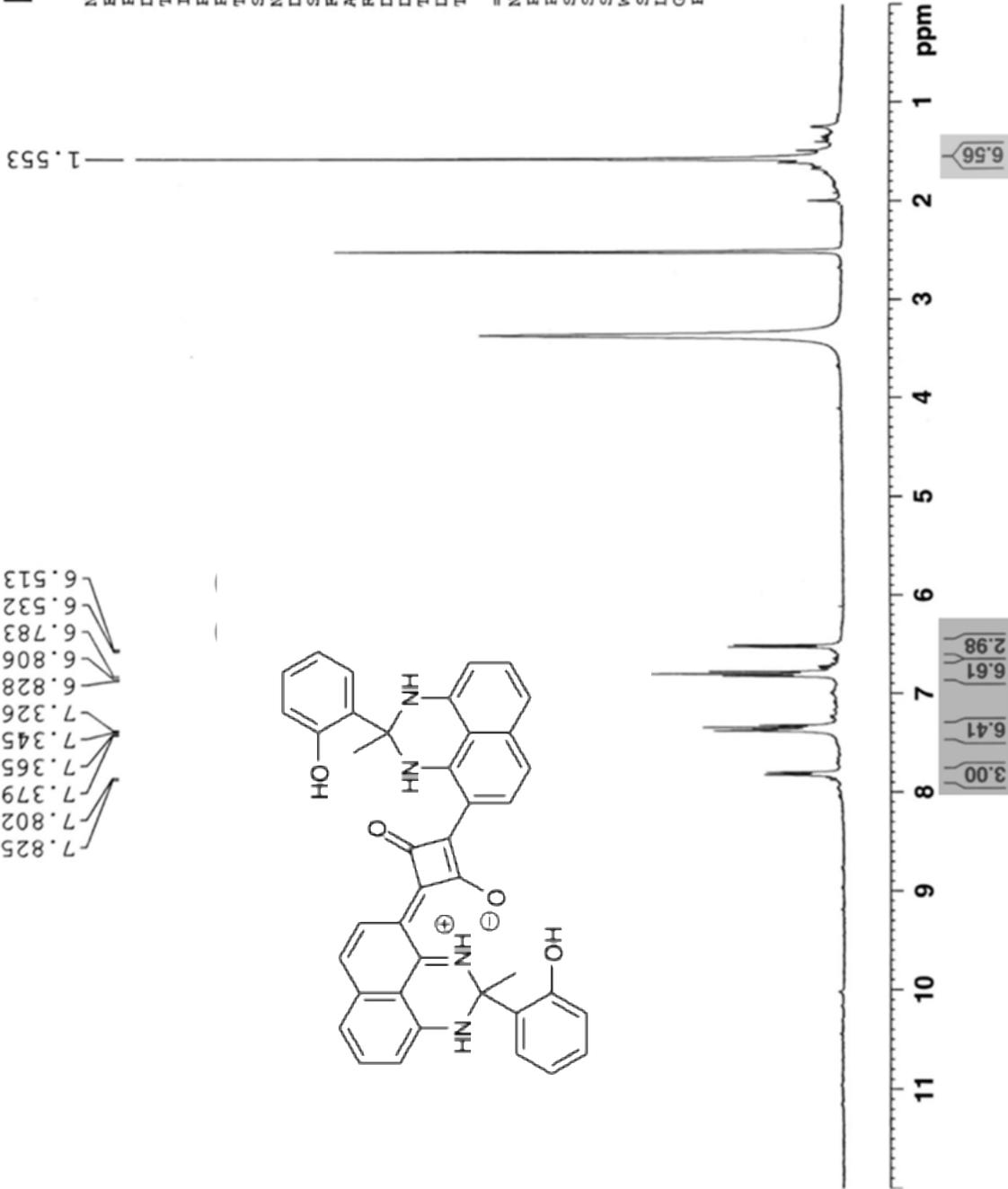
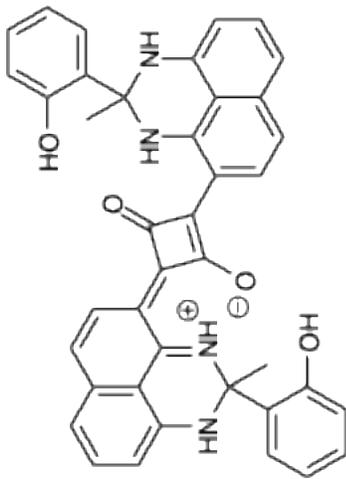


sample... 02/09/2022



NAME Shahir
EXPNO 32
PROCNO 1
Date_ 20220209
Time 15.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TDO 1
===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SF01 400.1324710 MHz
SI 32768
SF 400.1300032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.825
7.802
7.379
7.365
7.345
7.326
6.828
6.806
6.783
6.532
6.513



Shahirbluecap-06-23-22



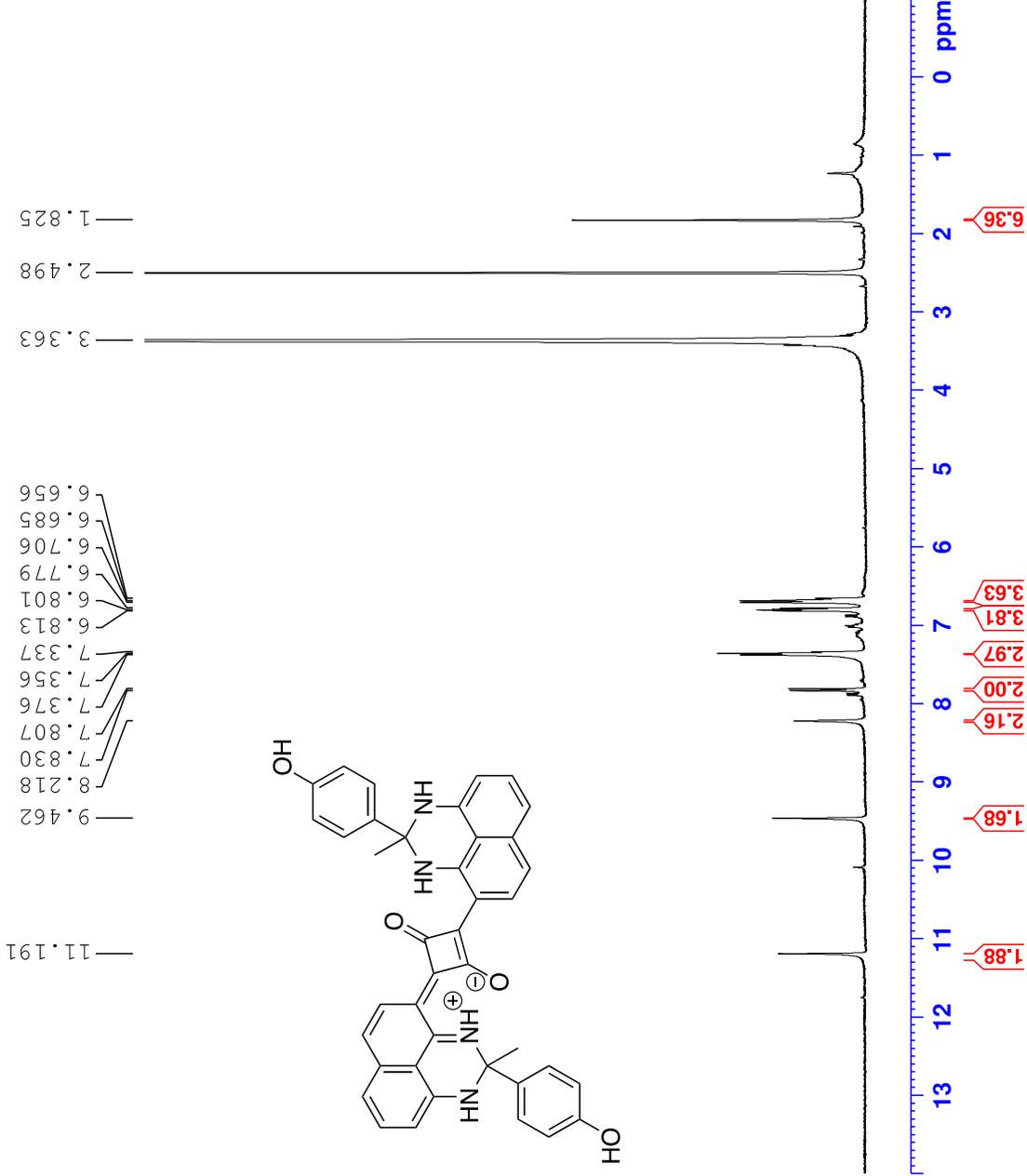
Current Data Parameters
NAME Shahirbluecap-06-23-22
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20220623
Time 16.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
DS 16
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.089465 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SF01 400.1424710 MHz
NUC1 1H
P1 13.55 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1400034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





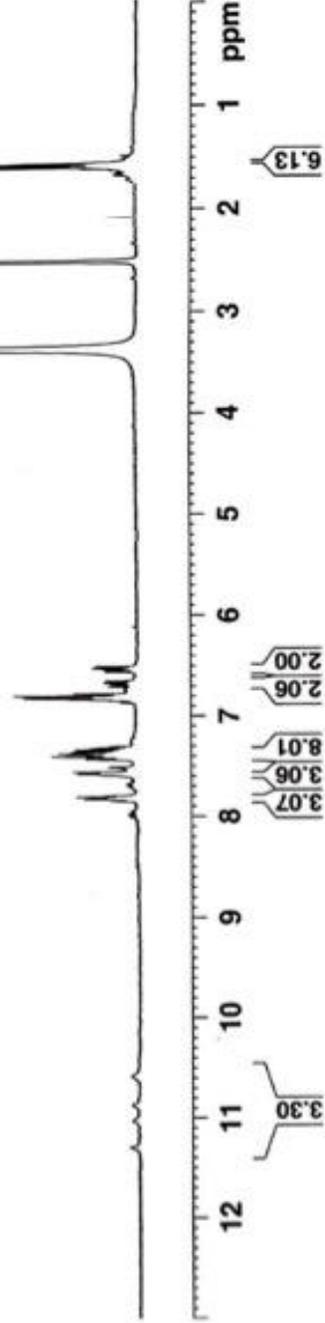
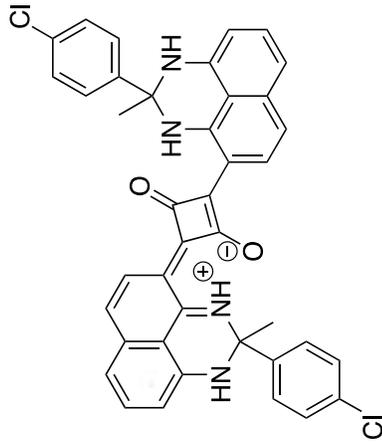
NAME Shahir
EXPNO 50
PROCNO 1
Date_ 20220310
Time 17.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz
SI 32768
SF 400.1300032 MHz
EM 0
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

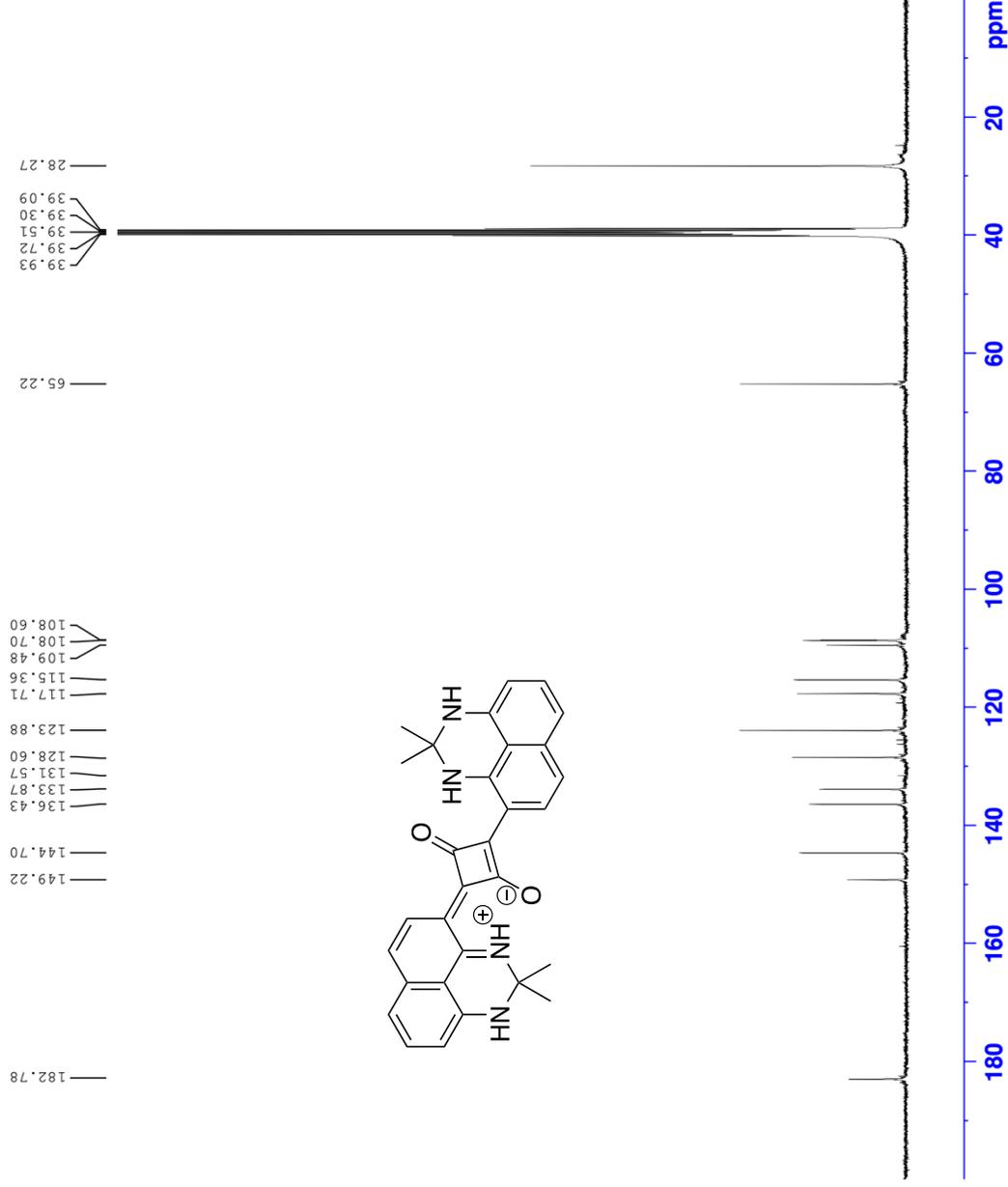
blue cap ... 03/10/2022

11.299
11.030
10.873
10.584
7.853
7.838
7.831
7.815
7.802
7.586
7.565
7.437
7.412
7.390
7.384
7.365
7.352
7.346
7.333
7.326
7.313
6.831
6.813
6.808
6.790
6.783
6.710
6.691
6.675
6.656
6.563
6.543
6.532
6.512

1.553



SS1carbon



Current Data Parameters
NAME ssl
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230213
Time 5.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 14336
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6253441 MHz
NUC1 13C
P1 9.25 usec
PLW1 62.00000000 W

==== CHANNEL f2 =====
SFO2 400.1416006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.36267000 W
PLW13 0.29376000 W

F2 - Processing parameters
SI 32768
SF 100.6153279 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

583carbon3

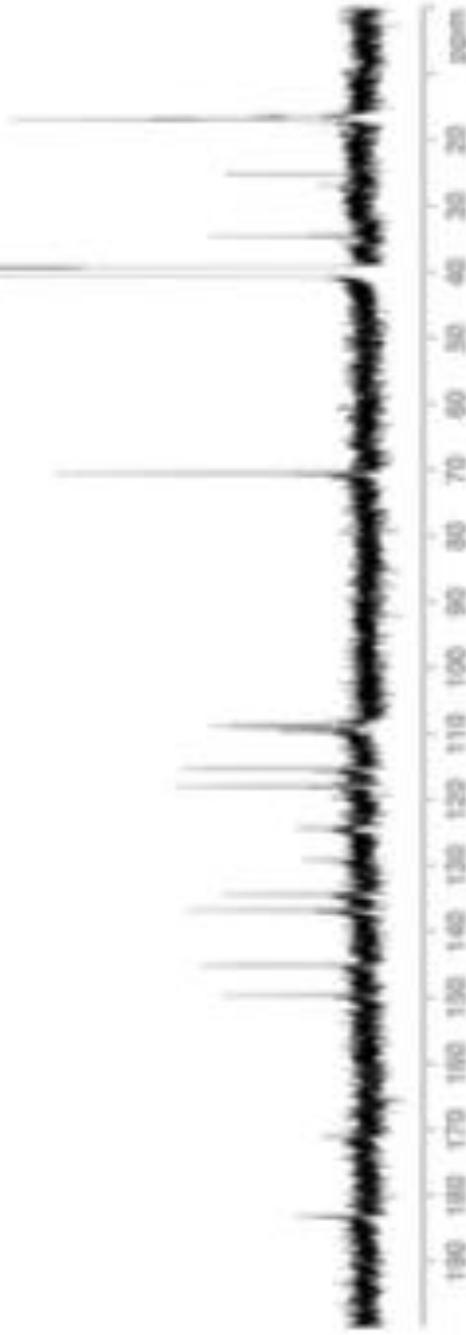
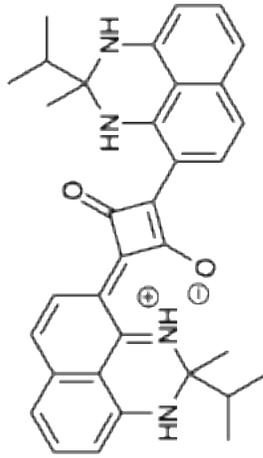


Current Data Parameters
 NAME: 583carbon3
 FNAME: 583
 PROCNO: 1
 FT - Acquisition Parameters
 Date_: 20120221
 Time: 4.32
 INSTRUM: spect
 PROBR: 5 mm HADAM SB-
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: DMSO
 NS: 5000
 DS: 4
 SWH: 24228.461 Hz
 FIDRES: 0.166769 Hz
 AQ: 1.1617448 sec
 RG: 253
 DM: 32768
 DE: 6.50 mm
 TE: 293.2 K
 SI: 2.0000000 sec
 SFO: 500.136000 MHz
 TPO: 1

===== CHANNEL F1 =====
 NUC1: 13C-6251442 MHz
 P1: 8.25 usec
 PL1: 0.0000000 dB

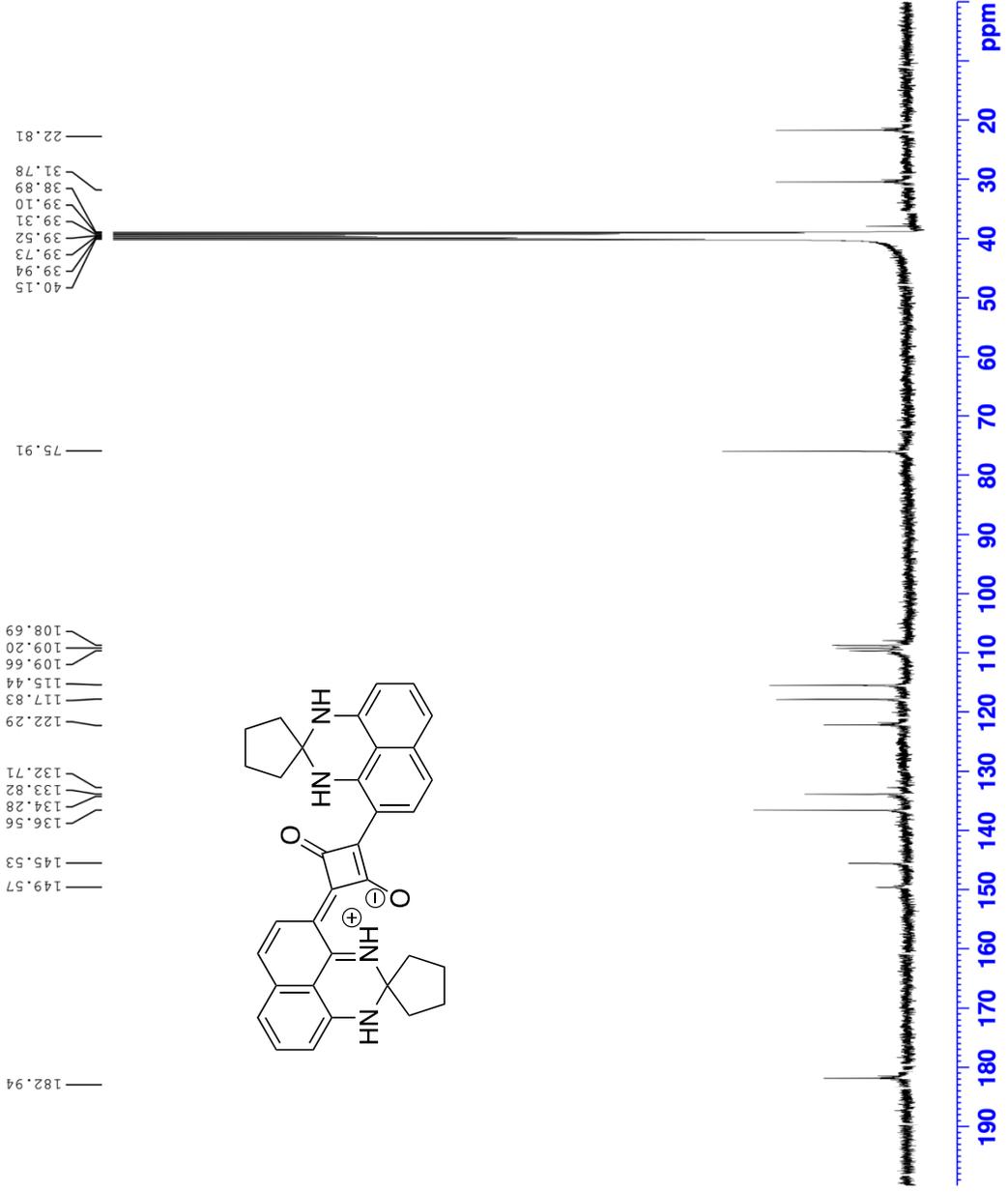
===== CHANNEL F2 =====
 NUC2: 400.1414000 MHz
 P2: 10
 PL2: 0.0000000 dB
 SFO2: 100.6132000 MHz
 NUC3: 13C-6251442 MHz
 P3: 8.25 usec
 PL3: 0.0000000 dB

FT - Processing parameters
 SI: 27748
 SF: 100.6132000 MHz
 N: 65536
 DSF: 0
 SW: 1.00 MHz
 WDS: 0.0156250 MHz
 FWHM: 1.42





SS5carbon



Current Data Parameters
NAME SS5carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230305
Time 8.42
INSTRUM spect
PROBHD 5 mm FABRO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15360
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DM 20.800 usec
DE 6.50 usec
TE 292.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

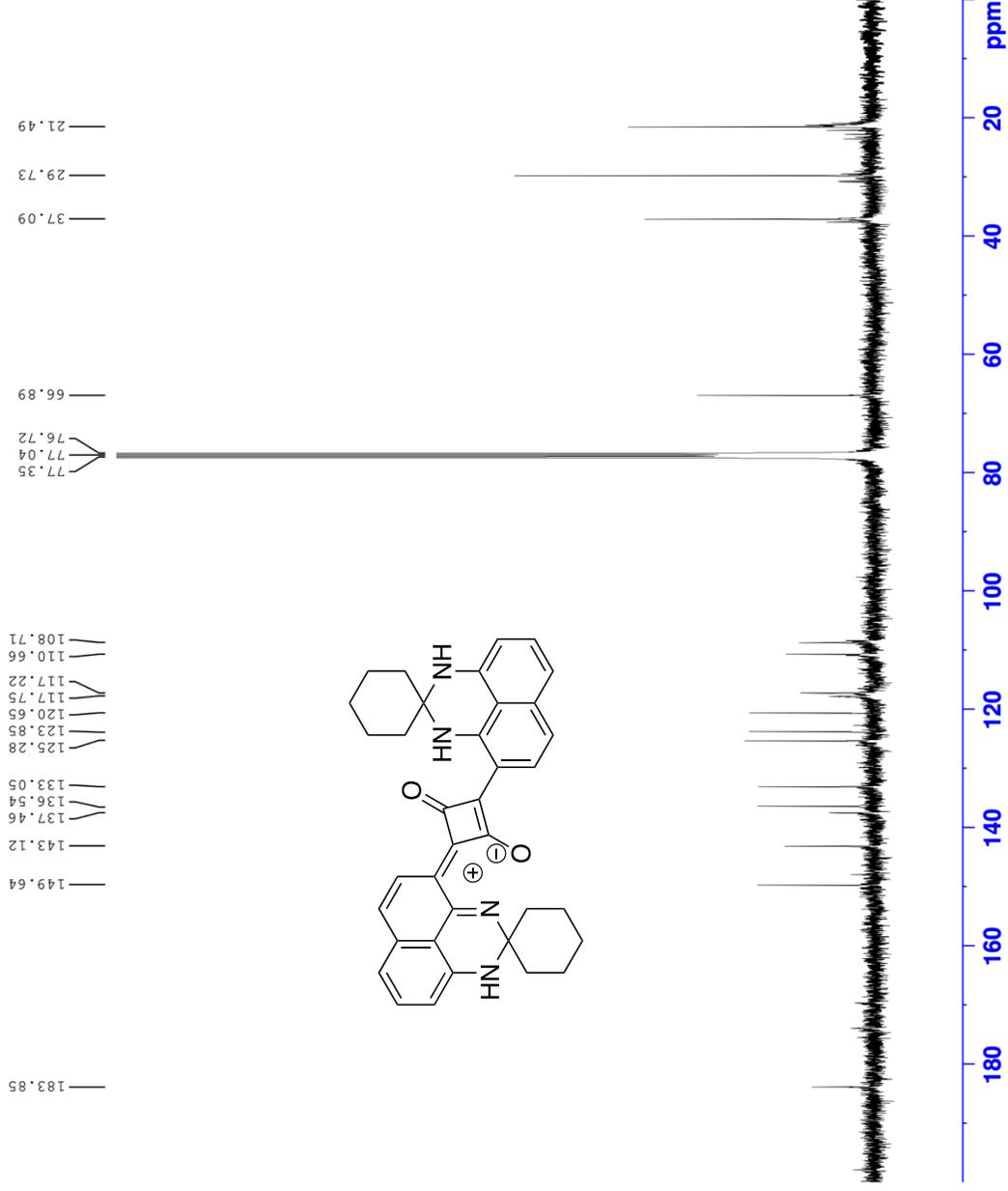
==== CHANNEL f1 =====
SF01 100.6253441 MHz
NUC1 13C
P1 9.25 usec
PLW1 62.00000000 W

==== CHANNEL f2 =====
SF02 400.1416006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.36267000 W
PLW13 0.29376000 W

F2 - Processing parameters
SI 32768
SF 100.6153207 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



SS8carbon2



Current Data Parameters
NAME SS8carbon2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230402
Time_ 6.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15360
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

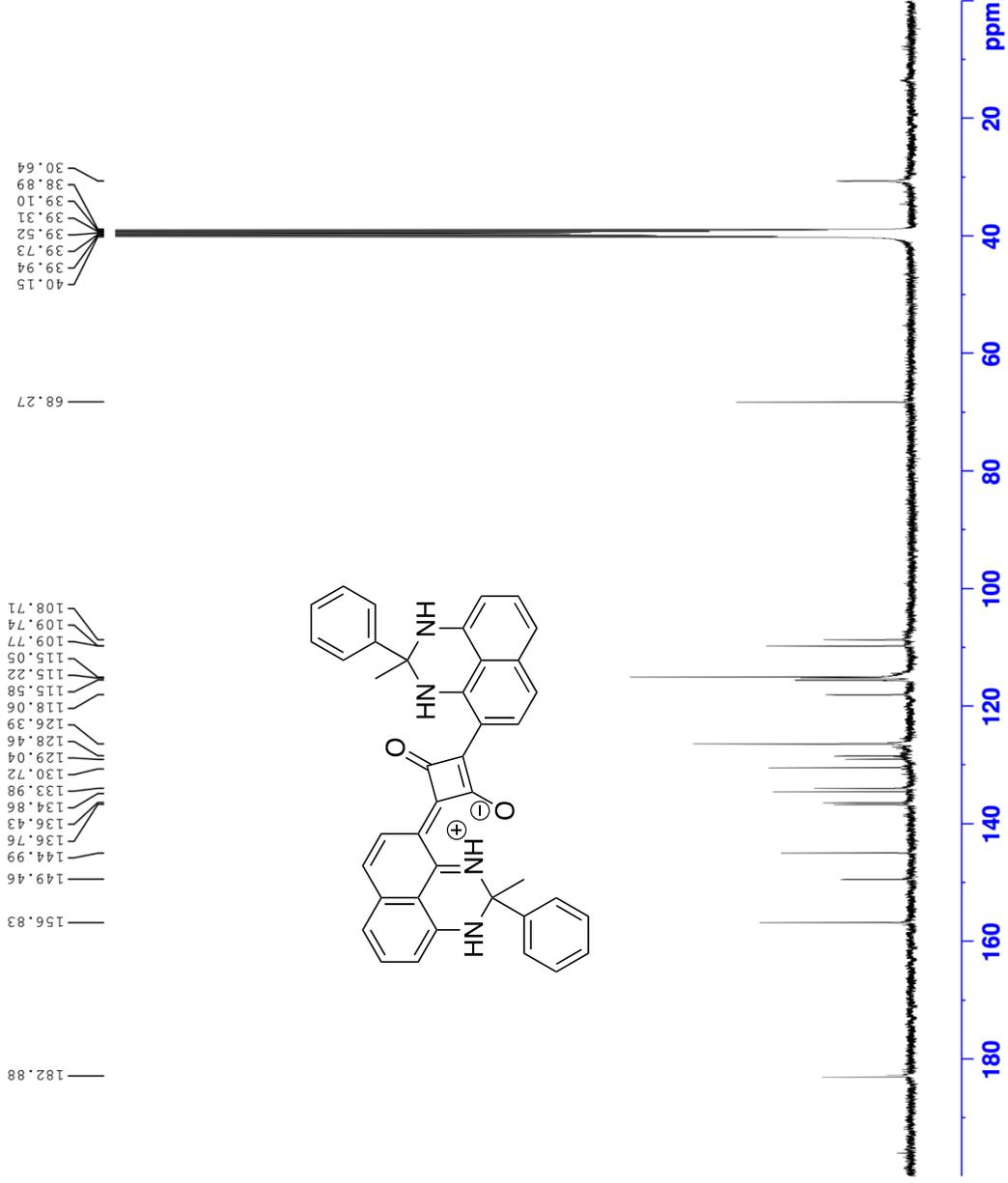
==== CHANNEL f1 =====
SFO1 100.625341 MHz
NUC1 13C
P1 9.25 usec
PLW1 62.0000000 W

==== CHANNEL f2 =====
SFO2 400.1416006 MHz
NUC2 1H
CFPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.3626700 W
PLW13 0.2937600 W

F2 - Processing parameters
SI 32768
SF 100.6152830 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



SS4carbon



Current Data Parameters
NAME SS12carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230326
Time 4.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15360
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 1290.2
DW 20.850 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

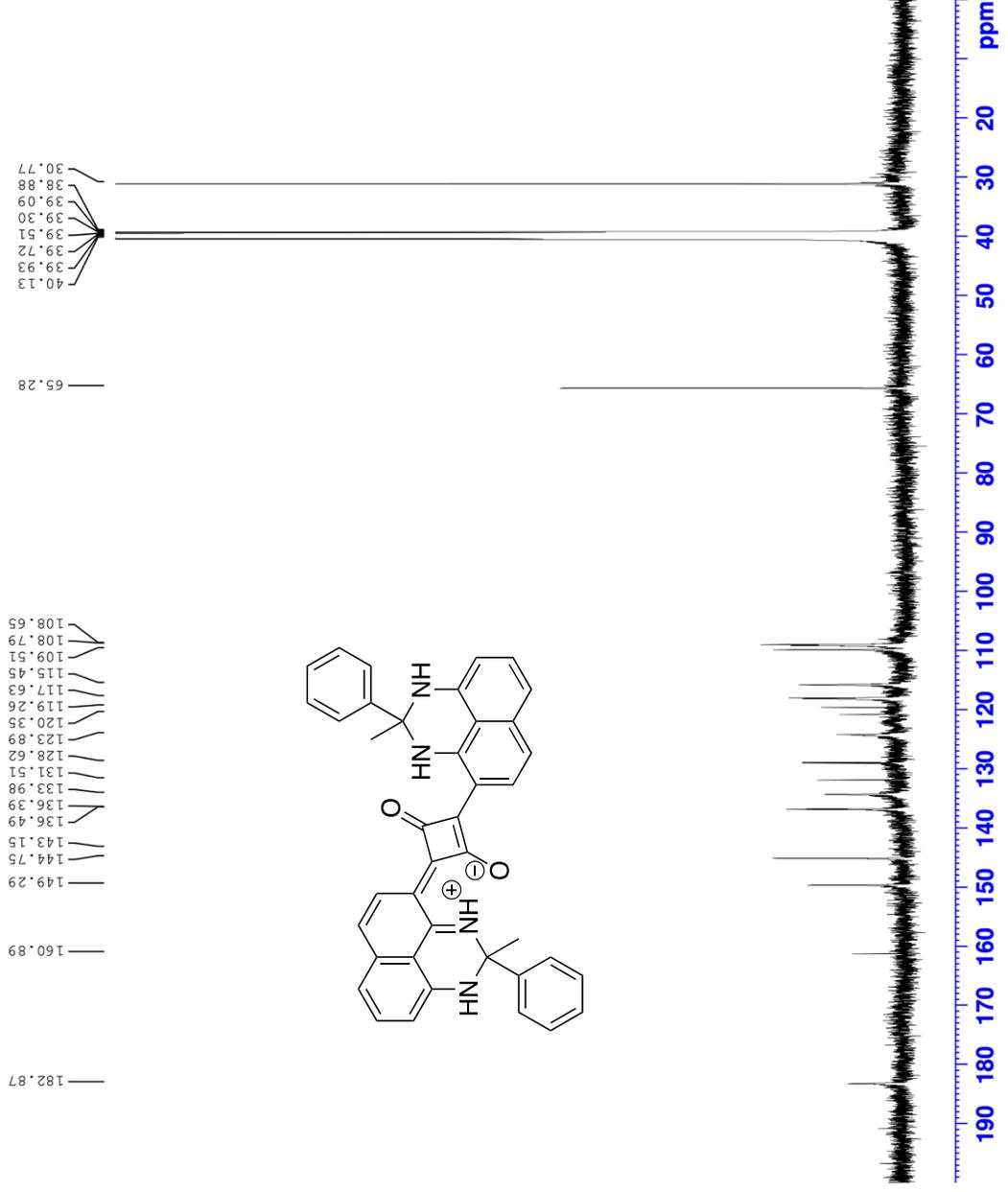
==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 3.00 dB
SFO1 100.6228298 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0 dB
PL12 19.17 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128148 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



SS7carbon



182.87
160.89
149.29
144.75
143.15
136.49
136.39
133.98
131.51
128.62
123.89
120.35
119.26
117.63
115.45
109.51
108.79
108.65

65.28

40.13
39.93
39.72
39.51
39.30
39.09
38.88
30.77

Current Data Parameters
NAME SS6carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230306
Time 2.04
INSTRUM spect
PROBHD 5 mm FAPBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 12288
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6253441 MHz
NUC1 13C
P1 9.25 usec
PLW1 62.00000000 W

==== CHANNEL f2 =====
SFO2 400.1416006 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLWI2 0.36267000 W
PLWI3 0.29376000 W

F2 - Processing parameters
SI 32768
SF 100.6152830 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

88cartbon



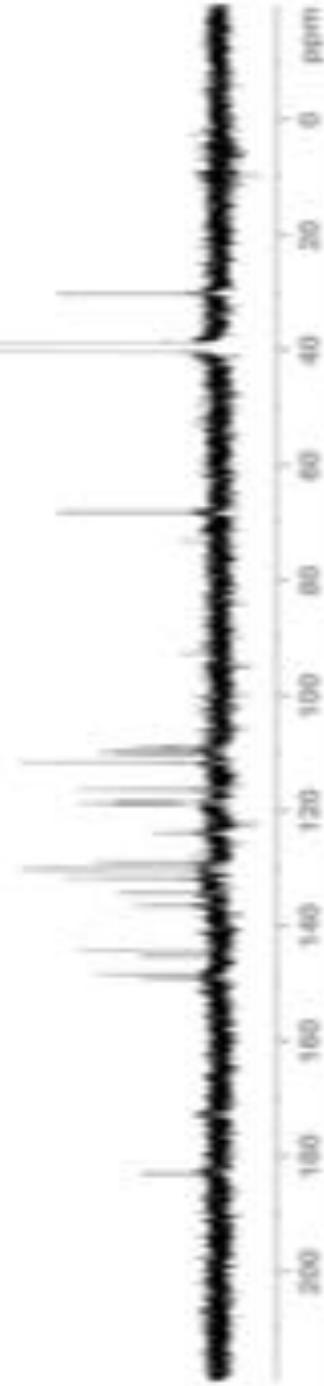
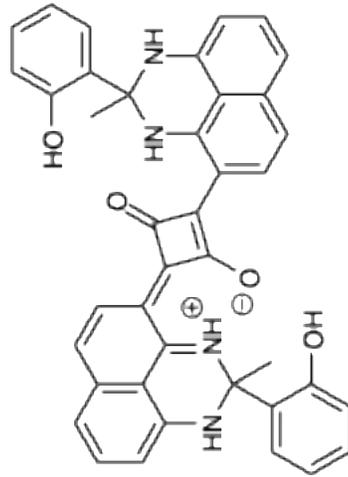
INSTRUM: spect
NAME: 88cartbon
EXPTNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_ 20231220
Time 8.11
INSTRUM spect
PROBHD 5 mm PABBY 4B-
PULPROG zgpg30
VS 3214
SOLVENT DMSO
NS 4
DS 4
SWH 40036.461 MHz
F2 100.6251843 MHz
AQ 1.1651488 sec
RG 327.5
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.0000000 sec
SFO 500.1362995 MHz

===== CHANNEL F1 =====
NUC1 13C-6251843 MHz
PULP 13C
PC 0.15 sec
PLM1 43.0000000 W

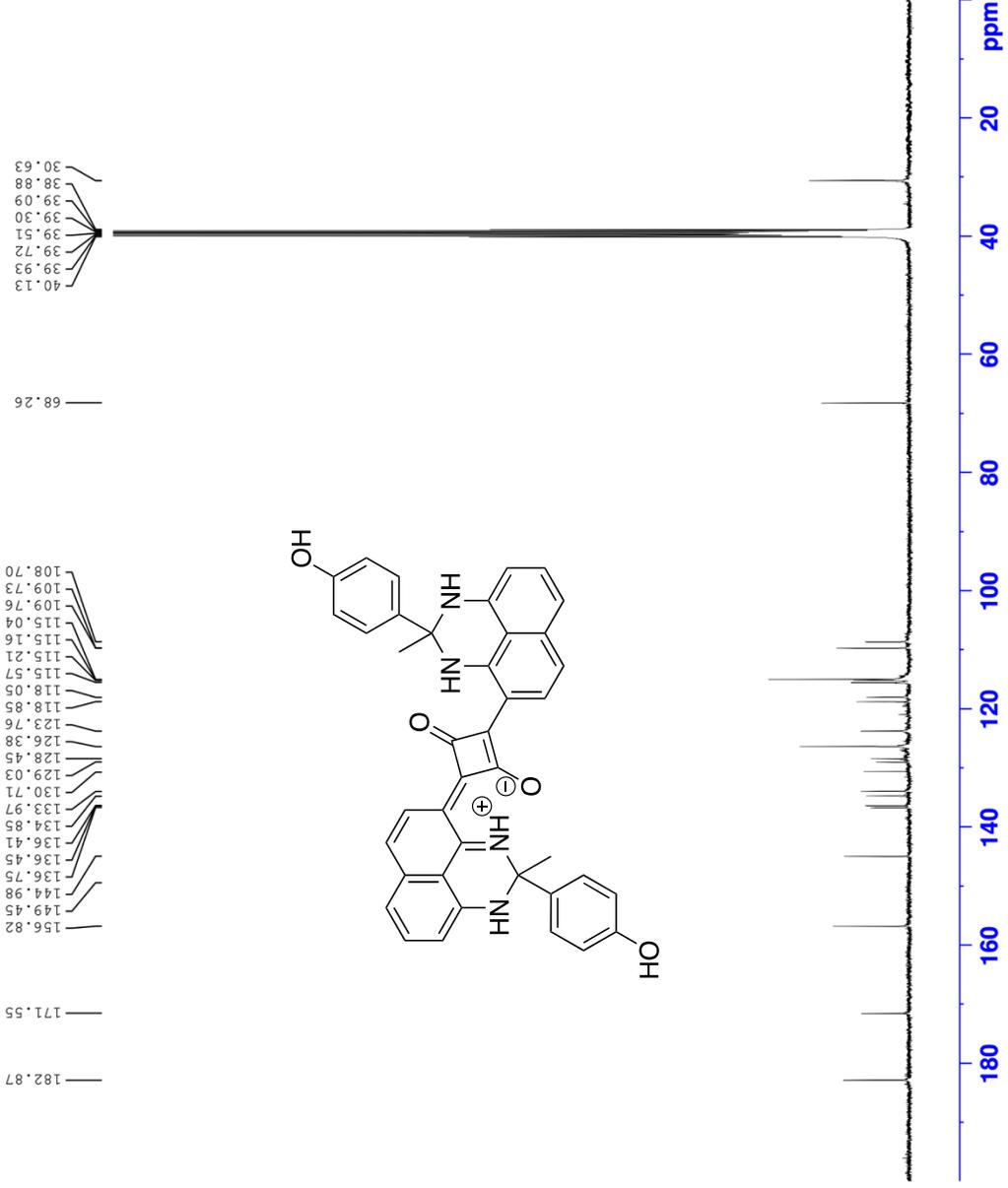
===== CHANNEL F2 =====
NUC2 1H-40036464 MHz
PULP 1H
PC 0.15 sec
PLM2 14.0000000 W
PCPD 0.1500000 W
PLM3 0.1500000 W
PLM4 0.1500000 W

F2 - Processing parameters
SI 32768
SF 100.6251843 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40





SS12carbon



Current Data Parameters
NAME SS12carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230326
Time_ 4.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15360
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 1290.2
DW 20.850 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

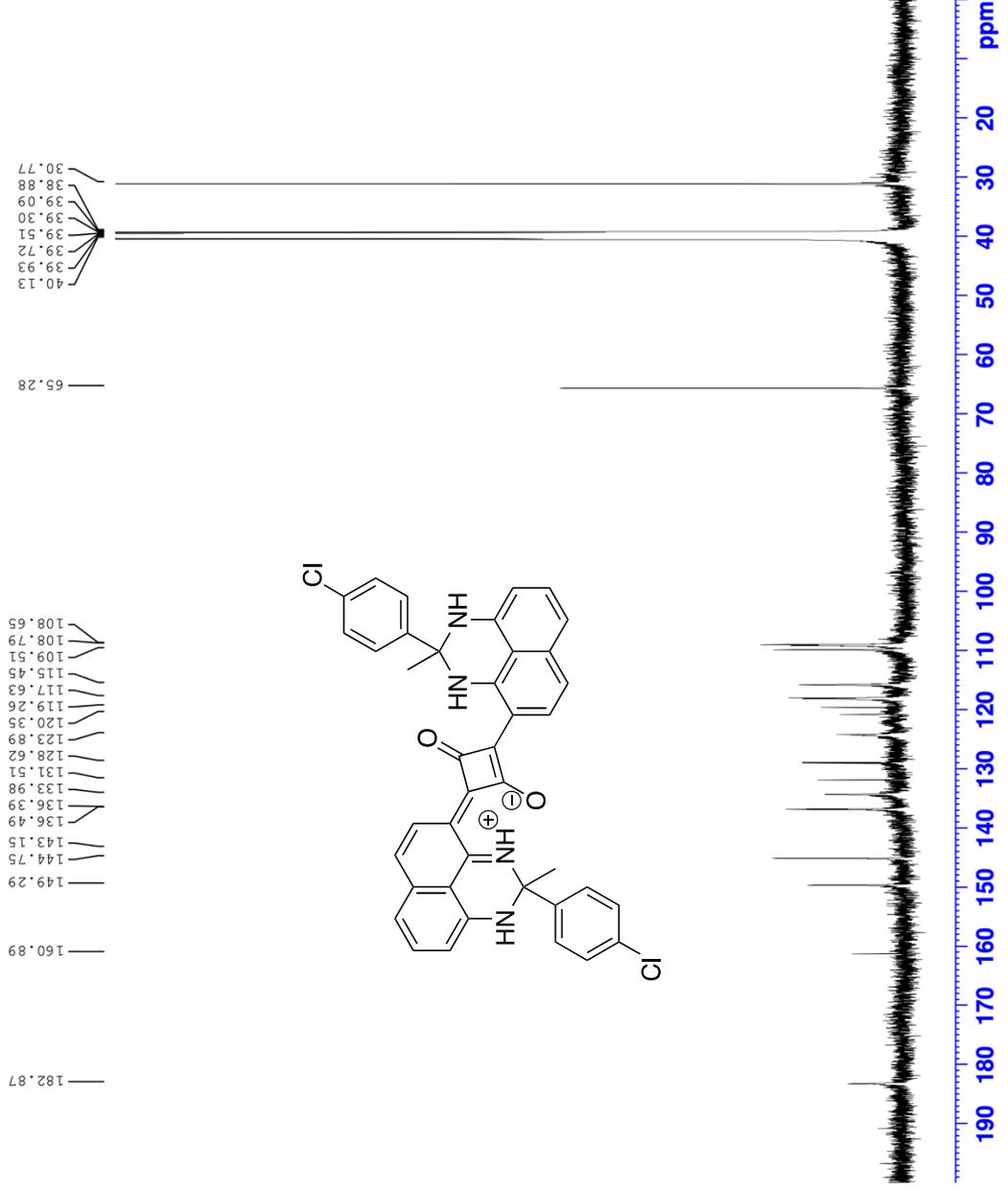
==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 3.00 dB
SFO1 100.6228298 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0 dB
PL12 19.17 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128158 MHz
EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



SS7carbon



Current Data Parameters
NAME SS6carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230306
Time 2.04
INSTRUM spect
PROBHD 5 mm FAPBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 12288
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6253441 MHz
NUC1 13C
P1 9.25 usec
PLW1 62.00000000 W

==== CHANNEL f2 =====
SFO2 400.1416006 MHz
NUC2 1H
CPDPRGf2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLWI2 0.36267000 W
PLWI3 0.29376000 W

F2 - Processing parameters
SI 32768
SF 100.6152830 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Reference: