

N-doped carbon quantum dots for the selective detection of OCl⁻ ion, bioimaging, and the production of Fe₃O₄ nanoparticles utilized in the synthesis of substituted imidazole

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S1 Quantum Yield Measurement:

Using quinine sulfate ($\phi = 0.54$ in $0.1\text{M H}_2\text{SO}_4$) as a standard reference, we determined the quantum yield of carbon dots. Using the following formula, the quantum yield was determined.

$$\Phi_{\text{CQD}} = \Phi_{\text{R}} \times \frac{I_{\text{CQD}}}{I_{\text{R}}} \times \frac{A_{\text{R}}}{A_{\text{CQD}}} \times \frac{\eta_{2\text{CQD}}}{\eta_{2\text{R}}}$$

The carbon dot and reference are denoted by CQD and R, respectively, in the equation above. " η " indicates the refractive index of the solvent medium (ethanol has a refractive index of 1.37), " I " stands for the integrated fluorescence intensity, and " A " for the absorbance value at the exciting wavelength. After calculating every value, the quantum Yield was found to be **40.5%**.

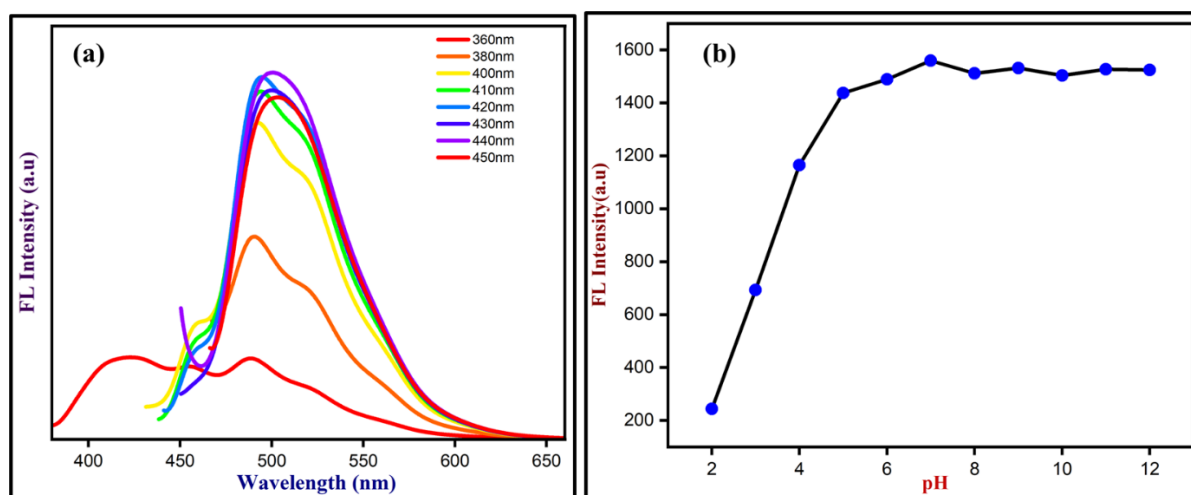


Figure S1. (a) represents the NCQD with different wavelengths, and (b) pH studies of the NCQD calibration plot of NCQD with varying concentrations of OCl^- ion ($0\text{--}8\mu\text{m}$).

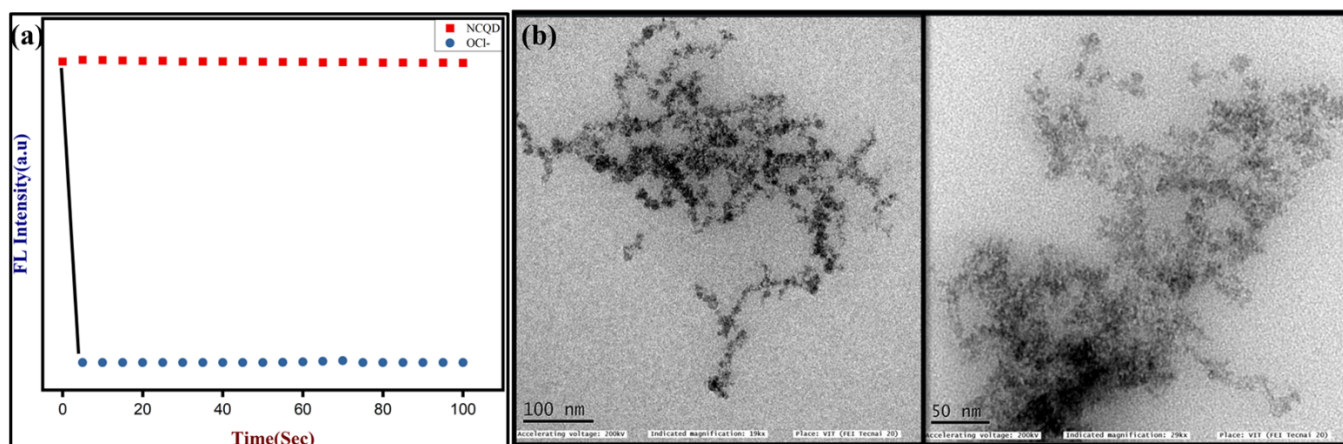


Figure S2. (a) Time response of NCQD with OCl^- , and (b) calibration plot of NCQD with different concentrations of OCl^- ion (0-8 μm).

Table S1: Comparison Table of different sensors for OCl^- detection:

Sensing Probe for OCl^-	Linear range (μm)	Lod (μm)	Ref.
CA and EDA/N-doped CQDs	1.0–10.0	0.43	[<i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , 279, 121456]
MoO_3 NPs-G-CDs	0.010–200	0.068	[<i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , 279, 121456]
Citric acid, GSH	0.1–0.8	0.016	[<i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , 242, 118721]
Red Pepper-based CQD	0.1 -300	0.06	[<i>Analyst</i> , 138(21), 6551-6557]
ammonium citrate and urea	10-150	1.82	[<i>Analytical and Bioanalytical Chemistry</i> , 414(8), 2651-2660]
L- Tartaric acid and o-phenylenediamine-based CQD	1-8	0.04	This work

Table S2: Comparison table of catalytic activity of Fe_3O_4 NPs for imidazole (4) Reaction:

Entry	Catalyst	Solvent	Temperature ($^{\circ}\text{C}$)	Time (min)	Yield (%)	Ref.
1	Cr_2O_3 nanoparticle	H_2O	MW, 200–500 W	6	97	[<i>Scientific Reports</i> , 12(1), 19942]

2	[P4-VP]-Fe ₃ O ₄	Solvent-free	100	35	91	[<i>Research on Chemical Intermediates</i> , 44, 6995-7011]
3	Cu ₂ O/ Fe ₃ O ₄ @guarana	EtOH	70	20	97	[<i>Inorganic Chemistry Communications</i> , 125, 108465]
4	Fe ₃ O ₄ /SiO ₂ /urea	EtOH	Reflux	50	90	[<i>Catalysis Communications</i> , 69, 29-33]
5	SA-MNPs	Dry petroleum ether	100, Microwave	35	88	[<i>Journal of Chemical Sciences</i> , 125, 835-841]
6	Fe ₃ O ₄ nanoparticles	Solvent-free	100	90	94	This Work

Table S3: Comparison table of catalytic activity of Fe₃O₄ NPs for imidazole (8) Reaction:

Entry	Catalyst	Solvent	Temperature (°C)	Time (min)	Yield (%)	Ref.
1	Ruthenium (II) catalyst	H ₂ O	100	5	66	[89(9), 6016-6026]
2	Iodine	EtOH	Reflux	60	80	[<i>Chinese Chemical Letters</i> , 20(1), 5-8]
3	TiO ₂	Solvent-free	120	45	88	[39(1), 142-154.]
	Fe₃O₄ nanoparticles	Solvent-free	110	100	88	This

free

Work

Table S4: Optimization table for substituted imidazole (4) Reaction:

Entry	Solvent	Nitrogen Source	Temp (°C)	Fe ₃ O ₄ (mol%)	Time(min)	Yield (%)
1	H ₂ O	NH ₄ OAc	100	3.3	90	45
2	DMF	NH ₄ OAc	100	3.3	90	Trace
3	Acetone	NH ₄ OAc	100	3.3	90	Trace
4	Acetonitrile	NH ₄ OAc	100	3.3	90	40
5	Toluene	NH ₄ OAc	100	3.3	90	20
6	EtOH	NH ₄ OAc	100	3.3	90	85
7	EtOH	NH ₄ OAc	100	3.3	90	80
8	THF	NH ₄ OAc	100	3.3	90	35
9	EtOH	NH ₄ OAc	100	3.3	90	75
10	EtOH	NH ₄ OAc	100	-	90	41
11	NEAT	NH ₄ OAc	100	-	90	40
12	NEAT	NH ₄ OAc	100	2	90	88
13	NEAT	NH ₄ OAc	100	4	90	96
14	NEAT	NH ₄ OAc	100	5	90	96
15	NEAT	NH₄OAc	100	3.3	90	96

Table S5: Optimization table for substituted imidazole (8) Reaction:

Entry	Solvent	Nitrogen Source	Temp (°C)	Fe ₃ O ₄ (mol%)	Time(min)	Yield (%)
1	THF	NH ₄ OAc	110	5	100	Trace
2	Acetone	NH ₄ OAc	110	5	100	20
3	H ₂ O	NH ₄ OAc	110	5	100	38
4	EtOH: H ₂ O	NH ₄ OAc	110	5	100	70
5	Acetonitrile	NH ₄ OAc	110	5	100	20
6	EtOH	NH ₄ OAc	110	5	100	78
7	EtOH	NH ₄ OAc	110	6	100	80
8	Toluene	NH ₄ OAc	110	5	100	35
9	EtOH	NH ₄ OAc	110	5	100	75
10	EtOH	NH ₄ OAc	110	-	100	39
11	NEAT	NH ₄ OAc	110	-	100	53
12	NEAT	NH ₄ OAc	110	4	100	82
13	NEAT	NH ₄ OAc	110	6	100	89
14	NEAT	NH ₄ OAc	110	5.5	100	88
15	NEAT	NH₄OAc	110	5	100	88

S2: Recyclability of Fe₃O₄ nanoparticles:

After the reaction was complete, the reaction mixture was allowed to cool to room temperature and moved to a centrifuge tube. After centrifuging for 10 minutes at 4000 RPM, the Fe₃O₄ NPs that had settled to the bottom of the reaction mixture were cleaned several times with water, ethanol, and acetone. They were then ground into a fine powder and allowed to dry in an oven. After that, the reactions were conducted using the catalyst once more till 4 cycles.

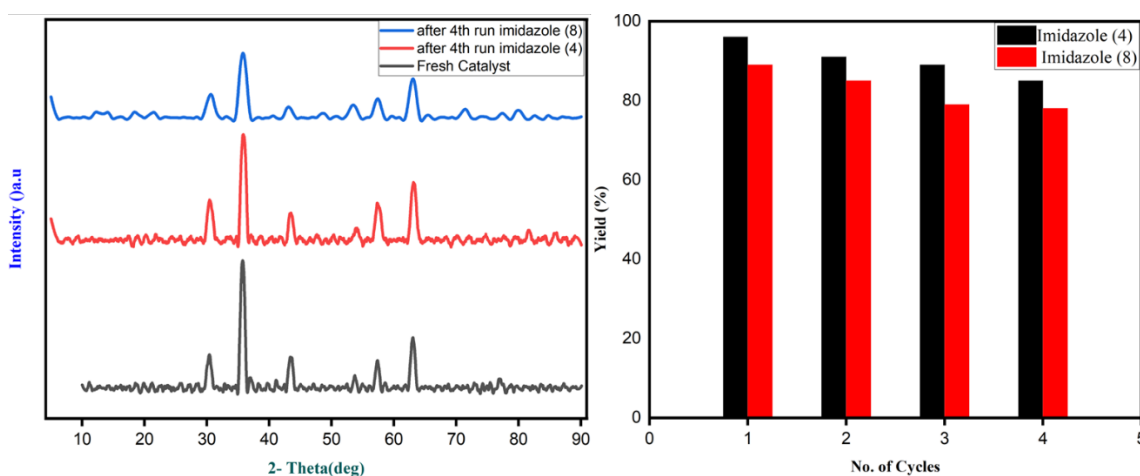


Figure S3: Recyclability study of the Fe₃O₄ NPs

S3: H¹ and C¹³ NMR analysis result of substituted Imidazole (4) Reaction:

1. 4,5-diphenyl-2-(p-tolyl)-1H-imidazole (4a): Off -White Powder. H¹ NMR (400 MHz, DMSO), δ (PPM) = 12.59 (s, 1H), 7.90 (d, J= Hz, 2H), 7.52 (m, 6H), 7.30 (t, 8 Hz, 6H), 2.36 (s, 3H). C13 NMR (100 MHz, CDCl₃) δ 21.39, 125.21, 126.48, 126.56, 127.37, 127.82, 128.17, 128.59, 129.59, 138.85, 146.21.
2. 4-(4,5-diphenyl-1H-imidazol-2-yl) benzonitrile (4f): white Powder. H¹ NMR (400 MHz, DMSO), δ (PPM) = 13.01 (s, 1H), 8.26 (d, J=8Hz, 2H), 7.96 (d, 8.4Hz, 2H), 7.56 (m, 4H), 7.49 (t, J=7.4Hz, 2H), 7.43(t, J= 8Hz, 1H), 7.34(t, J= 7.2Hz, 2H), 7.27 (t, J= 7.2Hz, 1H). C13 NMR (100 MHz, CDCl₃) δ 117.8, 118.69, 125.41, 127.84, 128.78, 132.76, 133.78.
3. 4,5-diphenyl-2-(o-tolyl)-1H-imidazole (4b): White powder. H¹ NMR (400 MHz, DMSO), δ (PPM) = 12.46 (s, 1H), 7.72 (t, J= 8.4 Hz, 1H), 7.56 (d, J= 7.2 Hz, 2H), 7.52 (d, J = 7.2 Hz, 2H), 7.45 (t, J= 7.2 Hz, 2H), 7.38 (m, 6H), 7.23 (t, J= 7.2 Hz, 1H), 2.64 (s, 3H). C13 NMR (100 MHz, CDCl₃) δ 21.19, 126.06, 127.76, 128.65, 128.87, 129.74, 131.35, 136.43, 146.31.
4. 2-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole (4c): White Powder. H¹ NMR (400 MHz, DMSO), δ (PPM) = 12.50 (s, 1H), 8.03 (d, J= 8.4Hz, 2H), 7.53 (d, J=8 Hz, 4H), 7.37 (s, 6H), 7.96 (d, J= 8.8 Hz, 2H), 3.82 (s, 3H). C13 NMR (100 MHz, CDCl₃) δ 55.39, 114.32, 122.73, 126.75, 127.37, 127.78, 128.61, 146.07, 160.21.
5. 2-(2-methoxyphenyl)-4,5-diphenyl-1H-imidazole(4d): white Powder. H¹ NMR (400 MHz, DMSO), δ (PPM) = 11.89 (s, 1H), 8.05 (m, 1H), 7.53 (m, 8H), 7.31 (t, J= 7.2 Hz, 2H), 7.23 (d, J= 8Hz, 1H), 7.18 (d, J= 8Hz, 1H), 7.09 (t, J= 7.2 Hz, 1H), 3.92 (s, 3H). C13 NMR (100 MHz, CDCl₃) δ 55.91, 111.21, 118.18, 121.71, 127.81, 128.66, 129.53, 144.65, 155.74.
6. 2-(4-nitrophenyl)-4,5-diphenyl-1H-imidazole (4e): Yellow Powder. H¹ NMR (400 MHz, DMSO), δ (PPM) = 13.16 (s, 1H), 8.37 (m, 4H), 7.57 (m, 4H), 7.49 (t, J= 8 Hz, 2H), 7.43 (d, J= 6.8 Hz, 1H), 7.35 (t, J= 7.2 Hz, 2H), 7.28 (t, J= 8Hz, 1H). C13 NMR (100 MHz, CDCl₃) δ 124.41, 125.51, 127.88, 128.01, 128.77, 135.52, 143.47, 147.41.
7. 4-(4,5-diphenyl-1H-imidazol-2-yl) benzonitrile (4f), white powder. H¹ NMR (400 MHz, DMSO), δ (PPM) = 13.01 (s, 1H), 8.26 (d, j= 8 Hz, 2H), 7.96 (d, J= 8.4 Hz, 2H), 7.56 (m, 4H), 7.49 (t, J= 7.2 Hz), 7.43 (d, J= 7.2 Hz, 1H), 7.34 (t, J= 8Hz, 2H), 7.27 (t, J= 7.2 Hz, 1H). C13 NMR (100 MHz, CDCl₃) δ
8. 1-(4,5-diphenyl-1H-imidazol-2-yl) naphthalen-2-ol (4g): Yellow Powder. H¹ NMR (400 MHz, DMSO), δ (PPM)= 12.5-11.5 (2H), 8.19 (d, J= 8Hz, 1H), 7.91 (t, J= 8.8Hz, 2H), 7.57 (d, J=

7.2Hz, 4H), 7.51 (t, $J=7.6$ Hz, 1H), 7.41 (m, 5H), 7.34 (m, 3H). C13 NMR (100 MHz, CDCl_3) δ 115.87, 116.09, 126.24, 127.21, 127.55, 127.80, 128.65, 145.18, 161.89.

9. 2-(4-fluorophenyl)-4,5-diphenyl-1H-imidazole (4h), Brown solid. H^1 NMR (400 MHz, DMSO), δ (PPM) = 12.69 (s, 1H), 8.14 (m, 2H), 7.55 (d, $J=7.2$ Hz, 2H), 7.51 (t, $J=8$ Hz, 2H), 7.47 (t, $J=7.2$ Hz, 2H), 7.40 (d, $J=7.2$ Hz, 1H), 7.35 (m, 4H), 7.24 (t, $J=7.6$ Hz, 1H). 2-(5-methylfuran-2-yl)-4,5-diphenyl-1H-imidazole (4i): brown powder. H^1 NMR (400 MHz, DMSO), δ (PPM) = 12.68 (s, 1H), 7.52 (t, $J=7.8$ Hz, 2H), 7.48 (d, $J=6.8$ Hz, 2H), 7.44 (t, $J=7.2$ Hz, 2H), 7.37 (t, $J=4.8$ Hz, 1H), 7.31 (t, $J=7.2$ Hz, 2H), 7.23 (t, $J=7.2$ Hz, 1H), 6.86 (d, $J=4$ Hz, 1H), 6.25 (t, $J=4$ Hz, 1H), 2.38 (s, 3H).

10. 2-(4,5-diphenyl-1H-imidazol-2-yl)-6-methoxy phenol (4j): white powder. H^1 NMR (400 MHz, DMSO), δ (PPM) = 13.05 (s, 1H), 13.01 (s, 1H), 7.65 (t, $J=4$ Hz, 1 H), 7.54 (m, 5H), 7.47 (t, $J=6.8$ Hz, 2H), 7.37 (t, $J=7.6$ Hz, 2H), 7.29 (t, $J=7.2$ Hz, 1H), 7.00 (d, $J=8$ Hz, 1H), 6.90 (t, $J=8$ Hz, 1H), 3.82 (s, 3H). C13 NMR (100 MHz, CDCl_3) δ 56.15, 112.07, 112.95, 115.59, 118.84, 127.72, 128.74, 145.54, 147.02, 148.89.

11. 2-(3-phenoxyphenyl)-4,5-diphenyl-1H-imidazole (4k): white powder. H^1 NMR (400 MHz, DMSO), δ (PPM) = 12.74 (s, 1H), 7.90 (d, $J=8$ Hz 1H), 7.78 (t, $J=4$ Hz, 1H), 7.75 (m, 4H), 7.45 (m, 5H), 7.31 (t, $J=7.2$ Hz, 2H), 7.24 (t, $J=7.2$ Hz, 1H), 7.18 (t, $J=7.6$ Hz, 1H), 7.08 (d, $J=7.6$ Hz, 2H), 7.04 (m, 1H), C13 NMR (100 MHz, CDCl_3) δ 115.64, 118.96, 119.32, 120.24, 123.48, 127.82, 128.74, 129.87, 130.38, 131.38, 131.69, 157.08, 157.80.

S4: H^1 NMR analysis result of imidazole (8):

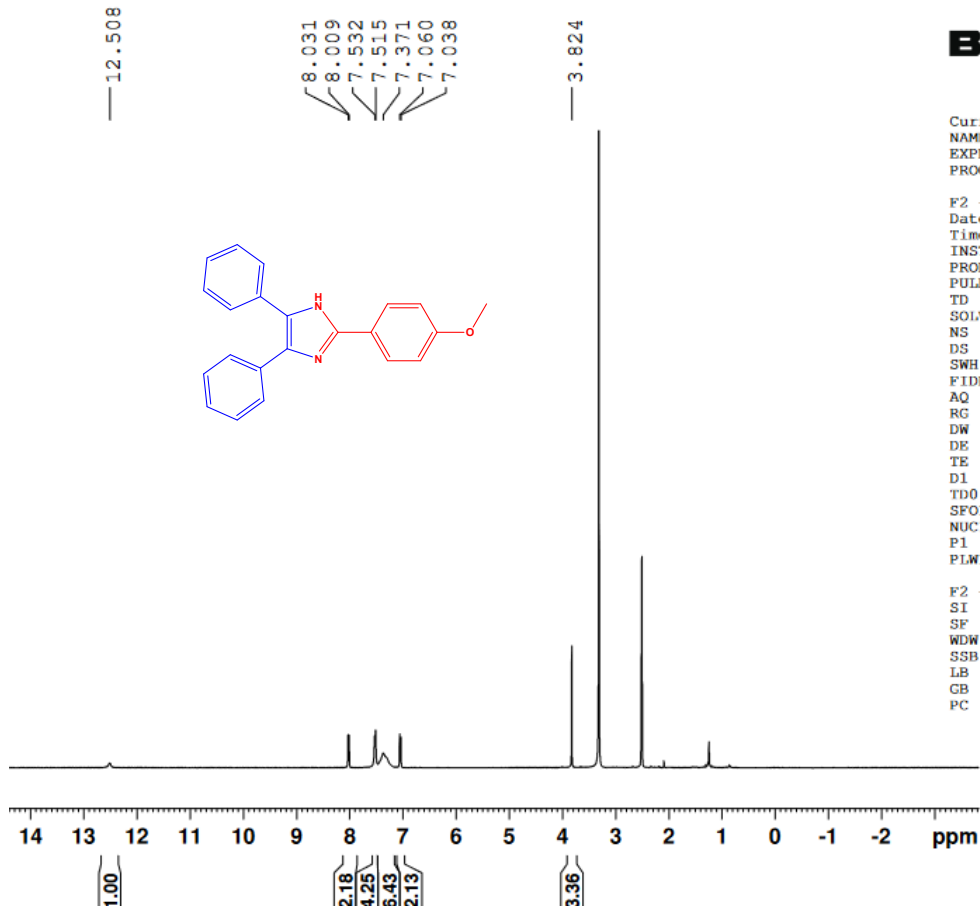
1. 2-(3-methoxyphenyl)-1H-phenanthro[9,10-d] imidazole (8a): yellow solid. H^1 NMR (400 MHz, DMSO), δ (PPM) = 13.42 (s, 1H), 8.89 (m, 2H), 8.61 (m, 2H), 7.92 (t, $J=8$ Hz, 2H), 7.78 (m, 2H), 7.67 (m, 2H), 7.54 (t, $J=8$ Hz, 1H), 7.09 (m, 1H), 3.93 (s, 3H). C13 NMR (100 MHz, CDCl_3) δ

2. 2-(4-ethoxy phenyl)-1H-phenanthro[9,10-d] imidazole (8b): light brown powder. H^1 NMR (400 MHz, DMSO), δ (PPM) = 13.29 (s, 1H), 8.86 (d, $J=8$ Hz, 2H), 8.56 (s, 2H), 8.25 (d, $J=8.8$ Hz, 2H), 7.75 (t, $J=6.8$ Hz, 2H), 7.64 (m, 2H), 7.16 (d, $J=8.8$ Hz, 2H), 4.16 (m, 2H), 1.40 (t, $J=6.8$ Hz, 3H). C13 NMR (100 MHz, CDCl_3) δ

3. 2-(3-fluorophenyl)-1H-phenanthro[9,10-d] imidazole (8c): yellow solid. H^1 NMR (400 MHz, DMSO), δ (PPM) = 13.54 (s, 1H), 8.89 (m, 2H), 8.61 (d, $J=7.8$ Hz, 1H), 8.55 (d, $J=8$ Hz, 1H), 8.19 (d, $J=8$ Hz, 1H), 8.12 (t, $J=8.4$ Hz, 1H), 7.79 (m, 2H), 7.68 (m, 3H), 7.36 (m, 3H). C13 NMR (100 MHz, CDCl_3) δ

4. 2-(2-ethoxy phenyl)-1H-phenanthro[9,10-d] imidazole (8d): ^1H NMR (400 MHz, CDCl_3), δ (PPM) = 11.40 (s, 1H), 8.80 (m, 4H), 7.87 (d, $J=8\text{ Hz}$, 1H), 7.73 (t, $J=6.8\text{ Hz}$, 1H), 7.63 (t, $J=7.2$, 3H), 7.38 (m, 1H), 7.19 (t, $J=7.6\text{ Hz}$, 1H), 7.04 (d, $J=8\text{ Hz}$, 1H), 4.35 (m, 2H), 1.76 (t, $J=7.2\text{ Hz}$, 3H).
5. 2-(4-chlorophenyl)-1H-phenanthro[9,10-d] imidazole (8e): white solid. ^1H NMR (400 MHz, DMSO), δ (PPM) = 13.54 (s, 1H), 8.86 (s, 2H), 8.56 (s, 2H), 8.34 (d, $J=8.8\text{ Hz}$), 7.75 (m, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ
6. 2-(naphthalen-1-yl)-1H-phenanthro[9,10-d] imidazole (8f): Yellow Powder. ^1H NMR (400 MHz, DMSO), δ (PPM) = 13.66 (s, 1H), 9.20 (d, $J=8.4\text{ Hz}$, 1H), 8.90 (d, $J=6.8\text{ Hz}$, 2H), 8.65 (s, 1H), 8.59 (s, 1H), 8.15 (t, $J=7.6\text{ Hz}$, 2H), 8.09 (d, $J=8\text{ Hz}$, 1H), 7.78 (m, 3H), 7.70 (m, 4H). ^{13}C NMR (100 MHz, CDCl_3) δ

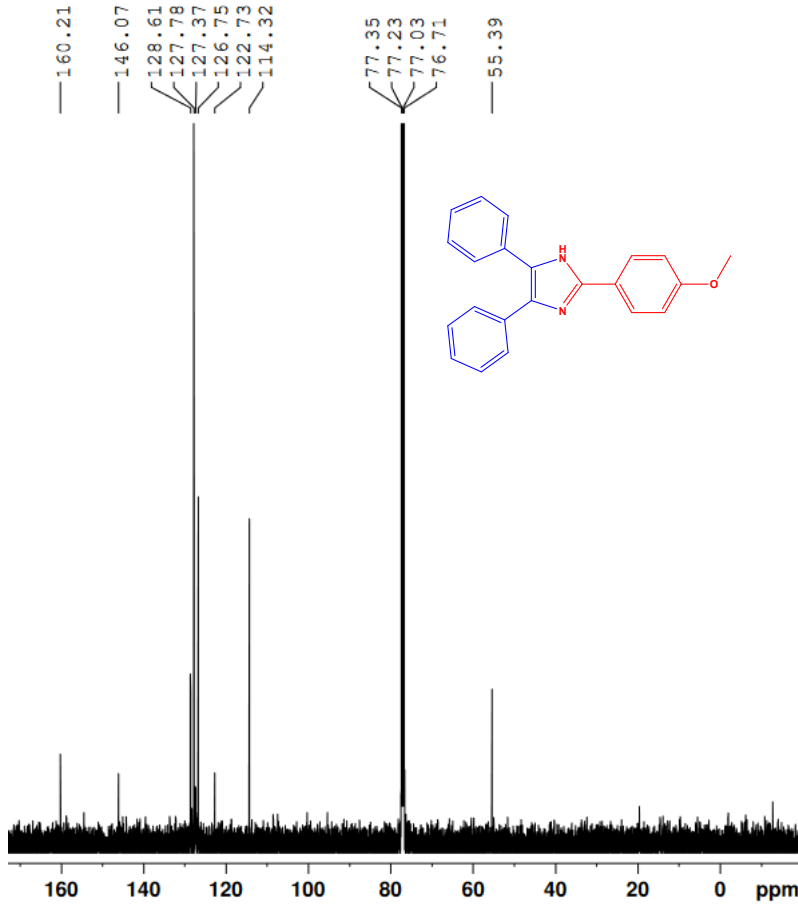
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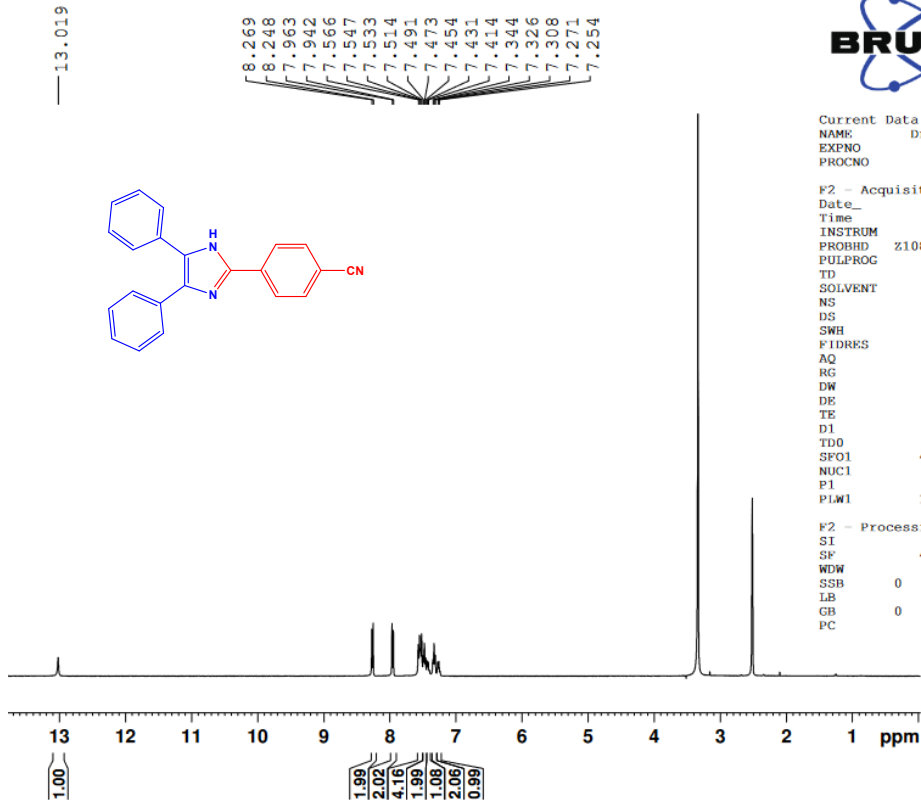
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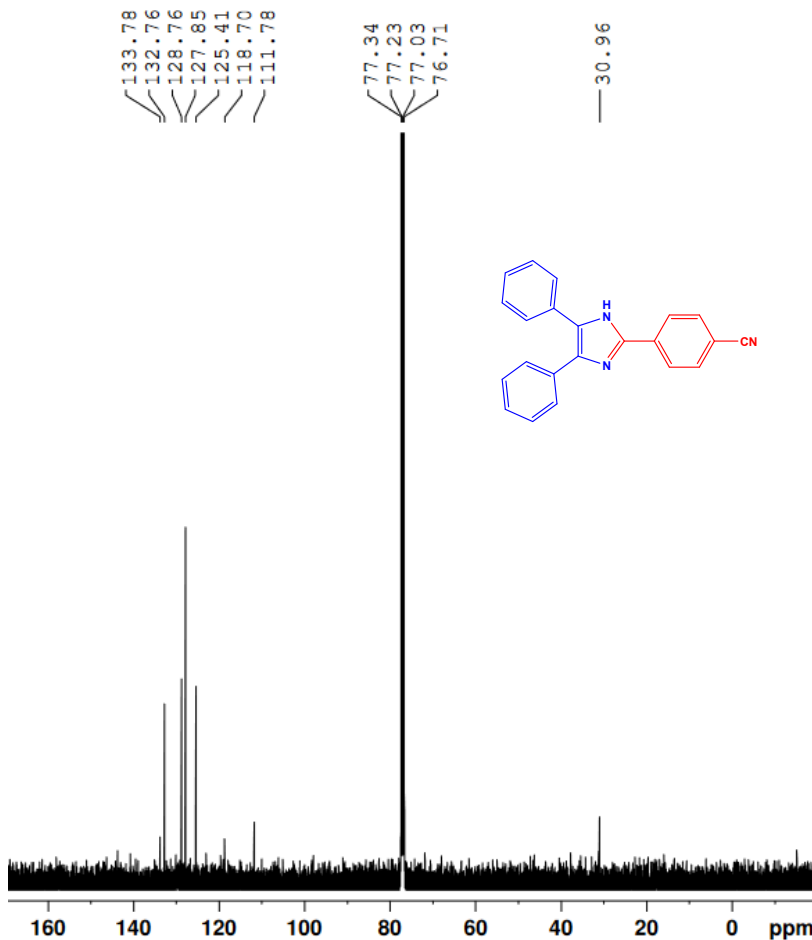
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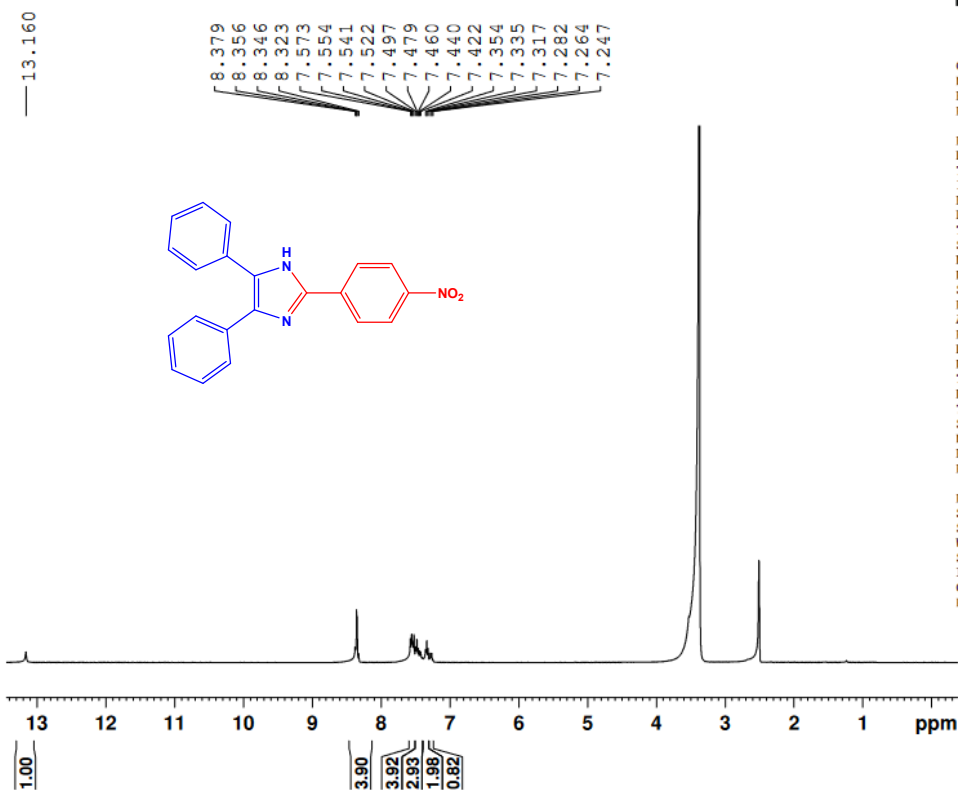
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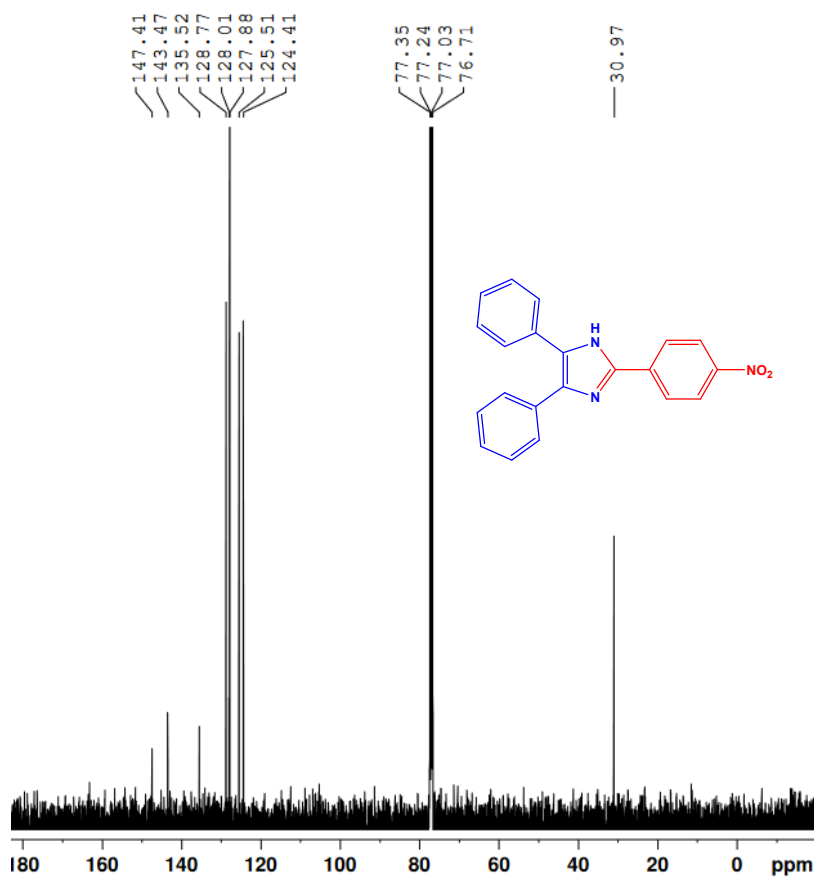
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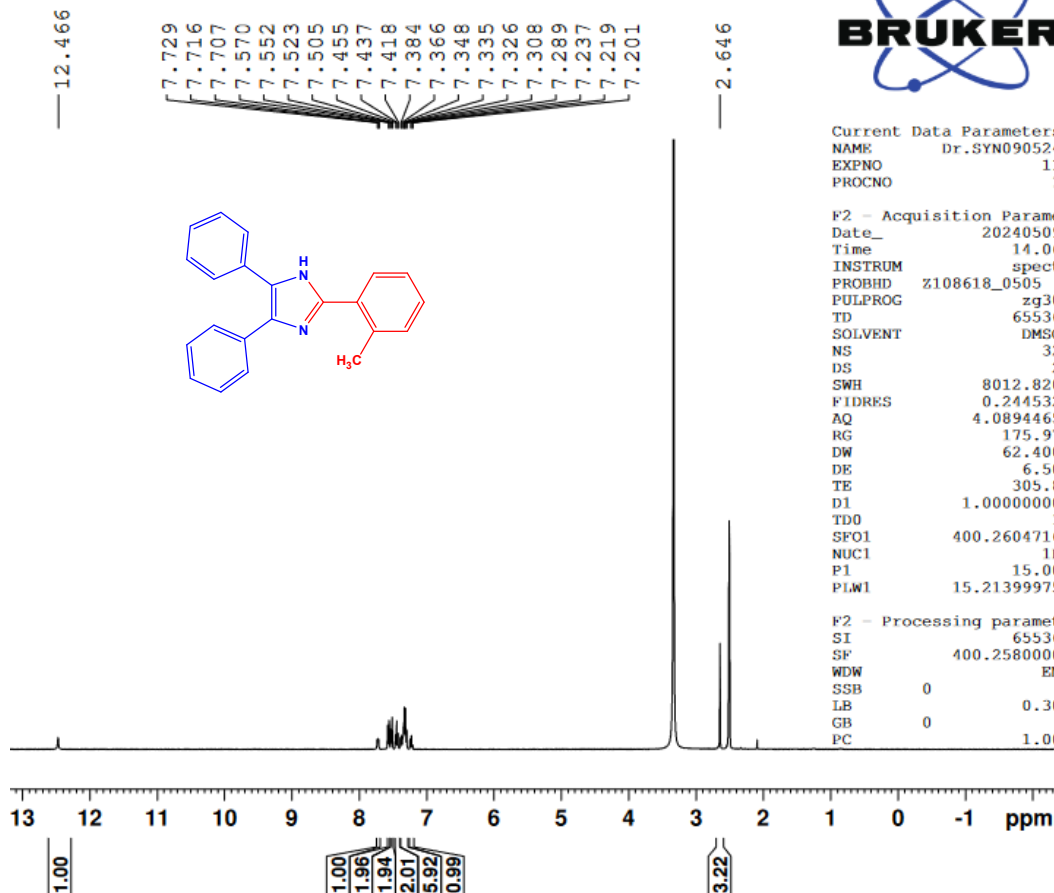
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Current Data Parameters
 NAME Dr.SYN230924
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240924
 Time 1.53 h
 INSTRUM spect
 PROBHD Z108618_0505 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 88.69
 DW 20.800 usec
 DE 6.50 usec
 TE 302.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1
 SFO1 100.6550186 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 56.49300003 W
 SFO2 400.2596010 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.21399975 W
 PLW12 0.42261001 W
 PLW13 0.21257000 W

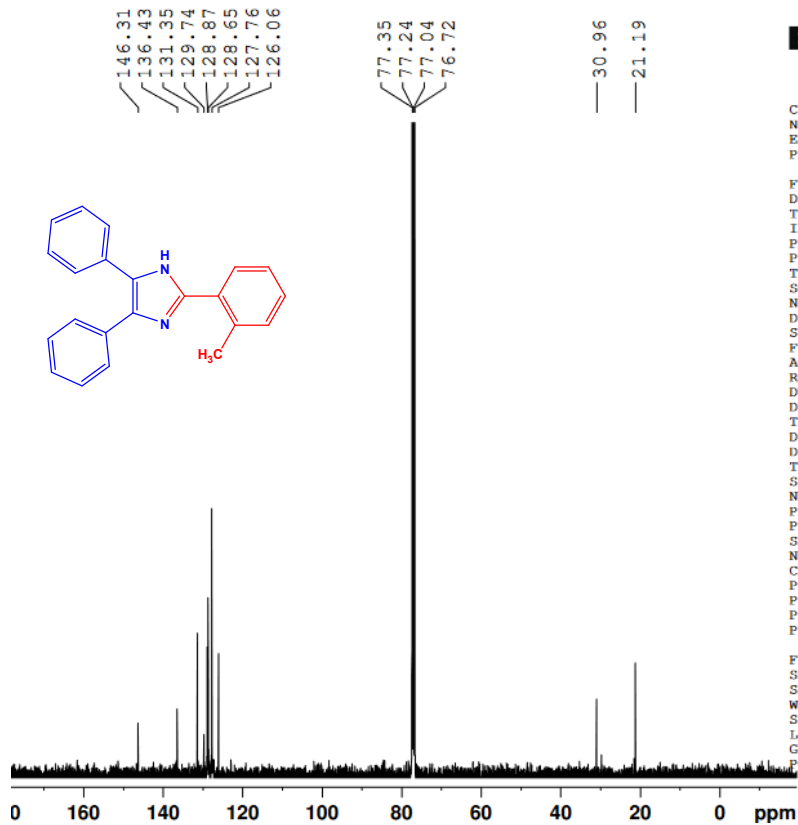
F2 - Processing parameters
 SI 32768
 SF 100.6449542 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME Dr.SYN090524
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240509
 Time 14.06 h
 INSTRUM spect
 PROBHD Z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 175.97
 DW 62.400 usec
 DE 6.50 usec
 TE 305.8 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

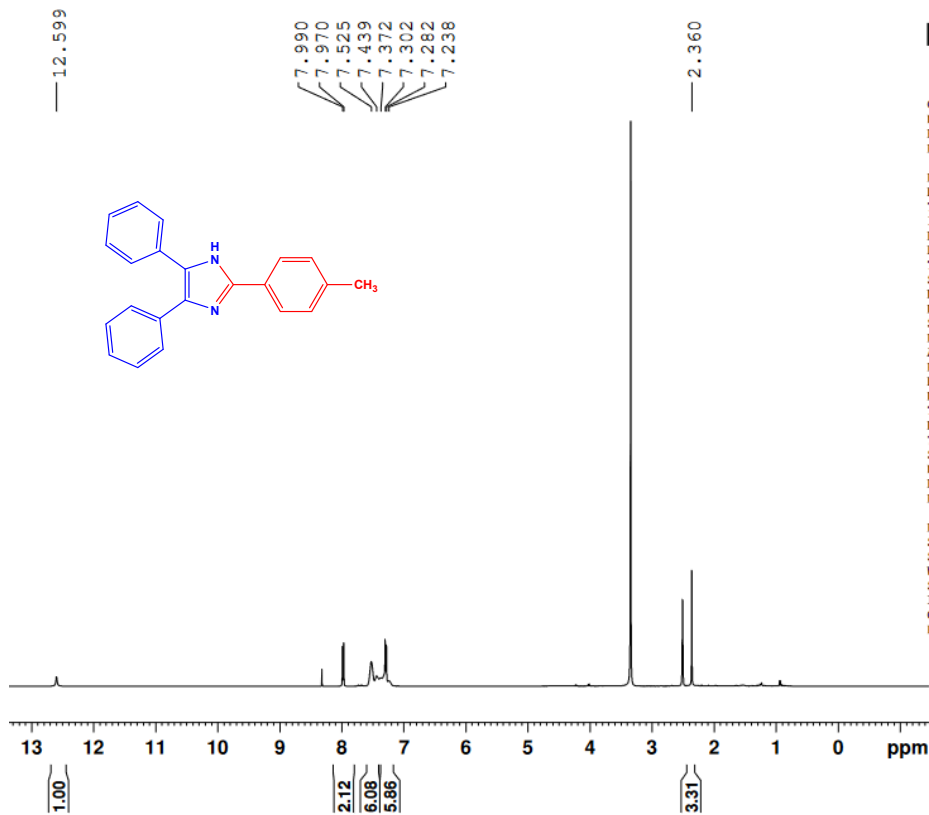
F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME: Dr.SYN230924
 EXPNO: 21
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20240924
 Time: 2.25 h
 INSTRUM: spect
 PROBHD: Z108618_0505 ()
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 512
 DS: 4
 SWH: 24038.461 Hz
 FIDRES: 0.733596 Hz
 AQ: 1.3631488 sec
 RG: 175.97
 DW: 20.800 usec
 DE: 6.50 usec
 TE: 302.4 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 TDO: 1
 SFO1: 100.6550186 MHz
 NUC1: 13C
 P1: 10.00 usec
 PLW1: 56.49300003 W
 SFO2: 400.2596010 MHz
 NUC2: 1H
 CPDPRG[2]: waltz16
 PCPD2: 90.00 usec
 PLW2: 15.21399975 W
 PLW12: 0.42261001 W
 PLW13: 0.21257000 W

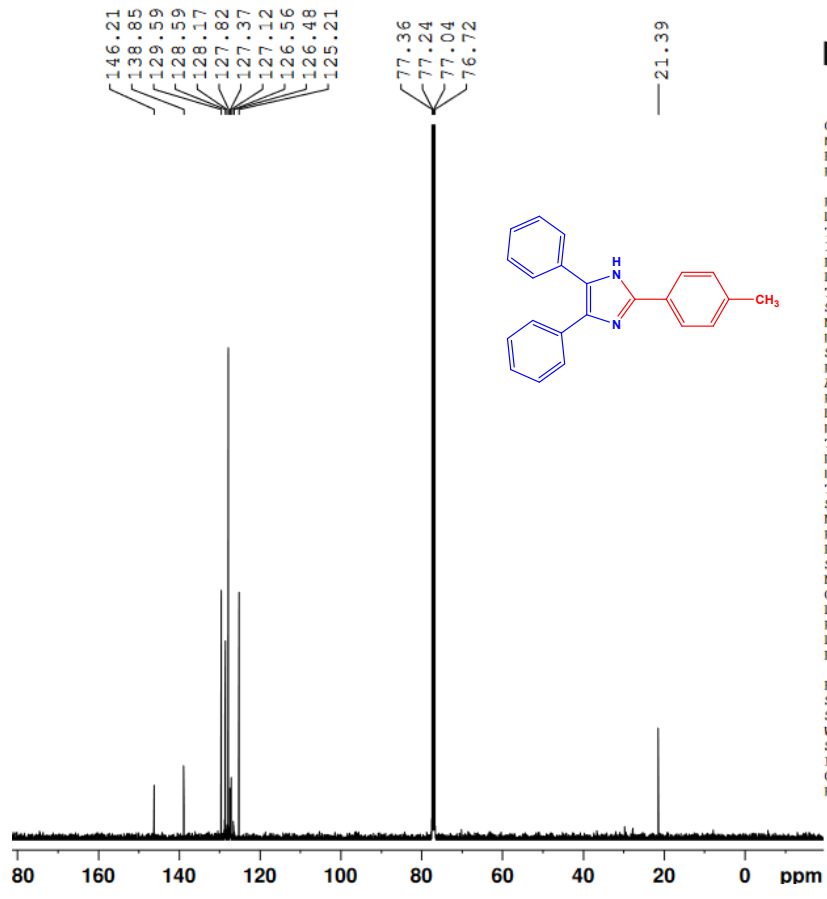
F2 - Processing parameters
 SI: 32768
 SF: 100.6449542 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40



Current Data Parameters
 NAME: Dr.SYN140524
 EXPNO: 19
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20240514
 Time: 13.16 h
 INSTRUM: spect
 PROBHD: Z108618_0505 ()
 PULPROG: zg30
 TD: 65536
 SOLVENT: DMSO
 NS: 64
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.244532 Hz
 AQ: 4.0894465 sec
 RG: 143.73
 DW: 62.400 usec
 DE: 6.50 usec
 TE: 303.7 K
 D1: 1.00000000 sec
 TDO: 1
 SFO1: 400.2604716 MHz
 NUC1: 1H
 P1: 15.00 usec
 PLW1: 15.21399975 W

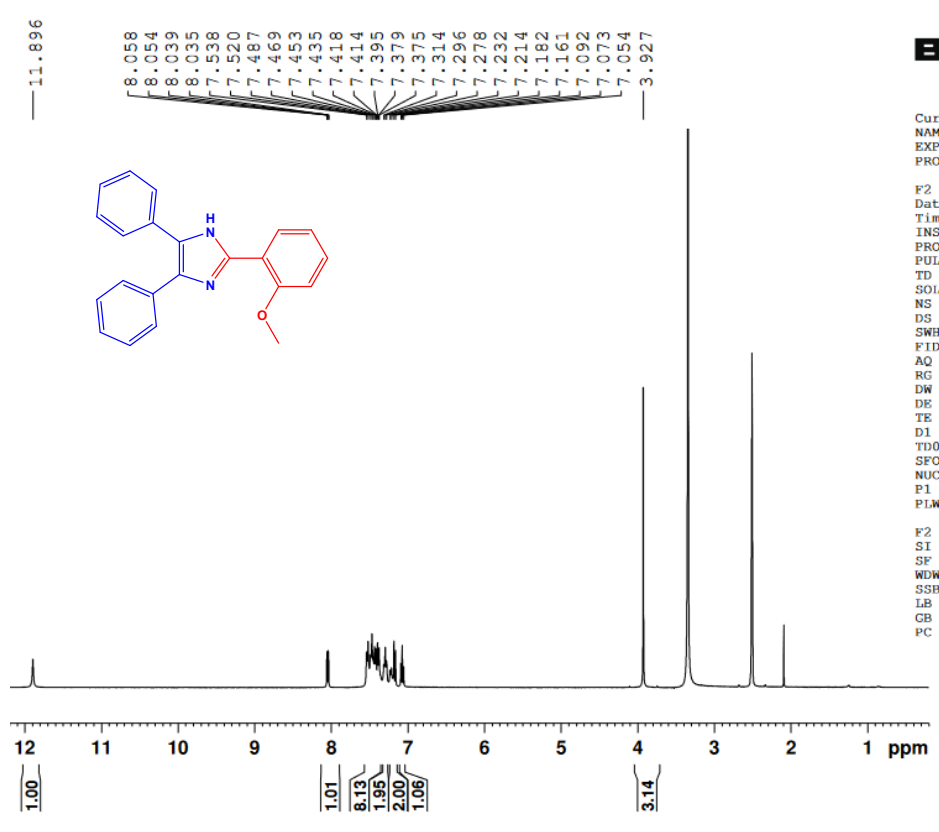
F2 - Processing parameters
 SI: 65536
 SF: 400.2580000 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00



Current Data Parameters
 NAME: Dr.SYN280924
 EXPNO: 36
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20240929
 Time: 5.33 h
 INSTRUM: spect
 PROBHD: Z108618_0505 (
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 512
 DS: 4
 SWH: 24038.461 Hz
 FIDRES: 0.733596 Hz
 AQ: 1.3631488 sec
 RG: 175.97
 DW: 20.800 usec
 DE: 6.50 usec
 TE: 302.8 K
 D1: 2.0000000 sec
 D11: 0.0300000 sec
 TD0: 1
 SFO1: 100.6550186 MHz
 NUC1: 13C
 P1: 10.00 usec
 PLW1: 56.4930003 W
 SFO2: 400.2596010 MHz
 NUC2: 1H
 CPDPRG[2]: waltz16
 PCPD2: 90.00 usec
 PLW2: 15.21399975 W
 PLW12: 0.42261001 W
 PLW13: 0.21257000 W

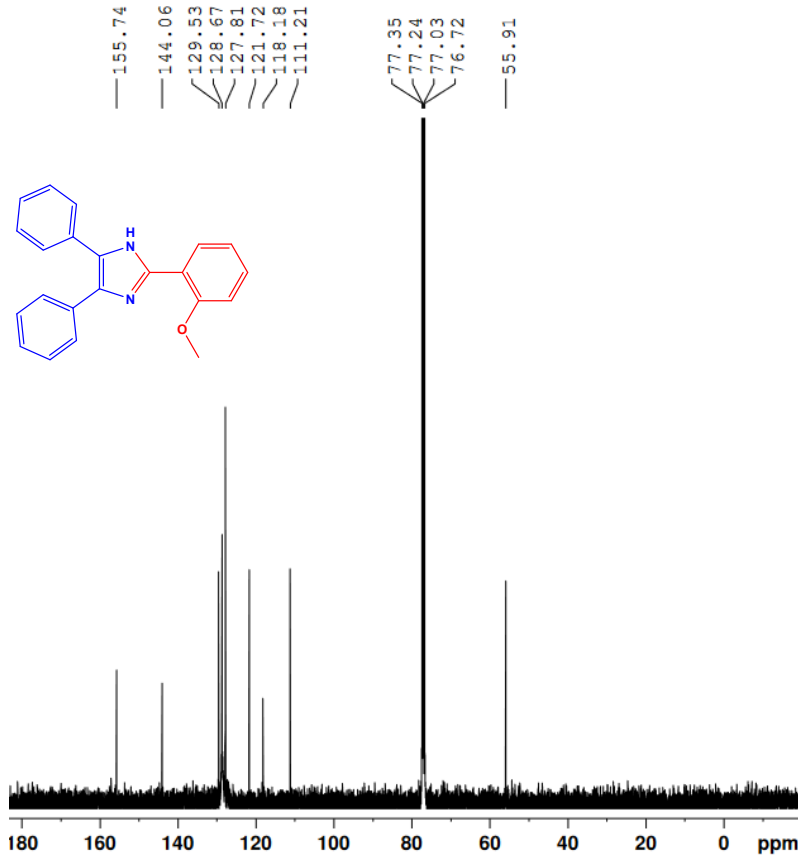
F2 - Processing parameters
 SI: 32768
 SF: 100.6449542 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40



Current Data Parameters
 NAME: Dr.SYN140524
 EXPNO: 20
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20240514
 Time: 13.23 h
 INSTRUM: spect
 PROBHD: Z108618_0505 (
 PULPROG: zg30
 TD: 65536
 SOLVENT: DMSO
 NS: 64
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.244532 Hz
 AQ: 4.0894465 sec
 RG: 156.91
 DW: 62.400 usec
 DE: 6.50 usec
 TE: 303.7 K
 D1: 1.0000000 sec
 TD0: 1
 SFO1: 400.2604716 MHz
 NUC1: 1H
 P1: 15.00 usec
 PLW1: 15.21399975 W

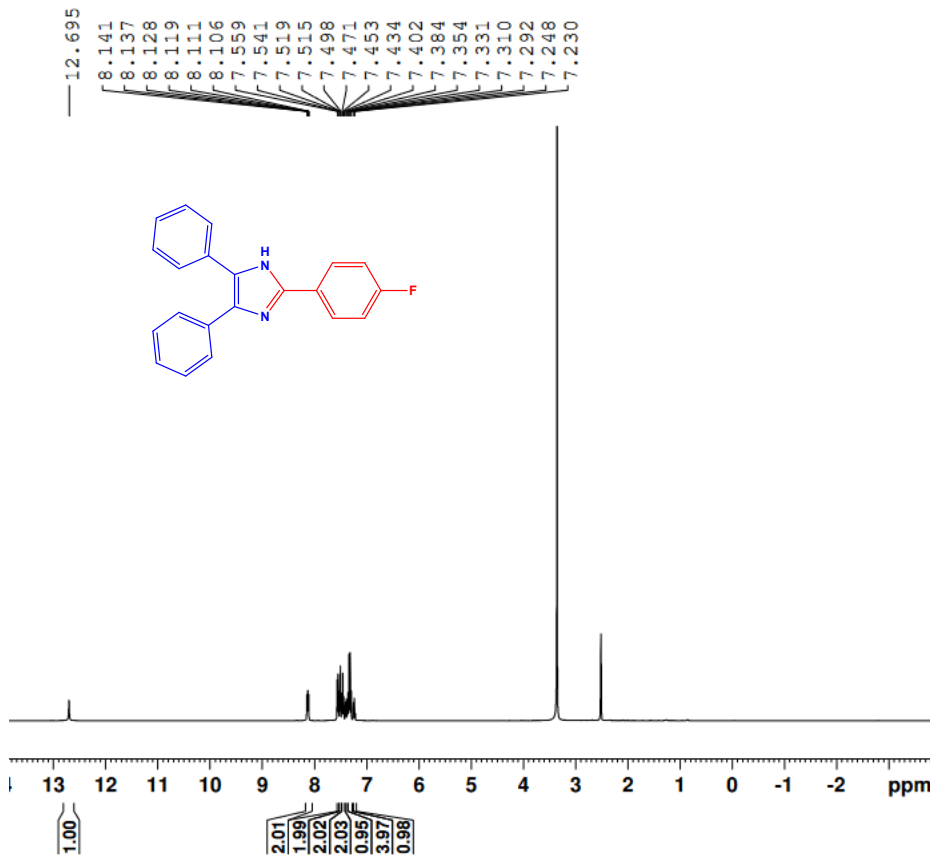
F2 - Processing parameters
 SI: 65536
 SF: 400.2580000 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00



Current Data Parameters
 NAME Dr.SYNI21024
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20241013
 Time 11.38 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 199.6
 DW 20.800 usec
 DE 6.50 usec
 TE 304.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6550186 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 56.49300003 W
 SFO2 400.2596010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 15.21399975 W
 PLW12 0.42261001 W
 PLW13 0.21257000 W

F2 - Processing parameters
 SI 32768
 SF 100.6449542 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



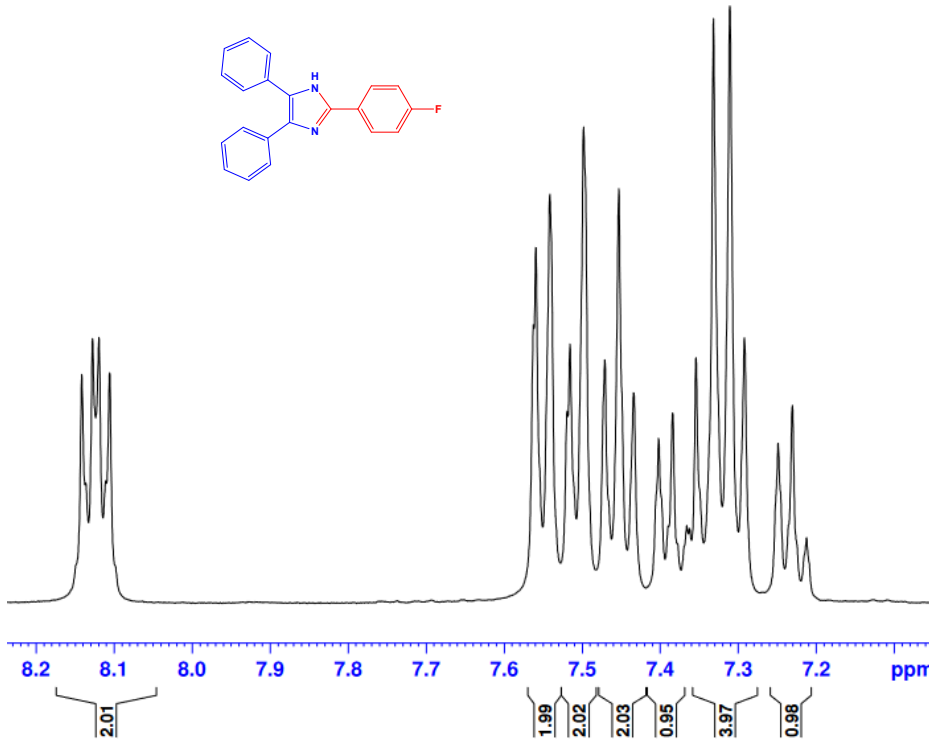
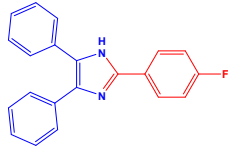
Current Data Parameters
 NAME Dr.SYNI70524
 EXPNO 23
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240517
 Time 15.42 h
 INSTRUM spect
 PROBHD Z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 143.73
 DW 62.400 usec
 DE 6.50 usec
 TE 304.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.141
8.137
8.128
8.119
8.111
8.106

7.559
7.541
7.519
7.515
7.498
7.471
7.433
7.434
7.402
7.384
7.354
7.331
7.310
7.292
7.248
7.230
7.212



Current Data Parameters
NAME Dr.SYN170524
EXPNO 23
PROCNO 1

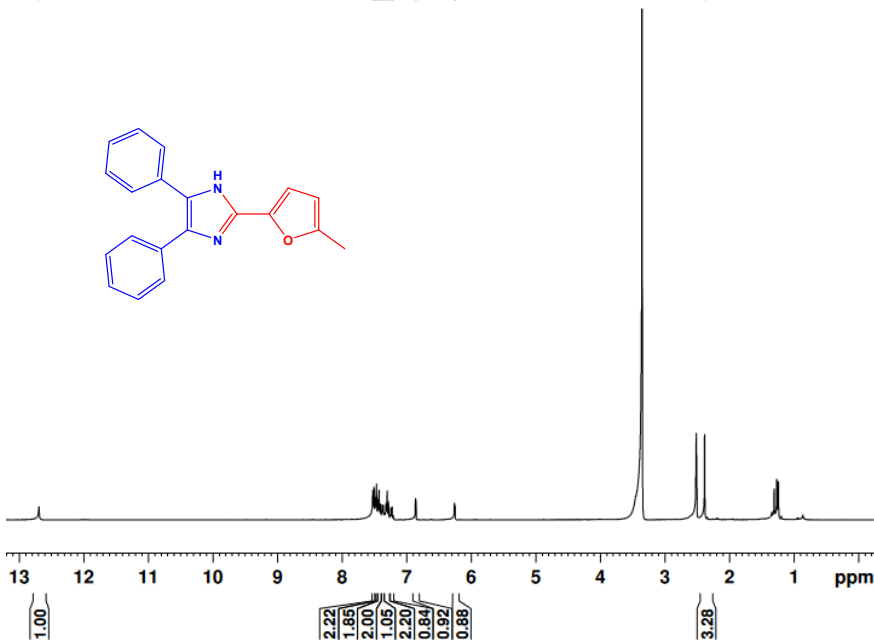
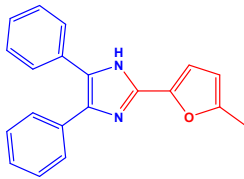
F2 - Acquisition Parameters
Date_ 20240517
Time 15.42 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 304.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

12.688

7.524
7.521
7.503
7.482
7.464
7.441
7.423
7.404
7.376
7.365
7.358
7.316
7.298
7.279
7.240
7.222
7.203
6.861
6.853
6.257
6.255
6.249

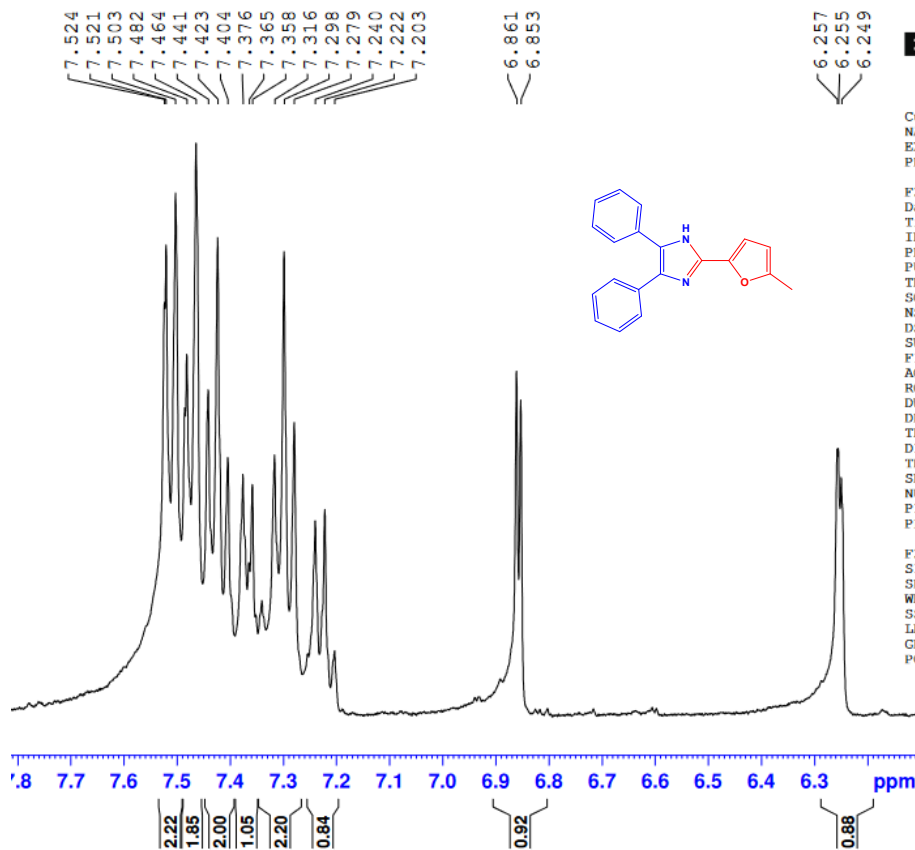
2.380



Current Data Parameters
NAME Dr.SYN210524
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240521
Time 15.13 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 303.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

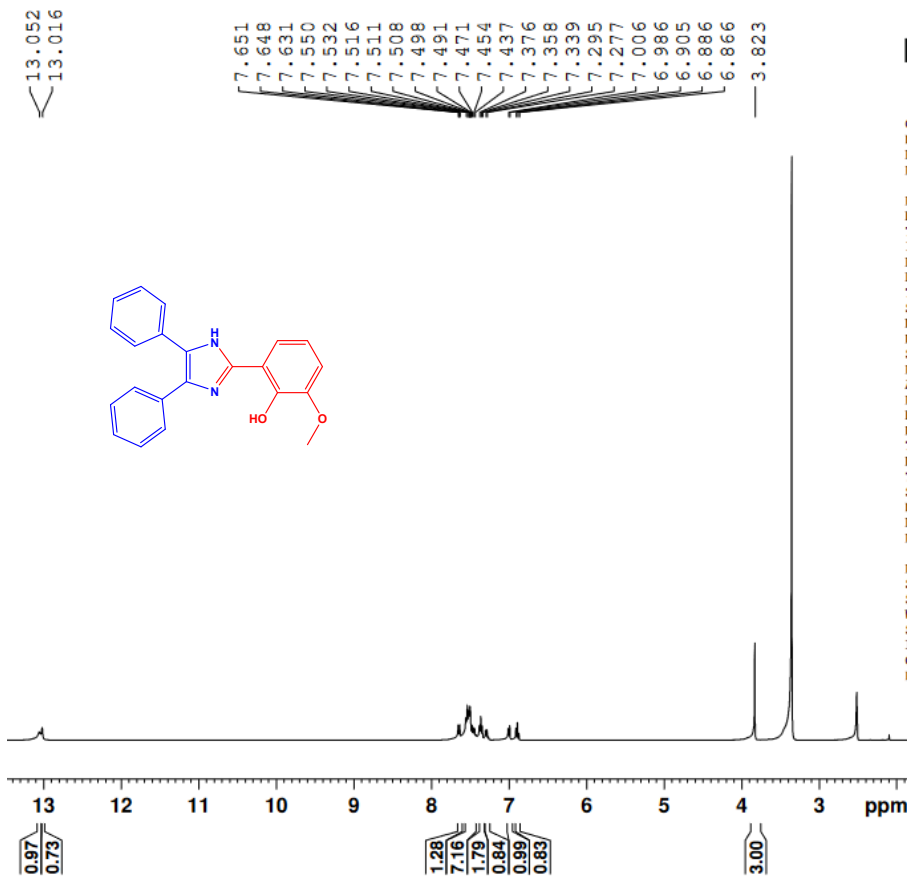
F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Dr.SYN210524
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240521
Time 15.13 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 303.5 K
D1 1.00000000 sec
TD0 1
SF01 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

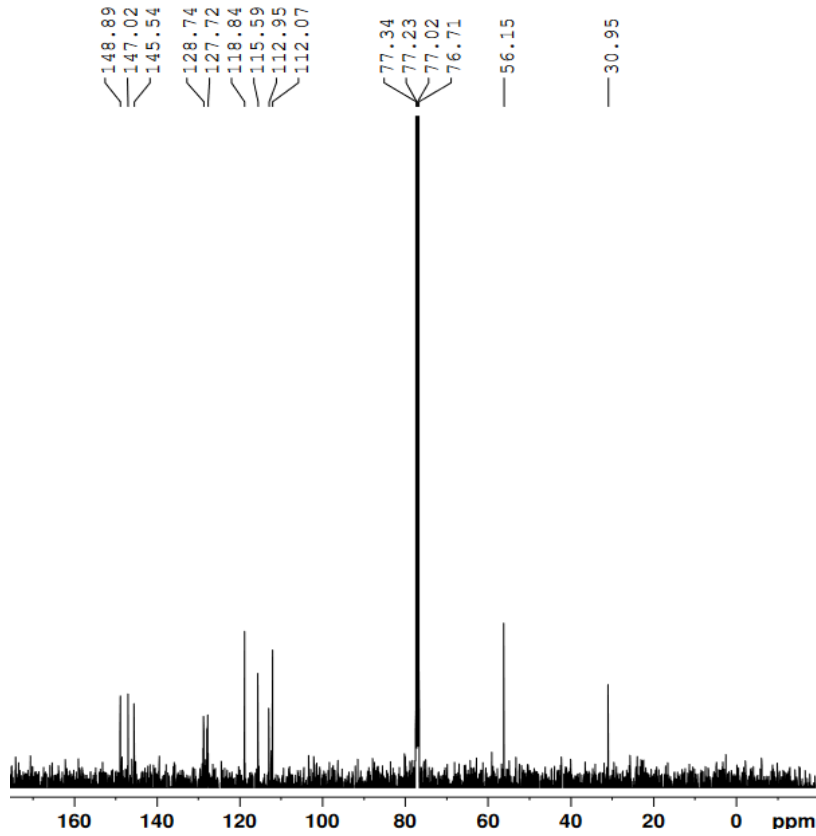
F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Dr.SYN230524
EXPNO 35
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240523
Time 15.53 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 303.4 K
D1 1.00000000 sec
TD0 1
SF01 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

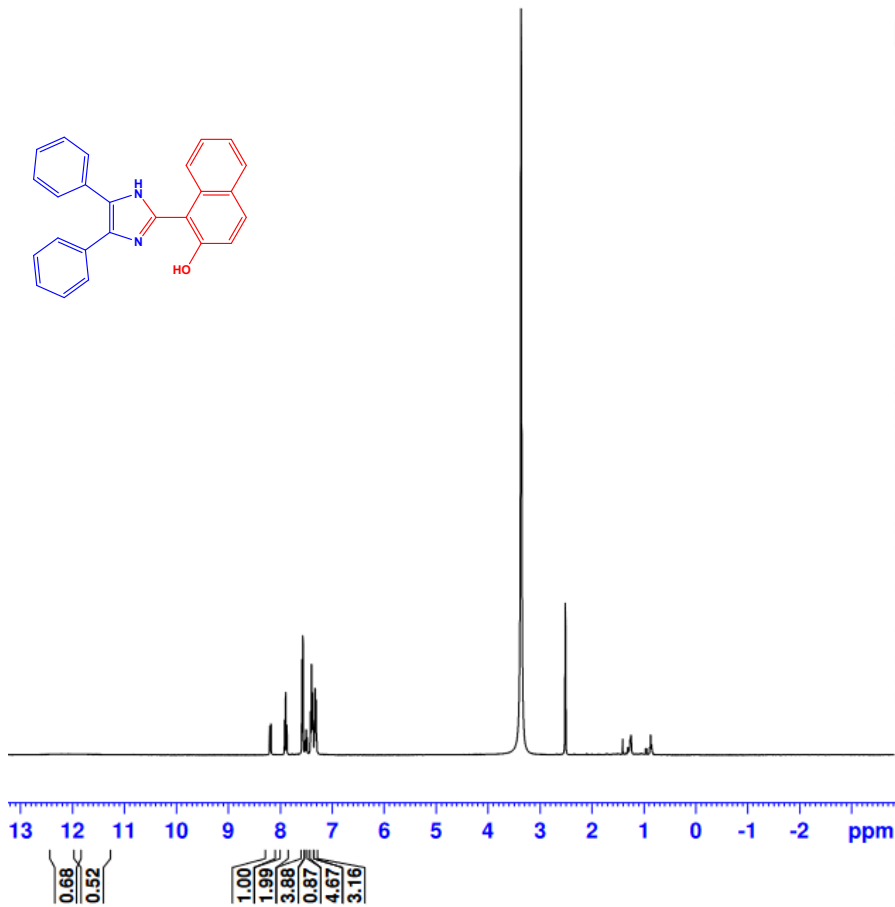
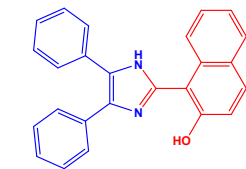
F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Dr.SYN280924
EXPNO 38
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240929
Time 11.43 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 303.9 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPCPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

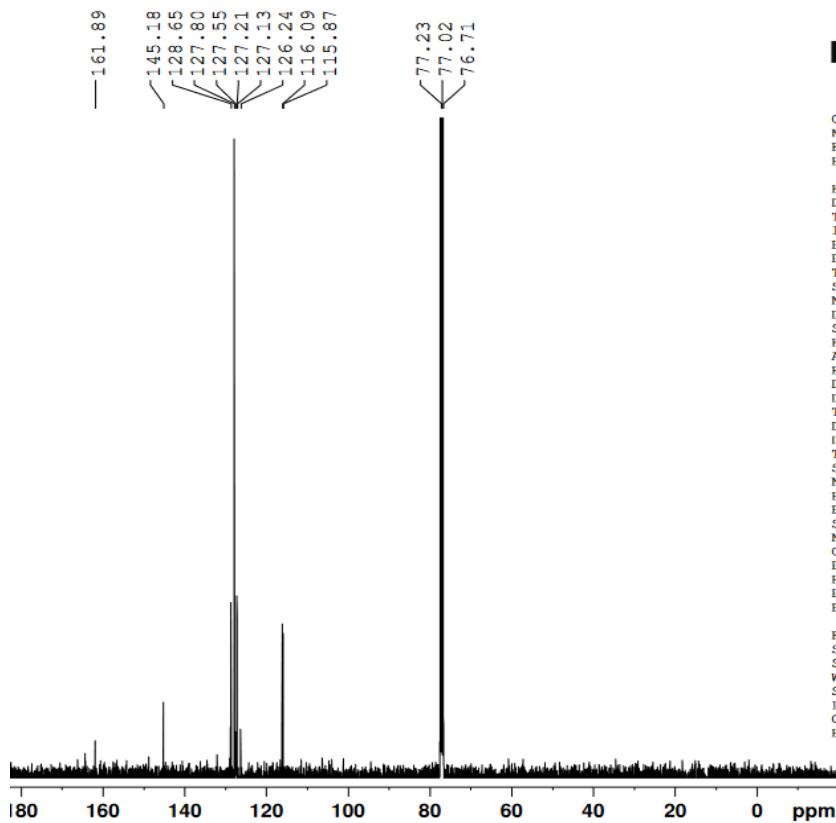
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME Dr.SYN170524 2
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240517
Time 18.48 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 303.5 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

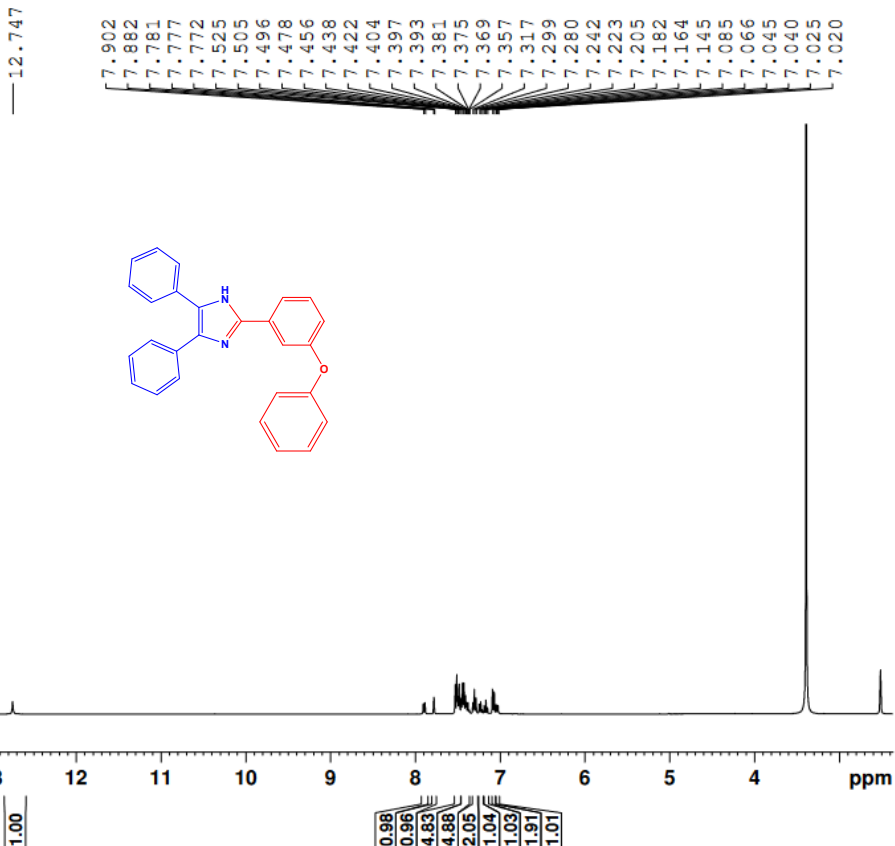
F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 32
 EXPNO 32
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240927
 Time 20.37 h
 INSTRUM spect
 PROBHD z108618_0505 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 199.6
 DW 20.800 usec
 DE 6.50 usec
 TE 304.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1
 SFO1 100.6550186 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 56.49300003 W
 SFO2 400.2596010 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 90.00 usec
 PLW2 15.21399975 W
 PLW12 0.42261001 W
 PLW13 0.21257000 W

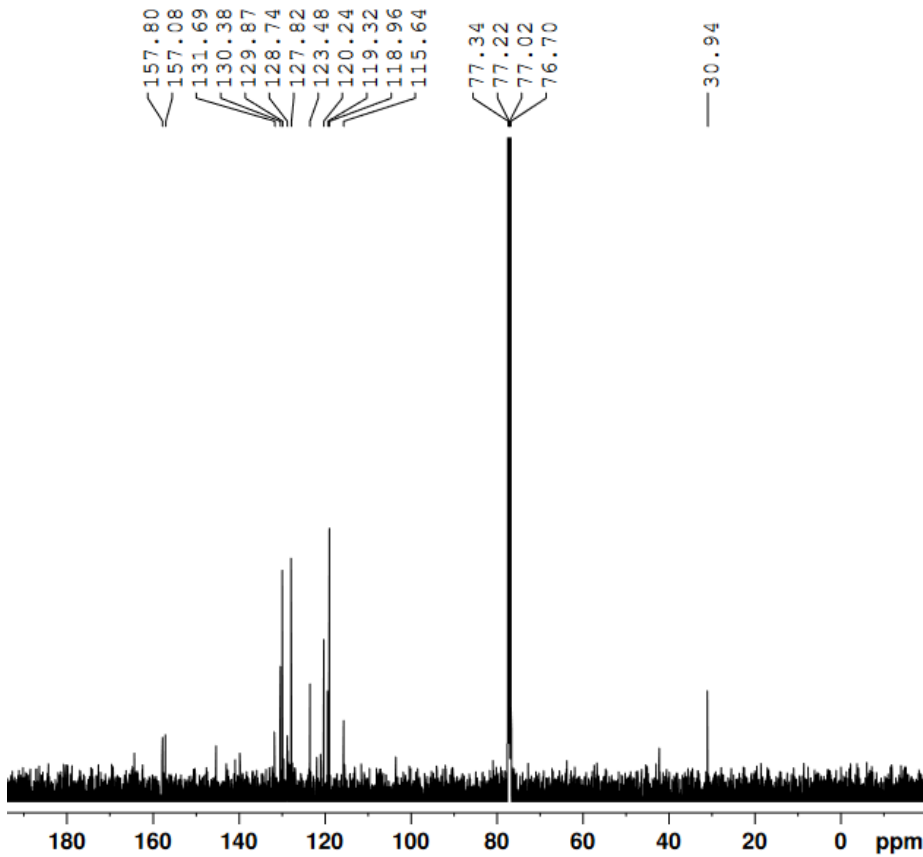
F2 - Processing parameters
 SI 32768
 SF 100.6449542 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME Dr.SYN240624
 EXPNO 36
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240624
 Time 12.07 h
 INSTRUM spect
 PROBHD z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 98.85
 DW 62.400 usec
 DE 6.50 usec
 TE 303.5 K
 D1 1.0000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

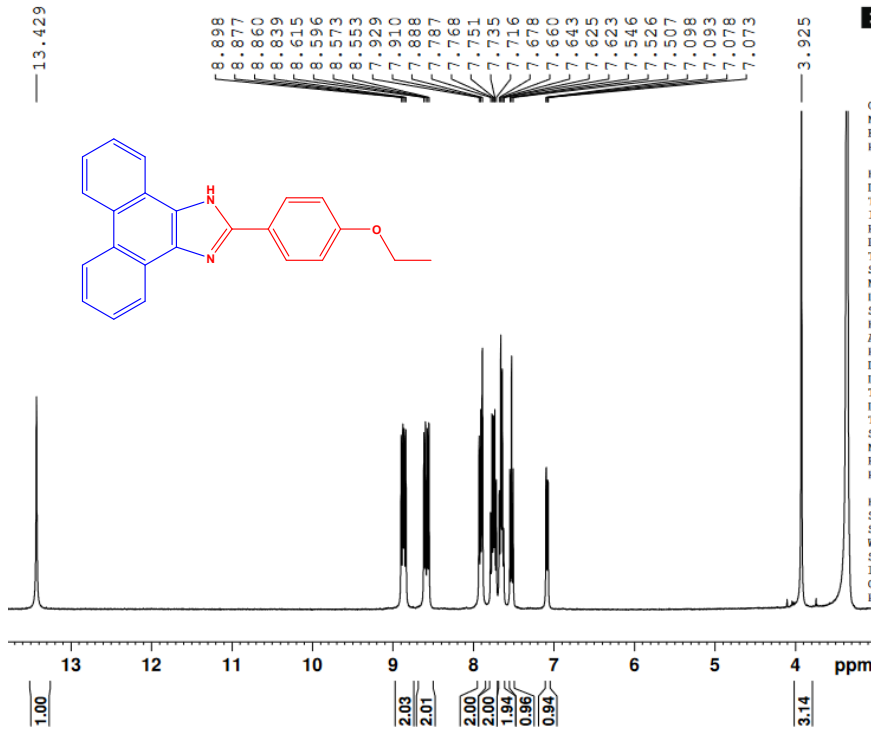
F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME Dr.SYN191024
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241019
Time 20.35 h
INSTRUM spect
PROBHD z108618_0505 ((
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 304.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
ELW12 0.42261001 W
ELW13 0.21257000 W

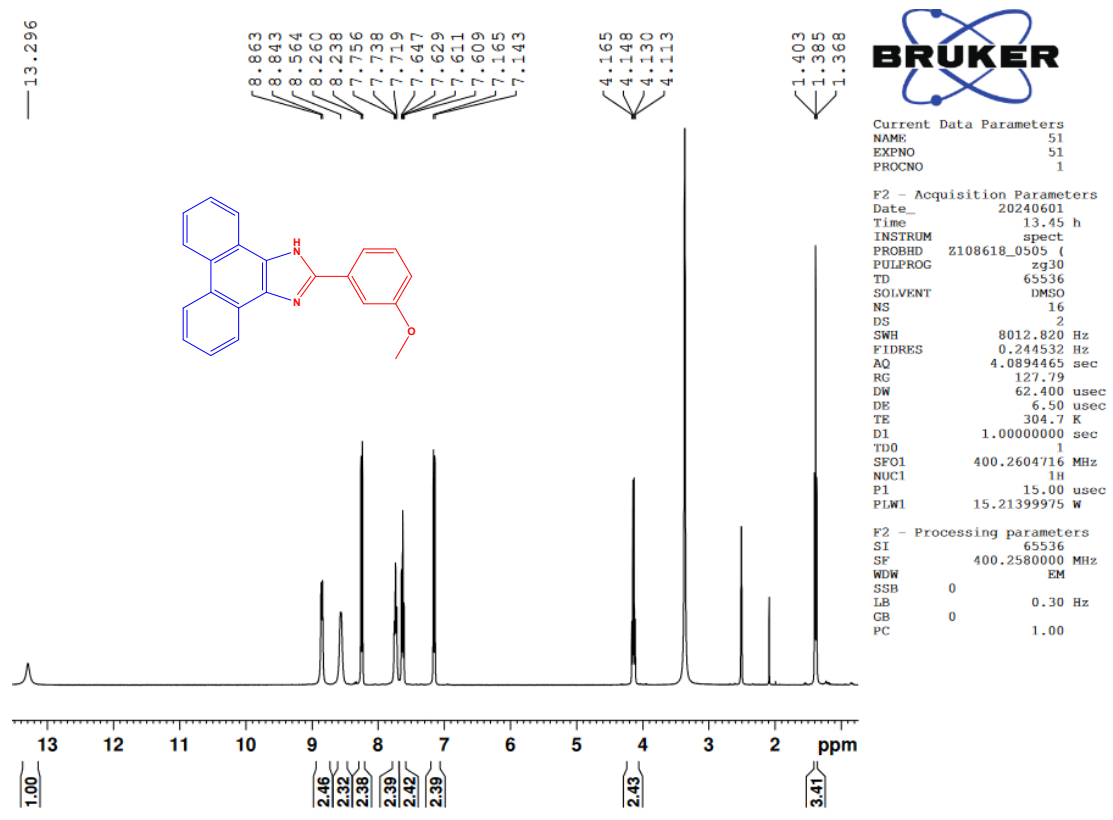
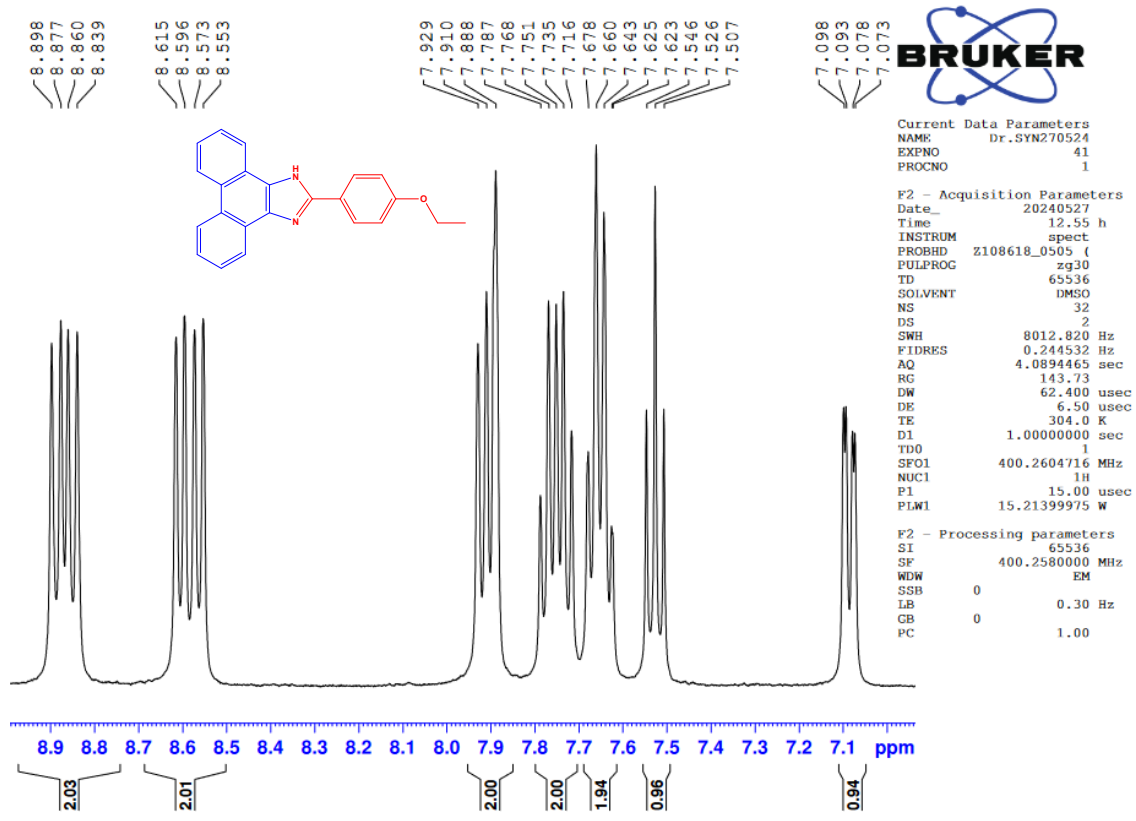
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

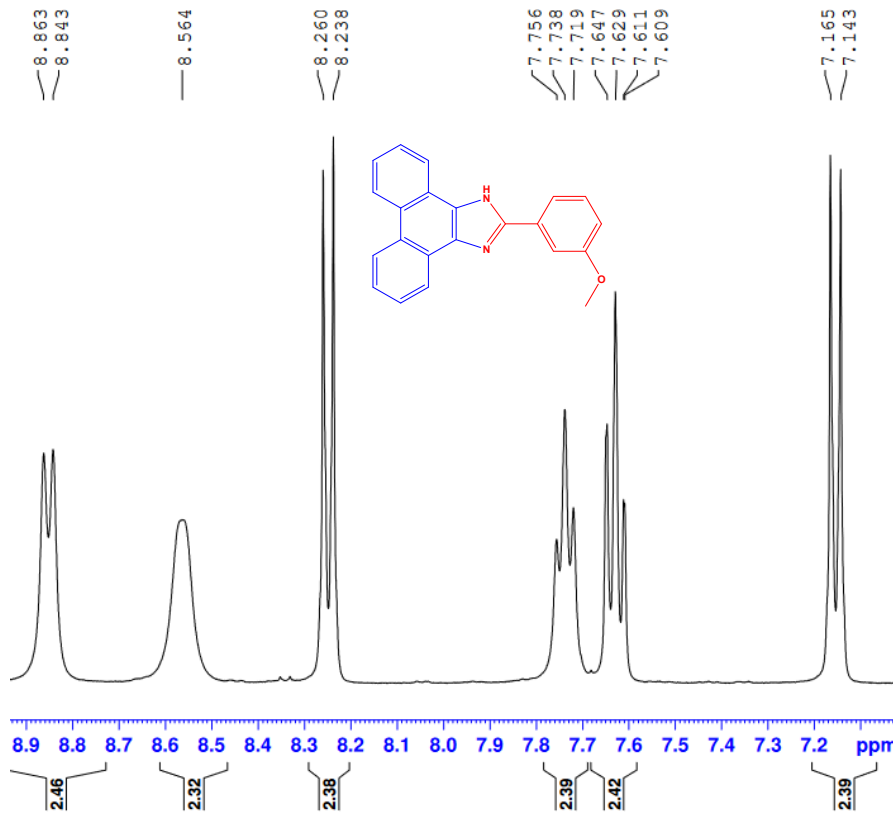


Current Data Parameters
NAME Dr.SYN270524
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240527
Time 12.55 h
INSTRUM spect
PROBHD z108618_0505 ((
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 304.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

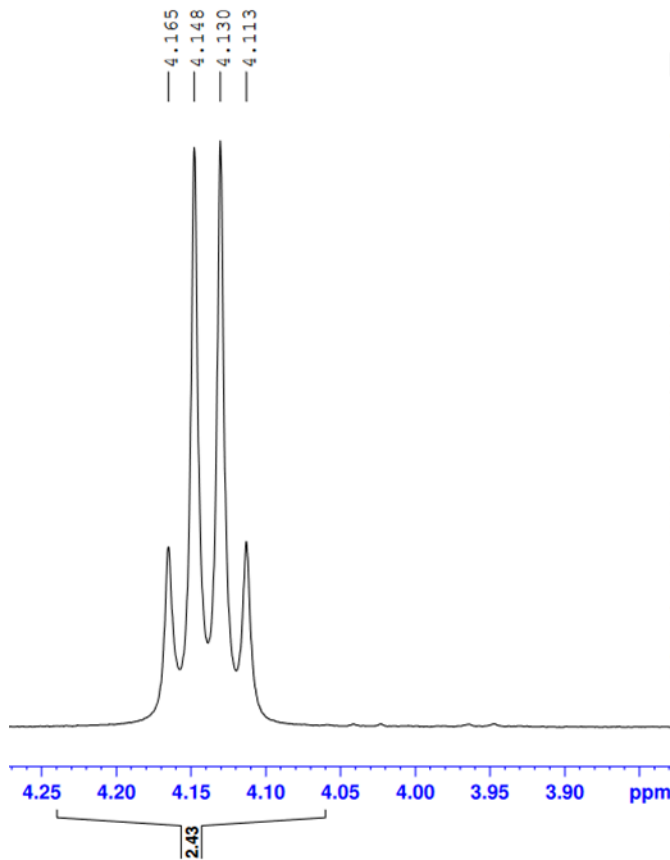




Current Data Parameters
 NAME: 51
 EXPNO: 51
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20240601
 Time: 13.45 h
 INSTRUM: spect
 PROBHD: Z108618_0505 ()
 PULPROG: zg30
 TD: 65536
 SOLVENT: DMSO
 NS: 16
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.244532 Hz
 AQ: 4.0894465 sec
 RG: 127.79
 DW: 62.400 usec
 DE: 6.50 usec
 TE: 304.7 K
 D1: 1.00000000 sec
 TD0: 1
 SFO1: 400.2604716 MHz
 NUC1: 1H
 P1: 15.00 usec
 PLW1: 15.21399975 W

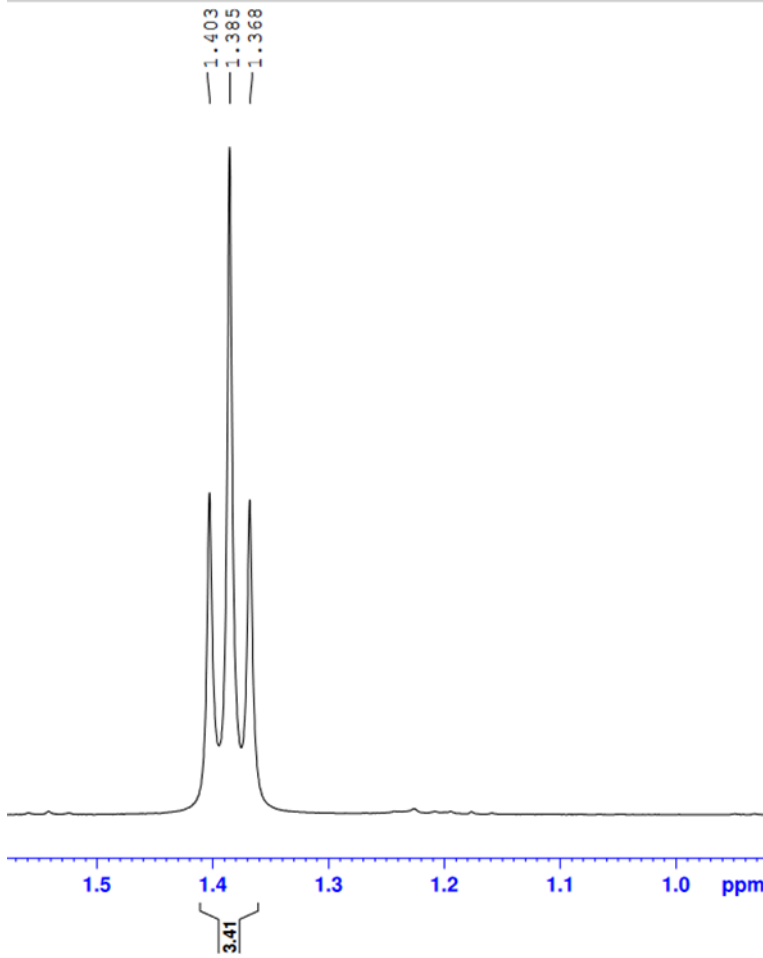
F2 - Processing parameters
 SI: 65536
 SF: 400.2580000 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00



Current Data Parameters
 NAME: 51
 EXPNO: 51
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20240601
 Time: 13.45 h
 INSTRUM: spect
 PROBHD: Z108618_0505 ()
 PULPROG: zg30
 TD: 65536
 SOLVENT: DMSO
 NS: 16
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.244532 Hz
 AQ: 4.0894465 sec
 RG: 127.79
 DW: 62.400 usec
 DE: 6.50 usec
 TE: 304.7 K
 D1: 1.00000000 sec
 TD0: 1
 SFO1: 400.2604716 MHz
 NUC1: 1H
 P1: 15.00 usec
 PLW1: 15.21399975 W

F2 - Processing parameters
 SI: 65536
 SF: 400.2580000 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00



Current Data Parameters
 NAME 51
 EXPNO 51
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240601
 Time 13.45 h
 INSTRUM spect
 PROBHD z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 127.79
 DW 62.400 usec
 DE 6.50 usec
 TE 304.7 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 13.664

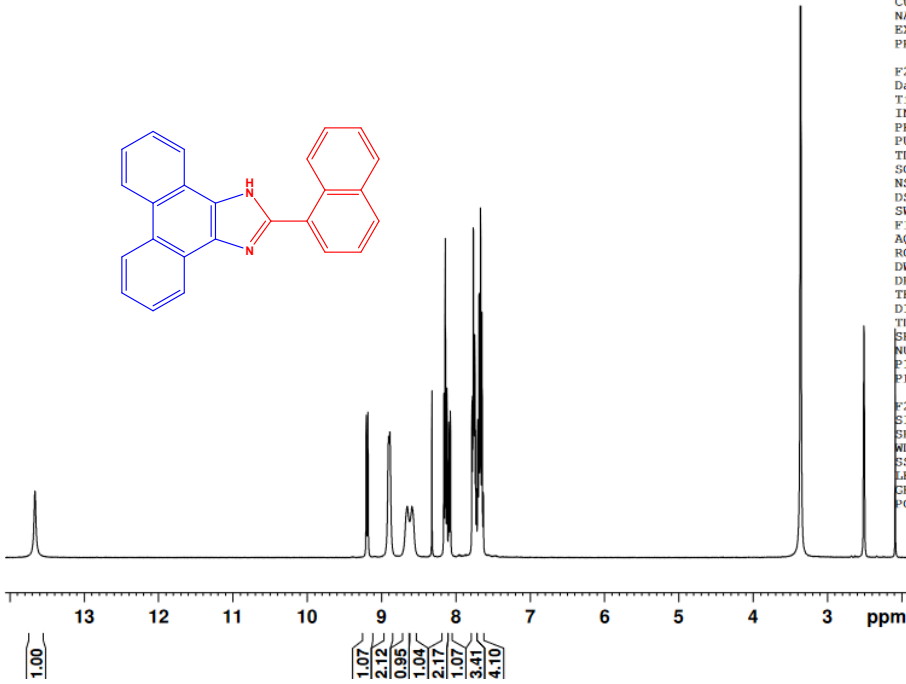
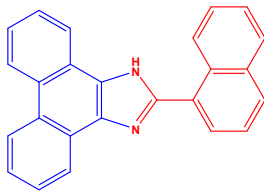
9.205
 9.184
 8.905
 8.888
 8.655
 8.591
 8.159
 8.141
 8.120
 8.094
 8.075
 7.782
 7.774
 7.764
 7.756
 7.746
 7.736
 7.707
 7.704
 7.687
 7.649
 7.632

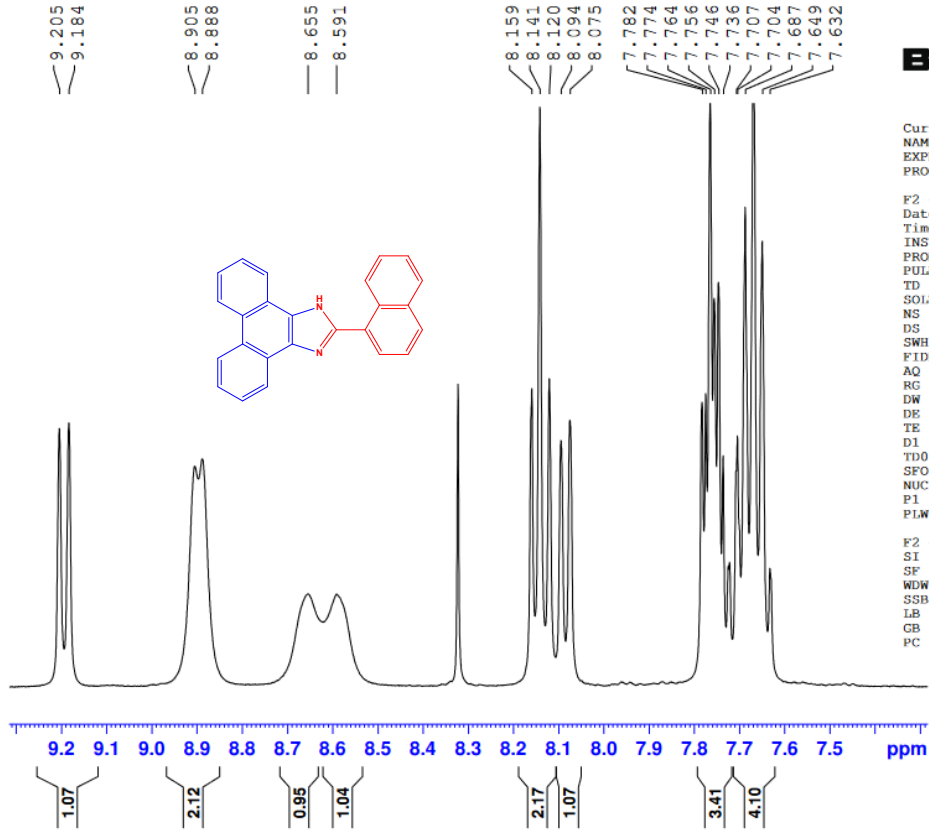


Current Data Parameters
 NAME 51
 EXPNO 52
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240601
 Time 13.48 h
 INSTRUM spect
 PROBHD z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 127.79
 DW 62.400 usec
 DE 6.50 usec
 TE 304.6 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

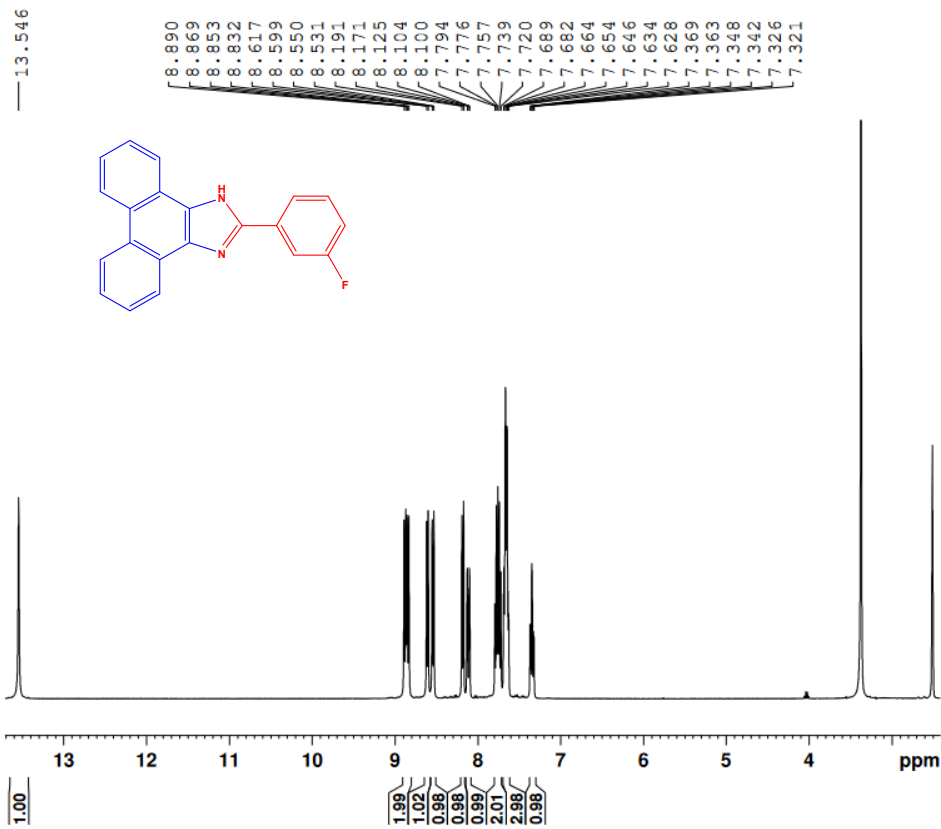




Current Data Parameters
 NAME 51
 EXPNO 52
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240601
 Time 13.48 h
 INSTRUM spect
 PROBHD z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 127.79
 DW 62.400 usec
 DE 6.50 usec
 TE 304.6 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 F1 15.00 usec
 PLW1 15.21399975 W

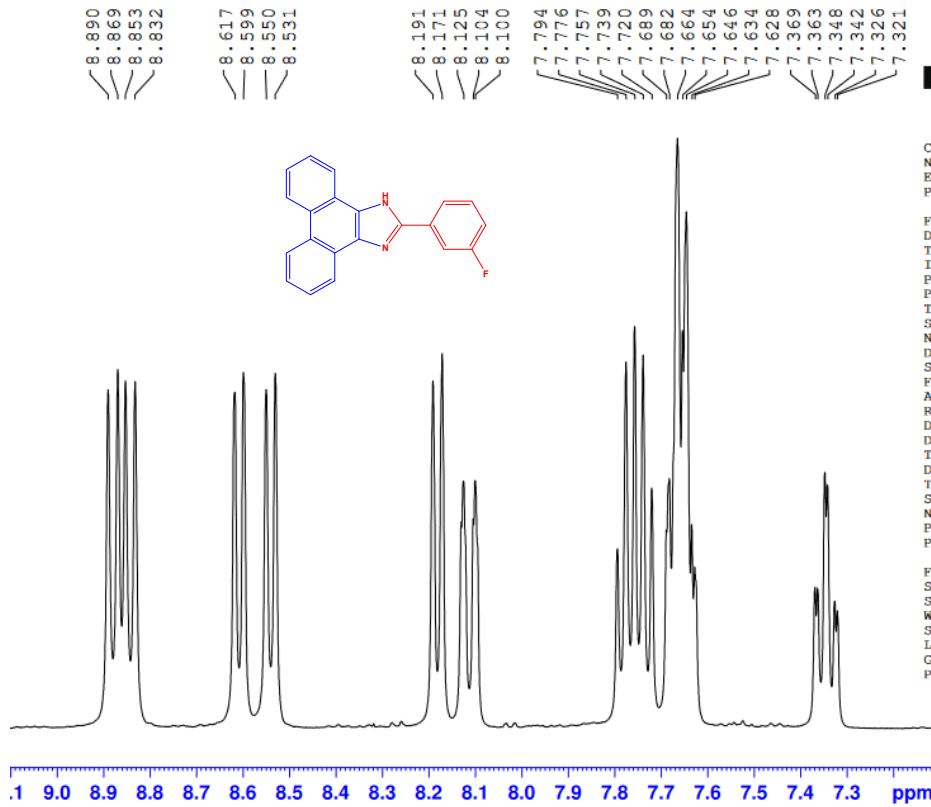
F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Dr.SYN300524
 EXPNO 48
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240530
 Time 16.47 h
 INSTRUM spect
 PROBHD z108618_0505 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 112.69
 DW 62.400 usec
 DE 6.50 usec
 TE 304.7 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 F1 15.00 usec
 PLW1 15.21399975 W

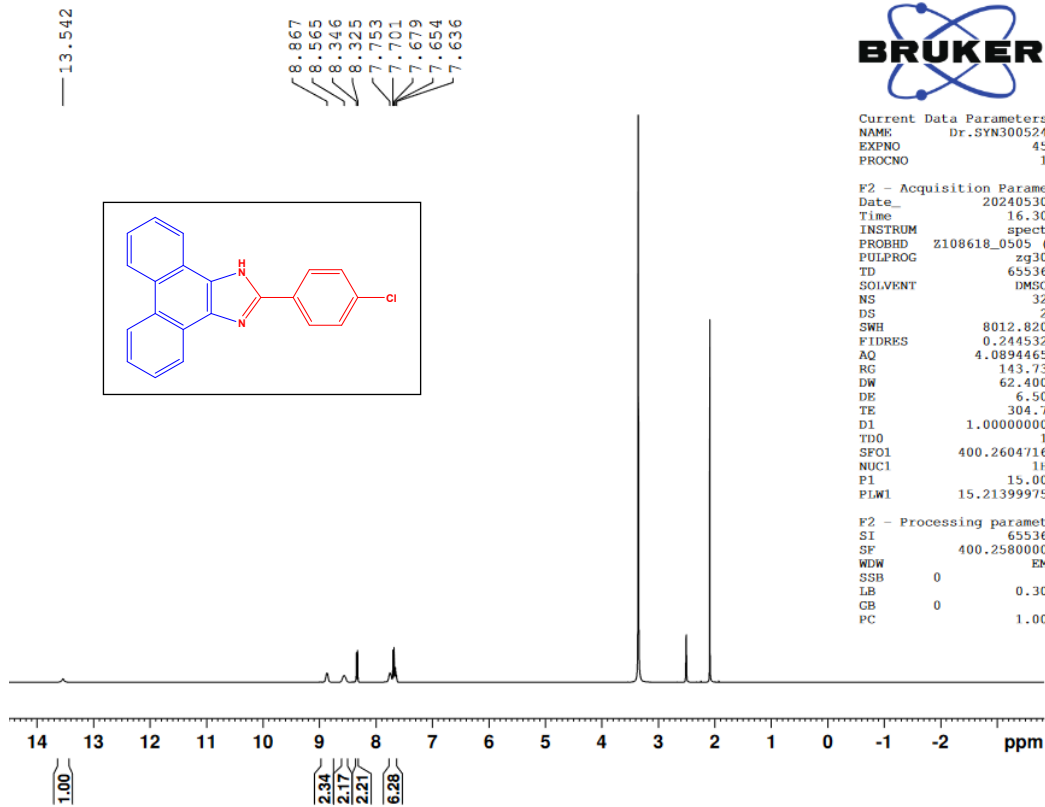
F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Dr.SYN300524
 EXPNO 48
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240530
 Time 16.47 h
 INSTRUM spect
 PROBHD Z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 112.69
 DW 62.400 usec
 DE 6.50 usec
 TE 304.7 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

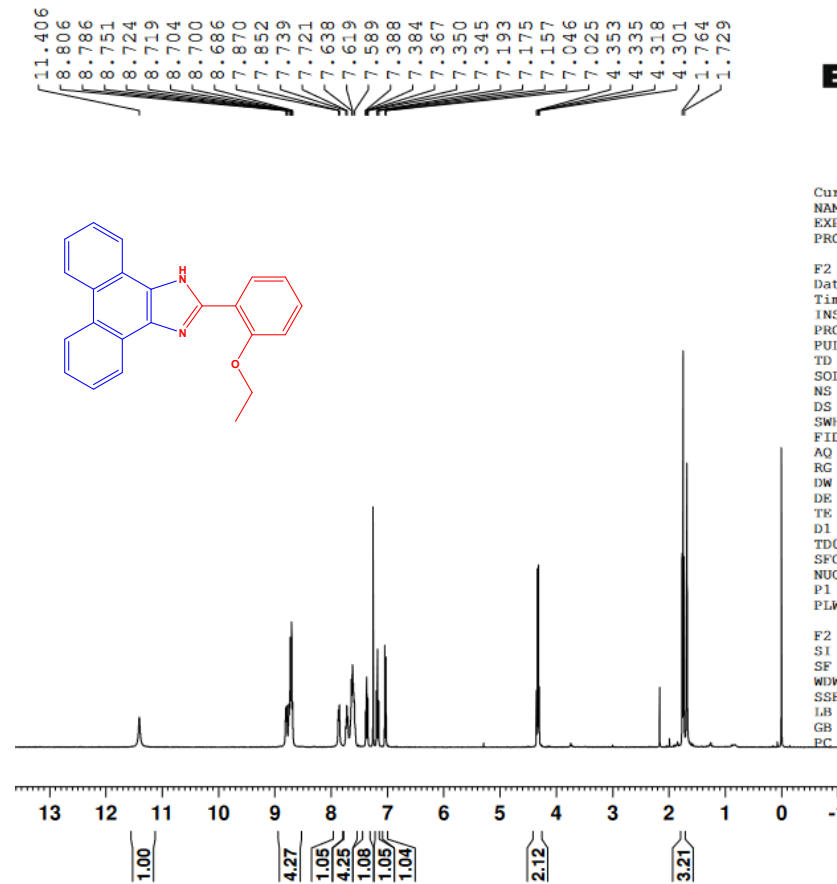
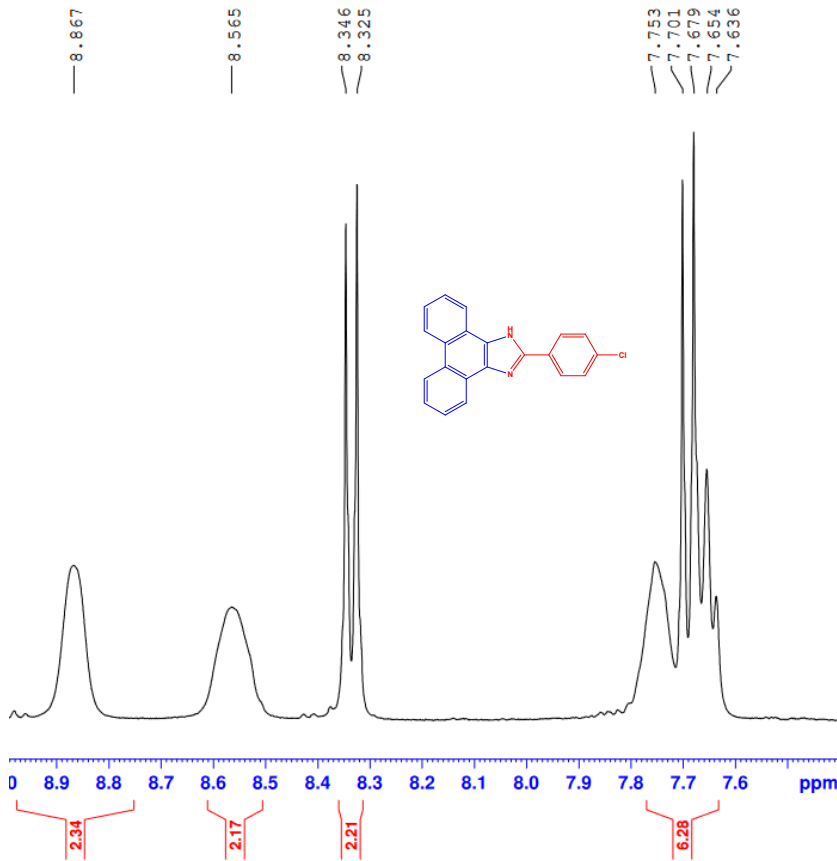
F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

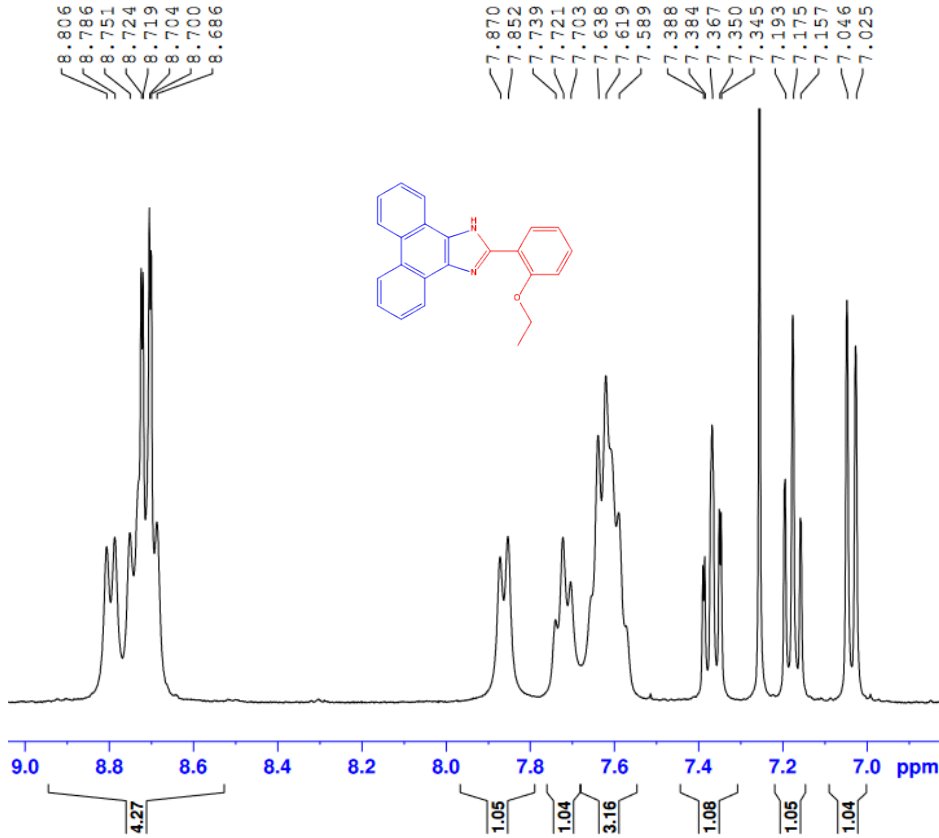


Current Data Parameters
 NAME Dr.SYN300524
 EXPNO 45
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240530
 Time 16.30 h
 INSTRUM spect
 PROBHD Z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 143.73
 DW 62.400 usec
 DE 6.50 usec
 TE 304.7 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

F2 - Processing parameters
 SI 65536
 SF 400.2580000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

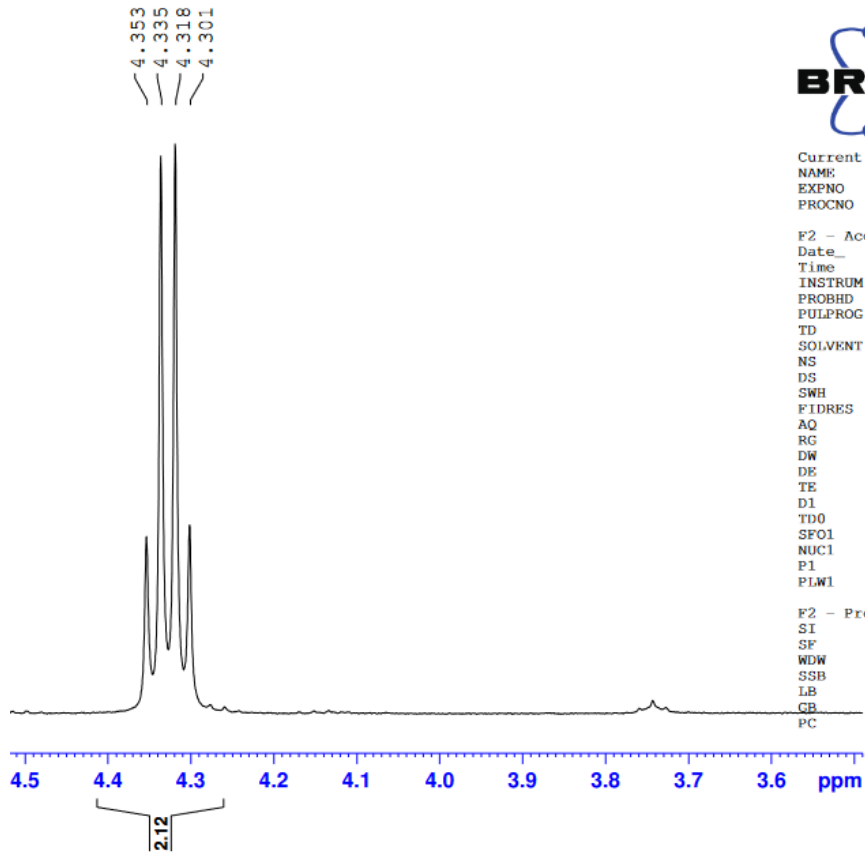




Current Data Parameters
 NAME Dr.SYN260624
 EXPNO 37
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240626
 Time 13.27 h
 INSTRUM spect
 PROBHD Z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 156.91
 DW 62.400 usec
 DE 6.50 usec
 TE 303.4 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

F2 - Processing parameters
 SI 65536
 SF 400.2580119 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME Dr.SYN260624
 EXPNO 37
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240626
 Time 13.27 h
 INSTRUM spect
 PROBHD Z108618_0505 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 156.91
 DW 62.400 usec
 DE 6.50 usec
 TE 303.4 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2604716 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 15.21399975 W

F2 - Processing parameters
 SI 65536
 SF 400.2580119 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME: Dr.SYN260624
EXPNO 37
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240626
Time 13.27 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 303.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

