Supplementary Information (SI) for ChemComm.
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Supporting Information

Unlocking Reactivity Potential of *Gem*-dihaloolefins: Access to Halo-Functionalized 1,4-Naphthoquinones via Intramolecular Radical Oxidative Cyclization

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1) X-Ray Crystallographic Studies

a) Crystal Structure of 3y

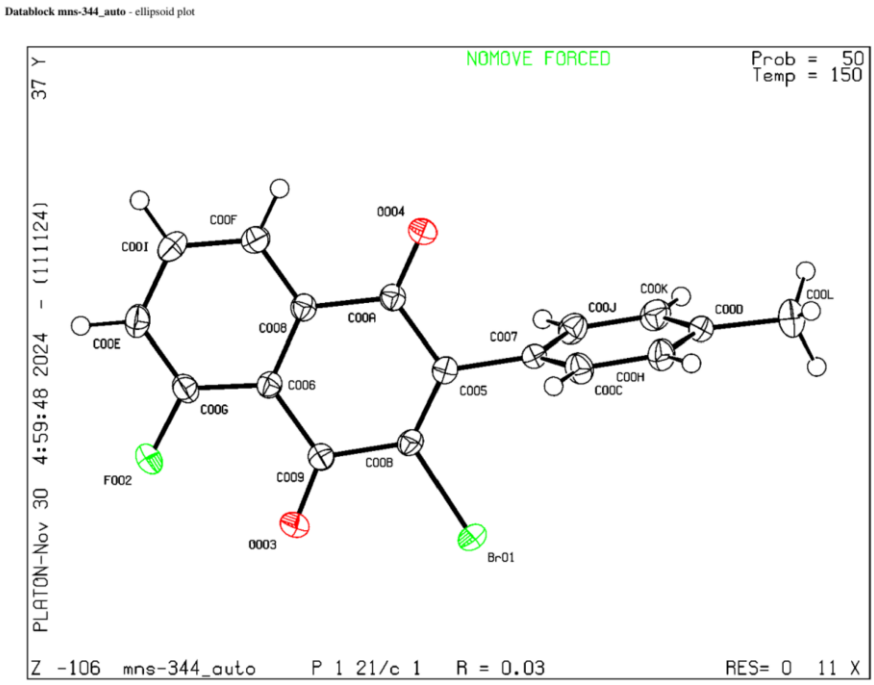


Figure SI. ORTEP structure of compound **3y**
(ellipsoid contours of probability level are 50%)

The crystals of **3y** of suitable quality were obtained from CH_2Cl_2/*n*-hexane. The compound **3y** crystallized in Monoclinic crystal system with space group P21/c. The single-crystal X-ray data were collected on an Oxford XCalibur CCD diffractometer using graphite monochromated Mo Kα radiation. The structures was solved using SIR-92 and refined by full matrix least square technique on F^2 using the SHELXL-97[1-4] program within the WinGX v 1.80.05 software package. Atomic coordinates, bond lengths, bond angles, and thermal parameters for compounds **3y** has been deposited at the Cambridge Crystallographic Data Centre. CCDC deposit number for **3y** is **2424439**.

Table SI. Crystallographic data and structure refinement for compounds 3y

Identification code	**MNS-344**
Empirical formula	$C_{17}H_{10}BrFO_2$
Formula weight	345.16
Temperature	150 K
Wavelength	0.71073 Å

Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.2785 (5) Å	α = 90.
	b = 14.3225 (6) Å	β = 105.808 (5).
	c = 9.8230 (5) Å	γ = 90.
Volume	1391.39 (12) $Å^3$	
Z	4	
Density (calculated)	1.648 g/cm^3	
Absorption coefficient	2.966 mm^{-1}	
F(000)	688.0	
Index ranges	h = 12, k = 20, l = 13	
Reflections collected	0.0342 (2853)	
Completeness to theta = 31.051 °	79.6 %	
Final R indices [I>2 sigma(I)][a,b]	R1 = 0.0342, wR2 = 0.0736	

[a] $R = \sum(\| Fo \| - \| Fc \|)/\sum | Fo |$; [b] $Rw = \{\sum[w(Fo^2 - Fc^2)^2]/\sum[w(Fo^2)^2]\}^{1/2}$

General Experimental Procedure General Method:

^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded in $CDCl_3$/DMSO-d_6. Chemical shifts for protons and carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet), coupling constants in Hertz and integration. High resolution mass spectra were recorded on electrospray mass spectrometer. Crystal structure analysis was accomplished on single needles X-ray diffractometer. The FT-IR analysis is carried out by Thermo Scientific Nicolet iS50 FT-IR using ATR method. TLC analysis was performed on commercially prepared 60 F254 silica gel plates and visualized by either UV irradiation or by staining with iodine. All purchased chemicals were used as received. All melting points are uncorrected.

Reagents:

All reagents were used directly as obtained commercially unless otherwise noted. HPLC grade ACN, THF, DMF, DMSO, Toluene, dioxane, hexanes, ethyl acetate, and DCM were purchased from Merck Chemical Co. $Pd(PPh_3)_2Cl_2$, Alkynes, TBHP, DTBP, PIDA, $K_2S_2O_8$, diphenyl diselenide and 2-bromobenzaldehyde derivatives were purchased from Aldrich Chemical Co., Inc.

2. Real time mass monitoring studies:

(2.1) Experimental Section

All chemicals were obtained from commercial sources. LC-MS grade solvents were obtained from Thermo Fisher Scientific.

Online ESI–MS Study. The real-time detection of reactive intermediates was carried out using online electrospray ionization mass spectrometry (ESI-MS), employing a custom-built pressurized sample infusion system, originally developed by McIndoe and colleagues. The schematic of the experimental setup is illustrated in the top panel of Figure 1. In brief, the reaction was conducted in a Schlenk flask, where 1.0 equivalent of diphenyl selenide and 3 equivalents of *tert*-butyl hydroperoxide (TBHP) were added to 5 mL of acetonitrile (ACN) along with the starting material and heated at 120 °C. The reaction mixture was transferred from the flask by applying a 5 psi backpressure of nitrogen gas, which pushed the solution through a borosilicate capillary to a T-junction. There, it was combined with acetonitrile delivered at a flow rate of 30 µL/min using a Hamilton syringe pump. This mixture was simultaneously subjected to a +5 kV DC high voltage to facilitate electrospray ionization.The diluted reaction stream from the T-junction was directed into a custom-designed electrospray source, where it was nebulized and sprayed into a high-resolution mass spectrometer (Orbitrap Exploris 120, Thermo Fisher Scientific). The spray system consisted of an inner fused silica capillary (100 µm i.d., 360 µm o.d.) for liquid delivery and an outer stainless steel coaxial capillary (0.5 mm i.d., 1.6 mm o.d.) for sheath gas delivery (nitrogen at 110 psi). To optimize nebulization, the inner silica capillary extended 1 mm beyond the orifice of the outer capillary.The resulting stream of charged microdroplets was directed toward the MS inlet, heated to 300 °C, which facilitated rapid desolvation and ion generation. The distance between the spray tip and the MS inlet was maintained at 15 mm. For data acquisition, the maximum ion injection time was set at 500 ms with a single microscan, and the mass resolution was configured to 120,000. Further tuning of ion optics was performed to maximize ion current. Data were collected using XCalibur software (Thermo Fisher Scientific). High mass accuracy and isotopic pattern analysis confirmed the identity of all key intermediates detected during the experiment.

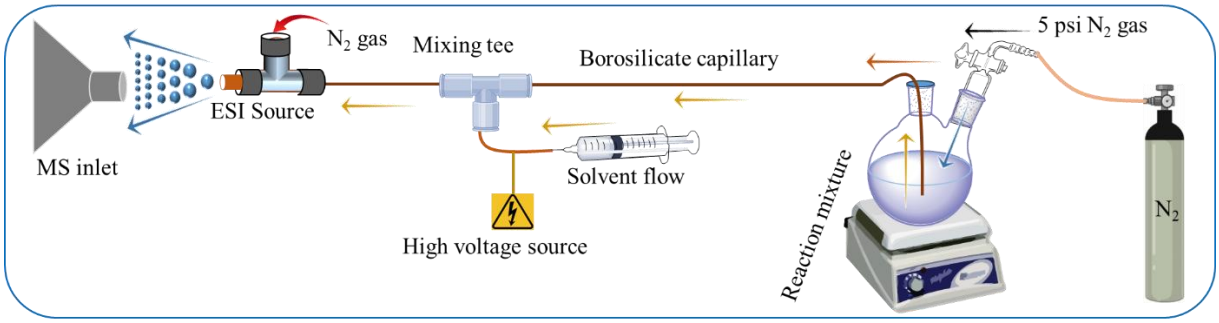


Figure S2. Custom-built online ESI-MS setup designed for real-time monitoring of reactants, intermediates, and products in positive ion mode throughout the course of the reaction.

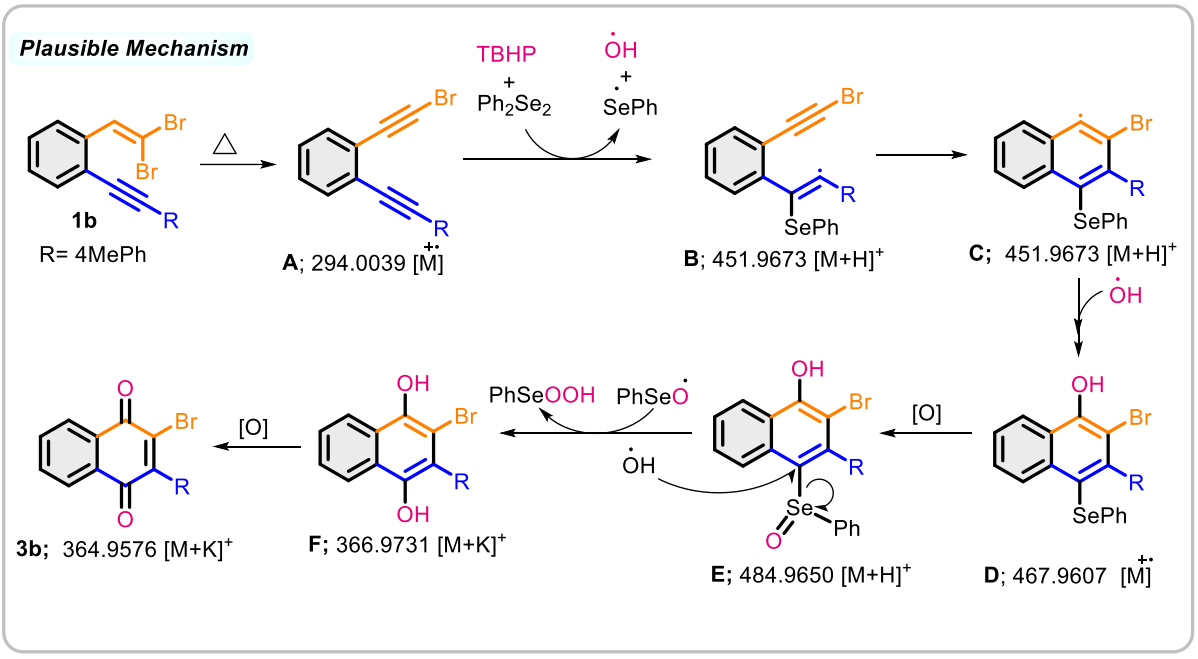
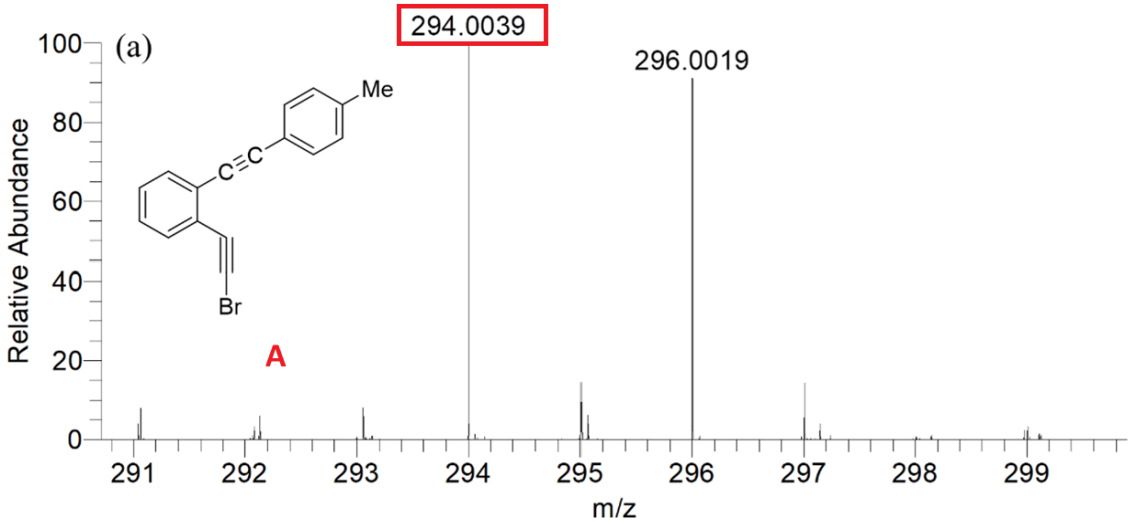
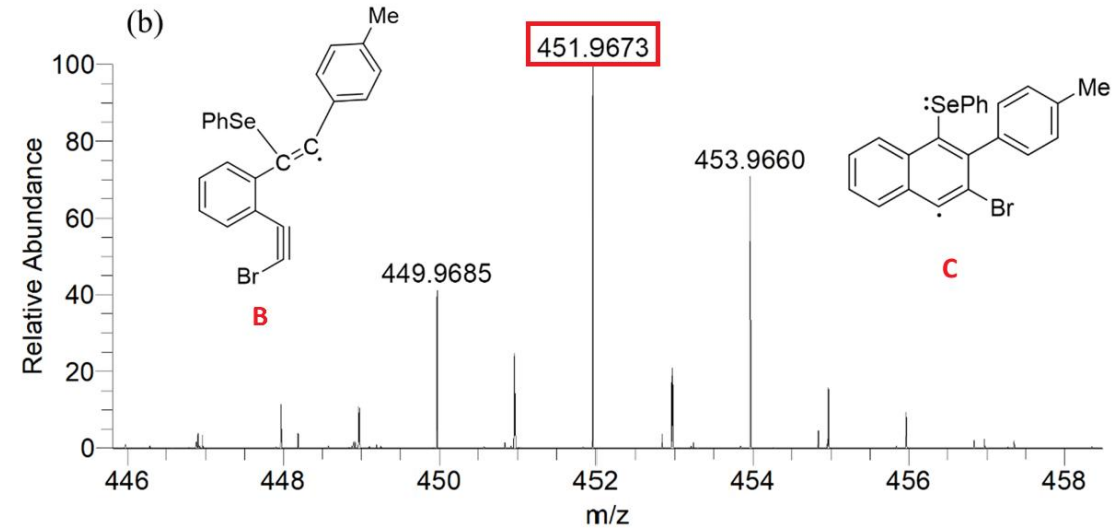
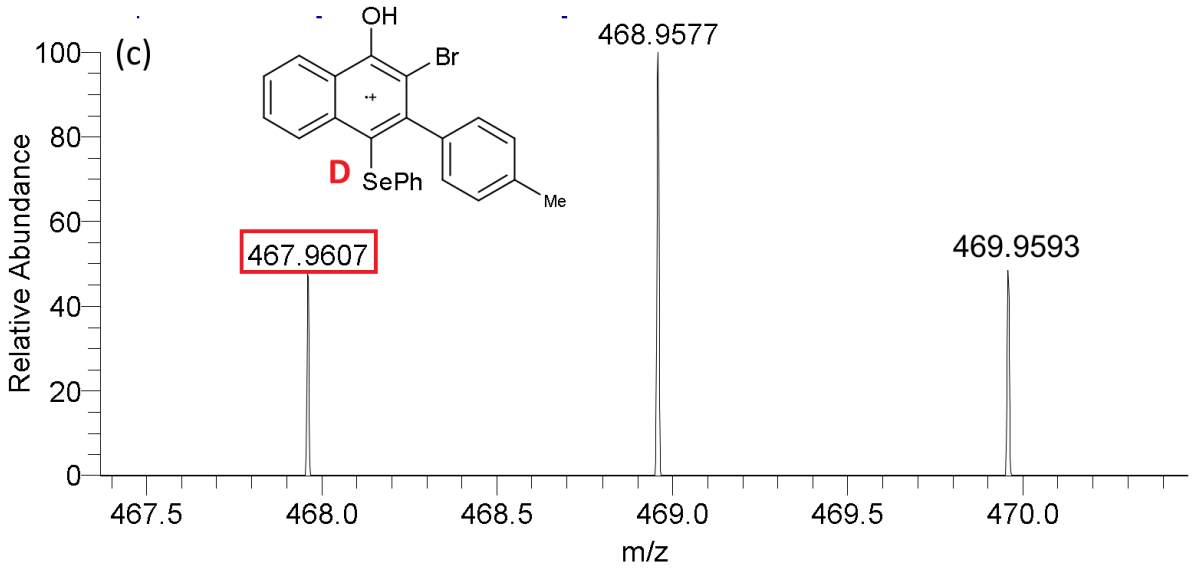


Figure S3. The proposed reaction mechanism includes all intermediate species identified via online mass spectrometry. Theoretical *m/z* values are in close agreement with the experimentally observed values.




(b)
Me
451.9673
PhSe
C
C
453.9660
:SePh
Me
Br
449.9685
Br
B
C
Relative Abundance
100
80
60
40
20
0
446
448
450
452
454
456
458
m/z


(c)
OH
Br
468.9577
D
SePh
Me
467.9607
469.9593
Relative Abundance
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60
40
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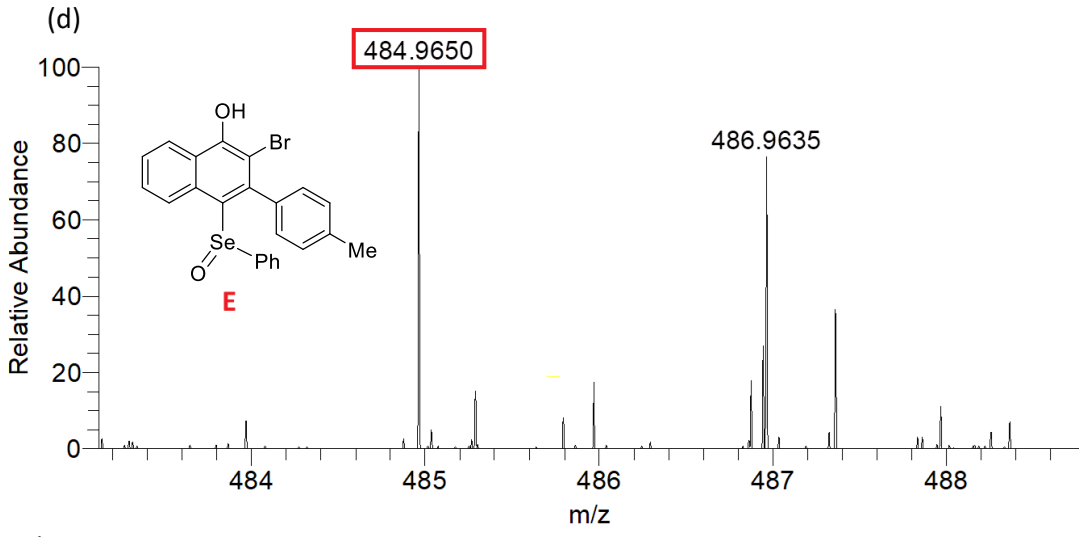
468.0
468.5
469.0
469.5
470.0
m/z


(d)
484.9650
OH
Br
486.9635
Se
Ph
O
Me
E
Relative Abundance
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60
40
20
0
484
485
486
487
488
m/z

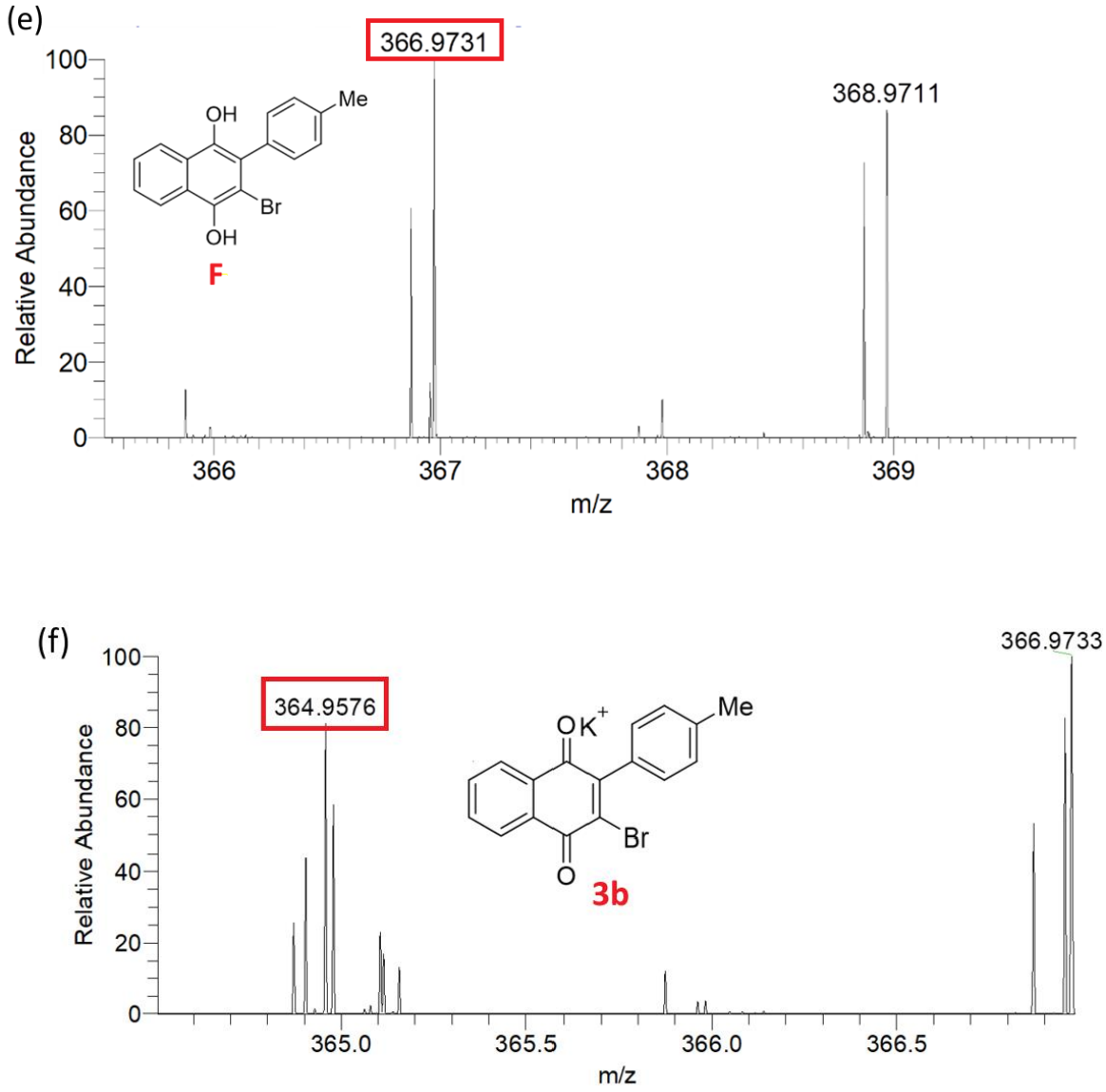


Figure S4. High-resolution ESI-MS spectra (a–f), acquired in positive ion mode during the reaction using the online mass spectrometric setup, are shown. The observed peaks correspond to various species generated over the course of the reaction (refer to Figure S3).

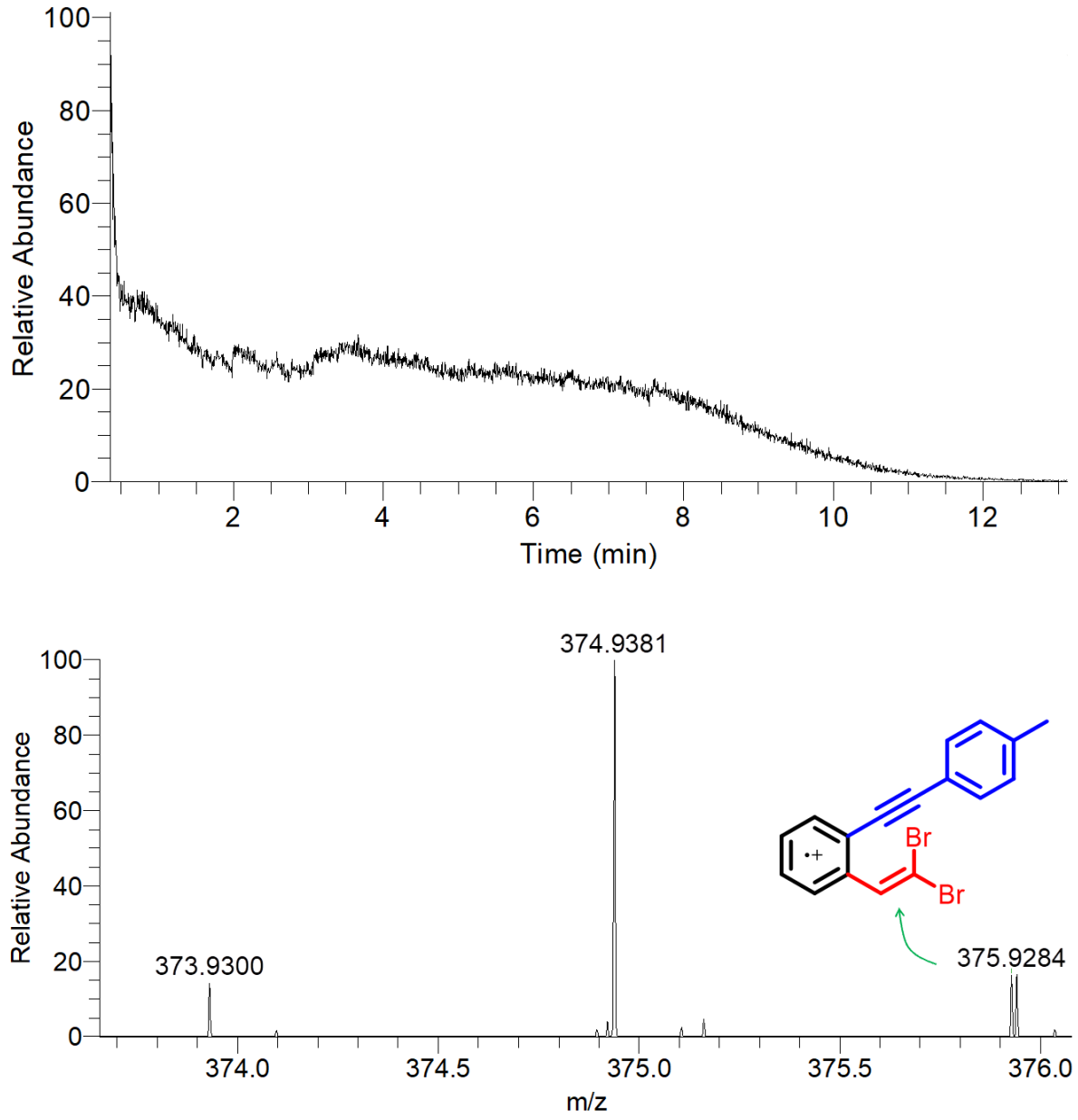


Figure S5. Graph showing consumption of the reactant **1b**

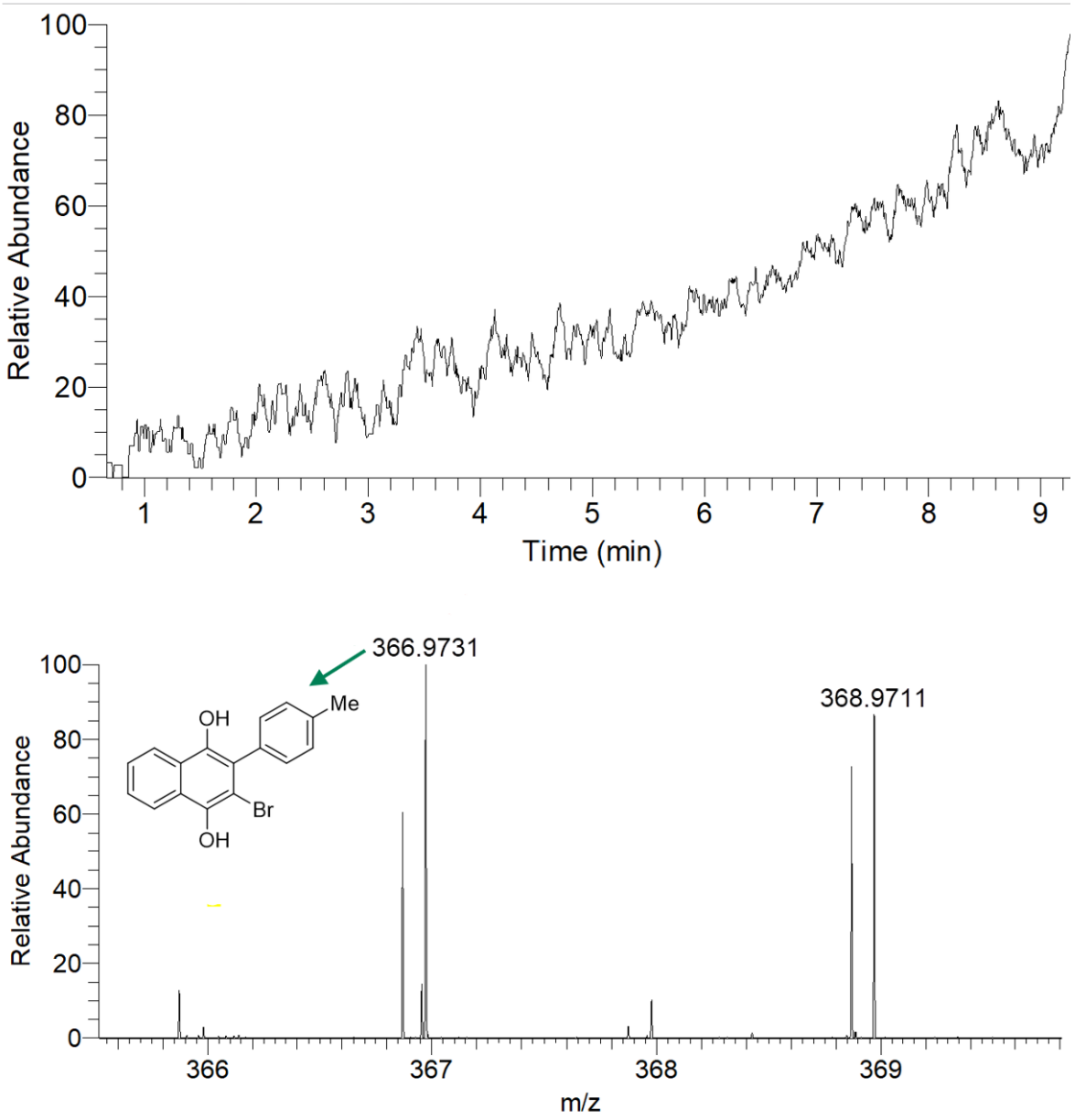
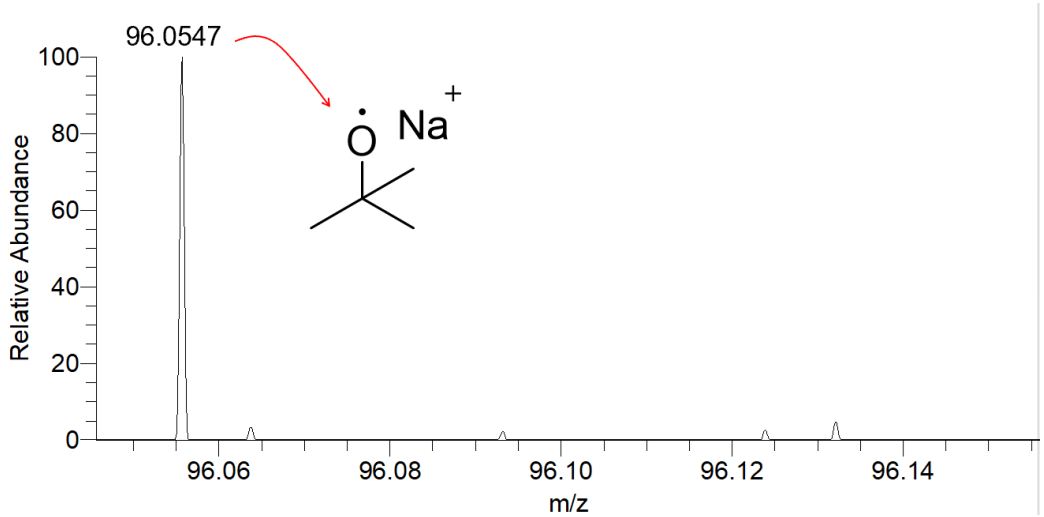


Figure S6. Graph showing formation of the intermediate **G**



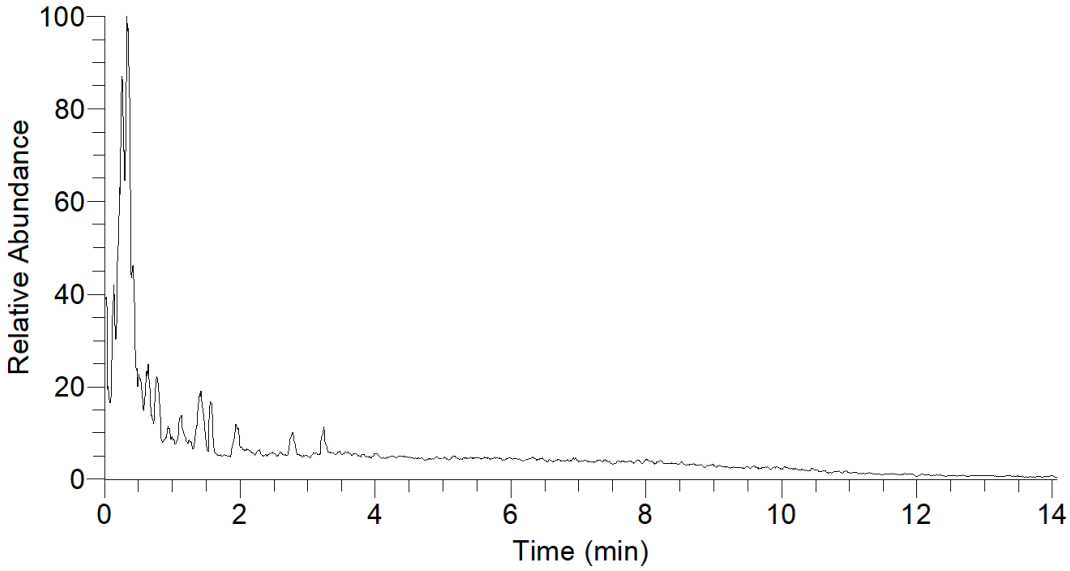
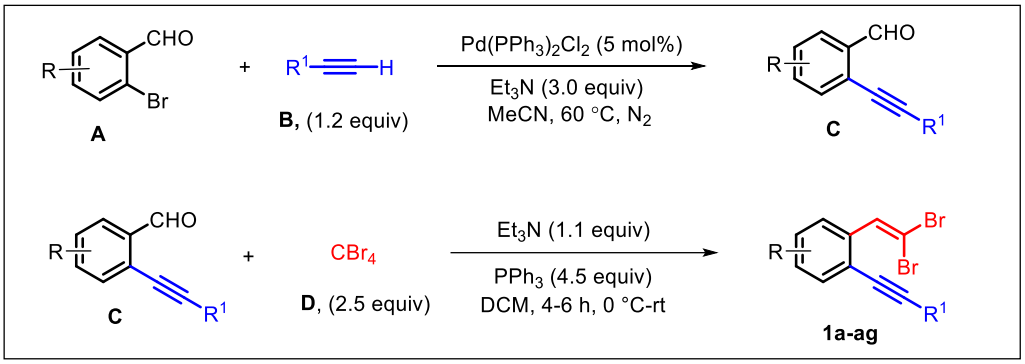


Figure S7. (i) Detection of tert-butyl radical through online ESI-MS; (ii) Graph showing the consumption of *tert*-butyl radical

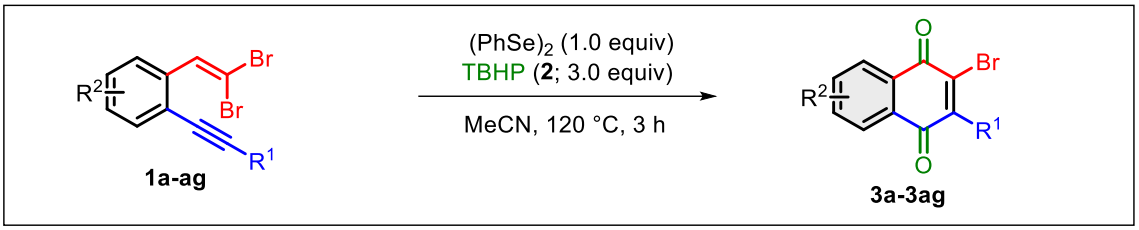
3. General Procedure for the Synthesis of 1-(2,2-dibromovinyl)-2-(alkynyl)benzene (1a-ag):



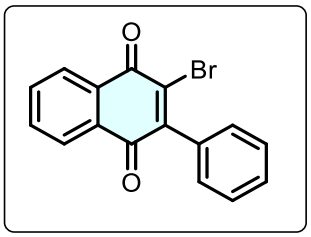
To an oven dried round bottom flask, substituted 2-bromobenzaldehyde **A** (1.0 mmol, 1.0 equiv), alkyne **B** (1.2 mmol, 1.2 equiv) and $Pd(PPh_3)_2Cl_2$ (5 mol%, 0.05 equiv) in 5.0 ml MeCN were added. The RB flask was then sealed and flushed with nitrogen. Then, Et_3N (3.0 mmol, 3.0 equiv) was added to the reaction mixture. Afterwards the reaction was stirred at 60 °C until TLC revealed complete conversion of the starting material. After completion of the reaction, the reaction mixture was allowed to cool. Then, organic layer was washed with aqueous saturated brine solution, and finally extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum. The crude material obtained was purified by column chromatography on silica gel (100−200 mesh) (hexane: ethyl acetate; 98/02) to afford the corresponding product **C**.

To an oven dried round bottomed flask charged with PPh_3 (4.5 mmol, 4.5 equiv) and Et_3N (1.1 mmol, 1.1 equiv) in DCM (10 mL) followed by slow addition of CBr_4 (2.5 mmol, 2.5 equiv) at 0 °C, 2 alkynylbenzaldehyde (**C**) (1 mmol, 1.0 equiv) was added to the mixture. This mixture was stirred at room temperature for 3-5 h. Then the reaction was quenched with water (20 mL), and extracted with ethyl acetate (20 mL x 2). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100−200 mesh size silica gel (hexane) to afford the corresponding product **1a-ag**. The structure and purity of known compounds were confirmed by comparison of their physical and NMR-spectral data (^{1}H NMR, ^{13}C NMR and HRMS) with those reported in the literature.

3. General Procedure for the Synthesis of 2-bromo-3-arylnaphthalene-1,4-dione (3a-3ag):

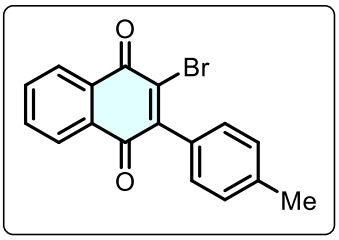


To an oven dried sealed tube, 1-(2,2-dibromovinyl)-2-(alkynyl)benzene derivatives (**1a-ag**, 0.278 mmol, 1.0 equiv), diphenyl selenide (0.278 mmol, 1.0 equiv) in MeCN was added. Then, 3.0 equiv (0.834 mmol; 0.01 M) of TBHP (**2**) was added to the reaction mixture. The reaction mixture was then stirred at 120 °C for 3 h in an oil bath. The reaction was monitored using thin layer chromatography. After completion of the reaction, the reaction mixture was allowed to cool. Then, organic layer was washed with aqueous saturated brine solution and finally extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum. The crude material obtained was purified by column chromatography on silica gel (100−200 mesh) (hexane: ethyl acetate; 98/02) to afford the corresponding product **3a-ag**.

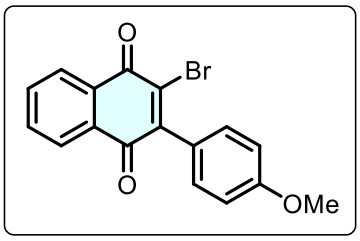


2-Bromo-3-phenylnaphthalene-1,4-dione (3a). The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3a** orange solid (74.35 mg, 86%); mp 88-90 °C; IR (ATR, neat) ν (cm^{-1}): 1664 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.16-8.11 (m, 1H), 8.08-8.03 (m, 1H), 7.73-7.67 (m, 2H), 7.45-7.38 (m, 3H), 7.29-7.25 (m, 2H); ^{13}C-NMR (100

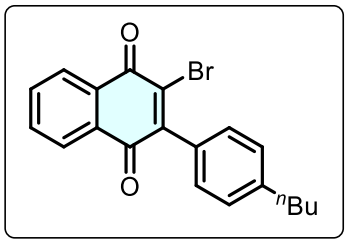
MHz, $CDCl_3$) δ 181.6, 178.2, 149.9, 139.2, 134.5, 134.2, 134.1, 131.7, 131.2, 129.4, 129.2, 128.2, 127.6, 127.4; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{16}H_{10}BrO_2]^+$ 312.9864, found 312.9861.



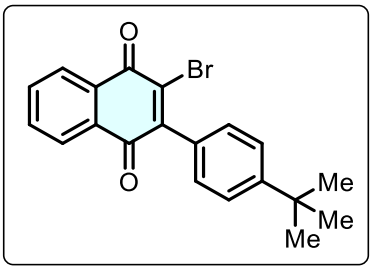
2-Bromo-3-(*p*-tolyl)naphthalene-1,4-dione (3b) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3b** as a orange solid (80.36 mg, 89%); mp 92-94 °C; IR (ATR, neat) ν (cm^{-1}): 1658 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.04-7.98 (m, 1H), 7.98-7.92 (m, 1H), 7.62-7.56 (m, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.3 Hz, 2H), 2.29 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.3, 177.9, 149.5, 139.2, 138.5, 134.1, 133.8, 131.3, 130.9, 130.8, 129.0, 128.6, 128.3, 127.2, 127.1, 21.3; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{12}BrO_2]^+$ 327.0021, found 327.0035.



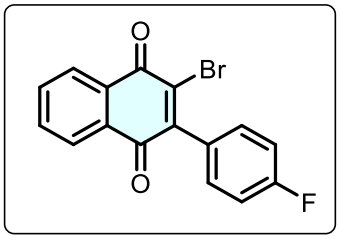
2-Bromo-3-(4-methoxyphenyl)naphthalene-1,4-dione (3c) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3c** as a orange solid (87.14 mg, 92%); mp 98-100 °C; IR (ATR, neat) ν (cm^{-1}): 1666 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15-8.11 (m, 1H), 8.08-8.03 (m, 1H), 7.72-7.66 (m, 2H), 7.24 (dt, *J* = 9.3, 2.4 Hz, 2H), 6.93 (dt, *J* = 9.3, 2.4 Hz, 2H), 3.79 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.8, 178.3, 160.4, 149.3, 138.5, 134.3, 134.0, 131.6, 131.2, 131.2, 130.9, 127.5, 127.4, 126.1, 113.5, 55.4; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{12}BrO_3]^+$ 342.9970, found 342.9982.



2-Bromo-3-(4-butylphenyl)naphthalene-1,4-dione (3d) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3d** as a orange solid (92.74 mg, 91%); mp 96-98 °C; IR (ATR, neat) ν (cm^{-1}): 1662 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.12-8.06 (m, 1H), 8.04-7.99 (m, 1H), 7.69-7.62 (m, 2H), 7.21-7.14 (m, 4H), 2.59 (t, *J* = 7.8 Hz, 2H), 1.60-1.53 (m, 2H), 1.35-1.25 (m, 2H), 0.86 (t, *J* = 7.4 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.6, 178.2, 149.8, 144.4, 138.8, 134.3, 134.0, 131.6, 131.3, 131.2, 129.3, 128.1, 127.5, 127.4, 35.6, 33.3, 22.5, 14.0; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{20}H_{18}BrO_2]^+$ 369.0490, found 369.0492.

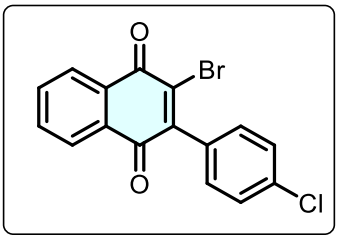


2-Bromo-3-(4-(*tert*-butyl)phenyl)naphthalene-1,4-dione (3e) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3e** as a orange solid (94.78 mg, 93%); mp 94-96 °C; IR (ATR, neat) ν (cm^{-1}): 1668 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15-8.09 (m, 1H), 8.07-8.02 (m, 1H), 7.71-7.65 (m, 2H), 7.42 (dt, *J* = 8.7, 2.0 Hz, 2H), 7.20 (dt, *J* = 8.6, 2.0 Hz, 2H), 1.29 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.6, 178.2, 152.4, 149.6, 138.7, 134.3, 134.0, 131.5, 131.1, 130.9, 129.0, 127.4, 127.3, 124.9, 34.8, 31.2; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{20}H_{18}BrO_2]^+$ 369.0490, found 369.0497.

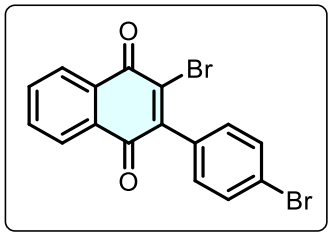


2-Bromo-3-(4-fluorophenyl)naphthalene-1,4-dione (3f) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3f** as a yellow solid (74.94 mg, 82%); mp 104-106 °C; IR (ATR, neat) ν (cm^{-1}): 1670 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.18-8.13 (m, 1H), 8.10-8.05 (m, 1H), 7.75-7.69 (m, 2H), 7.27 (ddd, *J* = 11.8, 5.1, 3.0 Hz, 2H), 7.14-7.08 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) 181.5, 178.1, 163.2 (d, $J_{C\text{-}F}$ = 250.7 Hz, 1C), 148.8, 139.4, 134.5, 134.2, 131.5, 131.4, 131.1, 129.9 (d, $J_{C\text{-}F}$ = 3.6 Hz, 1C), 127.6, 127.4, 115.4 (d,

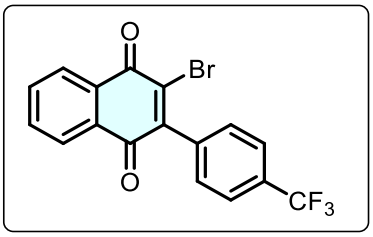
$J_{C\text{-}F}$ = 21.8 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ –110.83 (s); HRMS (ESI) $[M+H]^+$ Calcd for $[C_{16}H_9BrFO_2]^+$ 330.9770, found 330.9785.



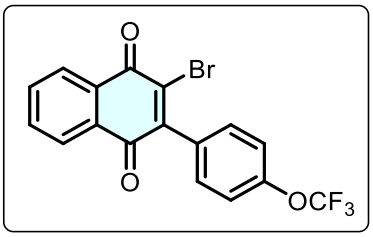
2-Bromo-3-(4-chlorophenyl)naphthalene-1,4-dione (3g) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3g** as a yellow solid (80.58 mg, 84%); mp 108-110 °C; IR (ATR, neat) ν (cm^{-1}): 1666 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15-8.10 (m, 1H), 8.07-8.02 (m, 1H), 7.73-7.67 (m, 2H), 7.40-7.36 (m, 2H), 7.21-7.18 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.4, 178.1, 148.8, 139.5, 135.7, 134.6, 134.3, 132.4, 131.6, 131.2, 130.9, 128.6, 127.8, 127.6; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{16}H_9BrClO_2]^+$ 346.9474, found 346.9472.



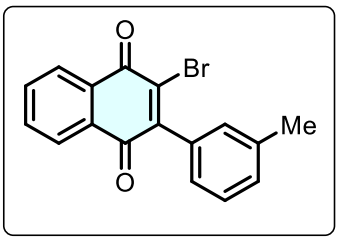
2-Bromo-3-(4-bromophenyl)naphthalene-1,4-dione (3h) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3h** as a yellow solid (89.81 mg, 83%); mp 108-110 °C; IR (ATR, neat) ν (cm^{-1}): 1662 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15-8.13 (m, 1H), 8.07-8.04 (m, 1H), 7.72-7.69 (m, 2H), 7.55 (d, J = 8.4 Hz, 2H), 7.14 (d, J = 8.5 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.2, 177.9, 148.7, 139.3, 134.5, 134.2, 132.7, 131.4, 131.0, 130.9, 127.6, 127.4, 123.8; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{16}H_9Br_2O_2]^+$ 390.8969, found 390.8973.



2-Bromo-3-(4-(trifluoromethyl)phenyl)naphthalene-1,4-dione (3i) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3i** as a yellow solid (75.74 mg, 72%); mp 142-144 °C; IR (ATR, neat) ν (cm^{-1}): 1672 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 1H), 8.11-8.06 (m, 1H), 7.77-7.72 (m, 2H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.39 (d, *J* = 8.1 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.2, 177.8, 148.5, 139.7, 137.5, 134.6, 134.3, 131.4, 131.0, 129.6, 127.7, 127.5, 125.2, 123.8 (q, $J_{C\text{-}F}$ = 272.9 Hz, 1C) ; ^{19}F NMR (376 MHz, $CDCl_3$) δ –62.62 (s, CF_3); HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_9BrF_3O_2]^+$ 380.9738, found 380.9735.

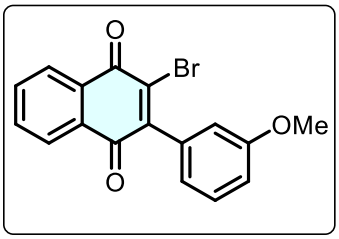


2-Bromo-3-(4-(trifluoromethoxy)phenyl)naphthalene-1,4-dione (3j) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3j** as a orange solid (76.73 mg, 70%); mp 148–150 °C; IR (ATR, neat) ν (cm^{-1}): 1664 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.14-8.09 (m, 1H), 8.06-8.01 (m, 1H), 7.73-7.67 (m, 2H), 7.30 (dt, *J* = 9.0, 2.3 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H*)*; ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.3, 177.9, 149.8, 148.5, 139.6, 134.5, 134.2, 132.4, 131.5, 131.1, 127.6, 127.4, 120.5 (q, $J_{C\text{-}F}$ = 258.9 Hz, 1C), 120.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ –57.52 (s, CF_3); HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_9BrF_3O_3]^+$ 396.9687, found 396.9693.

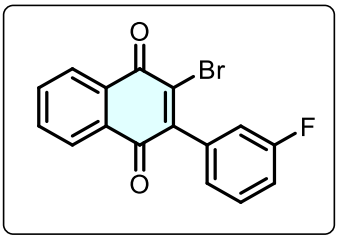


2-Bromo-3-(*m*-tolyl)naphthalene-1,4-dione (3m) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3m** as a orange solid (76.75 mg, 85%); mp 92-94 °C; IR (ATR, neat) ν (cm^{-1}): 1658 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.17-8.12 (m, 1H), 8.09-8.04 (m, 1H), 7.74-7.68 (m, 2H), 7.33-7.28 (m, 1H), 7.21 (d, *J* = 7.7 Hz, 1H), 7.05-7.04 (m, 2H), 2.35 (s, 3H) ; ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.6, 178.2, 150.0, 139.0,

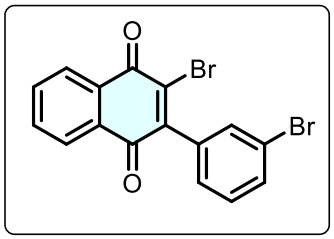
137.8, 134.4, 134.0, 131.5, 131.1, 130.1, 129.5, 128.0, 127.5, 127.3, 126.1, 21.5; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{12}BrO_2]^+$ 327.0021, found 327.0035.



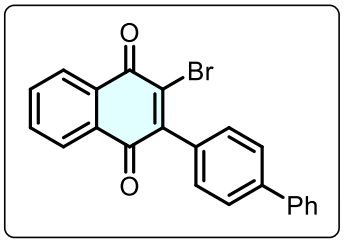
2-Bromo-3-(3-methoxyphenyl)naphthalene-1,4-dione (3n). The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3n** as a orange solid (80.50 mg, 85%); mp 98-100 °C; IR (ATR, neat) ν (cm^{-1}): 1667 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.19-8.13 (m, 1H), 8.10-8.05 (m, 1H), 7.75-7.69 (m, 2H), 7.34 (t, J = 8.0 Hz, 1H), 6.94 (dd, J = 8.3, 2.3 Hz, 1H), 6.82 (d, J = 7.6 Hz, 1H), 6.78-6.77 (m, 1H), 3.77 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.4, 178.2, 159.2, 149.7, 139.2, 135.3, 134.4, 134.1, 131.6, 129.3, 127.5, 127.4, 121.3, 114.9, 114.7, 55.3; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{12}BrO_3]^+$ 342.9970, found 342.9982.



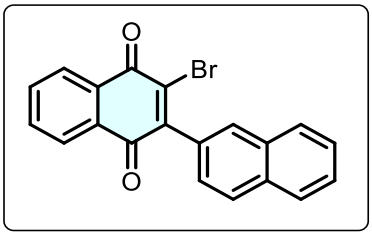
2-Bromo-3-(3-fluorophenyl)naphthalene-1,4-dione (3o) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3o** as a yellow solid (71.29 mg, 78%); mp 102-104 °C; IR (ATR, neat) ν (cm^{-1}): 1670 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.19-8.14 (m, 1H), 8.11-8.05 (m, 1H), 7.77-7.70 (m, 2H), 7.40 (td, J = 8.0, 5.8 Hz, 1H), 7.10 (tdd, J = 8.5, 2.6, 0.9 Hz, 1H), 7.05-7.02 (m, 1H), 6.98 (ddd, J = 9.3, 2.5, 1.6 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.2, 178.0, 162.3 (d, $J_{C\text{-}F}$ = 247.8 Hz, 1C), 148.6, 139.6, 135.9, 135.8, 134.5, 134.2, 131.2 (d, $J_{C\text{-}F}$ = 39.7 Hz, 1C), 129.8 (d, $J_{C\text{-}F}$ = 2.9 Hz, 1C), 127.6, 127.4, 124.9 (d, $J_{C\text{-}F}$ = 2.9 Hz, 1C), 116.5 (d, $J_{C\text{-}F}$ = 11.6 Hz, 1C), 116.3 (d, $J_{C\text{-}F}$ = 8.7 Hz, 1C); ^{19}F NMR (376 MHz, $CDCl_3$) δ –112.73 (s); HRMS (ESI) $[M+H]^+$ Calcd for $[C_{16}H_9BrFO_2]^+$ 330.9770, found 330.9785.



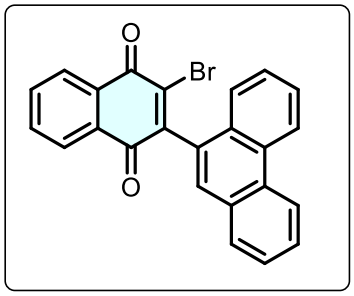
2-Bromo-3-(3-bromophenyl)naphthalene-1,4-dione (3p) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3p** as a yellow solid (81.15 mg, 75%); mp 106-108 °C; IR (ATR, neat) ν (cm^{-1}): 1662 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.19-8.14 (m, 1H), 8.10-8.05 (m, 1H), 7.77-7.70 (m, 2H), 7.54 (dq, *J* = 8.0, 1.0 Hz, 1H), 7.41 (t, *J* = 1.7 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 1H), 7.19 (dt, *J* = 7.6, 1.3 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.2, 177.9, 148.3, 139.6, 135.8, 134.6, 134.2, 132.3, 132.0, 131.4, 131.0, 129.7, 127.8, 127.7, 127.4, 122.0; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{16}H_9Br_2O_2]^+$ 390.8969, found 390.8973.



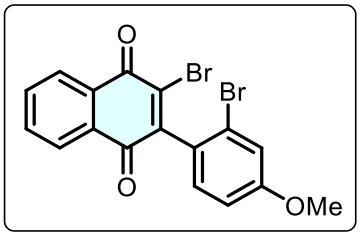
2-Bromo-3-(4-butylphenyl)naphthalene-1,4-dione (3q) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3q** as a orange solid (96.69 mg, 90%); mp 114-116 °C; IR (ATR, neat) ν (cm^{-1}): 1662 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.12-8.07 (m, 1H), 8.05-8.00 (m, 1H), 7.68-7.62 (m, 2H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.54-7.52 (m, 2H), 7.29-7.38 (m, 4H), 7.23-7.29 (m, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.5, 178.0, 149.3, 142.0, 140.2, 138.9, 134.3, 134.0, 132.7, 131.4, 131.0, 129.8, 128.8, 127.7, 127.4, 127.3, 127.1, 126.6; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{14}BrO_2]^+$ 389.0177, found 389.0171.



3-Bromo-[2,2'-binaphthalene]-1,4-dione (3r) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3r** as a red solid (85.21 mg, 85%); mp 116-118 °C; IR (ATR, neat) ν (cm^{-1}): 1664 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.17-8.11 (m, 1H), 8.10-8.09 (m, 1H), 7.88-7.82 (m, 3H), 7.77-7.71 (m, 3H), 7.49-7.48 (m, 2H), 7.35 (dd, *J* = 5.6, 1.6 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.7, 178.2, 149.7, 139.3, 134.4, 134.1, 133.4, 132.6, 131.5, 131.4, 131.1, 129.2, 128.5, 127.8, 127.7, 127.6, 127.4, 127.1, 126.5, 126.3; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{20}H_{12}BrO_2]^+$ 363.0021, found 363.0025.

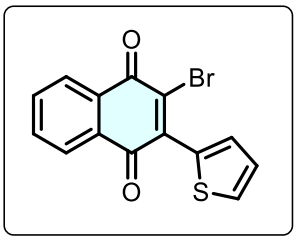


2-Bromo-3-(phenanthren-9-yl)naphthalene-1,4-dione (3s) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3s** as a red solid (99.23 mg, 87%); mp 120-122 °C; IR (ATR, neat) ν (cm^{-1}): 1662 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.69 (q, *J* = 8.5 Hz, 2H), 8.25-8.21 (m, 1H), 8.11-8.08 (m, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.76-7.71 (m, 2H), 7.67-7.54 (m, 5H), 7.47 (t, *J* = 7.5 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.5, 178.0, 150.1, 141.3, 134.5, 134.2, 131.7, 131.3, 131.2, 130.8, 130.7, 130.4, 129.1, 128.8, 127.7, 127.6, 127.5, 127.0, 127.0, 125.3, 123.3, 122.7; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{24}H_{14}BrO_2]^+$ 413.0177, found 413.0184.

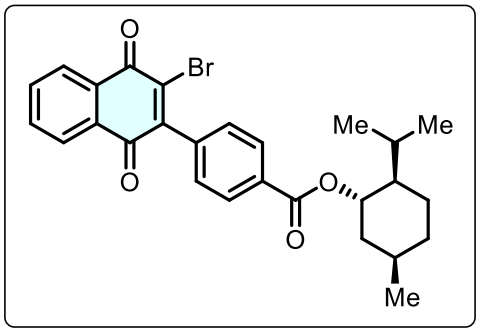


2-Bromo-3-(2-bromo-4-methoxyphenyl)naphthalene-1,4-dione (3t) The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3t** as a orange solid (83.87 mg, 72%); mp 128-130 °C; IR (ATR, neat) ν (cm^{-1}): 1666 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.21-8.15 (m, 1H), 8.12-8.08 (m, 1H), 7.77-7.71 (m, 2H), 7.50 (d, *J* = 8.9 Hz, 1H), 6.82 (dd, *J* = 8.9, 3.0 Hz, 1H), 6.68 (d, *J* = 3.0 Hz, 1H), 3.75 (s, 3H); ^{13}C-NMR (100 MHz,

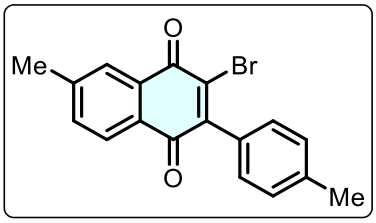
$CDCl_3$) δ 180.4, 177.9, 158.8, 149.9, 140.3, 136.7, 134.5, 134.2, 133.5, 131.5, 131.1, 127.7, 127.5, 116.5, 115.2, 112.1, 55.6; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{11}Br_2O_3]^+$ 420.9075, found 420.9072.



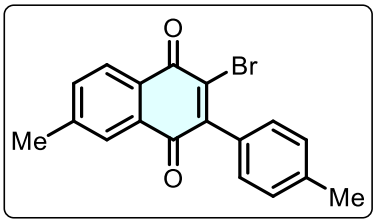
2-Bromo-3-(thiophen-2-yl)naphthalene-1,4-dione (3u) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3u** as a orange solid (57.26 mg, 65%); mp 90-92 °C; IR (ATR, neat) ν (cm^{-1}): 1666 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.22-8.16 (m, 1H), 8.16-8.11 (m, 1H), 7.80-7.74 (m, 2H), 7.68 (q, *J* = 1.4 Hz, 1H), 7.42 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.30 (dd, *J* = 5.0, 1.3 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.4, 178.2, 144.7, 138.1, 134.3, 134.1, 132.9, 131.6, 131.0, 129.3, 129.1, 127.5, 127.4, 124.6; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{14}H_8BrO_2S]^+$ 318.9428, found 318.9441.



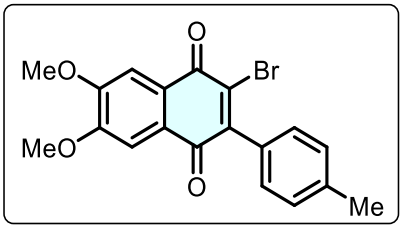
2-Isopropyl-5-methylcyclohexyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl) benzoate (3v) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3v** as a yellow solid (92.97 mg, 68%); mp 90-92 °C; IR (ATR, neat) ν (cm^{-1}): 1707 (s, C=O ester), 1672 (s, C=O ketone); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.19-8.15 (m, 1H), 8.11-8.06 (m, 3H), 7.76-7.71 (m, 2H), 7.33 (dd, *J* = 6.7, 1.7 Hz, 2H), 4.90 (td, *J* = 10.9, 4.4 Hz, 1H), 2.10-2.06 (m, 1H), 1.97-1.88 (m, 1H), 1.69-1.65 (m, 2H), 1.55-1.47 (m, 3H), 1.13-1.00 (m, 2H), 0.87 (dd, *J* = 6.8, 3.0 Hz, 7H), 0.75 (s, 1H), 0.73 (s, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.1, 177.7, 165.3, 149.0, 139.3, 138.2, 134.4, 134.1, 131.5, 131.4, 131.0, 129.3, 129.1, 127.5, 127.3, 113.6, , 75.1, 47.2, 40.9, 34.2, 31.4, 26.4, 23.5, 22.0, 20.7, 16.4; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{27}H_{28}BrO_4]^+$ 495.1171, found 495.1165.



3-Bromo-6-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3w) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3w** as a yellow solid (84.75 mg, 90%); mp 92-94 °C; IR (ATR, neat) ν (cm^{-1}): 1658 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.90 (t, *J* = 8.1 Hz, 2H), 7.46 (dd, *J* = 7.8, 0.9 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.16-7.13 (m, 2H), 2.42 (s, 3H), 2.33 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.3, 178.4, 149.6, 145.2, 139.3, 138.4, 134.9, 131.1, 130.9, 129.2, 129.1, 129.0, 128.7, 127.7, 127.4, 21.8, 21.4; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{18}H_{14}BrO_2]^+$ 341.0177, found 341.0185.

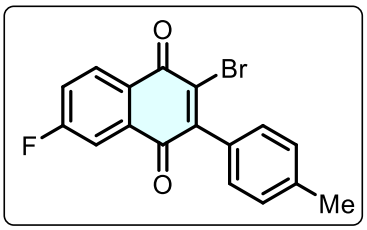


3-Bromo-6-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3x) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3x** as a orange solid (83.81 mg, 89%); mp 92-94°C; IR (ATR, neat) ν (cm^{-1}): 1656 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.8 Hz, 1H), 7.80 (s, 1H), 7.44 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.15-7.12 (m, 2H), 2.40 (s, 3H), 2.33 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.7, 177.8, 149.4, 145.5, 139.2, 138.8, 134.6, 131.3, 131.1, 129.1, 128.7, 128.7, 127.5, 127.5, 21.8, 21.4; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{18}H_{14}BrO_2]^+$ 341.0177, found 341.0196.

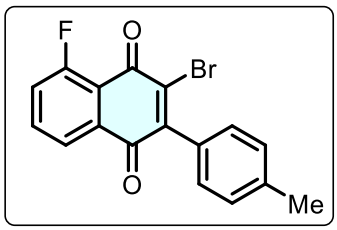


2-Bromo-6,7-dimethoxy-3-(*p*-tolyl)naphthalene-1,4-dione (3y) The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3y** as a orange solid (99.39 mg, 93%); mp 104-106 °C; IR (ATR, neat) ν (cm^{-1}): 1656 (s, C=O); ^{1}H-NMR (400 MHz,

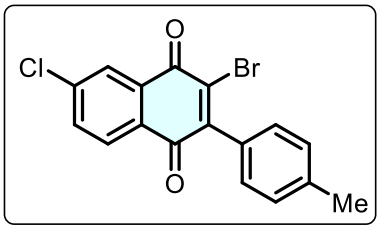
$CDCl_3$) δ 7.49 (s, 1H), 7.41 (s, 1H), 7.22-7.19 (m, 2H), 7.15 (d, J = 8.2 Hz, 2H), 3.95 (s, 3H), 3.92 (s, 3H), 2.35 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.0, 177.5, 153.7, 153.4, 149.1, 139.3, 138.0, 131.2, 129.2, 128.7, 126.2, 125.7, 108.7, 108.4, 56.5, 56.5, 21.4; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{19}H_{16}BrO_4]^+$ 387.0232, found 387.0235.



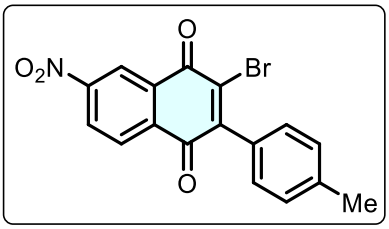
2-Bromo-6-fluoro-3-(*p*-tolyl)naphthalene-1,4-dione (3z) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3z** as a yellow solid (79.07 mg, 83%); mp 104-106 °C; IR (ATR, neat) ν (cm^{-1}): 1660 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, J = 8.6, 5.2 Hz, 1H), 7.67 (dd, J = 8.5, 2.6 Hz, 1H), 7.35-7.31 (m, 1H), 7.21 (d, J = 8.0 Hz, 2H), 7.13 (dd, J = 6.4, 1.7 Hz, 2H), 2.34 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 180.5, 176.9, 166.2 (d, $J_{C\text{-}F}$ = 260.4 Hz, 1C), 149.8, 139.6, 139.0, 134.2, 134.1,130.7 (d, $J_{C\text{-}F}$ = 7.8 Hz, 1C), 129.1, 128.8, 127.6, 121.3, 121.1, 114.0 (d, $J_{C\text{-}F}$ = 24.1 Hz, 1C), 21.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ –100.46 (s); HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{11}BrFO_2]^+$ 344.9926, found 344.9924.



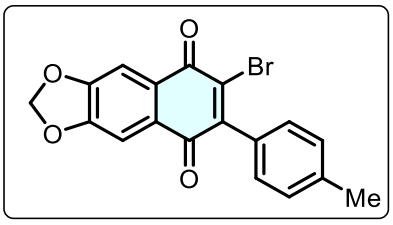
3-Bromo-5-fluoro-2-(*p*-tolyl)naphthalene-1,4-dione (3aa) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3aa** as a yellow solid (80.98 mg, 85%); mp 106-108 °C; IR (ATR, neat) ν (cm^{-1}): 1662 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, J = 7.7, 1.0 Hz, 1H), 7.66 (td, J = 8.0, 4.6 Hz, 1H), 7.38 (ddd, J = 10.6, 8.4, 1.1 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 7.13 (dd, J = 6.3, 1.8 Hz, 2H), 2.34 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 180.6, 175.6, 160.9 (d, $J_{C\text{-}F}$ = 271.9 Hz, 1C), 148.8, 139.7 , 135.8, 135.7 (d, $J_{C\text{-}F}$ = 27.1 Hz, 1C), 133.2, 130.7, 129.0, 128.8, 123.7, 123.7, 122.9, 122.7, 118.7 (d, $J_{C\text{-}F}$ = 4.8 Hz, 1C), 21.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ –110.19 (s); HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{11}BrFO_2]^+$ 344.9926, found 344.9924.



3-Bromo-6-chloro-2-(*p*-tolyl)naphthalene-1,4-dione (3ab) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3ab** as a yellow solid (77.85 mg, 78%); mp 108-110 °C; IR (ATR, neat) ν (cm^{-1}): 1660 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 2.0 Hz, 1H), 7.99 (d, *J* = 8.3 Hz, 1H), 7.63 (dd, *J* = 8.3, 2.3 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.3 Hz, 2H), 2.34 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 180.6, 177.3, 149.9, 141.0, 139.7, 138.3, 134.3, 132.1, 130.7, 129.7, 129.1, 129.0, 128.8, 127.3, 21.5; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{11}BrClO_2]^+$ 360.9631, found 360.9635.

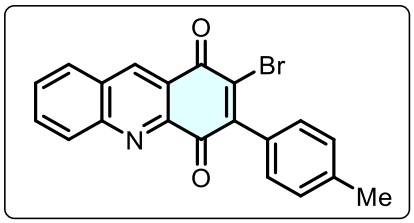


3-Bromo-6-nitro-2-(*p*-tolyl)naphthalene-1,4-dione (3ac) The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3ac** as a yellow solid (61.63 mg, 60%); mp 116-118 °C; IR (ATR, neat) ν (cm^{-1}): 1664 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.94 (d, *J* = 2.2 Hz, 1H), 8.52 (dd, *J* = 8.5, 2.3 Hz, 1H), 8.28 (d, *J* = 8.5 Hz, 1H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.19-7.16 (m, 2H), 2.37 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 180.1, 176.5, 151.0, 150.3, 140.1, 139.3, 135.0, 132.1, 130.3, 129.3, 129.1, 128.9, 128.3, 122.7, 21.5; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{11}BrNO_4]^+$ 371.9871, found 371.9879.

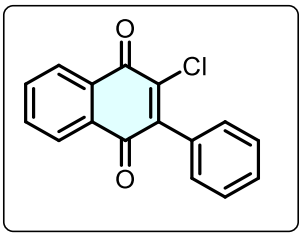


6-Bromo-7-(*p*-tolyl)naphtho[2,3-*d*][1,3]dioxole-5,8-dione (3ad) The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3ad** as a orange solid (88.10 mg, 86%); mp 106-108 °C; IR (ATR, neat) ν (cm^{-1}): 1658 (s, C=O); ^{1}H-NMR (400

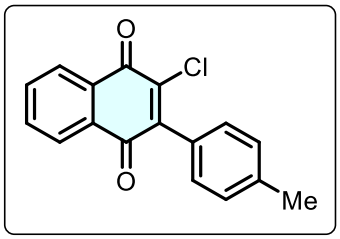
MHz, $CDCl_3$) δ 7.47 (s, 1H), 7.39 (s, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.14 (dd, *J* = 6.4, 1.9 Hz, 2H), 6.08 (s, 2H), 2.35 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 180.6, 177.1, 152.7, 152.4, 149.0, 139.4, 138.0, 131.0, 129.2, 128.7, 128.6, 128.0, 106.7, 106.5, 102.8, 21.5; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{18}H_{12}BrO_4]^+$ 370.9919, found 370.9918.



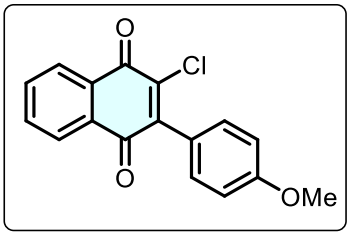
2-Bromo-3-(*p*-tolyl)acridine-1,4-dione (3ae) The crude product was purified by column chromatography (hexane/EtOAc = 85/15) to afford **3ae** as a yellow solid (67.85 mg, 65%); mp 148-150 °C; IR (ATR, neat) ν (cm^{-1}): 1668 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.38 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.2 Hz, 1H), 7.92-7.88 (m, 1H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.27-7.22 (m, 3H), 7.19 (s, 1H), 2.38 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 179.8, 177.7, 151.7, 150.0, 146.0, 139.9, 139.8, 138.0, 133.6, 131.6, 130.9, 130.2, 129.6, 129.3, 128.9, 128.7, 124.7, 21.6; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{20}H_{13}BrNO_2]^+$ 378.0130, found 378.0129.



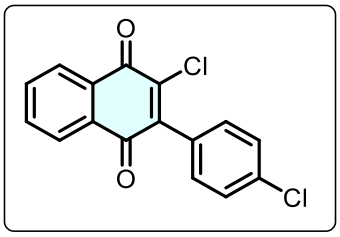
2-Chloro-3-phenylnaphthalene-1,4-dione (5a). The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **5a** as a yellow solid (74.99 mg, 75%); mp 94-96 °C; IR (ATR, neat) ν (cm^{-1}): 1668 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.16-8.12 (m, 1H), 8.10-8.05 (m, 1H), 7.74-7.69 (m, 2H), 7.44-7.37 (m, 3H), 7.30-7.26 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 182.1, 178.2, 145.9, 143.1, 134.4, 134.1, 131.8, 131.6, 131.3, 129.5, 129.4, 128.1, 127.3, 127.2; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{16}H_{10}ClO_2]^+$ 269.0369, found 269.0376.



2-Chloro-3-(*p*-tolyl)naphthalene-1,4-dione (5b). The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **5b** as a yellow solid (80.52 mg, 78%); mp 94-96 °C; IR (ATR, neat) ν (cm^{-1}): 1660 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.17-8.13 (m, 1H), 8.11-8.06 (m, 1H), 7.74-7.69 (m, 2H), 7.25-7.18 (m, 4H), 2.36 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 182.2, 178.3, 146.0, 142.8, 139.7, 134.4, 134.0, 131.7, 131.4, 129.6, 128.8, 127.3, 127.2, 21.5; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{12}ClO_2]^+$ 283.0526, found 283.0526.

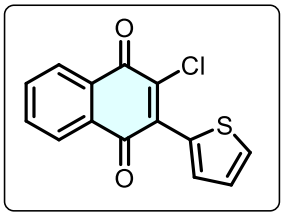


2-Chloro-3-(4-methoxyphenyl)naphthalene-1,4-dione (5c). The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **5c** as an orange solid (86.98 mg, 80%); mp 96-98 °C; IR (ATR, neat) ν (cm^{-1}): 1660 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.18-8.13 (m, 1H), 8.11-8.07 (m, 1H), 7.74-7.70 (m, 2H), 7.30-7.26 (m, 2H), 6.98-6.92 (m, 2H), 3.81 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 182.4, 178.4, 160.5, 145.5, 142.4, 134.3, 134.0, 131.8, 131.6, 131.4, 127.3, 127.1, 123.8, 113.5, 55.3; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{12}ClO_3]^+$ 299.0475, found 299.0487.



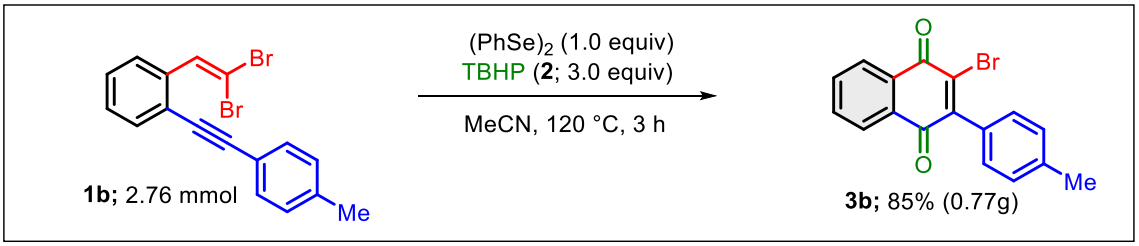
2-Chloro-3-(4-chlorophenyl)naphthalene-1,4-dione (5d). The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **5d** as a yellow solid (77.13 mg, 70%); mp 94-96 °C; IR (ATR, neat) ν (cm^{-1}): 1670 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.16-8.12 (m, 1H), 8.09-8.05 (m, 1H), 7.75-7.69 (m, 2H), 7.41-7.38 (m, 2H), 7.25-7.21 (m,

2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 181.8, 177.9, 144.8, 143.3, 135.6, 134.5, 134.2, 131.5, 131.2, 131.1, 130.0, 128.4, 127.3, 127.3; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{16}H_9Cl_2O_2]^+$ 302.9980, found 302.9981.



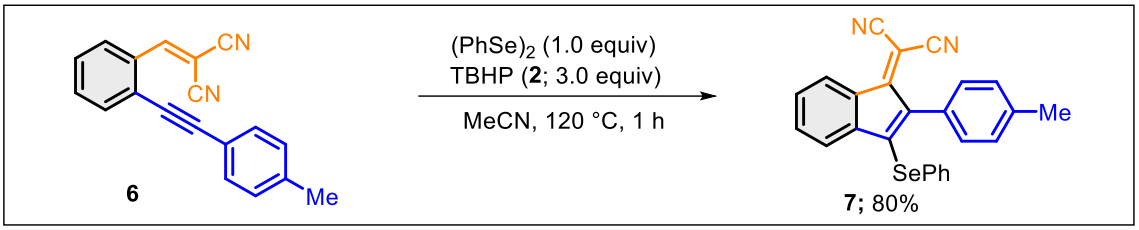
2-chloro-3-(thiophen-2-yl)naphthalene-1,4-dione (5e). The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **5e** as an orange solid (68.45 mg, 68%); mp 94-96 °C; IR (ATR, neat) ν (cm^{-1}): 1666 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15-8.11 (m, 1H), 8.10-8.08 (m, 1H), 7.74-7.69 (m, 2H), 7.68 (dd, J = 2.8, 1.2 Hz, 1H), 7.35 (dd, J = 5.0, 3.0 Hz, 1H), 7.28 (dd, J = 5.1, 1.1 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) 182.0, 178.2, 141.9, 140.7, 134.4, 134.1, 131.7, 131.2, 130.9, 130.1, 129.3, 127.3, 127.1, 124.5; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{14}H_8ClO_2S]^+$ 274.9934, found 274.9940.

3.1. Gram Scale Synthesis of 3b:

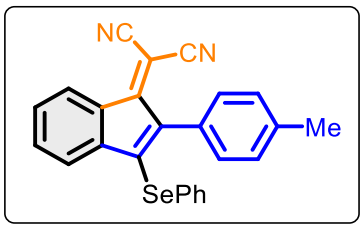


To an oven dried sealed tube, 1-(2,2-dibromovinyl)-2-(*p*-tolyl)benzene (**1b**, 2.76 mmol, 1.0 equiv), diphenyl selenide (2.76 mmol, 1.0 equiv) in MeCN was added. Then, 3.0 equiv (8.28 mmol; 0.01 M) of TBHP (**2**) was added to the reaction mixture. The reaction mixture was then stirred at 120 °C for 3 h in an oil bath. The reaction was monitored using thin layer chromatography. After completion of the reaction, the reaction mixture was allowed to cool. Then, organic layer was washed with aqueous saturated brine solution and finally extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum. The crude material obtained was purified by column chromatography on silica gel (100−200 mesh) (hexane: ethyl acetate; 98/02) to afford the corresponding product **3b** in 85% yield (0.77 g).

4. General Procedure for the Synthesis of 2-(3-(Phenylselanyl)-2-(*p*-tolyl)-1*H*-inden-1-ylidene)malononitrile (7):

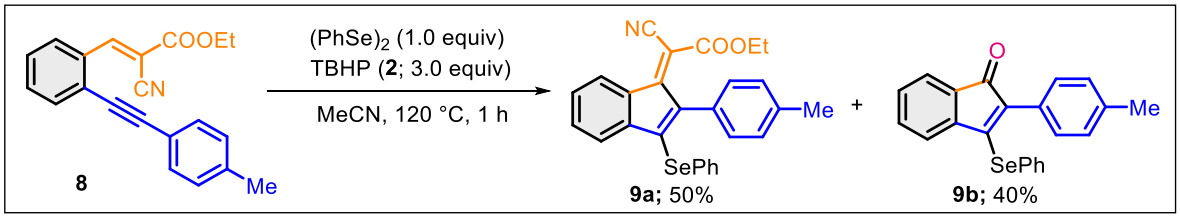


To an oven dried sealed tube, 2-(2-(*p*-tolylethynyl)benzylidene)malononitrile (**6**, 0.373 mmol, 1.0 equiv), diphenyl selenide (0.373 mmol, 1.0 equiv) in 2.0 ml MeCN was added. Then, 3.0 equiv (1.119 mmol; 0.01 M) of TBHP (**2**) was added to the reaction mixture. The reaction mixture was then stirred at 120 °C for 1 h in an oil bath. The reaction was monitored using thin layer chromatography. After completion of the reaction, the reaction mixture was allowed to cool. Then, organic layer was washed with aqueous saturated brine solution and finally extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum. The crude material obtained was purified by column chromatography on silica gel (100−200 mesh) (hexane: ethyl acetate; 98/02) to afford the corresponding product **7.**

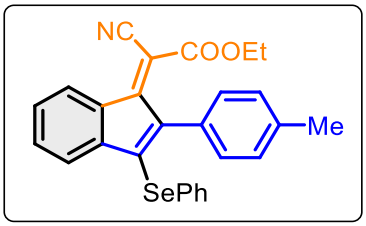


2-(3-(Phenylselanyl)-2-(*p*-tolyl)-1*H*-inden-1-ylidene)malononitrile (7). The crude product was purified by column chromatography (hexane/EtOAc = 98/2) to afford **7** as a deep red solid (126.23 mg, 80%); IR (ATR, neat) ν (cm^{-1}): 2223 (s, CN), 2213 (s, CN); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.16-8.12 (m, 1H), 7.38-7.36 (m, 2H), 7.28-7.23 (m, 1H), 7.20-7.10 (m, 6H), 7.08-7.05 (m, 2H), 6.63-6.59 (m, 1H), 2.34 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 160.5, 150.3, 141.0, 138.6, 133.4, 131.8, 128.9, 128.5, 127.8, 127.7, 127.6, 125.4, 123.5, 122.1, 113.1, 110.5, 21.7; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{25}H_{17}N_2Se]^+$ 425.0557, found 425.0567.

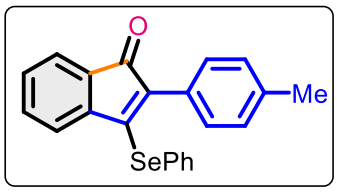
5. General Procedure for the Synthesis of 9a and 9b:



To an oven dried sealed tube, ethyl (*E*)-2-cyano-3-(2-(*p*-tolylethynyl)phenyl)acrylate (**8**, 0.317 mmol, 1.0 equiv), diphenyl selenide (0.317 mmol, 1.0 equiv) in 2.0 ml MeCN was added. Then, 3.0 equiv (0.951 mmol; 0.01M) of TBHP (**2**) was added to the reaction mixture. The reaction mixture was then stirred at 120 °C for 1 h in an oil bath. The reaction was monitored using thin layer chromatography. After completion of the reaction, the reaction mixture was allowed to cool. Then, organic layer was washed with aqueous saturated brine solution and finally extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum. The crude material obtained was purified by column chromatography on silica gel (100−200 mesh) (hexane: ethyl acetate; 98/02) to afford the corresponding product **9a-b.**



Ethyl (*Z*)-2-cyano-2-(3-(phenylselanyl)-2-(*p*-tolyl)-1H-inden-1-ylidene)acetate (9a). The crude product was purified by column chromatography (hexane/EtOAc = 98/2) to afford **9a** as a deep red solid (74.76 mg, 50%); IR (ATR, neat) ν (cm^{-1}): 2210 (s, CN), 1724 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 7.6 Hz, 1H), 7.31-7.28 (m, 2H), 7.18-7.03 (m, 9H), 6.72 (d, *J* = 7.0 Hz, 1H), 3.42 (q, *J* = 7.2 Hz, 2H), 2.29 (s, 3H), 1.00 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 161.6, 153.6, 145.3, 142.2, 141.6, 138.0, 133.8, 132.9, 131.4, 131.3, 129.5, 129.3, 128.7, 128.1, 128.0, 127.8, 123.7, 122.8, 116.1, 100.0, 62.7, 21.3, 13.5; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{27}H_{22}NO_2Se]^+$ 472.0816, found 472.0803.

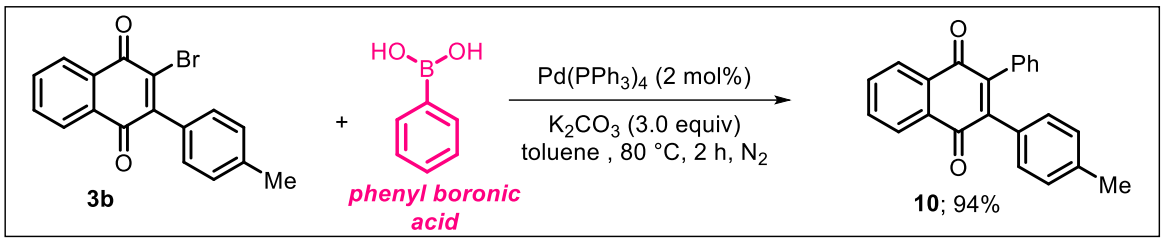


3-(Phenylselanyl)-2-(p-tolyl)-1H-inden-1-one (9b). The crude product was purified by column chromatography (hexane/EtOAc = 98/2) to afford **9b** as an orange liquid (23.93 mg, 40%); IR (ATR, neat) ν (cm^{-1}): 1670 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.56-7.54 (m, 1H), 7.40-7.37 (m, 2H), 7.35-7.29 (m, 2H), 7.20-7.05 (m, 7H), 6.62-6.58 (m, 1H), 2.29 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 193.2, 150.0, 144.4, 138.5, 138.4, 133.5, 133.3, 132.7, 130.7,

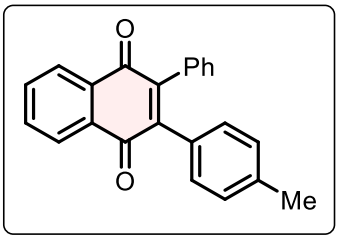
130.4, 129.7, 129.6, 129.3, 128.7, 128.6, 128.0, 127.5, 122.5, 121.9, 21.4; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{22}H_{17}OSe]^+$ 377.0445, found 377.0443.

6. General Procedure for Synthetic Applications of Product 3b.

(6a) Suzuki Coupling Reaction:

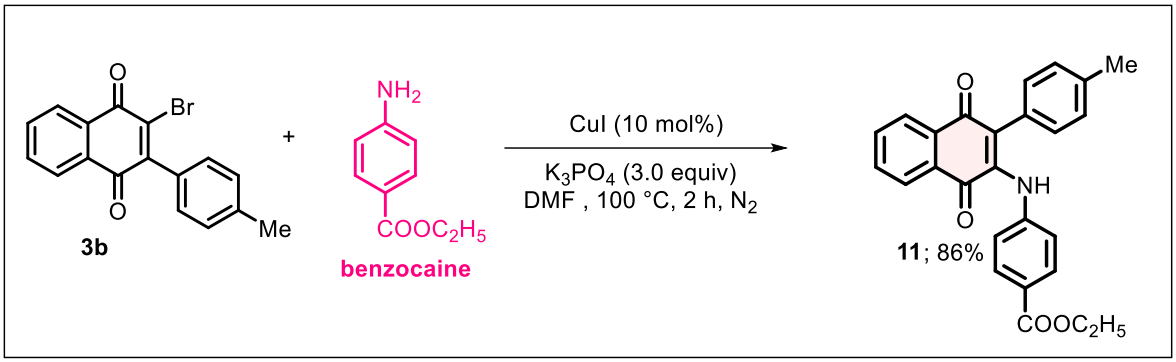


In an oven dried 25 mL round bottom flask, **3b** (0.266 mmol, 1.0 mmol) was taken, to this phenyl boronic acid (0.319 mmol, 1.2 equiv), $Pd(PPh_3)_4$ (2 mol%, 0.02 equiv) and K_2CO_3 (0.798 mmol, 3.0 equiv) was added in 2 mL of toluene. The reaction mixture was then purged with nitrogen and stirred at 80 °C for 2 h. Progress of reaction was monitored with TLC. After the consumption of starting material, the reaction mixture was washed with brine, extracted with ethyl acetate, and evaporated. The residue was purified by column chromatography (hexane/ethyl acetate) (95/5) to afford the corresponding coupled product **10**.

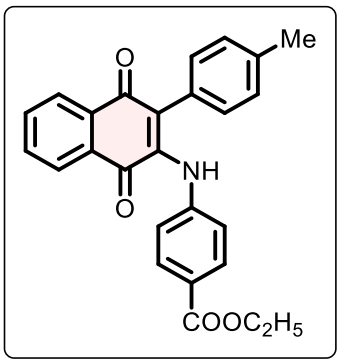


2-Phenyl-3-(*p*-tolyl)naphthalene-1,4-dione (10) The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **10** as a orange solid (81.12 mg, 94%); mp 134-136 °C; IR (ATR, neat) ν (cm^{-1}): 1654 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.13-8.08 (m, 2H), 7.72-7.68 (m, 2H), 7.18-7.14 (m, 3H), 7.04-7.00 (m, 2H), 6.95 (d, J = 8.0 Hz, 2H), 6.89 (dd, J = 6.4, 1.9 Hz, 2H), 2.21 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 184.9, 184.8, 145.7, 145.4, 138.2, 133.7, 133.4, 132.1, 132.1, 130.5, 130.1, 128.4, 128.1, 127.6, 126.6, 126.5, 21.3; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{23}H_{17}O_2]^+$ 325.1229 , found 325.1235.

(6b) Buchwald Coupling Reaction:

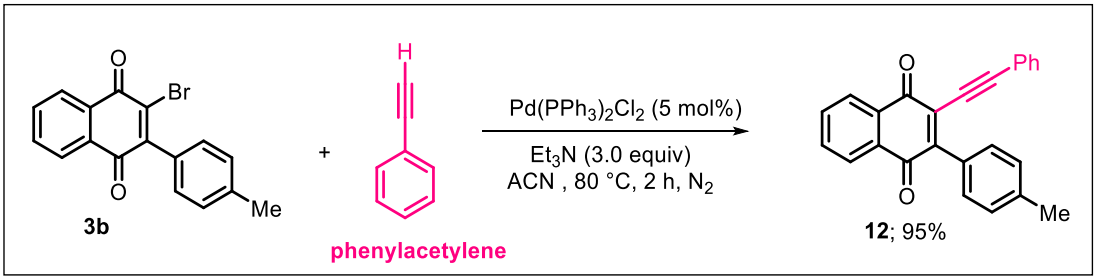


In an oven dried 25 mL round bottom flask, **3b** (0.266 mmol, 1.0 mmol) was taken, to this benzocaine (0.319 mmol, 1.2 equiv), CuI (10 mol%, 0.1 equiv) and K_3PO_4 (0.798 mmol, 3.0 equiv) was added in 2 mL of DMF. The reaction mixture was then purged with nitrogen and stirred at 100 °C for 2 h. Progress of reaction was monitored with TLC. After the consumption of starting material, the reaction mixture was washed with brine, extracted with ethyl acetate, and evaporated. The residue was purified by column chromatography (hexane/ethyl acetate) (95/5) to afford the corresponding coupled product **11**.

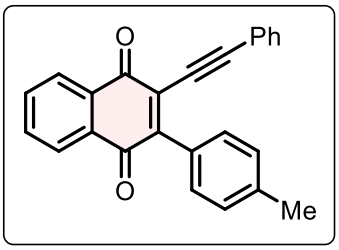


Ethyl 4-((1,4-dioxo-3-(*p*-tolyl)-1,4-dihydronaphthalen-2-yl)amino)benzoate (11) The product was obtained as a red solid (94.12 mg, 86%); mp 96-98 °C; IR (ATR, neat) ν (cm^{-1}): 3311 (s, N-H), 1704 (s, C=O ester), 1664 (s, C=O ketone); ^{1}H-NMR (400 MHz, DMSO-d_6) δ 9.12 (s, 1H), 8.08 (dd, J = 19.0, 7.2 Hz, 2H), 7.87 (dt, J = 22.7, 7.1 Hz, 2H), 7.44 (d, J = 8.5 Hz, 2H), 6.97-6.79 (m, 6H), 4.22 (q, J = 7.1 Hz, 2H), 2.12 (s, 3H), 1.26 (t, J = 7.1 Hz, 3H); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 182.6, 182.1, 165.3, 143.6, 141.3, 136.4, 134.7, 133.1, 132.5, 130.5, 130.1, 128.6, 127.7, 126.0, 125.8, 122.7, 121.5, 120.5, 60.2, 20.7, 14.2; HRMS (ESI) $[M+Na]^+$ Calcd for $[C_{26}H_{21}NNaO_4]^+$ 434.1368, found 434.1381.

(6c) Sonogashira Coupling Reaction:

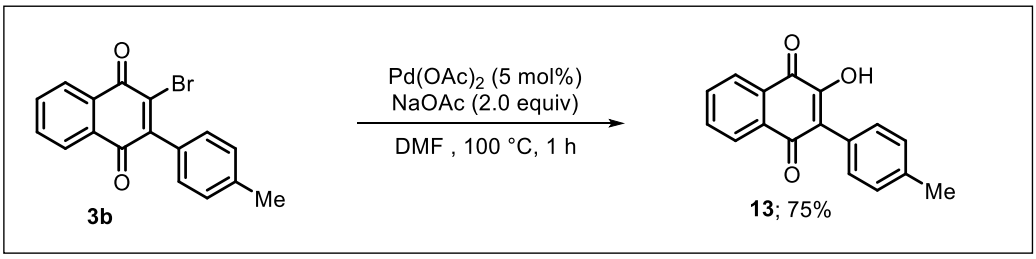


In an oven dried 25 mL round bottom flask, **3b** (0.266 mmol, 1.0 equiv) was taken, to this $Pd(PPh_3)_2Cl_2$ (5 mol%, 0.05 equiv) and phenylacetylene (0.319 mmol, 1.2 equiv) in 3.0 Ml MeCN was added. The reaction mixture was then purged with nitrogen and to this Et_3N (0.798 mmol, 3.0 equiv) was added. The reaction mixture was then stirred at 60 °C for 2 h. Progress of reaction was monitored with TLC. After the consumption of starting material, the reaction mixture was quenched with brine, extracted with ethyl acetate, and evaporated. The residue was purified by column chromatography (hexane/ethyl acetate) (95/5) to afford the corresponding coupled product **12**.

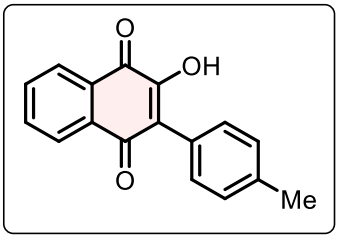


2-(Phenylethynyl)-3-(*p*-tolyl)naphthalene-1,4-dione (12) The product was obtained as a yellow liquid (88.04 mg, 95%); IR (ATR, neat) ν (cm^{-1}): 2213 (s, C≡C), 1666 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.09-8.02 (m, 2H), 7.67-7.62 (m, 2H), 7.43 (dd, *J* = 6.5, 1.7 Hz, 2H), 7.31-7.28 (m, 2H), 7.27-7.18 (m, 5H), 2.35 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 183.5, 181.8, 148.2, 139.7, 134.0, 133.6, 132.2, 132.1, 131.7, 130.5, 129.9, 129.8, 129.5, 128.3, 126.8, 126.5, 122.1, 105.8, 84.5, 21.5; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{25}H_{17}O_2]^+$ 349.1229, found 349.1225.

(6d) Functional group interconversion:



In an oven dried 25 mL round bottom flask, **3b** (0.266 mmol, 1.0 equiv) was taken, to this $Pd(OAc)_2$ (5 mol%, 0.05 equiv), NaOAc (0.532 mmol, 2.0 equiv) in 3.0 mL DMF was added. The reaction mixture was then stirred at 100 °C for 12 h. Progress of reaction was monitored with TLC. After the consumption of starting material, the reaction mixture was quenched with brine, extracted with ethyl acetate, and evaporated. The residue was purified by column chromatography (hexane/ethyl acetate) (90/10) to afford the corresponding coupled products **13**.



2-hydroxy-3-(*p*-tolyl)naphthalene-1,4-dione (13) The product was obtained as a yellow solid (52.72 mg, 75%); mp 146-148 °C; IR (ATR, neat) ν (cm^{-1}): 3350 (br, O-H), 1647 (s, C=O); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 7.6, 0.9 Hz, 1H), 8.07 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.73 (td, *J* = 7.5, 1.3 Hz, 1H), 7.66 (td, *J* = 7.5, 1.3 Hz, 1H), 7.51 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 2.33 (s, 3H) ; ^{13}C-NMR (100 MHz, $CDCl_3$) δ 183.8, 181.8, 152.0, 138.7, 135.2, 133.1, 132.8, 130.5, 129.3, 128.7, 127.2, 126.9, 126.1, 122.2, 21.4; HRMS (ESI) $[M+H]^+$ Calcd for $[C_{17}H_{13}O_3]^+$ 265.0865 , found 265.0871.

7. References:

1. Claus; V.; Monilari, L.; Büllmann, S.; Thusek, J.; Rudolph, M.; Rominger, F.; Hashmi; S. K. Gold Catalyzed Cyclisation by 1,4-Dioxidation. *Chem. Eur. J.* **2019**, *25*, 9385 – 9389.

2. Ye, X.; Yang, X.; Wu, J. Rapid access to 1-methyleneindenes via palladium-catalyzed tandem reactions of 1-(2,2-dibromovinyl)-2-alkynylbenzenes with arylboronic acids. *Chem. Commun*. **2010**, *46*, 2950–2952.

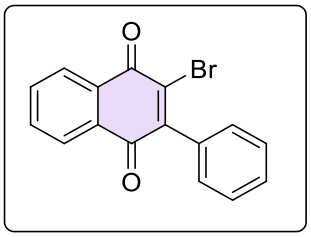
3. Wurm, T.; Bucher, J.; Duckworth, S. B.; Rudolph, M.; Rominger, F.; Hashmi, A. S. K., On the Gold Catalyzed Generation of Vinyl Cations from 1,5-Diynes. *Angew. Chem*. **2017**, *56*, 3364-3368.

4. Rivera-Fuentes, P.; Rekowski, M. v. W.; Schweizer, W. B.; Gisselbrecht, J.-P.; Boudon, C.; Diederich, F., Cascade Carbopalladation Reaction between Alkynes and *gem*-Dibromoolefins: Facile Access to Monoannelated Pentalenes. *Org. Lett*. **2012**, *14*, 4066-4069.

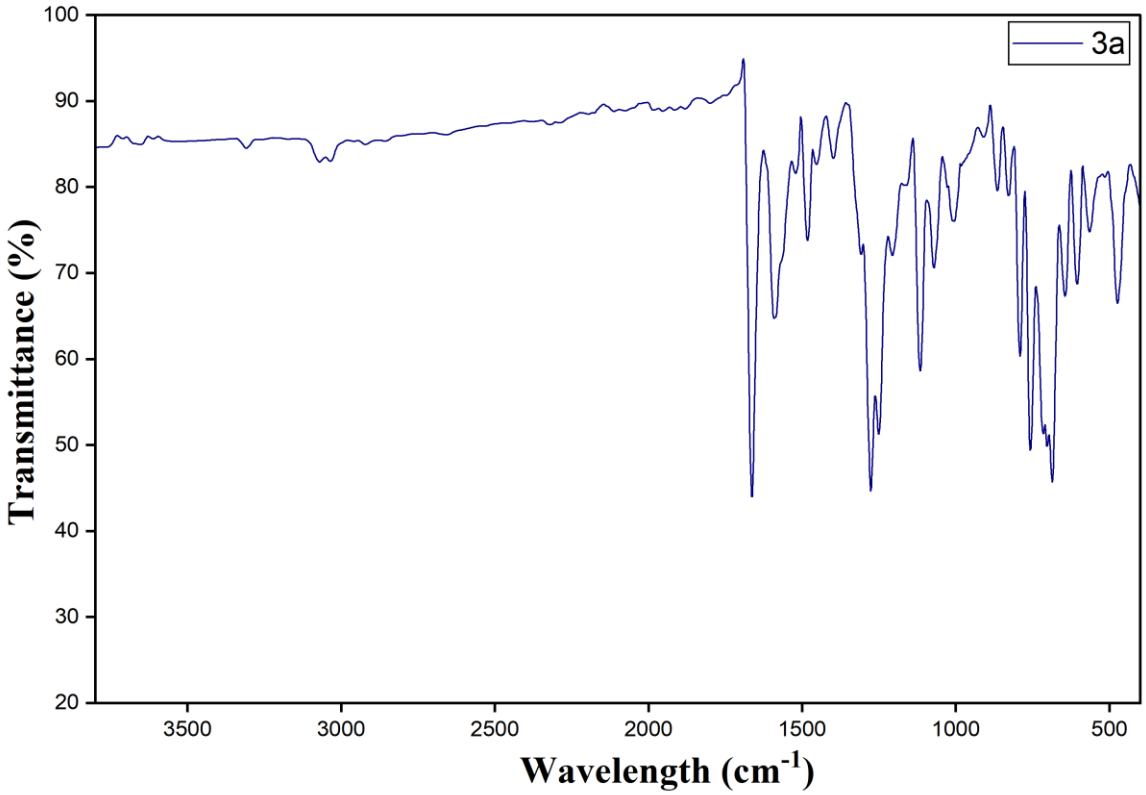
5. London, G.; von Wantoch Rekowski, M.; Dumele, O.; Schweizer, W. B.; Gisselbrecht, J.-P.; Boudon, C.; Diederich, F., Pentalenes with Novel Topologies: Exploiting the Cascade Carbopalladation Reaction Between Alkynes and *gem*-Dibromoolefins. *Chem. Sci*. **2014**, *5*, 965-972.

Copies of FT-IR, ^{1}H NMR, ^{13}C{^{1}H} NMR and HRMS

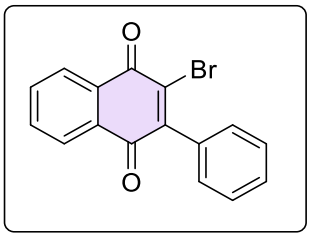
IR Spectra



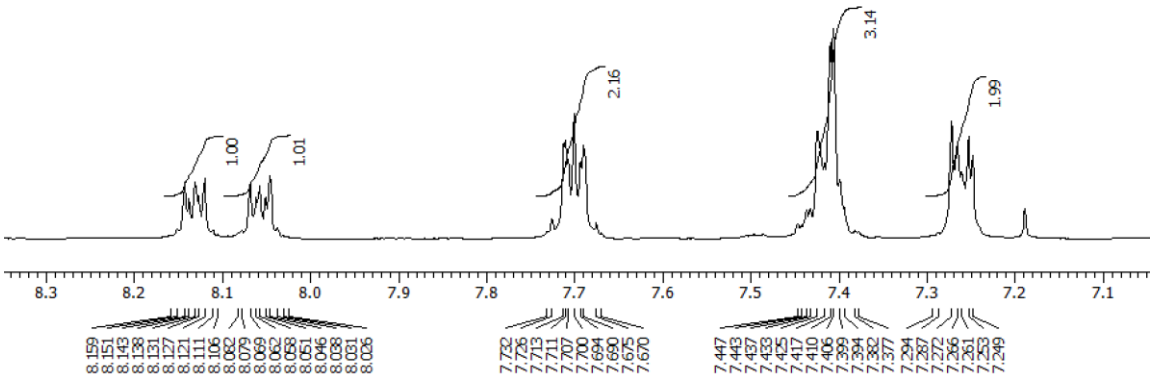
2-bromo-3-phenylnaphthalene-1,4-dione (3a)

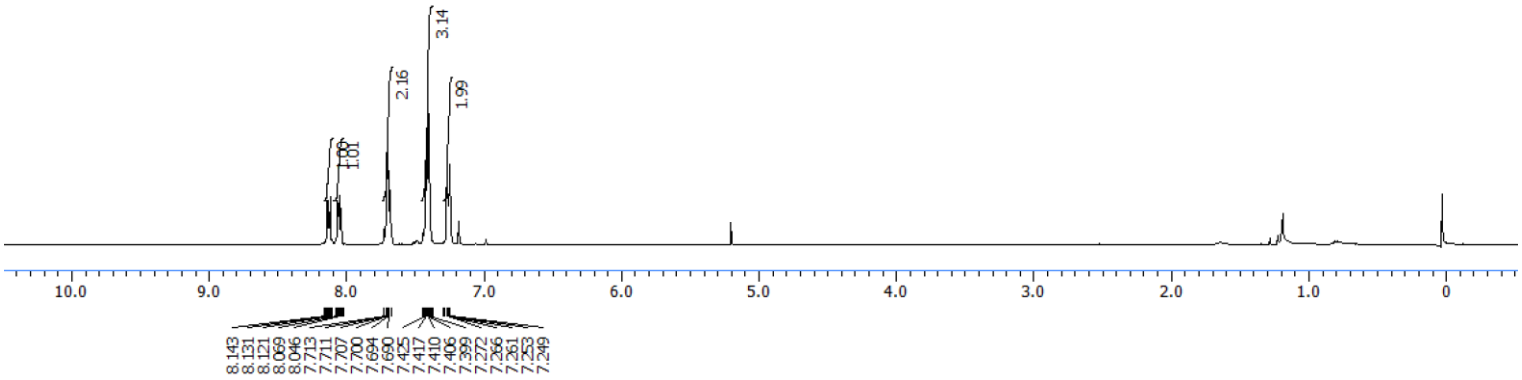


^{1}H NMR (400 MHz, $CDCl_3$)

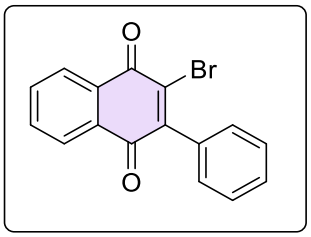


2-bromo-3-phenylnaphthalene-1,4-dione (3a)

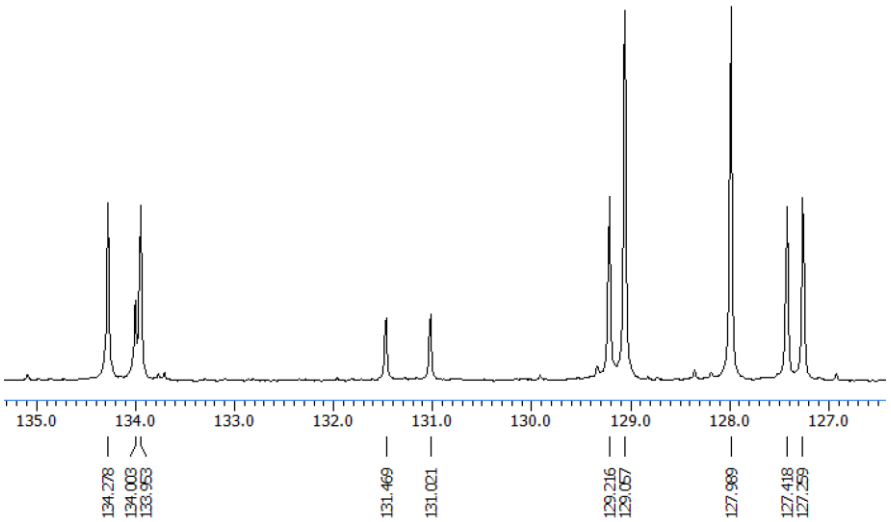


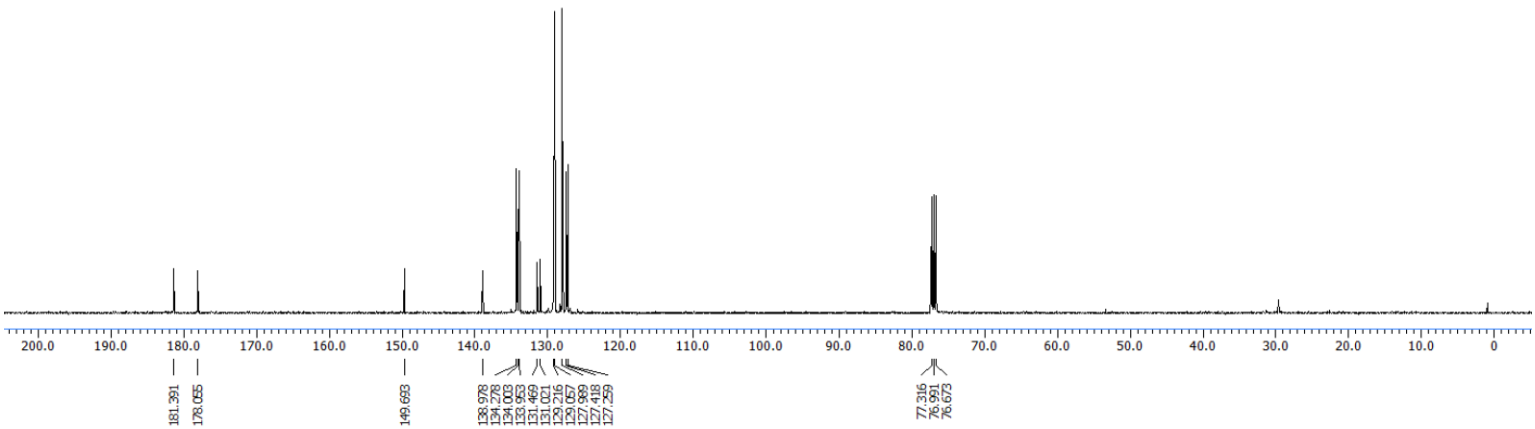


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

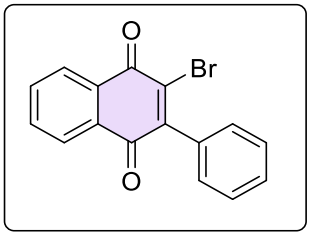


2-bromo-3-phenylnaphthalene-1,4-dione (3a)





HRMS



2-bromo-3-phenylnaphthalene-1,4-dione (3a)

Qualitative Compound Report

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Sample Type	Sample	Position	P1-A7
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IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group	Info.	3	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
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Compound Label	m/z	RT	Algorithm	Mass
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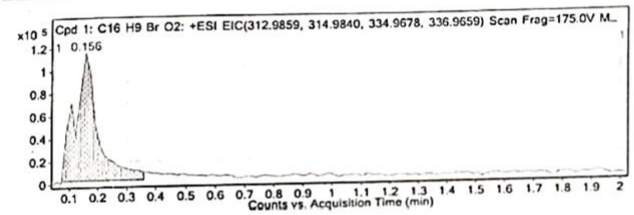
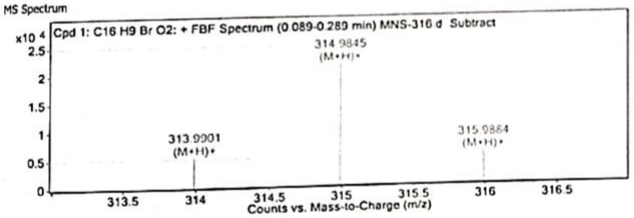
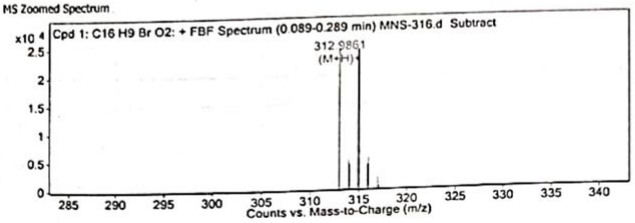


MS Spectrum



MS Zoomed Spectrum

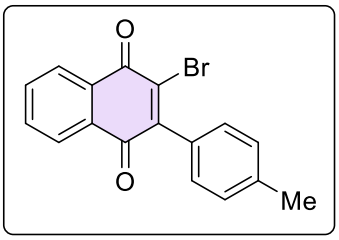


MS Spectrum Peak List

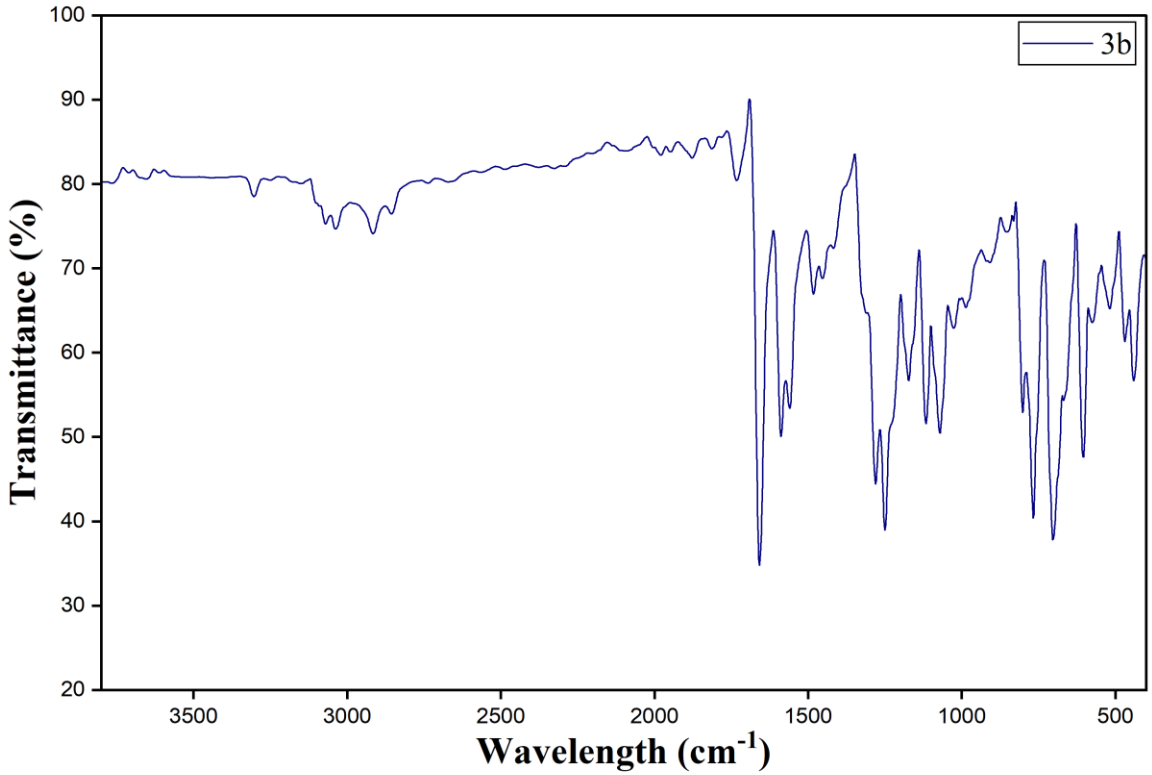
m/z	z	Abund	Formula	Ion
312.9861	1	22859.24	C16H10BrO2	(M+H)+
313.9901	1	5249	C16H10BrO2	(M+H)+
314.9845	1	22504.3	C16H10BrO2	(M+H)+
315.9884	1	5434.67	C16H10BrO2	(M+H)+
316.9849	1	1874.18	C16H10BrO2	(M+H)+

--- End Of Report ---

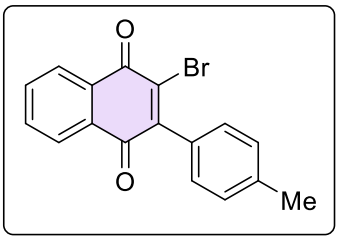
IR Spectra



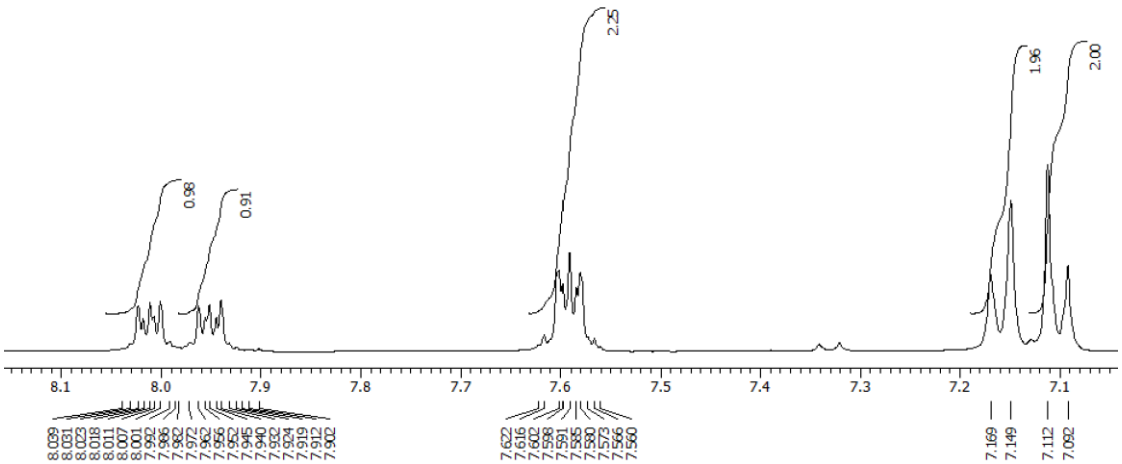
2-bromo-3-(*p*-tolyl)naphthalene-1,4-dione (3b)

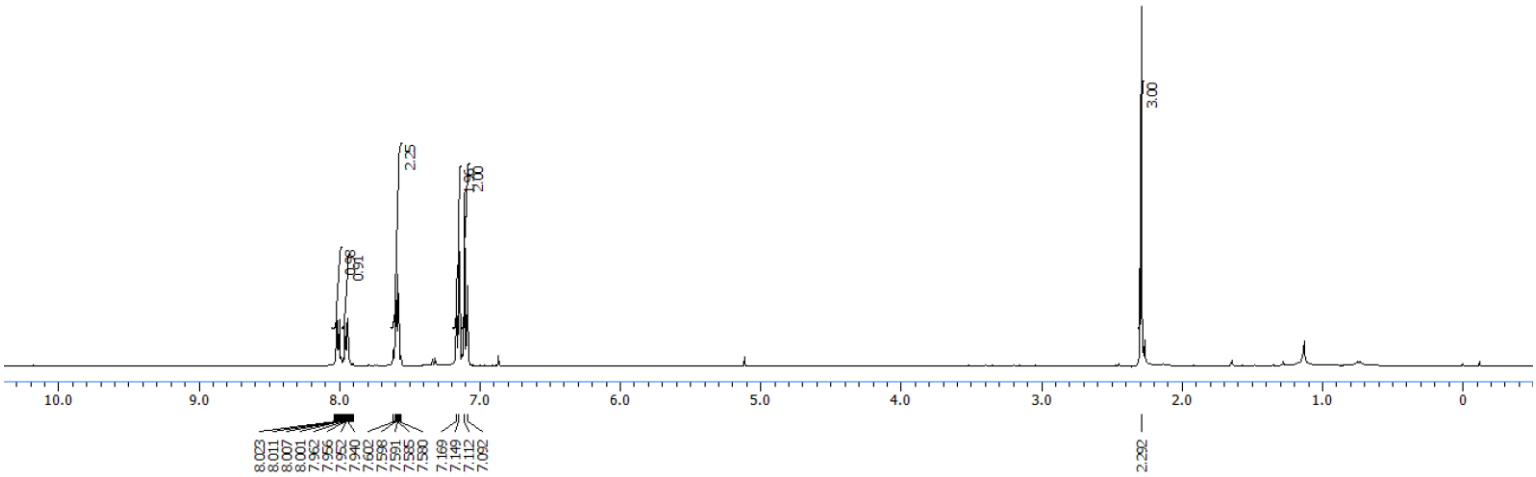


^{1}H NMR (400 MHz, $CDCl_3$)

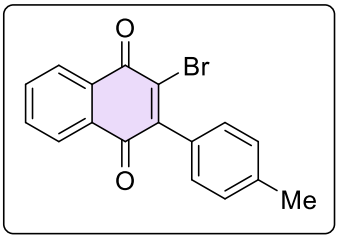


2-bromo-3-(*p*-tolyl)naphthalene-1,4-dione (3b)

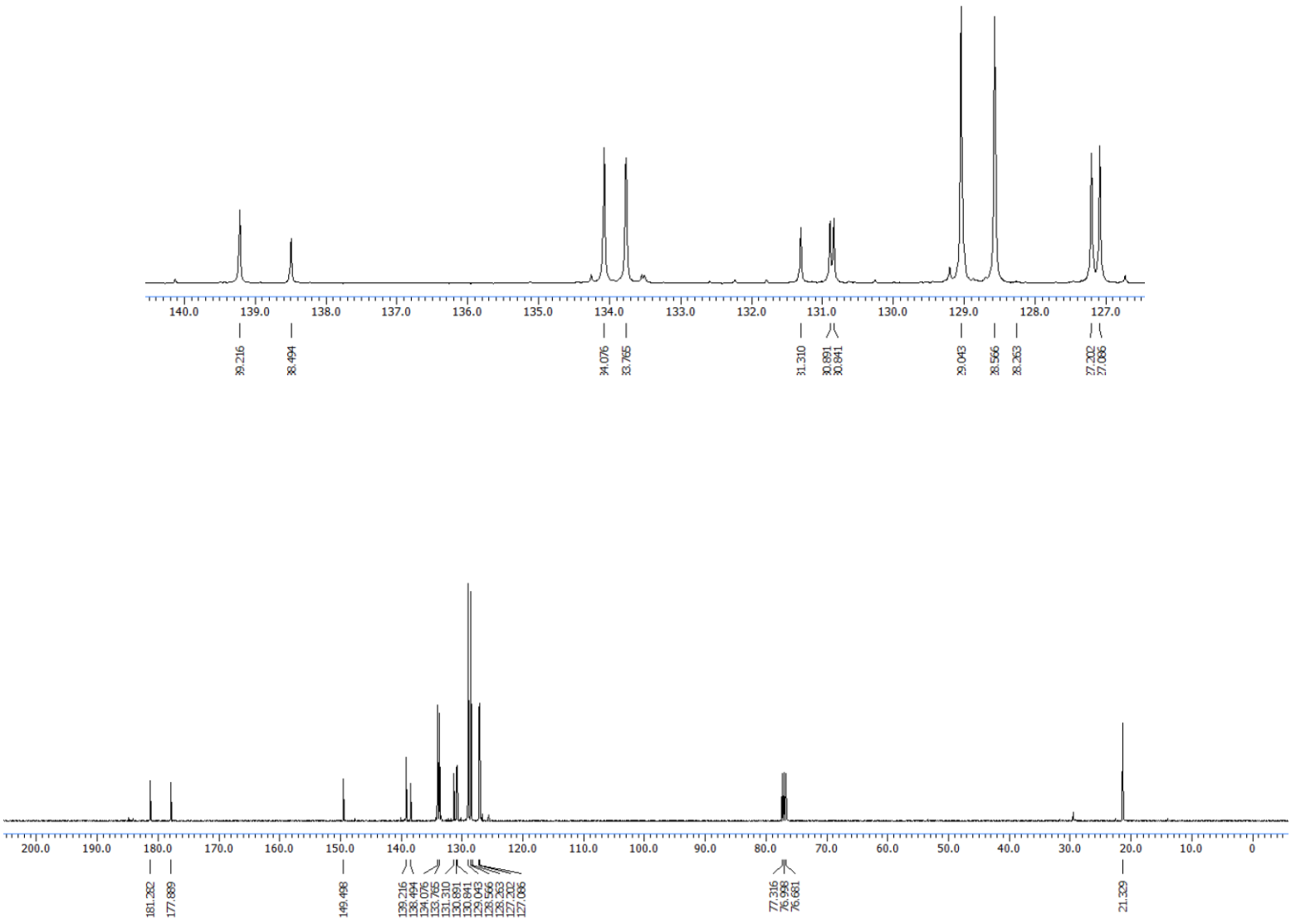




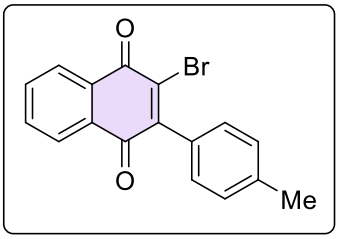
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-bromo-3-(*p*-tolyl)naphthalene-1,4-dione (3b)



HRMS



2-bromo-3-(*p*-tolyl)naphthalene-1,4-dione (3b)

Qualitative Compound Report

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IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group	Info.	3	
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Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H11 Br O2	0.157	325.9963	20071	C17 H11 Br O2	325.9942	6.27	C17 H11 Br O2	C17 H11 Br O2

Compound Label	m/z	RT	Algorithm	Mass
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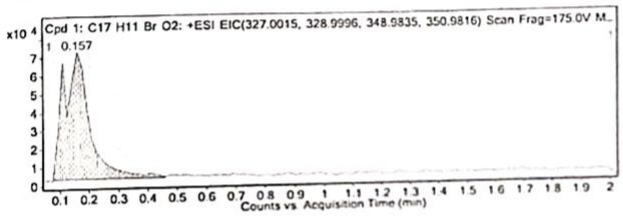
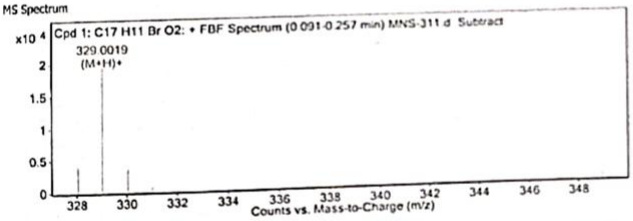
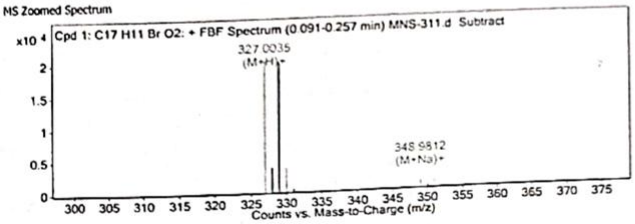


MS Spectrum



MS Zoomed Spectrum

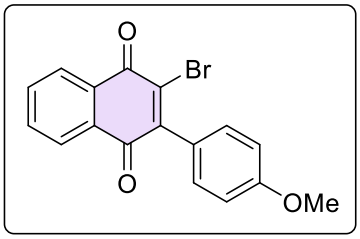


MS Spectrum Peak List

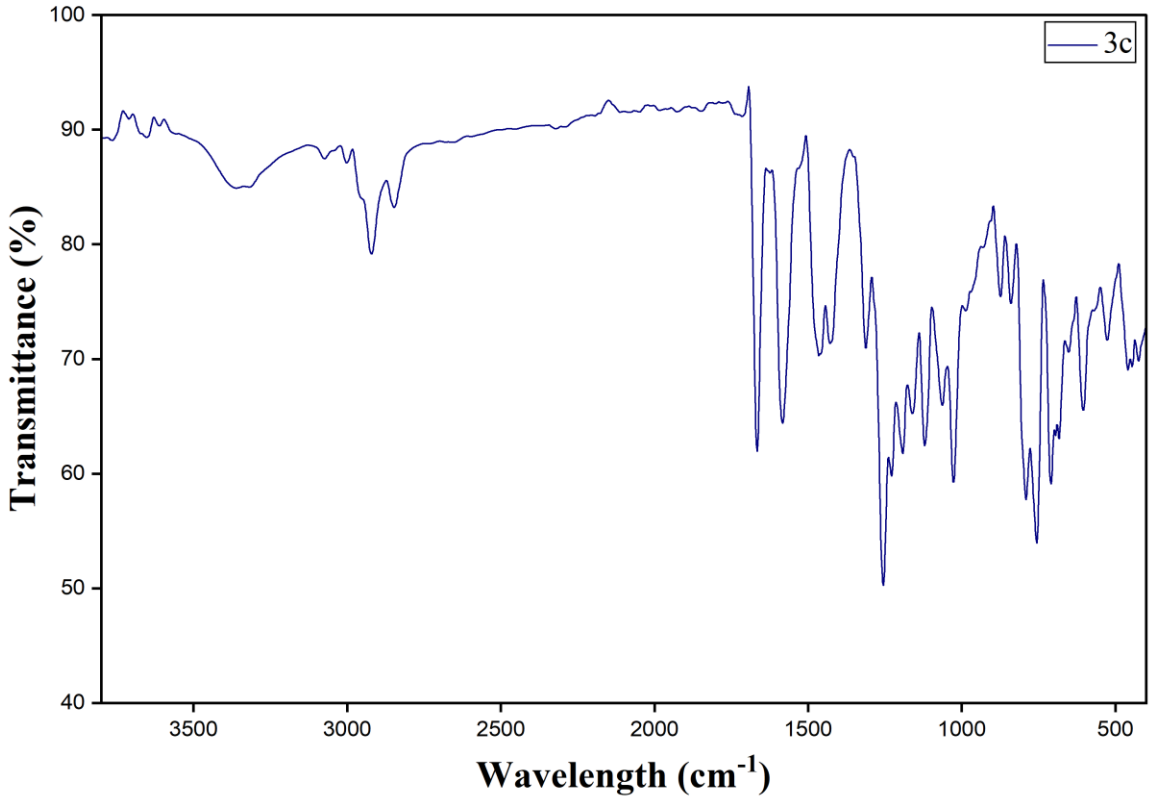
m/z	z	Abund	Formula	Ion
327.0035	1	20070.81	C17H12BrO2	(M+H)+
328.0067	1	3905.27	C17H12BrO2	(M+H)+
329.0019	1	19387.96	C17H12BrO2	(M+H)+
330.0055	1	3731.68	C17H12BrO2	(M+H)+
331.0089	1	899.03	C17H12BrO2	(M+H)+
332.0095	1	66.73	C17H12BrO2	(M+H)+
348.9812	1	914.41	C17H11BrNaO2	(M+Na)+
349.9818	1	284.85	C17H11BrNaO2	(M+Na)+

--- End Of Report ---

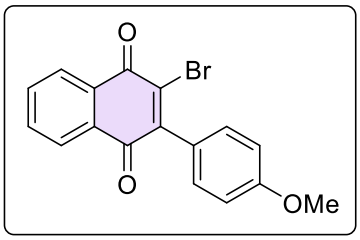
IR Spectra



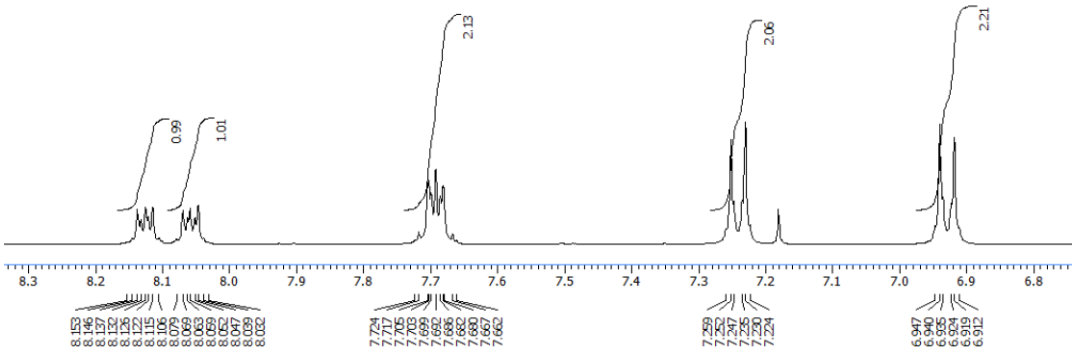
2-bromo-3-(4-methoxyphenyl)naphthalene-1,4-dione (3c)

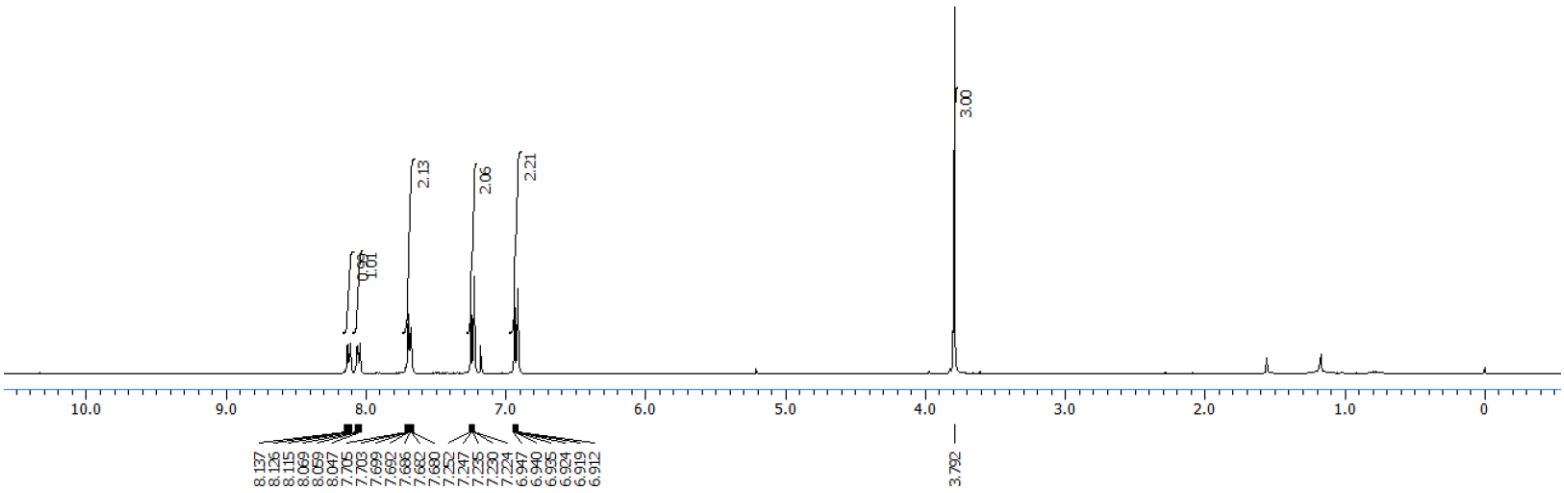


^{1}H NMR (400 MHz, $CDCl_3$)

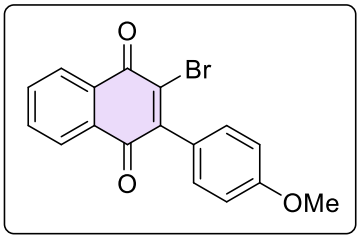


2-bromo-3-(4-methoxyphenyl)naphthalene-1,4-dione (3c)

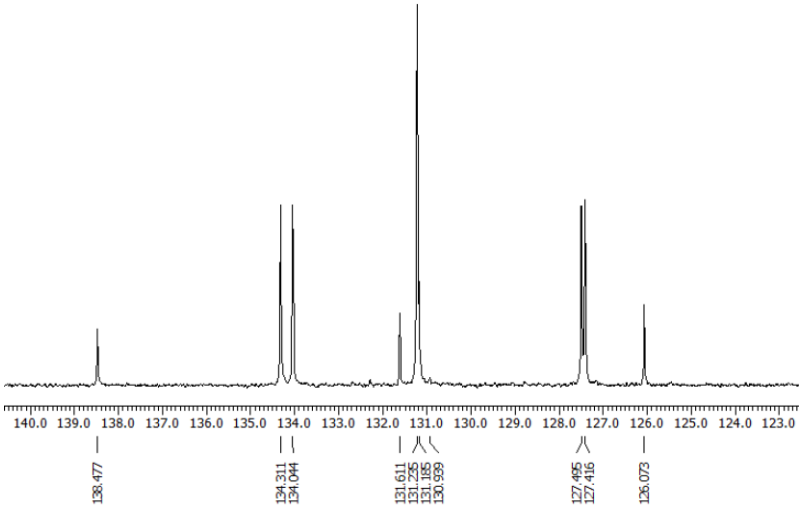


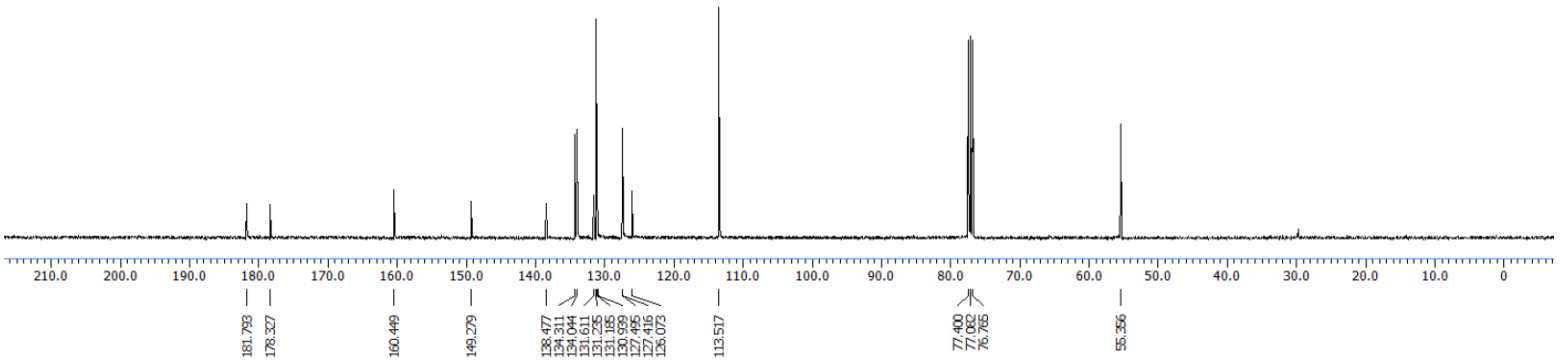


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

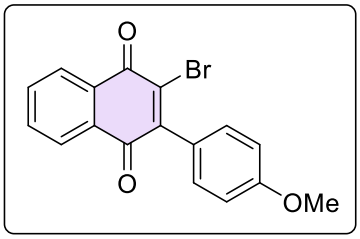


2-bromo-3-(4-methoxyphenyl)naphthalene-1,4-dione (3c)





HRMS



2-bromo-3-(4-methoxyphenyl)naphthalene-1,4-dione (3c)

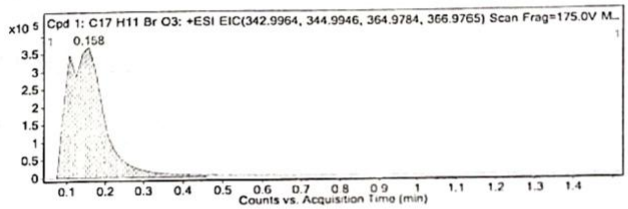
Qualitative Compound Report

Data File	MNS-300.d	Sample Name	MNS-300
Sample Type	Sample	Position	P1-A3
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	13-05-2024 14:16:22
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group	Info.	3	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

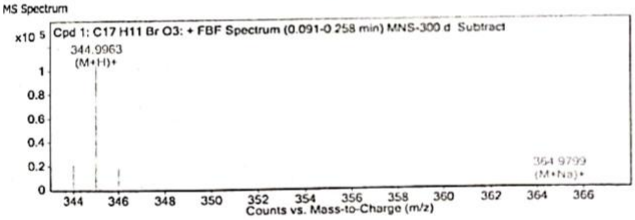
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H11 Br O3	0.158	341.991	106321	C17 H11 Br O3	341.9892	5.44	C17 H11 Br O3	C17 H11 Br O3

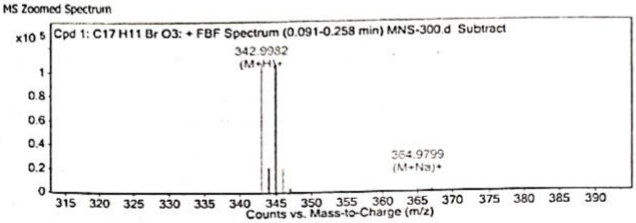
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H11 Br O3	342.9982	0.158	Find By Formula	341.991



MS Spectrum



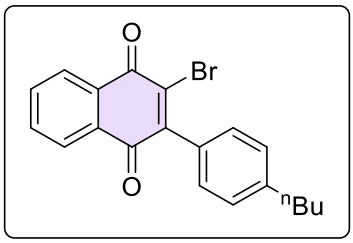
MS Zoomed Spectrum



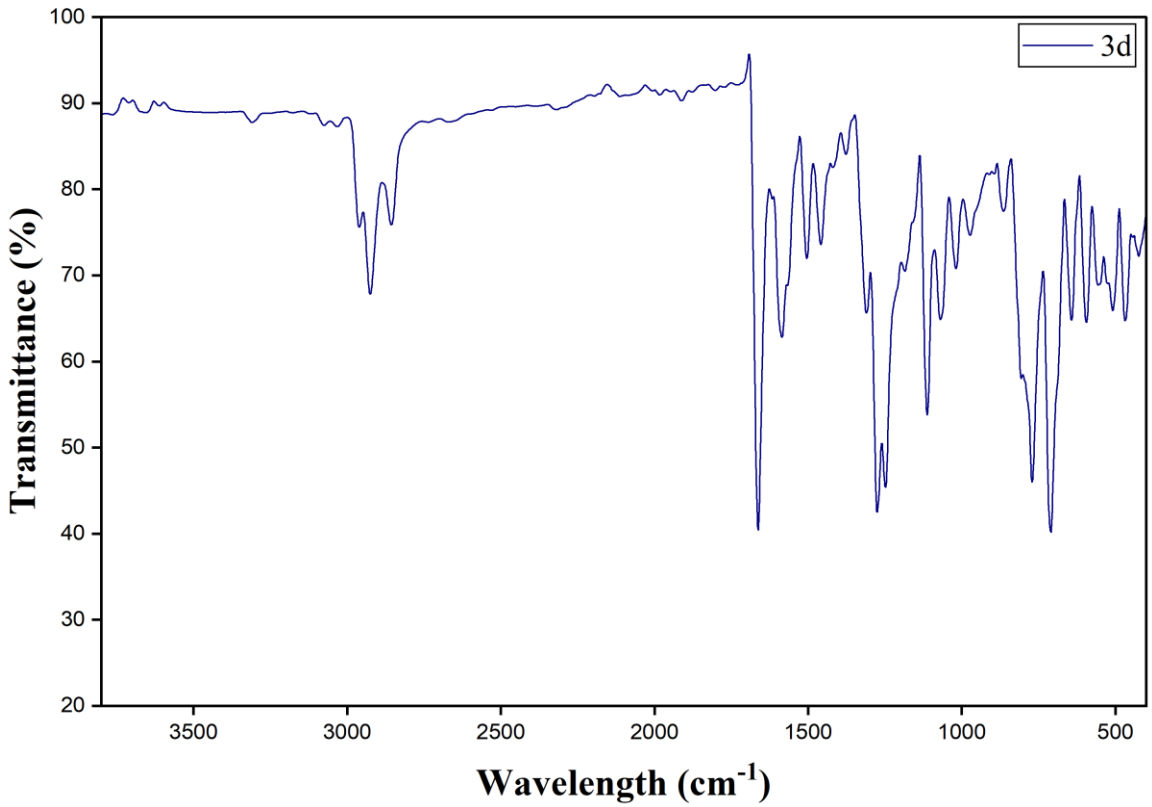
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
342.9982	1	106321.27	C17H12BrO3	(M+H)+
344.0027	1	21468.66	C17H12BrO3	(M+H)+
344.9963	1	105363.95	C17H12BrO3	(M+H)+
345.9996	1	18958.19	C17H12BrO3	(M+H)+
347.003	1	2561.77	C17H12BrO3	(M+H)+
348.0029	1	187.86	C17H12BrO3	(M+H)+
364.9799	1	1568.85	C17H11BrNaO3	(M+Na)+
365.9823	1	326.81	C17H11BrNaO3	(M+Na)+
366.978	1	1550.11	C17H11BrNaO3	(M+Na)+
367.9867	1	314.61	C17H11BrNaO3	(M+Na)+

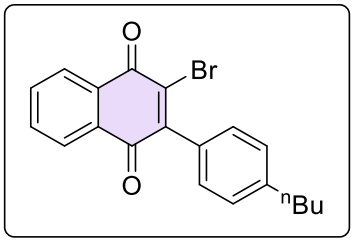
IR Spectra



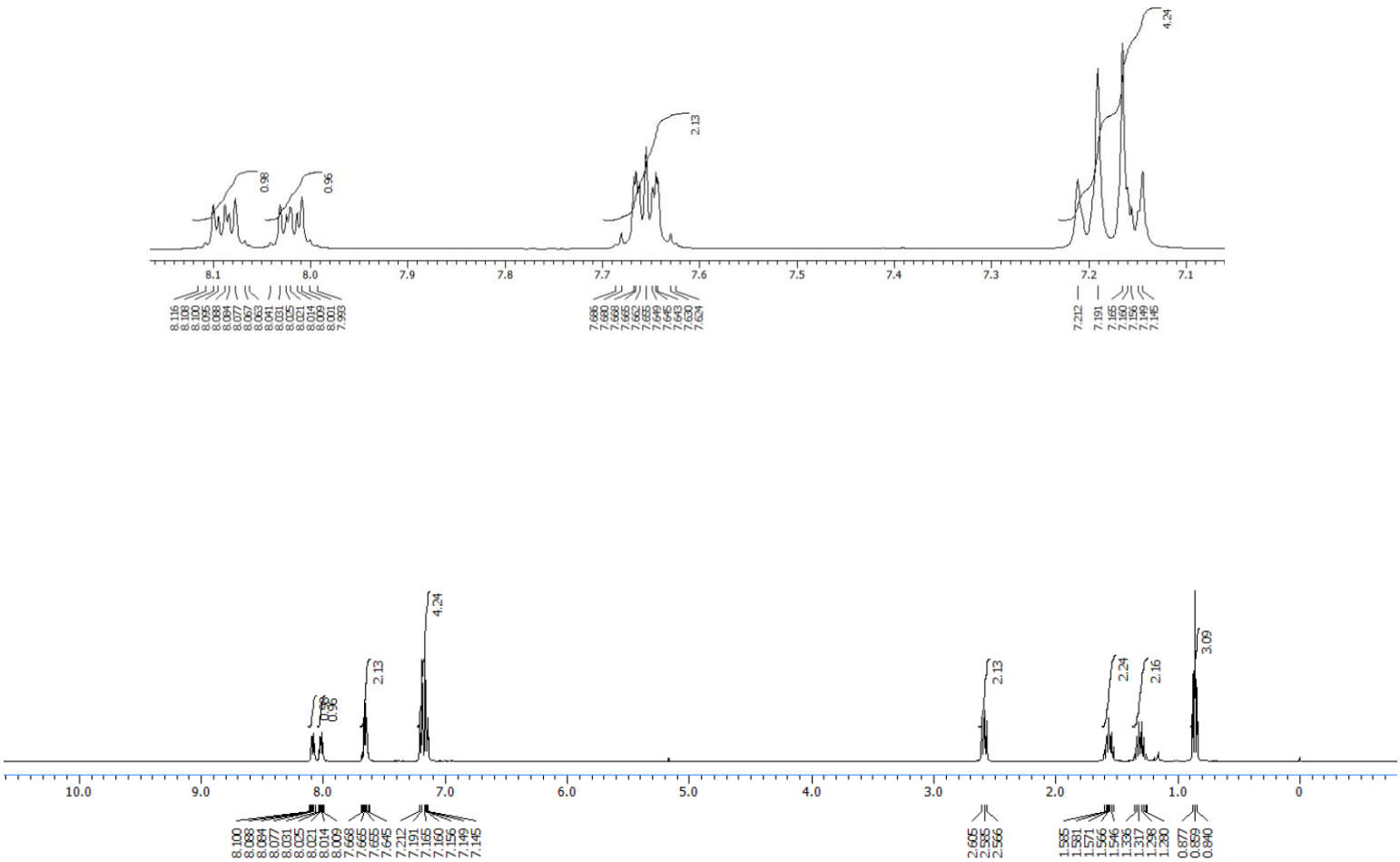
2-bromo-3-(4-butylphenyl)naphthalene-1,4-dione (3d)



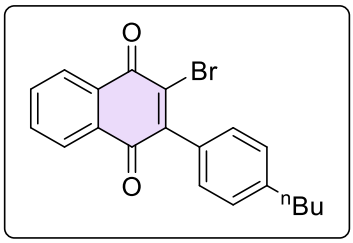
^{1}H NMR (400 MHz, $CDCl_3$)



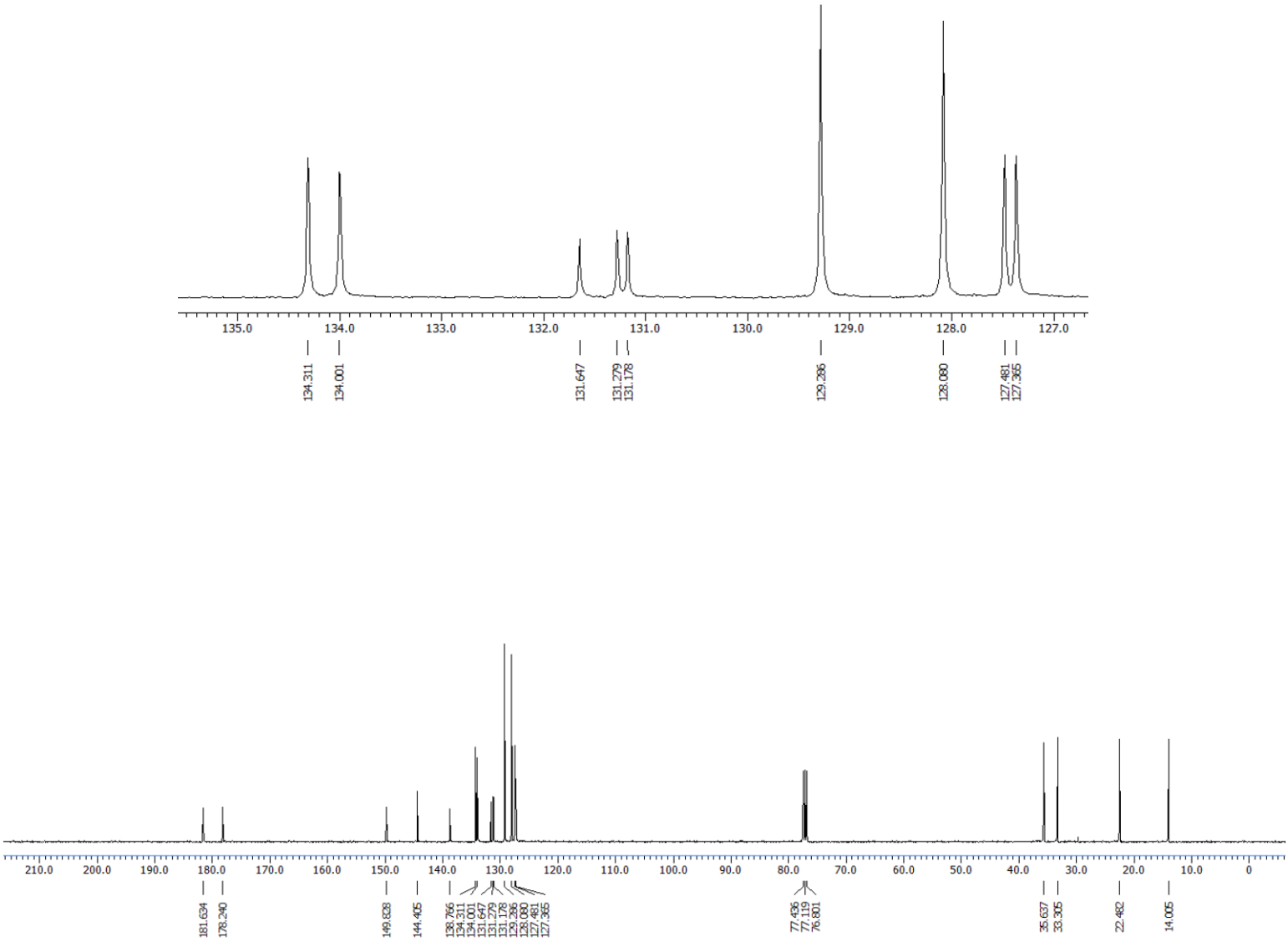
2-bromo-3-(4-butylphenyl)naphthalene-1,4-dione (3d)



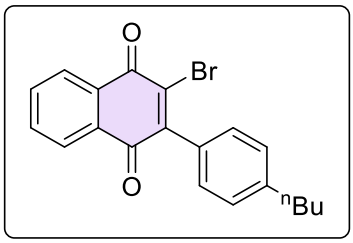
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-bromo-3-(4-butylphenyl)naphthalene-1,4-dione (3d)



HRMS



2-bromo-3-(4-butylphenyl)naphthalene-1,4-dione (3d)

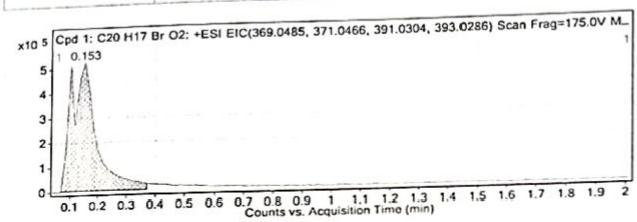
Qualitative Compound Report

Data File	MNS-317.d	Sample Name	MNS-317
Sample Type	Sample	Position	P1-A8
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	04-03-2025 13:02:59
IRM Calibration Status	Success	DA Method	Default.m
Comment			
	Info.	3	
Sample Group			
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

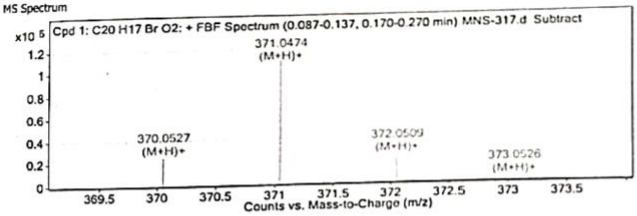
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H17 Br O2	0.153	368.042	112600	C20 H17 Br O2	368.0412	2.06	C20 H17 Br O2	C20 H17 Br O2

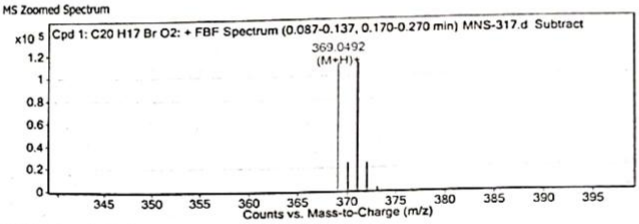
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H17 Br O2	369.0492	0.153	Find By Formula	368.042



MS Spectrum



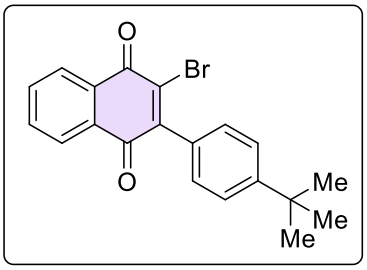
MS Zoomed Spectrum



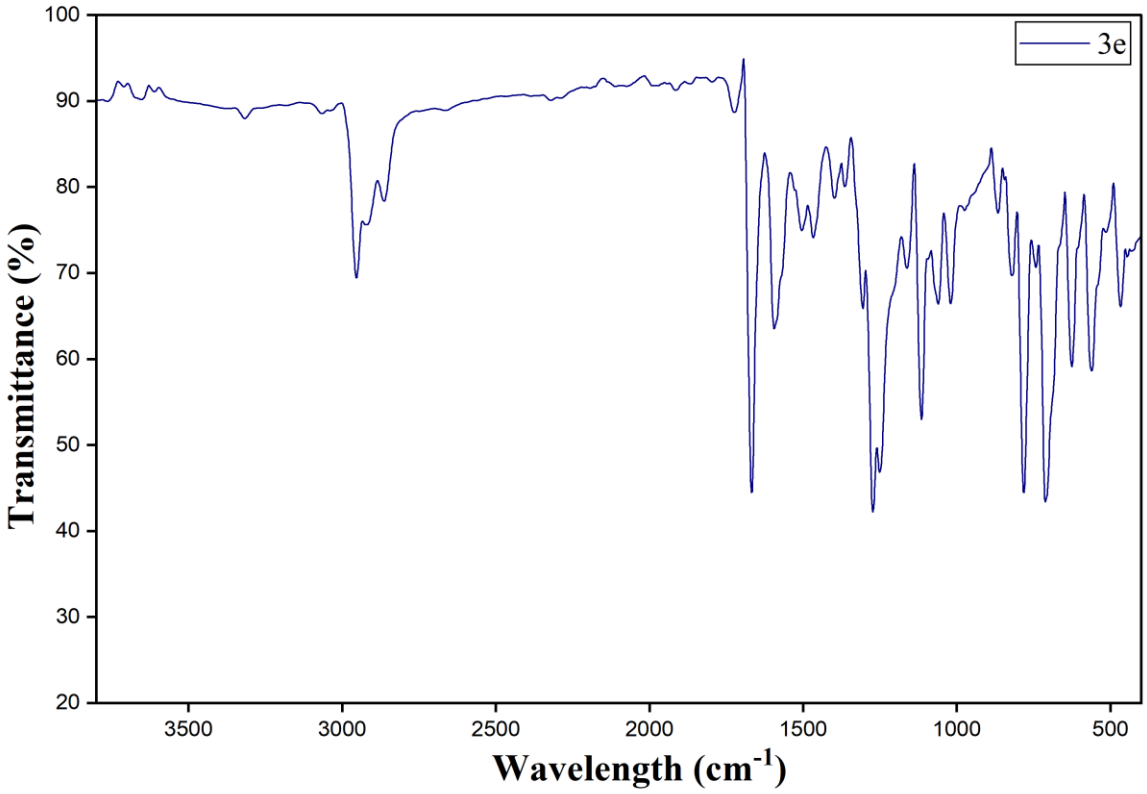
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
369.0492	1	112600.45	C20H18BrO2	(M+H)+
370.0527	1	24693.54	C20H18BrO2	(M+H)+
371.0474	1	111579.8	C20H18BrO2	(M+H)+
372.0509	1	23795.92	C20H18BrO2	(M+H)+
373.0526	1	3040.17	C20H18BrO2	(M+H)+
374.0448	1	326.97	C20H18BrO2	(M+H)+

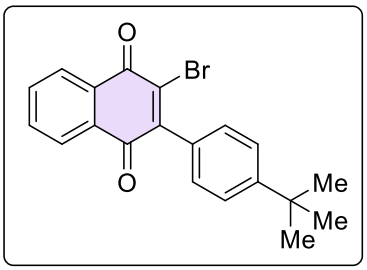
IR Spectra



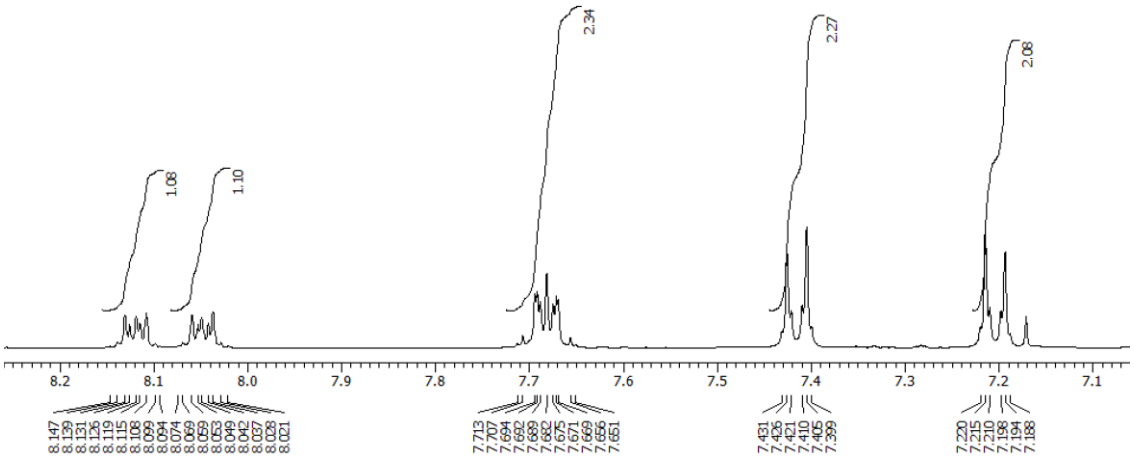
2-bromo-3-(4-(*tert*-butyl)phenyl)naphthalene-1,4-dione (3e)

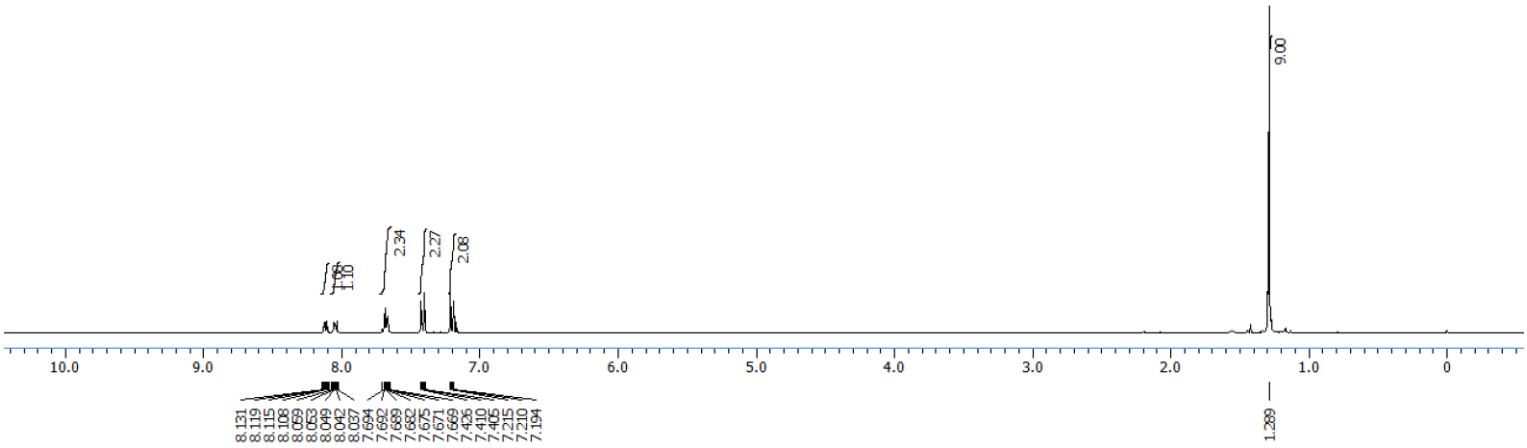


^{1}H NMR (400 MHz, $CDCl_3$)

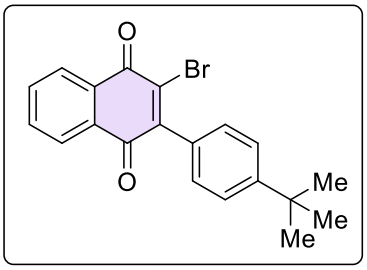


2-bromo-3-(4-(*tert*-butyl)phenyl)naphthalene-1,4-dione (3e)

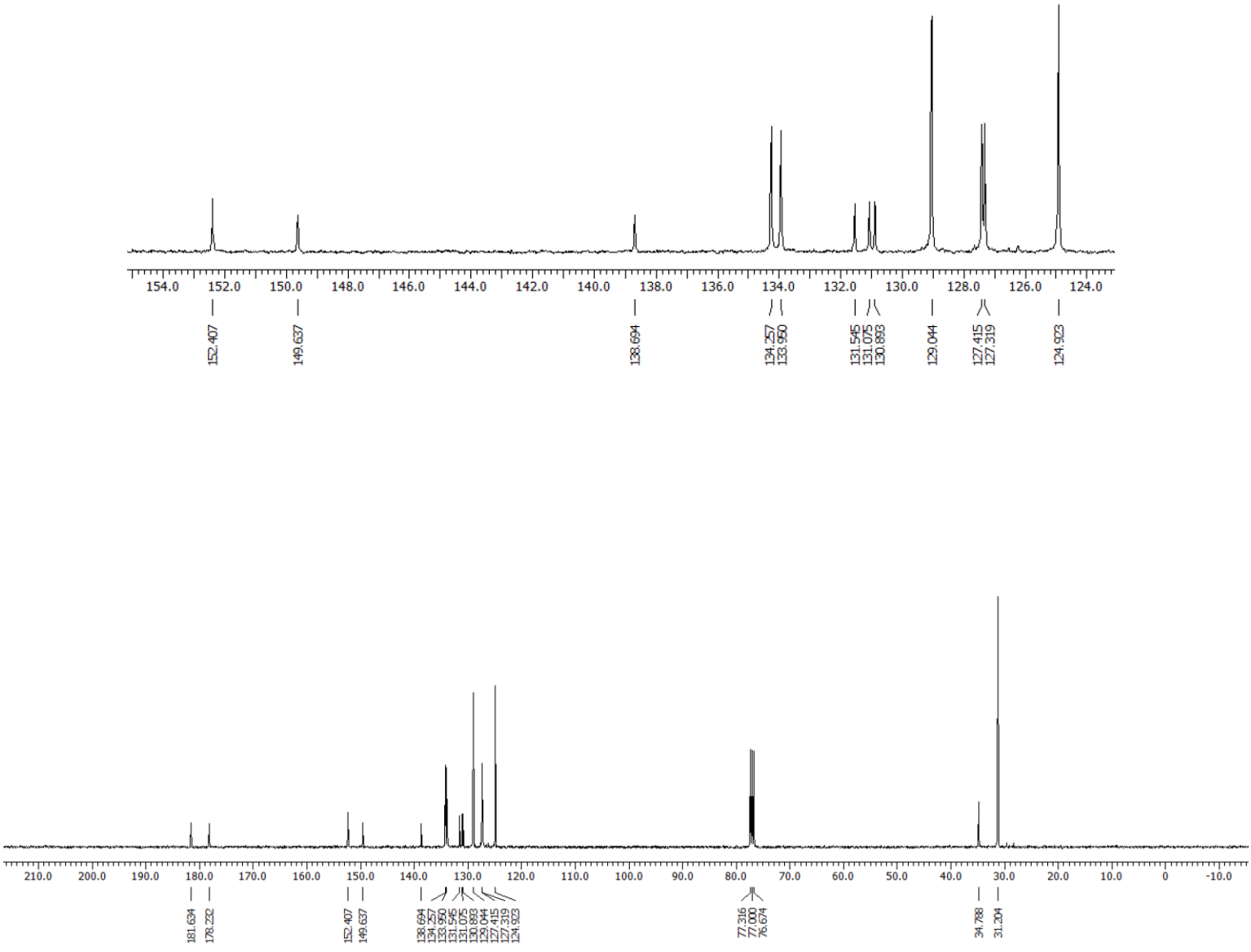




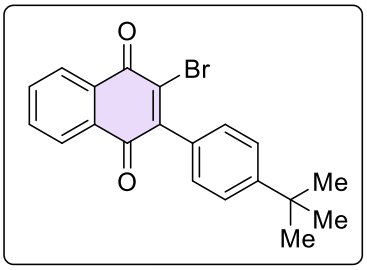
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-bromo-3-(4-(*tert*-butyl)phenyl)naphthalene-1,4-dione (3e)



HRMS



2-bromo-3-(4-(*tert*-butyl)phenyl)naphthalene-1,4-dione (3e)

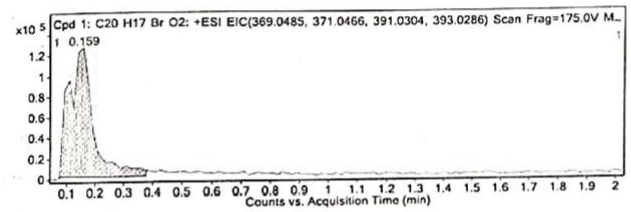
Qualitative Compound Report

Data File	MNS-313.d	Sample Name	MNS-313
Sample Type	Sample	Position	P1-A6
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	04-03-2025 12:57:15
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group	Info.	3	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

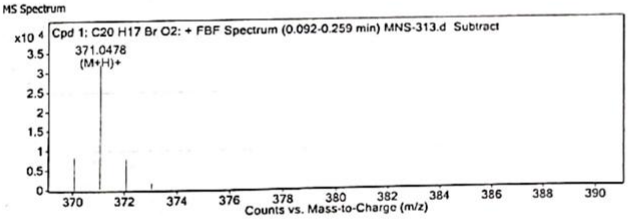
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H17 Br O2	0.159	368.0424	32372	C20 H17 Br O2	368.0412	3.28	C20 H17 Br O2	C20 H17 Br O2

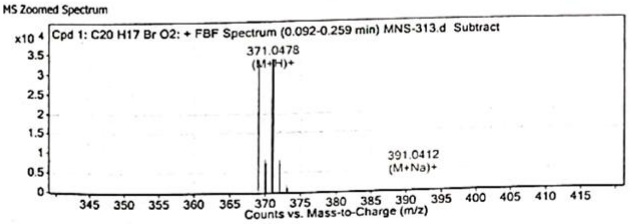
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H17 Br O2	371.0478	0.159	Find By Formula	368.0424



MS Spectrum



MS Zoomed Spectrum

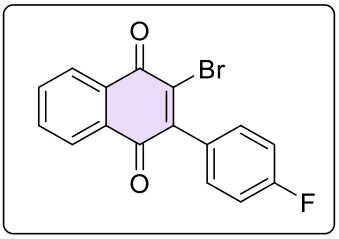


MS Spectrum Peak List

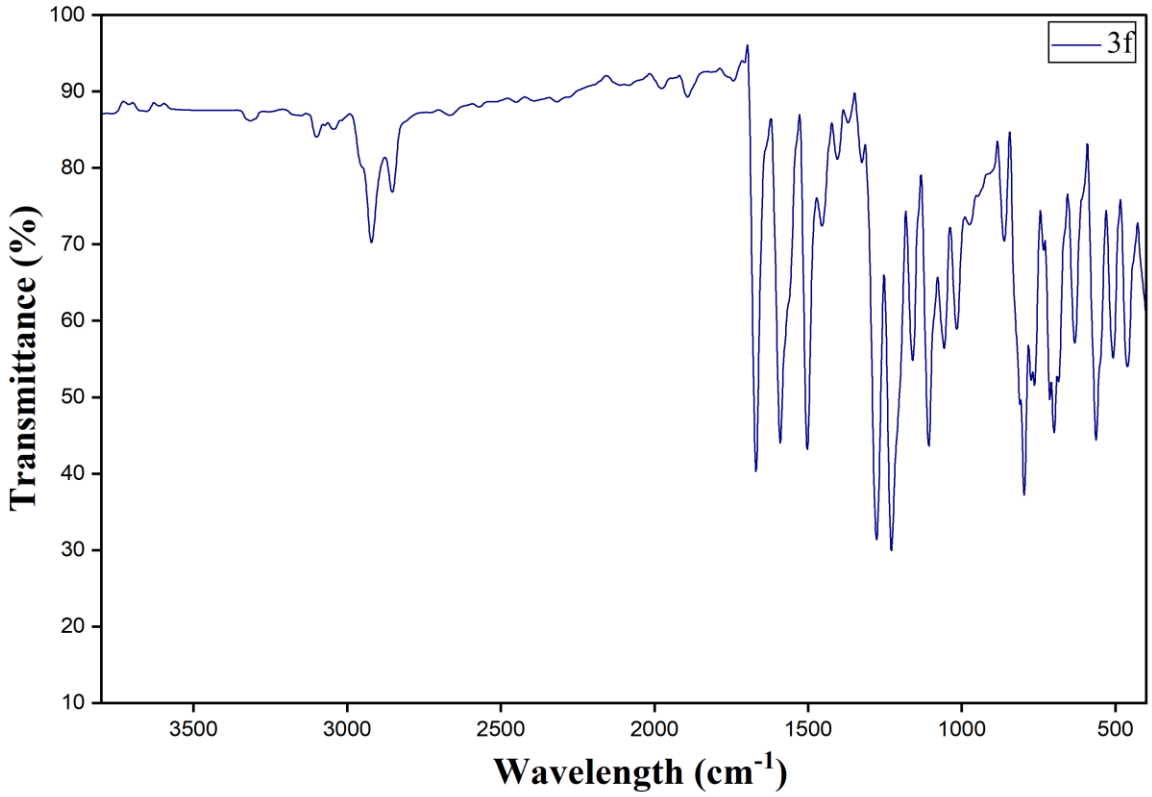
m/z	z	Abund	Formula	Ion
369.0497	1	32357.64	C20H18BrO2	(M+H)+
370.0532	1	8269.11	C20H18BrO2	(M+H)+
371.0478	1	32372.27	C20H18BrO2	(M+H)+
372.0517	1	8049.56	C20H18BrO2	(M+H)+
373.0504	1	1769.93	C20H18BrO2	(M+H)+
391.0412	1	178.22	C20H17BrNaO2	(M+Na)+

--- End Of Report ---

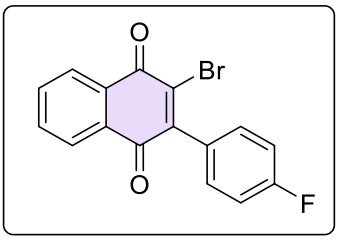
IR Spectra



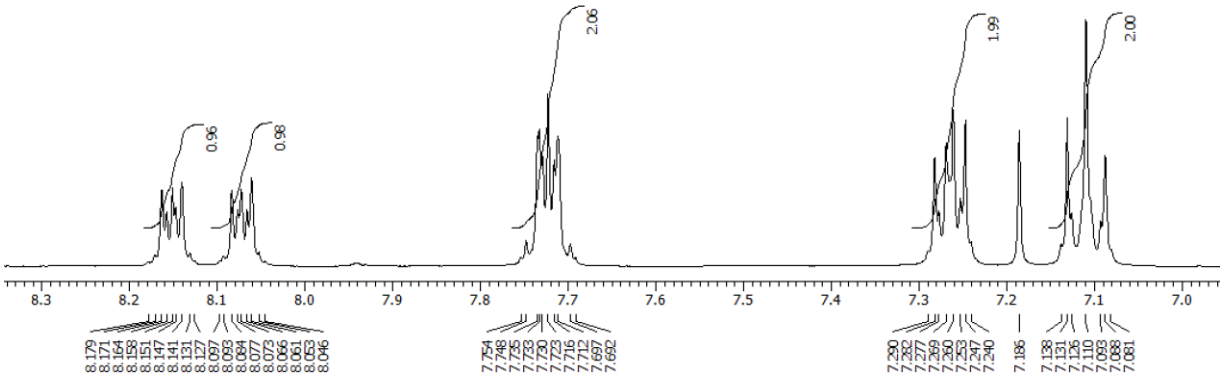
2-bromo-3-(4-fluorophenyl)naphthalene-1,4-dione (3f)

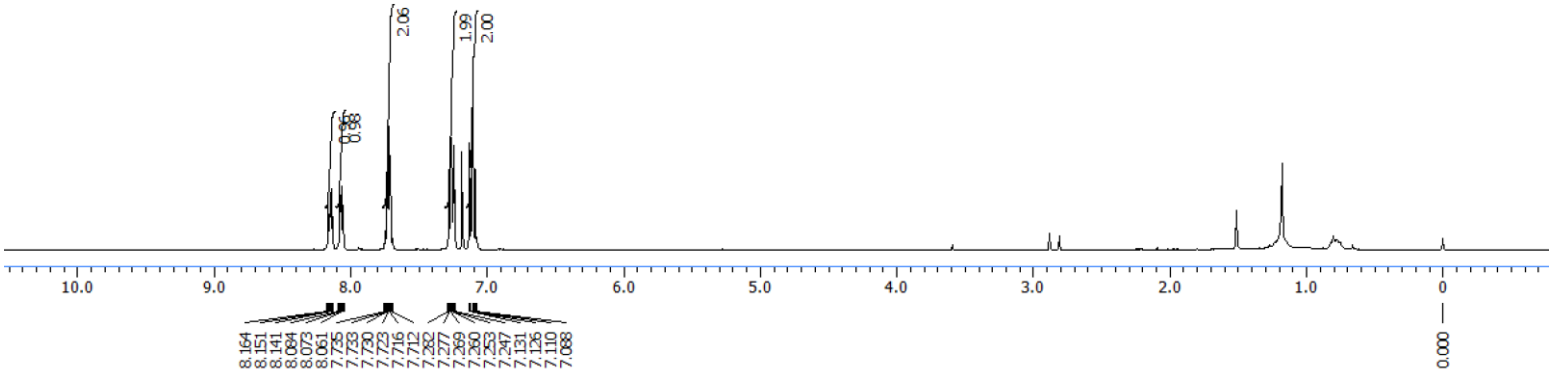


^{1}H NMR (400 MHz, $CDCl_3$)

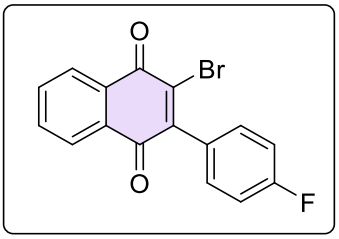


2-bromo-3-(4-fluorophenyl)naphthalene-1,4-dione (3f)

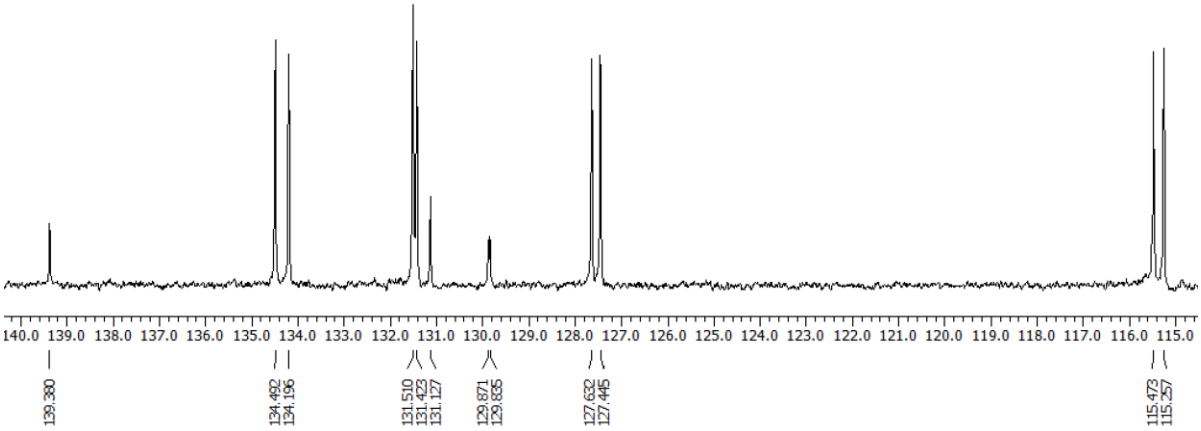


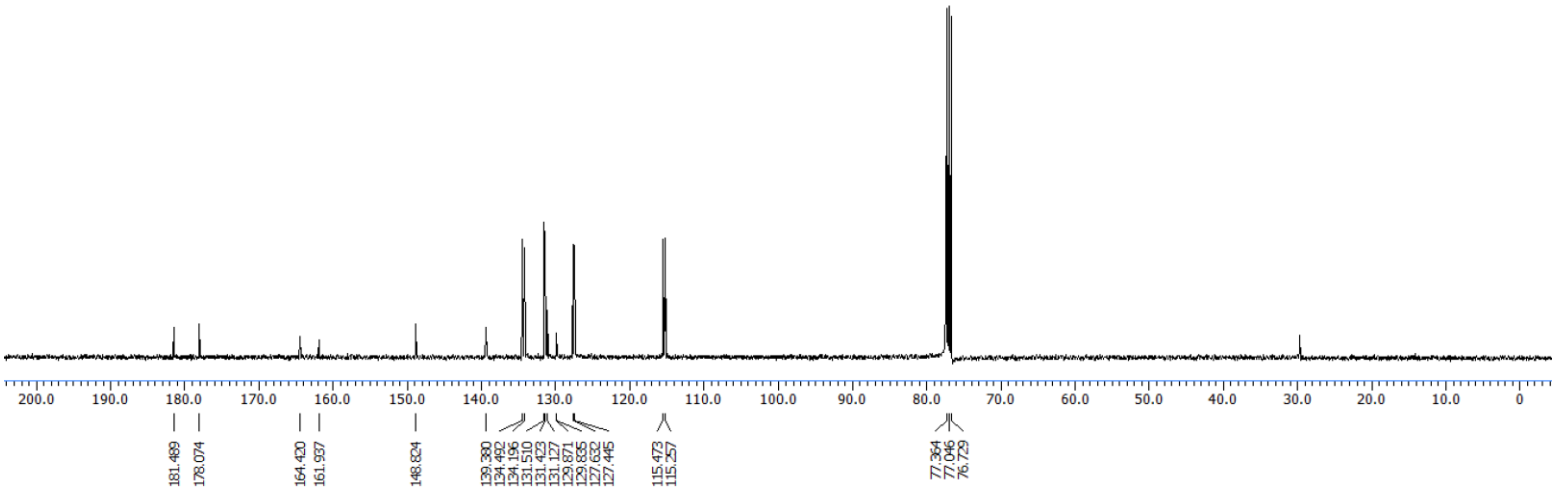


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

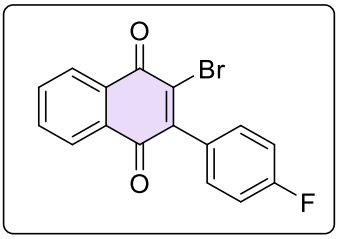


2-bromo-3-(4-fluorophenyl)naphthalene-1,4-dione (3f)

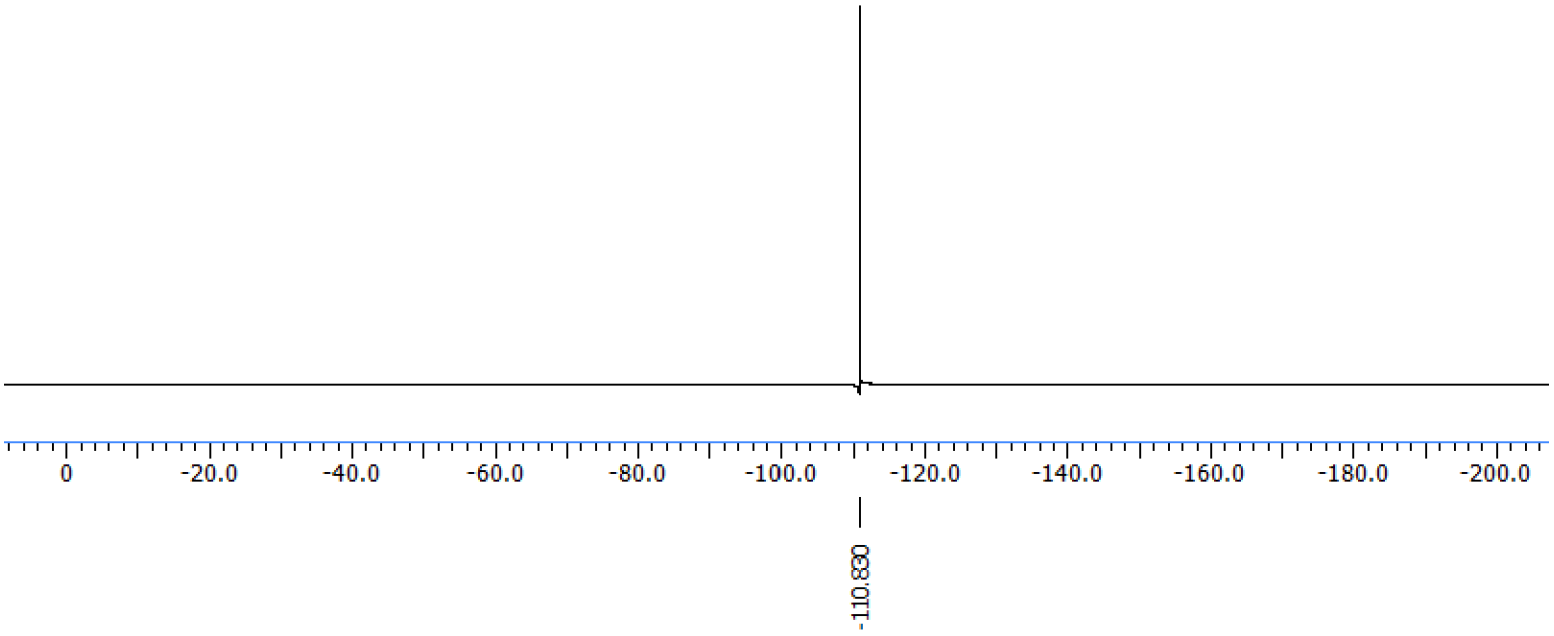




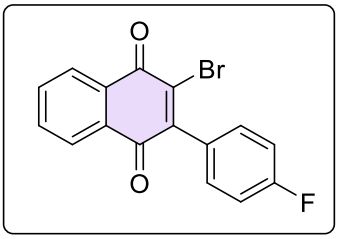
^{19}F NMR (376 MHz, $CDCl_3$)



2-bromo-3-(4-fluorophenyl)naphthalene-1,4-dione (3f)



HRMS



2-bromo-3-(4-fluorophenyl)naphthalene-1,4-dione (3f)

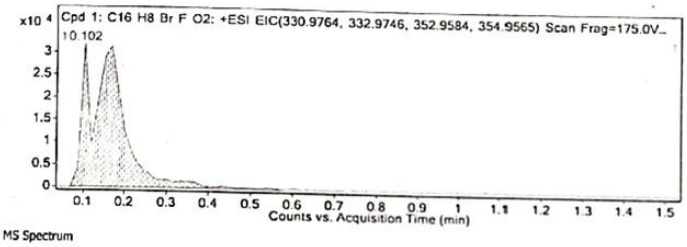
Qualitative Compound Report

Data File	MNS-302.d	**Sample Name**	MNS-302
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	13-05-2024 14:20:15
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

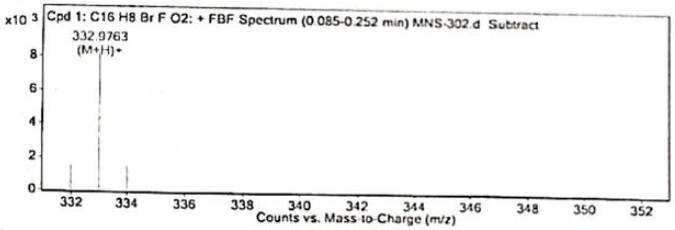
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C16 H8 Br F O2	0.102	329.9712	8767	C16 H8 Br F O2	329.9692	6.09	C16 H8 Br F O2	C16 H8 Br F O2

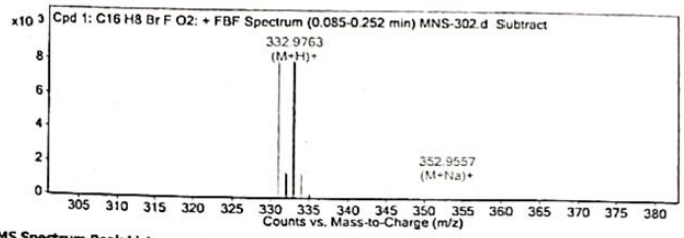
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C16 H8 Br F O2	332.9763	0.102	Find By Formula	329.9712



MS Spectrum



MS Zoomed Spectrum

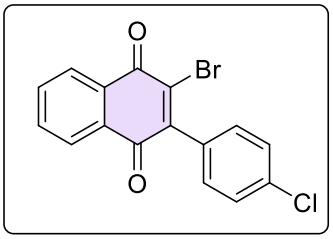


MS Spectrum Peak List

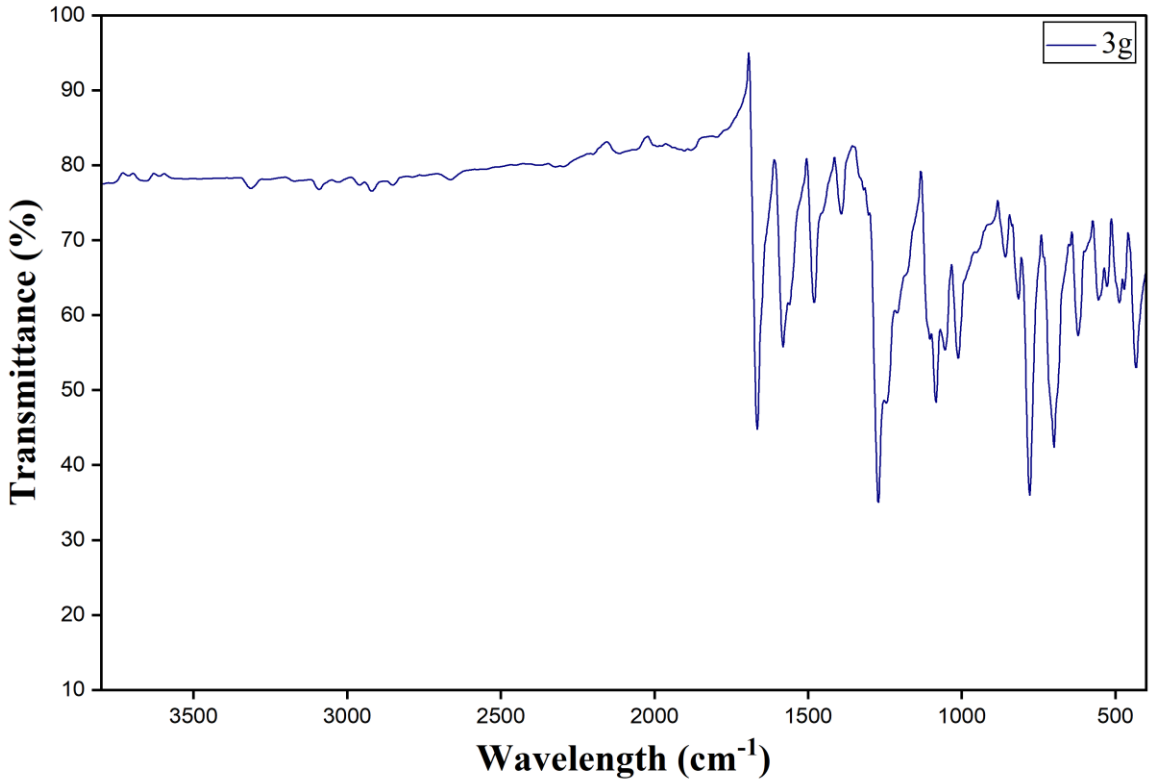
m/z	z	Abund	Formula	Ion
330.9785	1	7443.49	C16H9BrFO2	(M+H)+
331.9829	1	1502.41	C16H9BrFO2	(M+H)+
332.9763	1	8267.29	C16H9BrFO2	(M+H)+
333.9802	1	1465.49	C16H9BrFO2	(M+H)+
334.9861	1	220.44	C16H9BrFO2	(M+H)+
352.9557	1	61.64	C16H8BrFNaO2	(M+Na)+

--- End Of Report ---

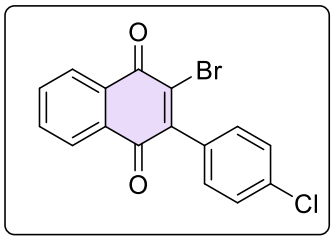
IR Spectra



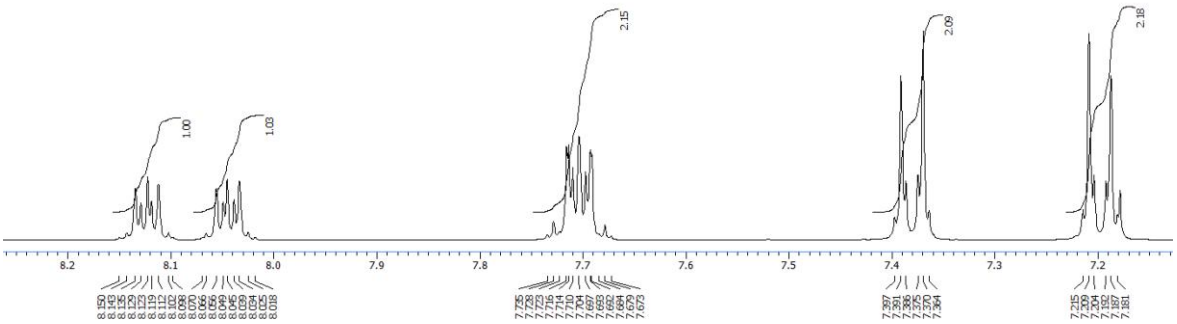
2-bromo-3-(4-chlorophenyl)naphthalene-1,4-dione (3g)

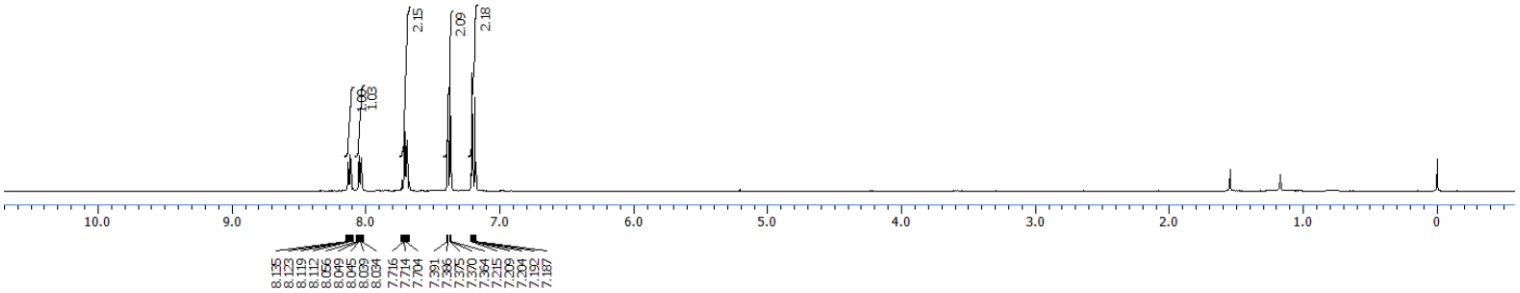


^{1}H NMR (400 MHz, $CDCl_3$)

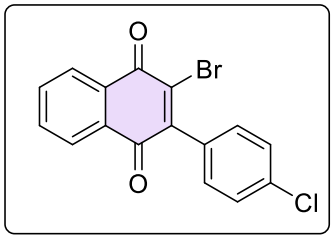


2-bromo-3-(4-chlorophenyl)naphthalene-1,4-dione (3g)

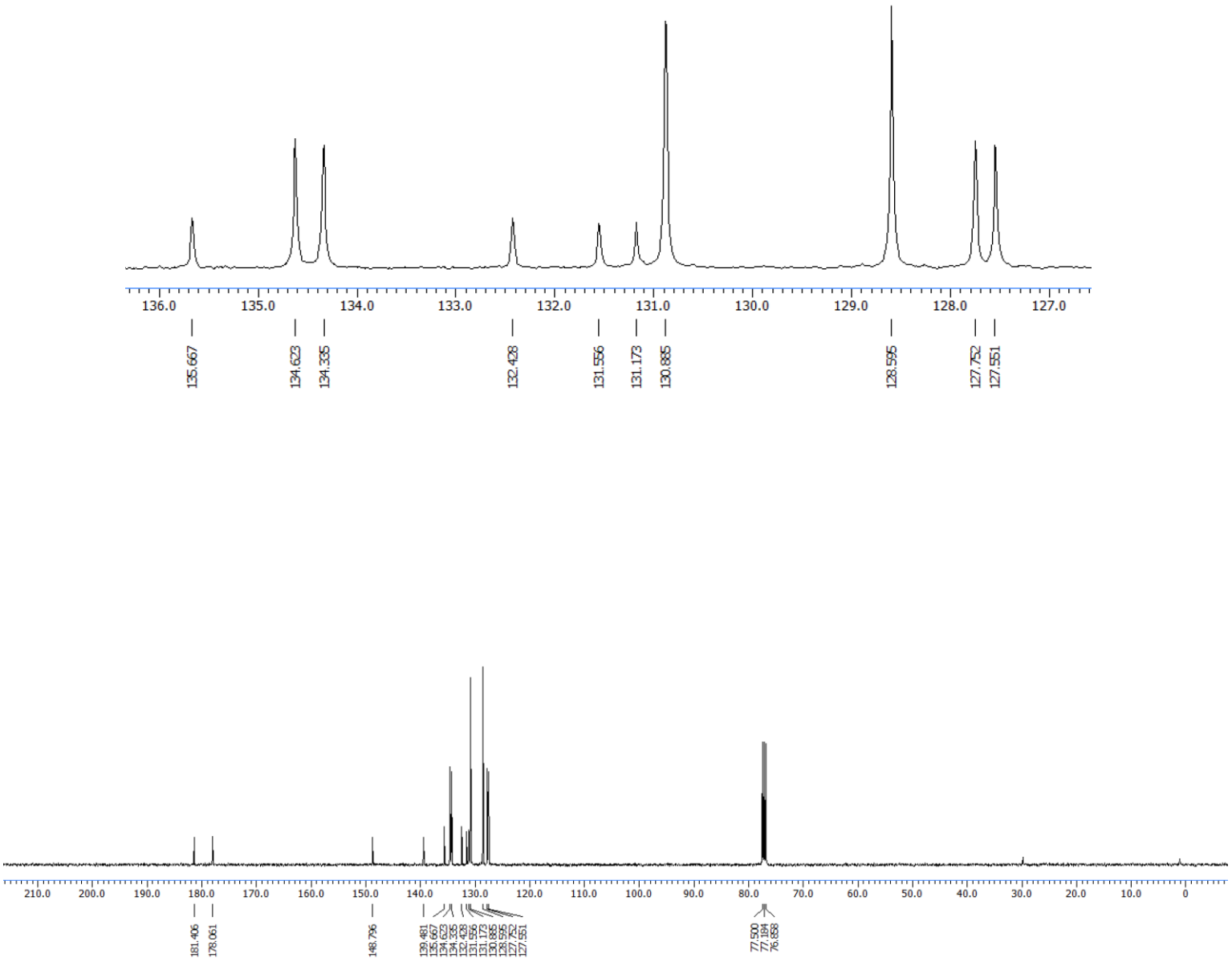




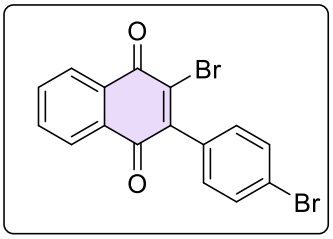
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



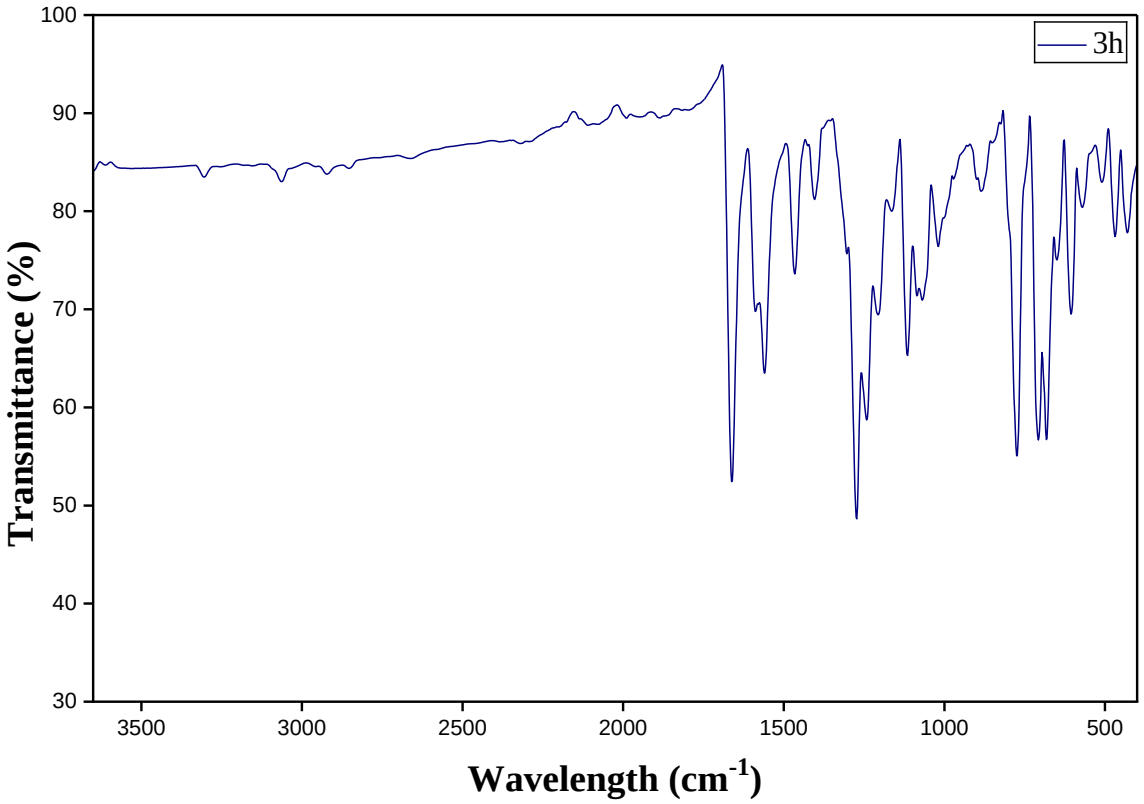
2-bromo-3-(4-chlorophenyl)naphthalene-1,4-dione (3g)



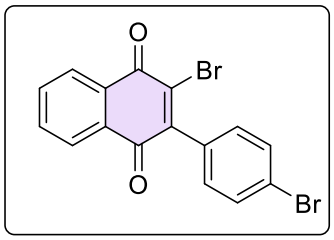
IR Spectra



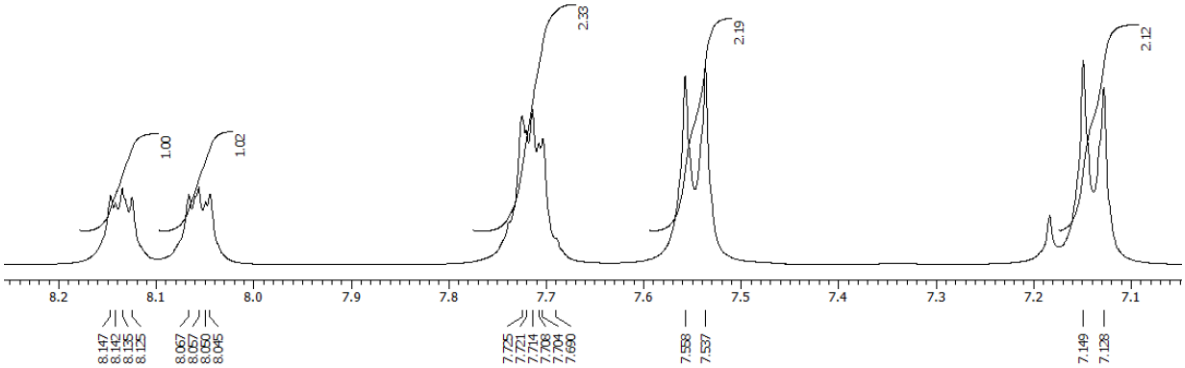
2-bromo-3-(4-bromophenyl)naphthalene-1,4-dione (3h)

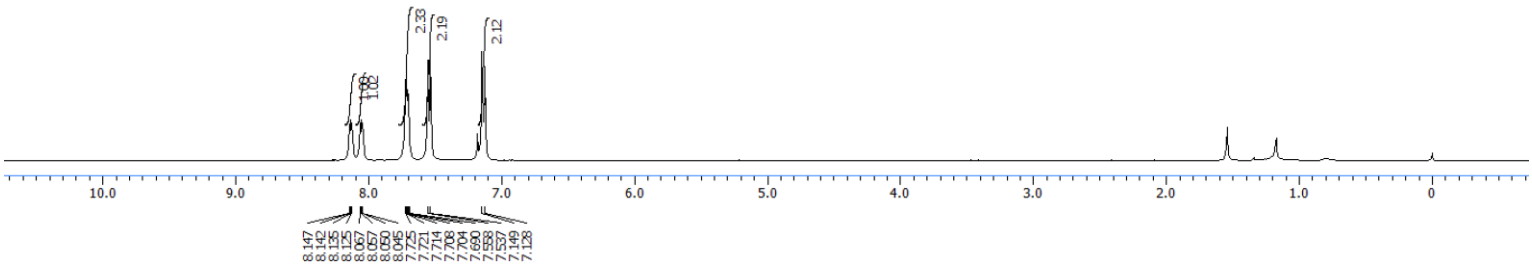


^{1}H NMR (400 MHz, $CDCl_3$)

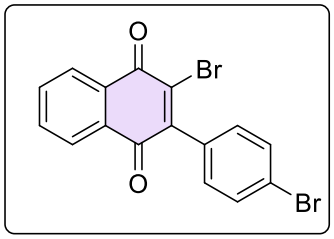


2-bromo-3-(4-bromophenyl)naphthalene-1,4-dione (3h)

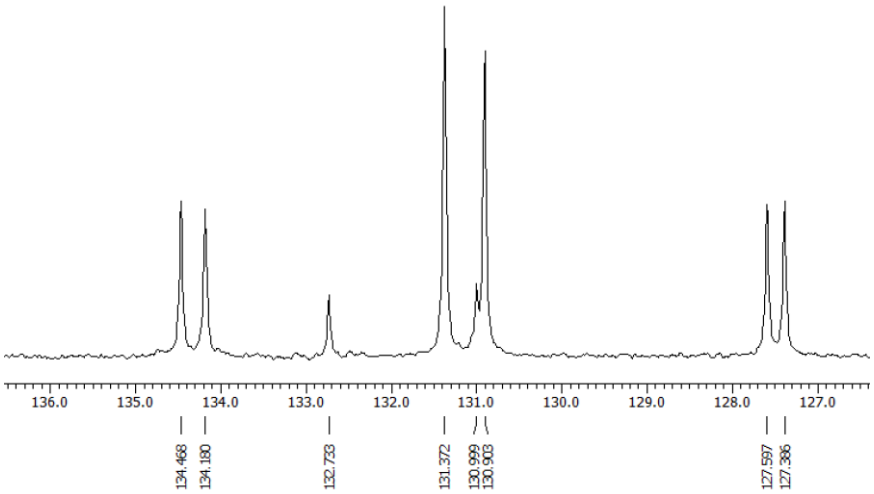


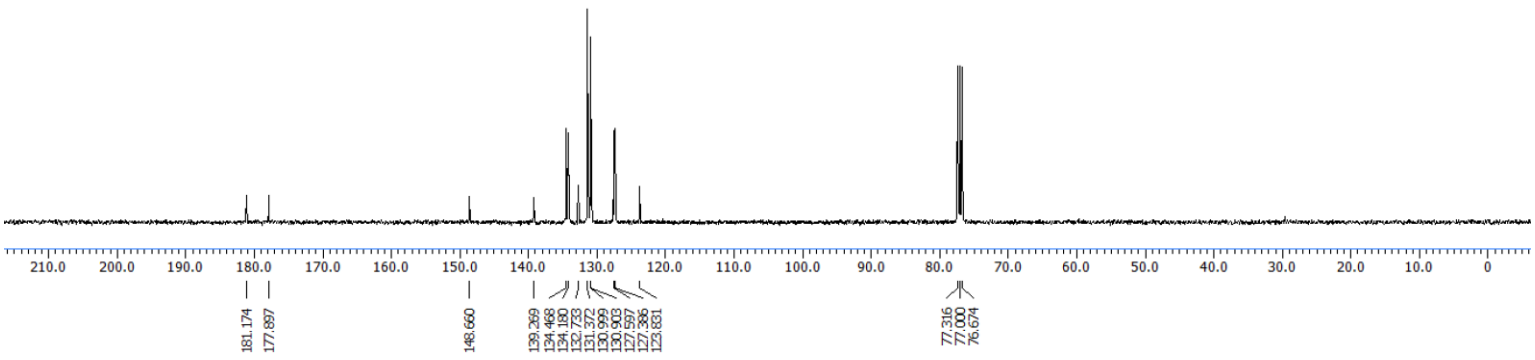


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

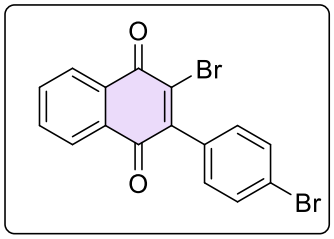


2-bromo-3-(4-bromophenyl)naphthalene-1,4-dione (3h)





HRMS



2-bromo-3-(4-bromophenyl)naphthalene-1,4-dione (3h)

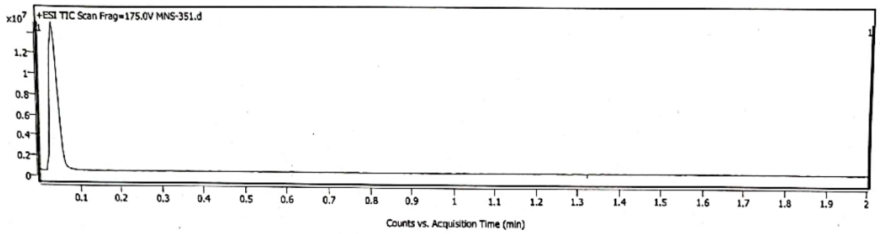
Compound Screening Report

Agilent

Sample Information

Sample Name	MNS-351	Data File Path	D:\Projects\demo & training\Data\MNS-351.d
Sample ID		Acq Time (Local)	01-08-2025 13:07:08 (UTC+05:30)
Instrument	BIO-QTOF	Acq Method Path	D:\Projects\demo & training\Methods\demo.m
MS Type	QTOF	Acq SW Version	6500 series Q-TOF (12.1.98.0)
Inj Vol (ul)	1	IRM Status	Success
Sample Position	P1-A4	DA Method Path	D:\Projects\Instrument_Verification\Methods\default.m
Plate Position		Target Source Path	
Acq Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Chromatograms



Compound Summary

Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
1		C16 H8 Br2 O2		0.042	389.8903	389.8891	3.16	67.25	FBF

Compound Details

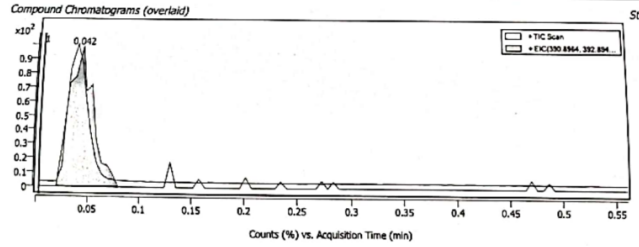
Cpd 1: C16 H8 Br2 O2

Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C16 H8 Br2 O2	0.042		389.8903	3.16		FBF	67.25	FBF

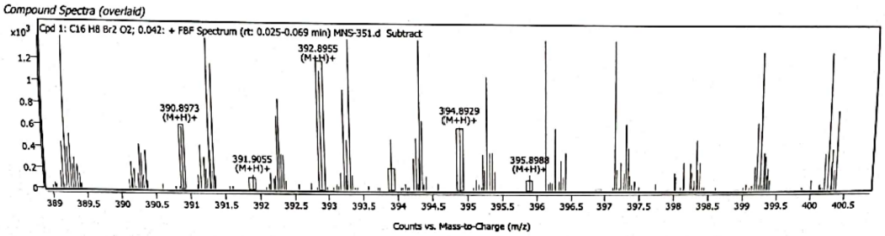
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+H)+	390.8973	67.25				

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

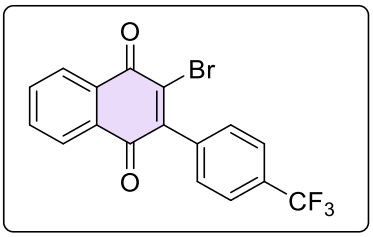


Compound ID Table

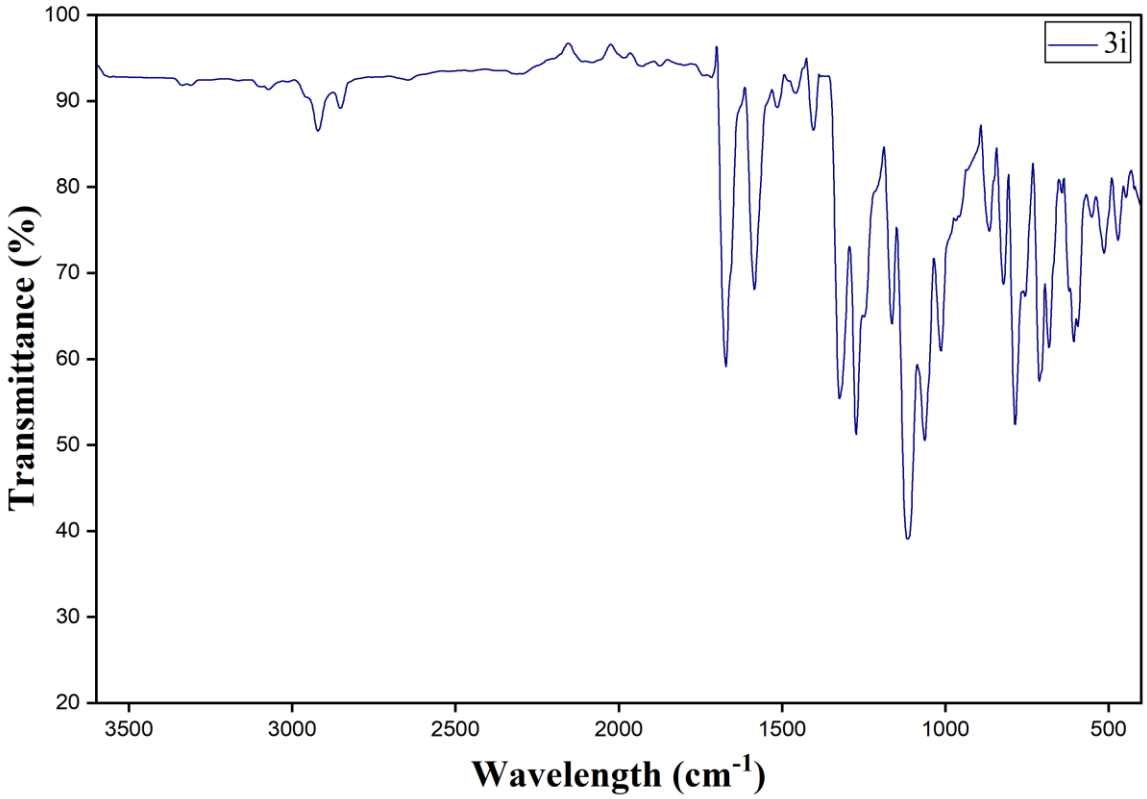
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C16 H8 Br2 O2	(M+H)+	0.042		389.8903		FBF	67.25		67.25

MassHunter Qual 12.0
(End of Report)

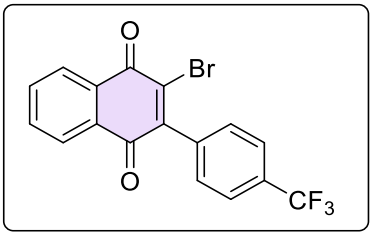
IR Spectra



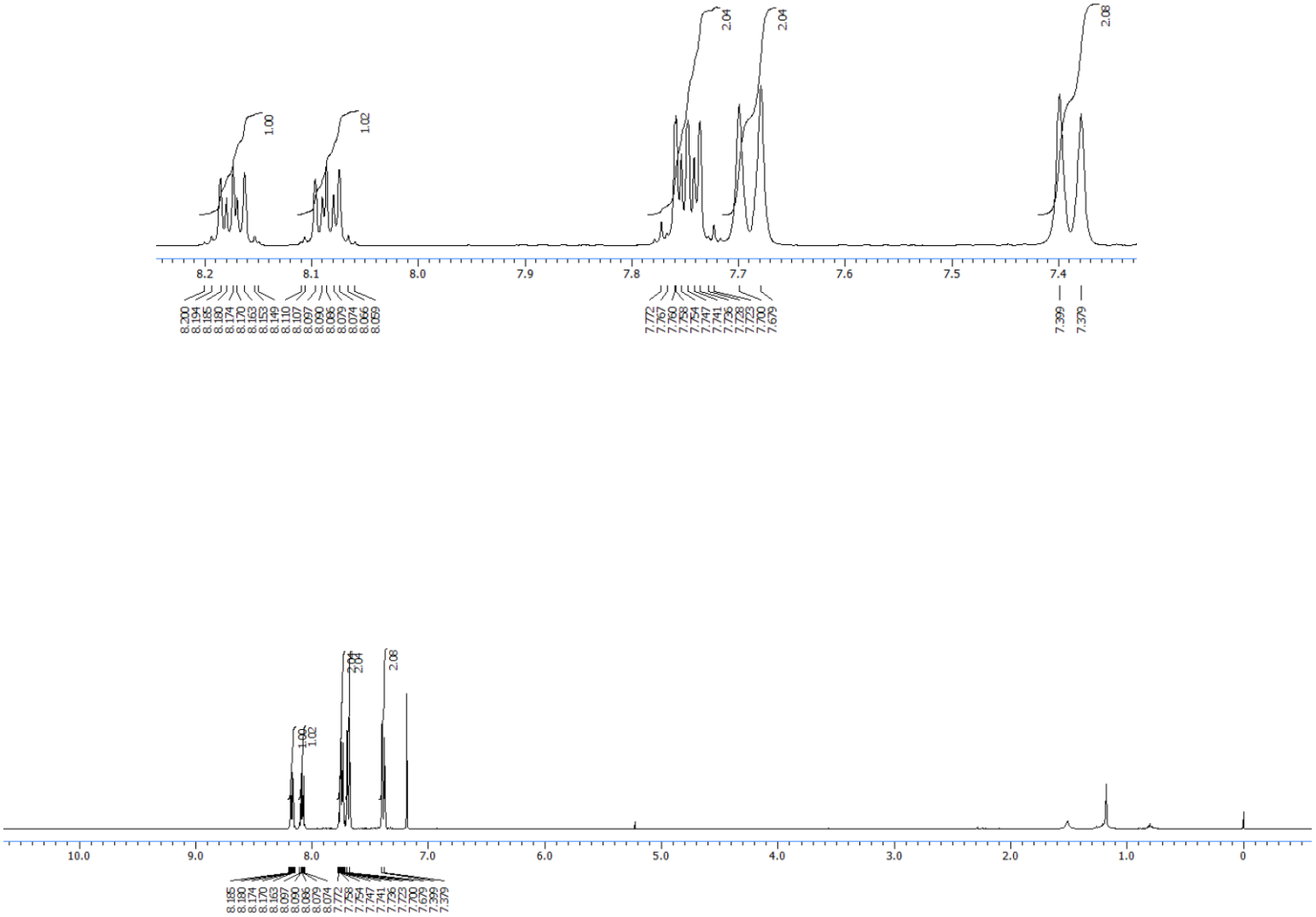
2-bromo-3-(4-(trifluoromethyl)phenyl)naphthalene-1,4-dione (3i)



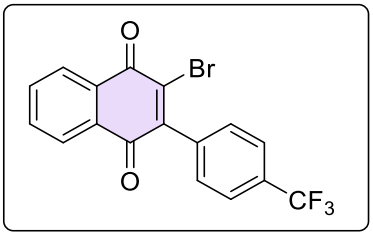
^{1}H NMR (400 MHz, $CDCl_3$)



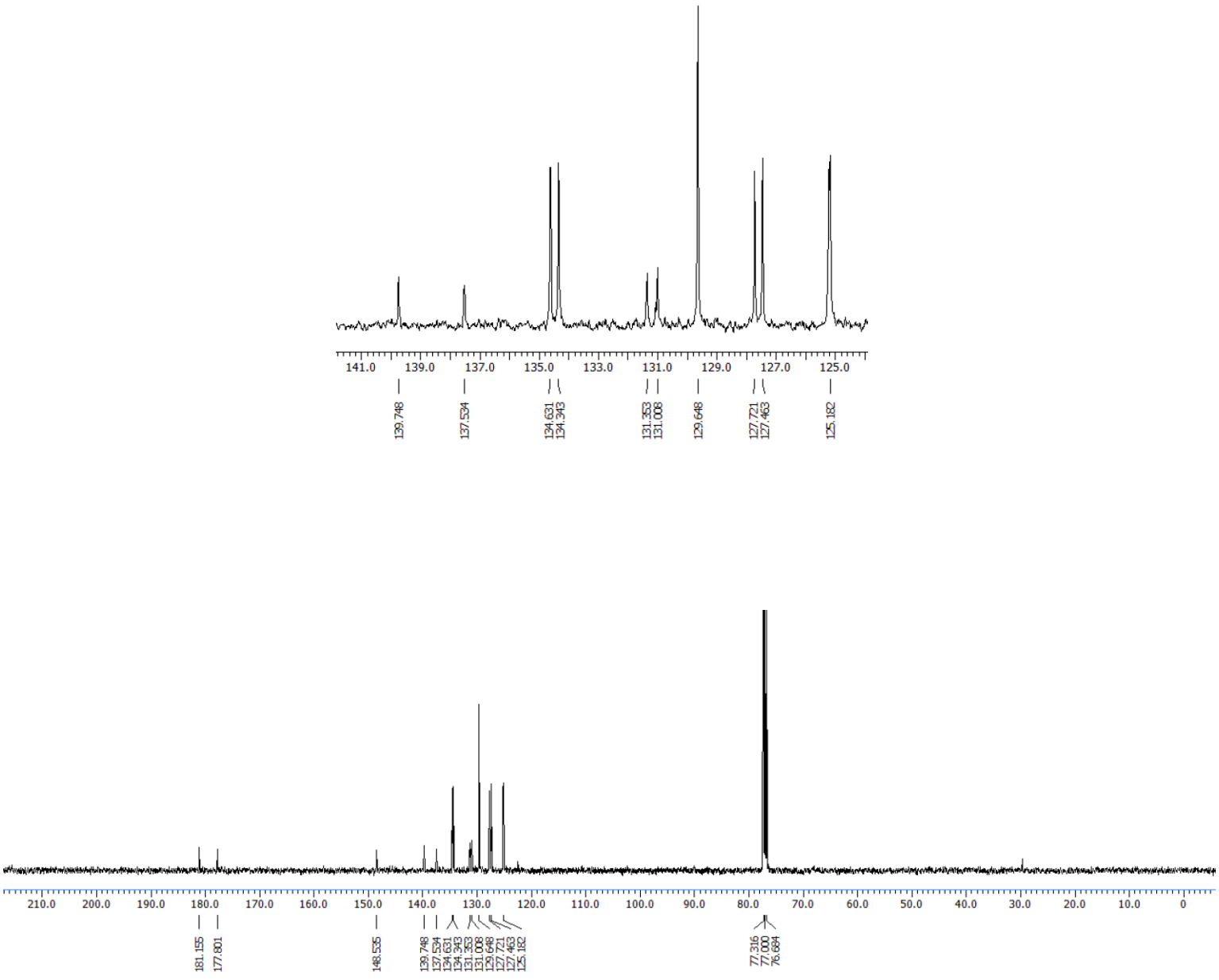
2-bromo-3-(4-(trifluoromethyl)phenyl)naphthalene-1,4-dione (3i)



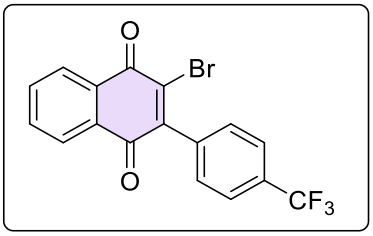
^{13}C NMR (100 MHz, $CDCl_3$)



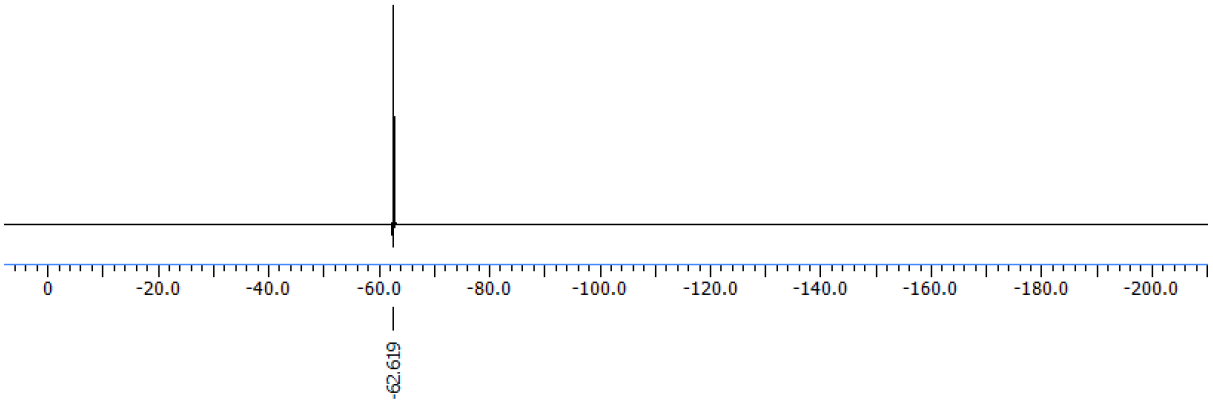
2-bromo-3-(4-(trifluoromethyl)phenyl)naphthalene-1,4-dione (3i)



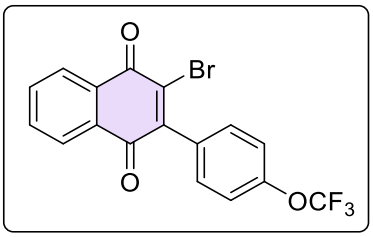
^{19}F NMR (376 MHz, $CDCl_3$)



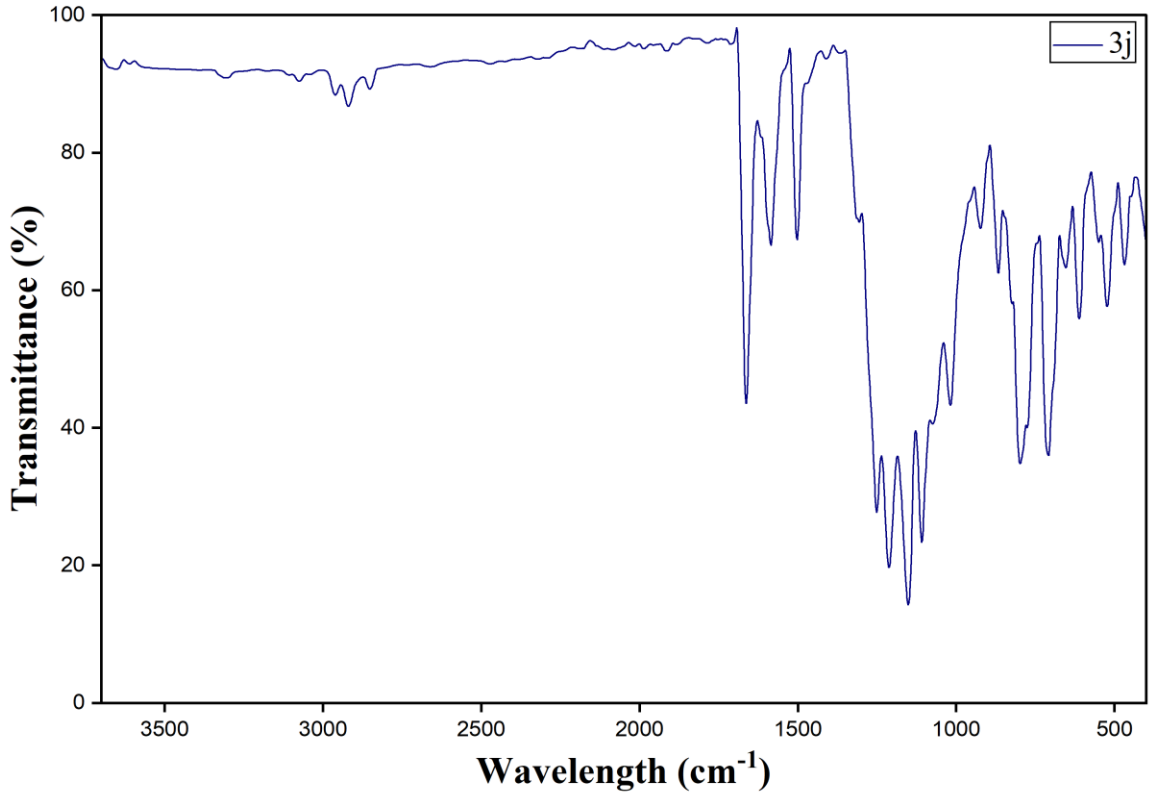
2-bromo-3-(4-(trifluoromethyl)phenyl)naphthalene-1,4-dione (3i)



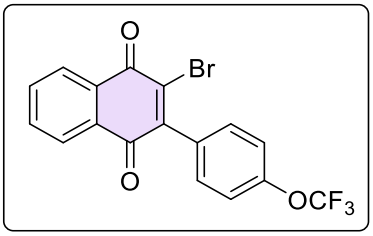
IR Spectra



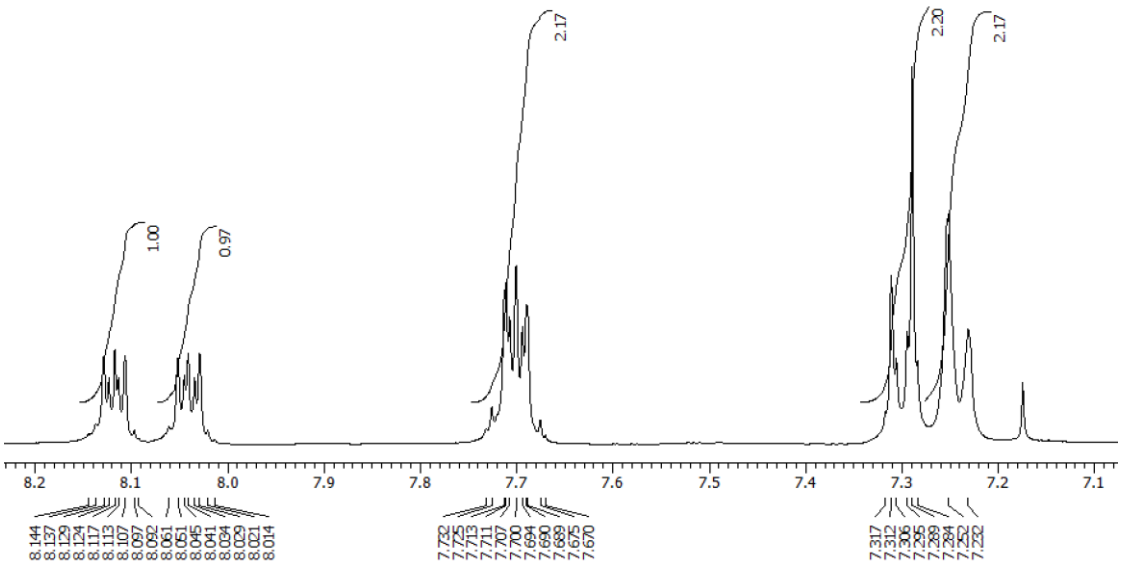
2-bromo-3-(4-(trifluoromethoxy)phenyl)naphthalene-1,4-dione (3j)

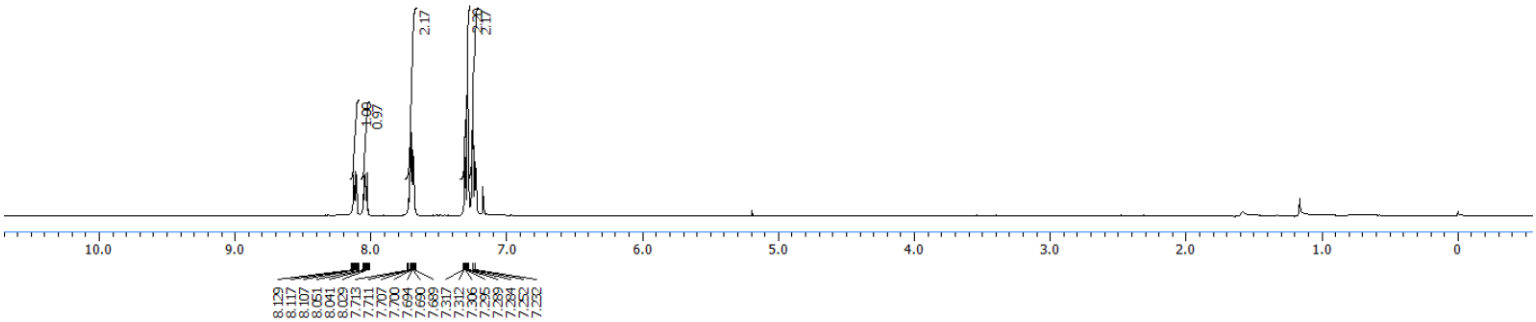


^{1}H NMR (400 MHz, $CDCl_3$)

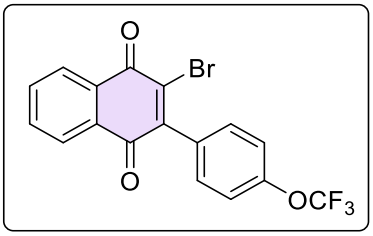


2-bromo-3-(4-(trifluoromethoxy)phenyl)naphthalene-1,4-dione (3j)

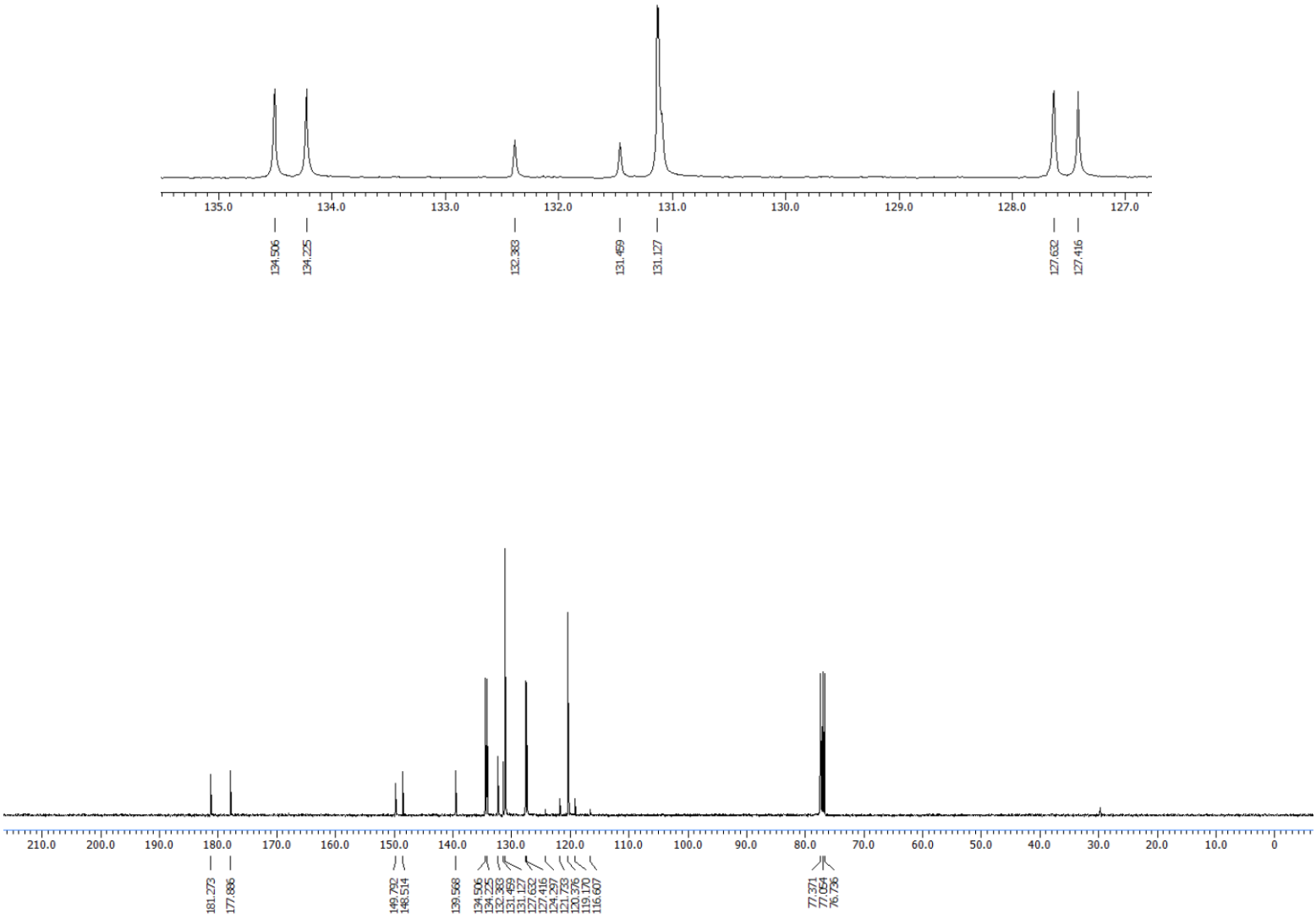




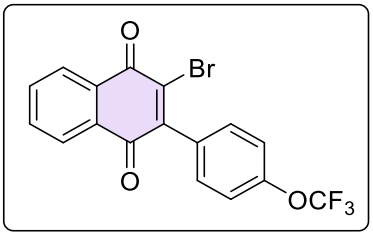
^{13}C NMR (100 MHz, $CDCl_3$)



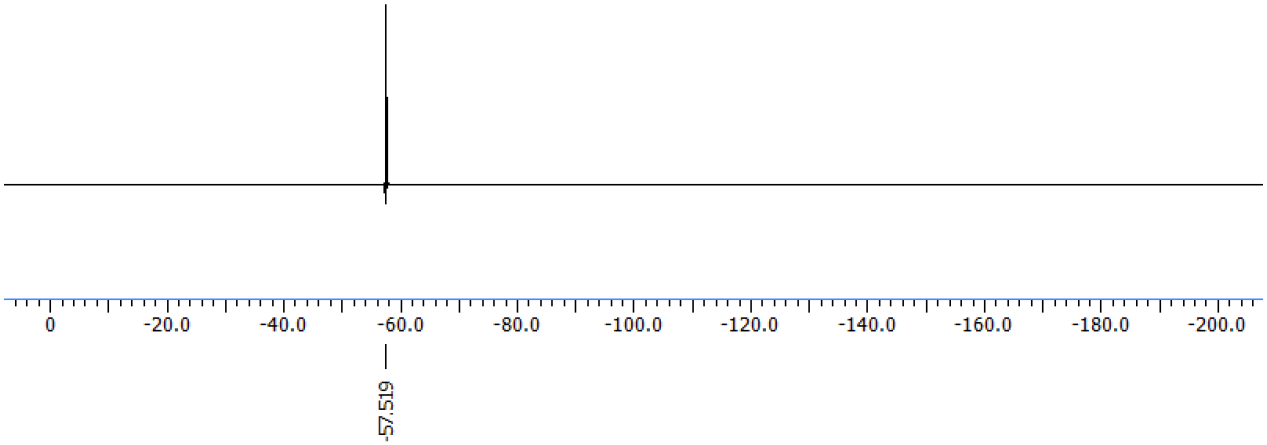
2-bromo-3-(4-(trifluoromethoxy)phenyl)naphthalene-1,4-dione (3j)



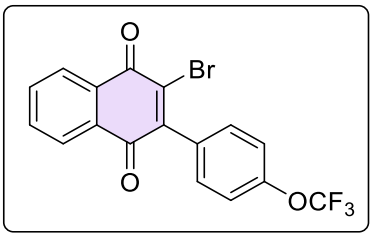
^{19}F NMR (376 MHz, $CDCl_3$)



2-bromo-3-(4-(trifluoromethoxy)phenyl)naphthalene-1,4-dione (3j)



HRMS



2-bromo-3-(4-(trifluoromethoxy)phenyl)naphthalene-1,4-dione (3j)

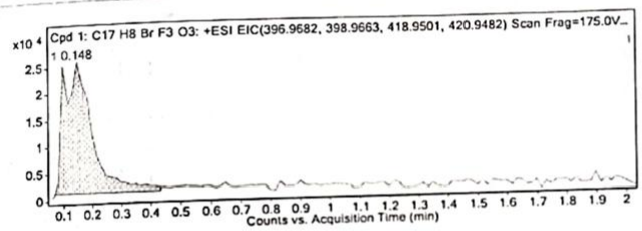
Qualitative Compound Report

Data File	MNS-318.d	Sample Name	MNS-318
Sample Type	Sample	Position	P1-C1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	03-03-2025 13:08:58
IRM Calibration Status	Success	DA Method	Default.m
Comment			
	Info.	3	
Sample Group	6200 series TOF/6500 series		
Acquisition SW Version	Q-TOF B.05.01 (B5125)		

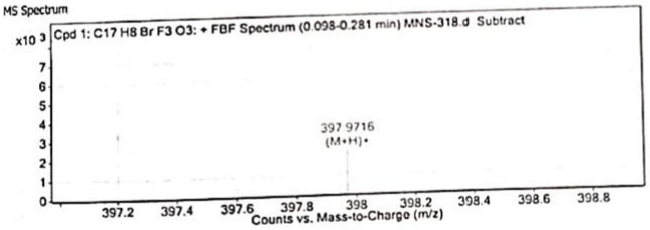
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H8 Br F3 O3	0.148	395.962	7226	C17 H8 Br F3 O3	395.9609	2.86	C17 H8 Br F3 O3	C17 H8 Br F3 O3

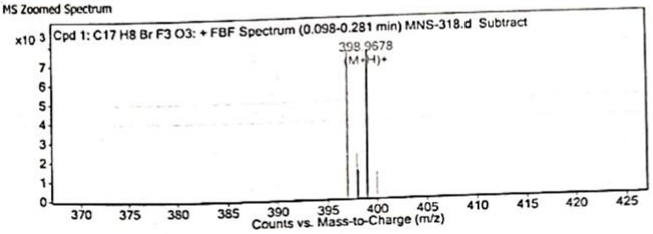
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H8 Br F3 O3	398.9678	0.148	Find By Formula	395.962



MS Spectrum



MS Zoomed Spectrum

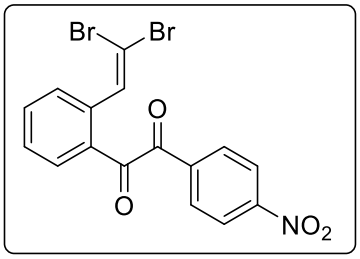


MS Spectrum Peak List

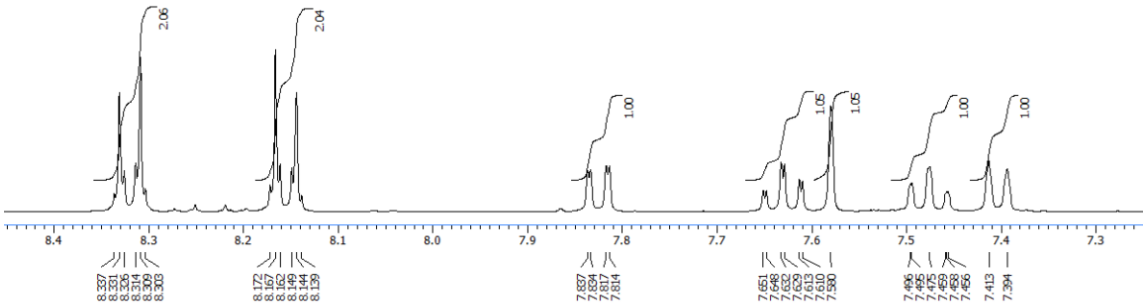
m/z	z	Abund	Formula	Ion
396.9693	1	7029.91	C17H9BrF3O3	(M+H)+
397.9716	1	2301.97	C17H9BrF3O3	(M+H)+
398.9678	1	7225.93	C17H9BrF3O3	(M+H)+

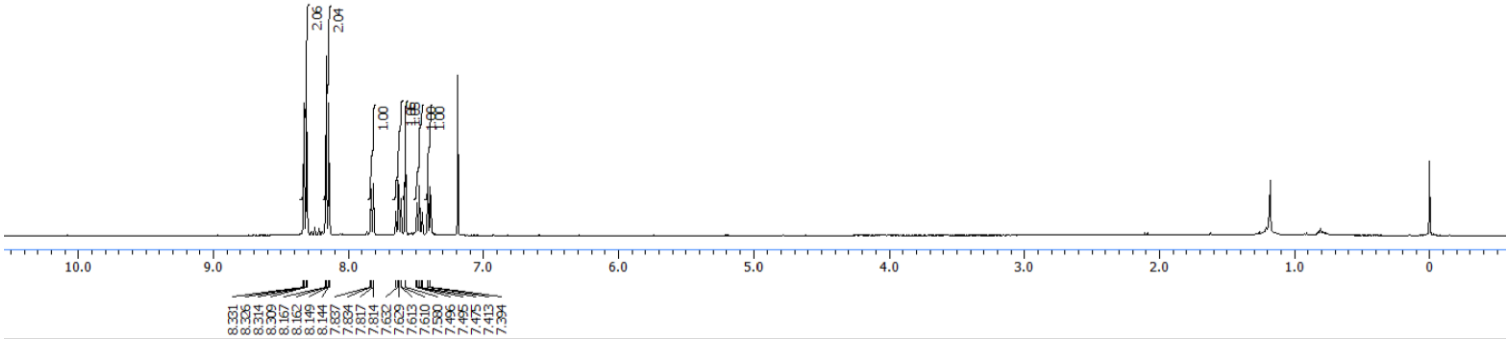
— End Of Report —

^{1}H NMR (400 MHz, $CDCl_3$)

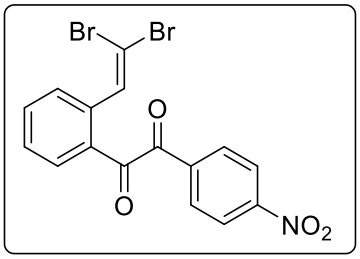


1-(2-(2,2-dibromovinyl)phenyl)-2-(4-nitrophenyl)ethane-1,2-dione (3k')

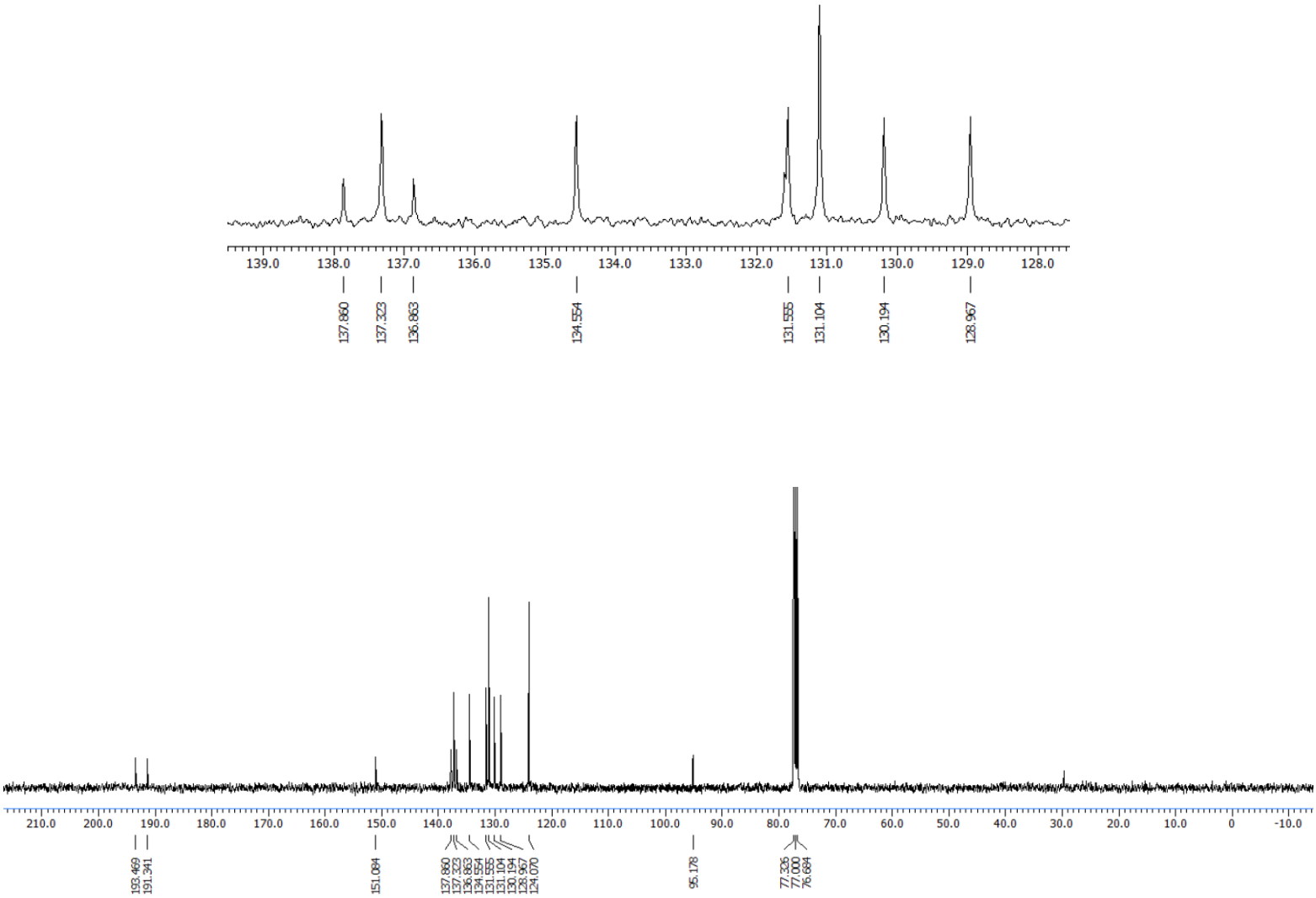




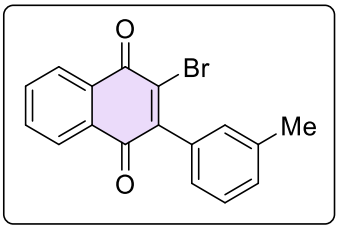
^{13}C NMR (100 MHz, $CDCl_3$)



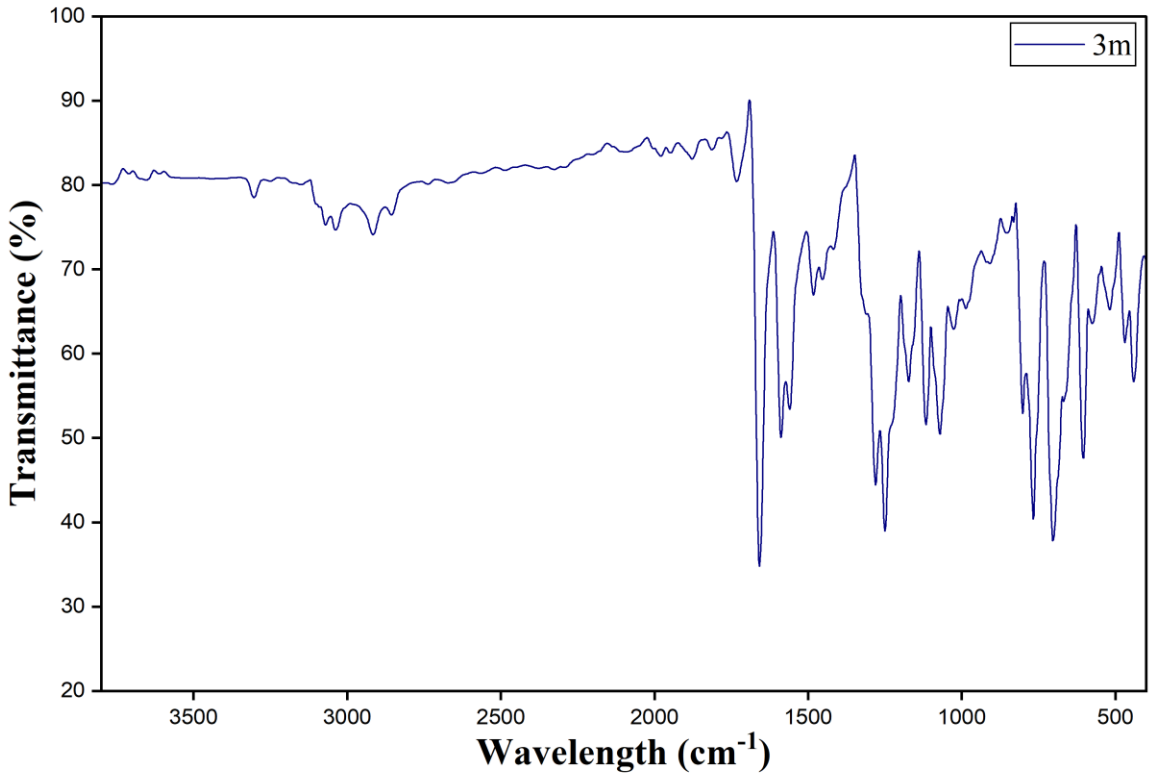
1-(2-(2,2-dibromovinyl)phenyl)-2-(4-nitrophenyl)ethane-1,2-dione (3k')



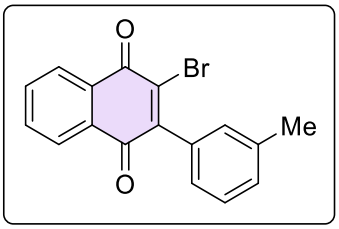
IR Spectra



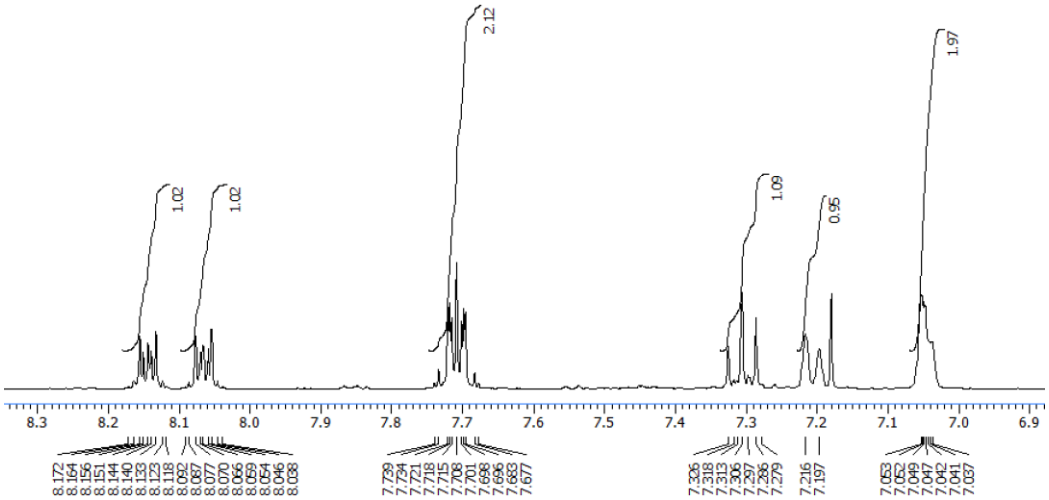
2-bromo-3-(*m*-tolyl)naphthalene-1,4-dione (3m)

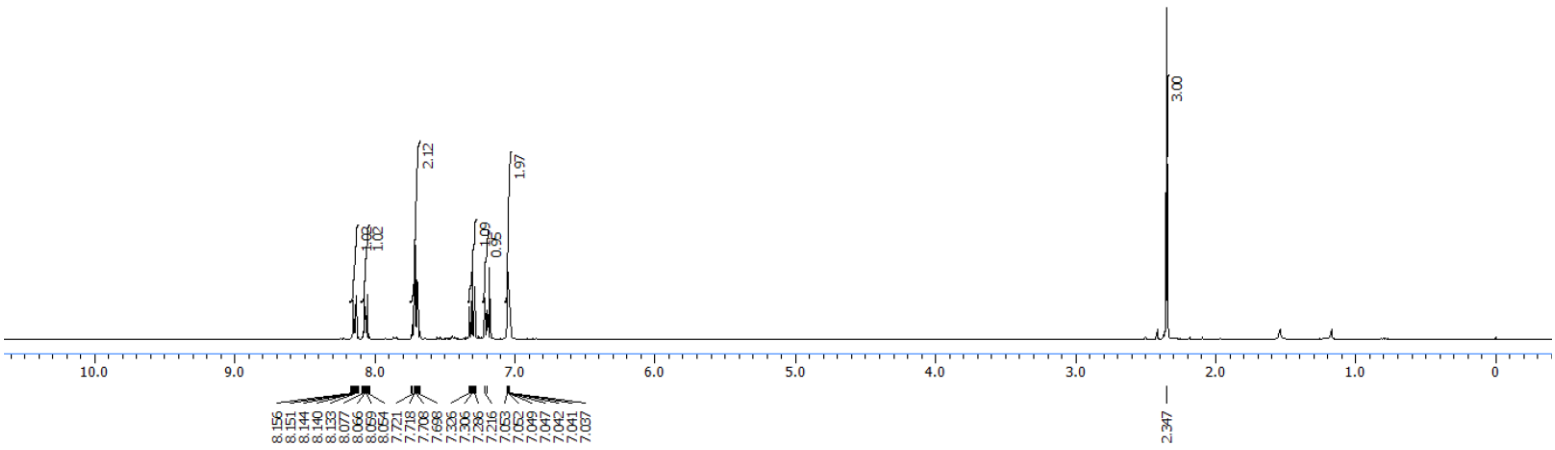


^{1}H NMR (400 MHz, $CDCl_3$)

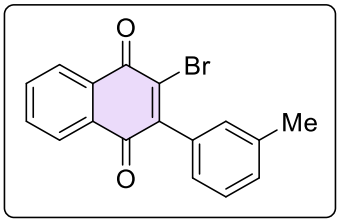


2-bromo-3-(*m*-tolyl)naphthalene-1,4-dione (3m)

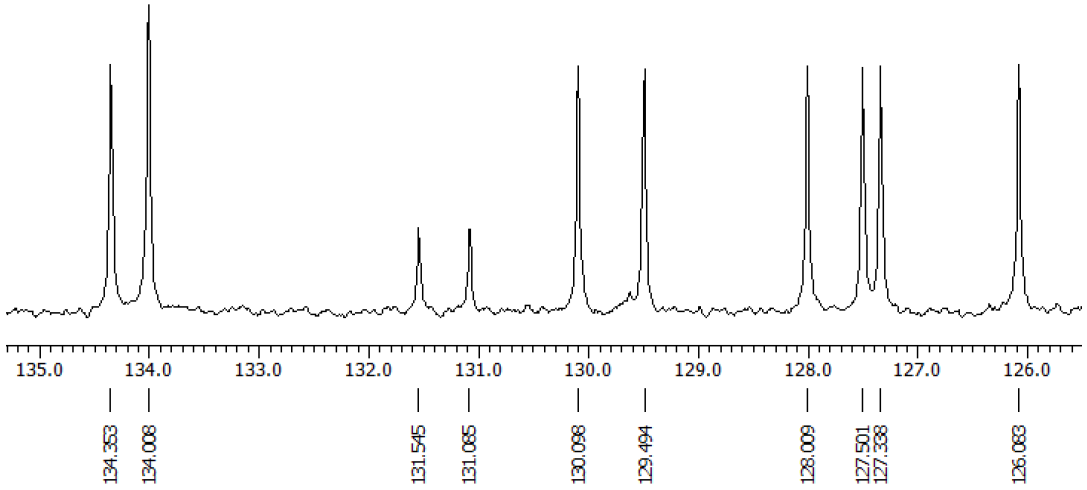


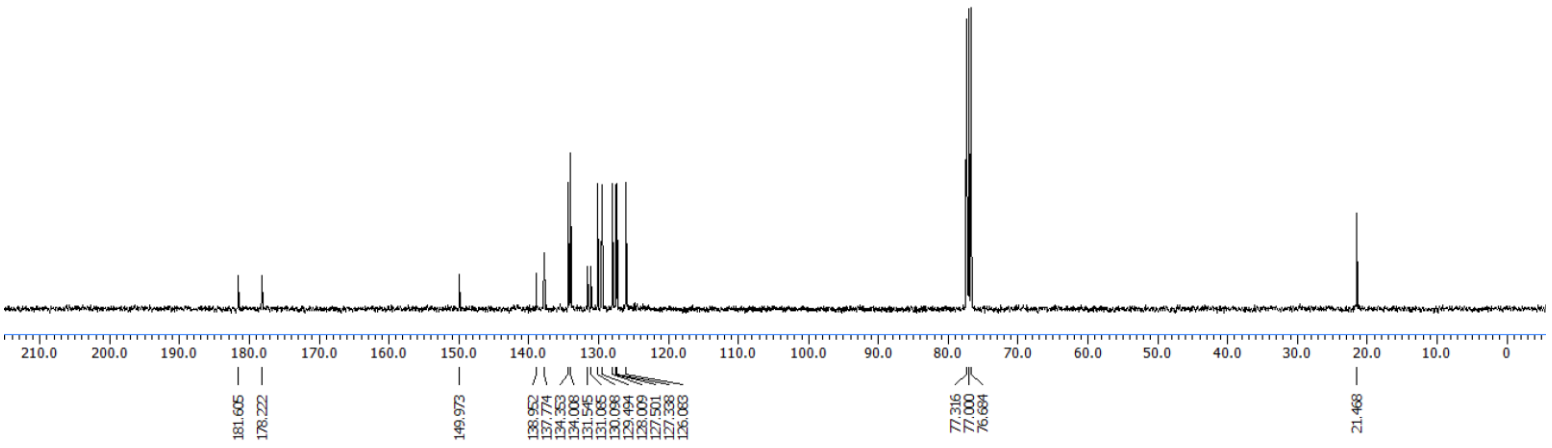


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

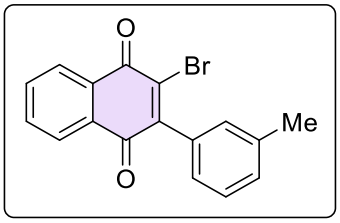


2-bromo-3-(*m*-tolyl)naphthalene-1,4-dione (3m)





HRMS



2-bromo-3-(*m*-tolyl)naphthalene-1,4-dione (3m)

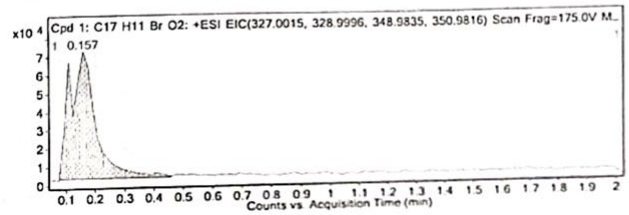
Qualitative Compound Report

Data File	MNS-311.d	Sample Name	MNS-311
Sample Type	Sample	Position	P1-B1
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	11-06-2024 13:23:20
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

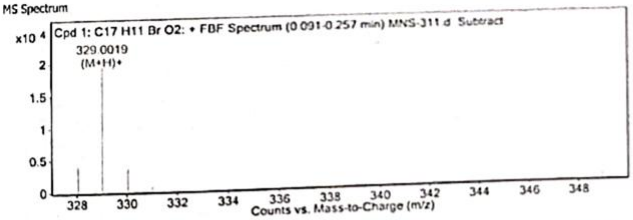
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H11 Br O2	0.157	325.9963	20071	C17 H11 Br O2	325.9942	6.27	C17 H11 Br O2	C17 H11 Br O2

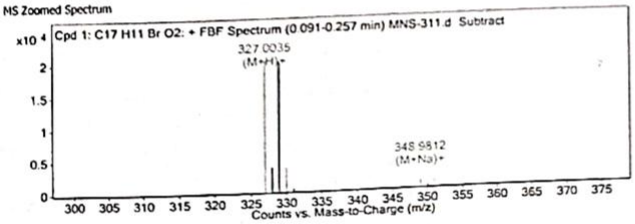
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H11 Br O2	327.0035	0.157	Find By Formula	325.9963



MS Spectrum



MS Zoomed Spectrum

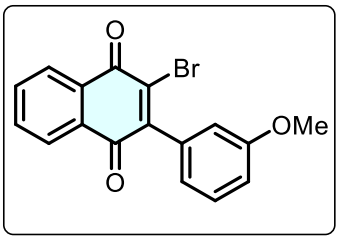


MS Spectrum Peak List

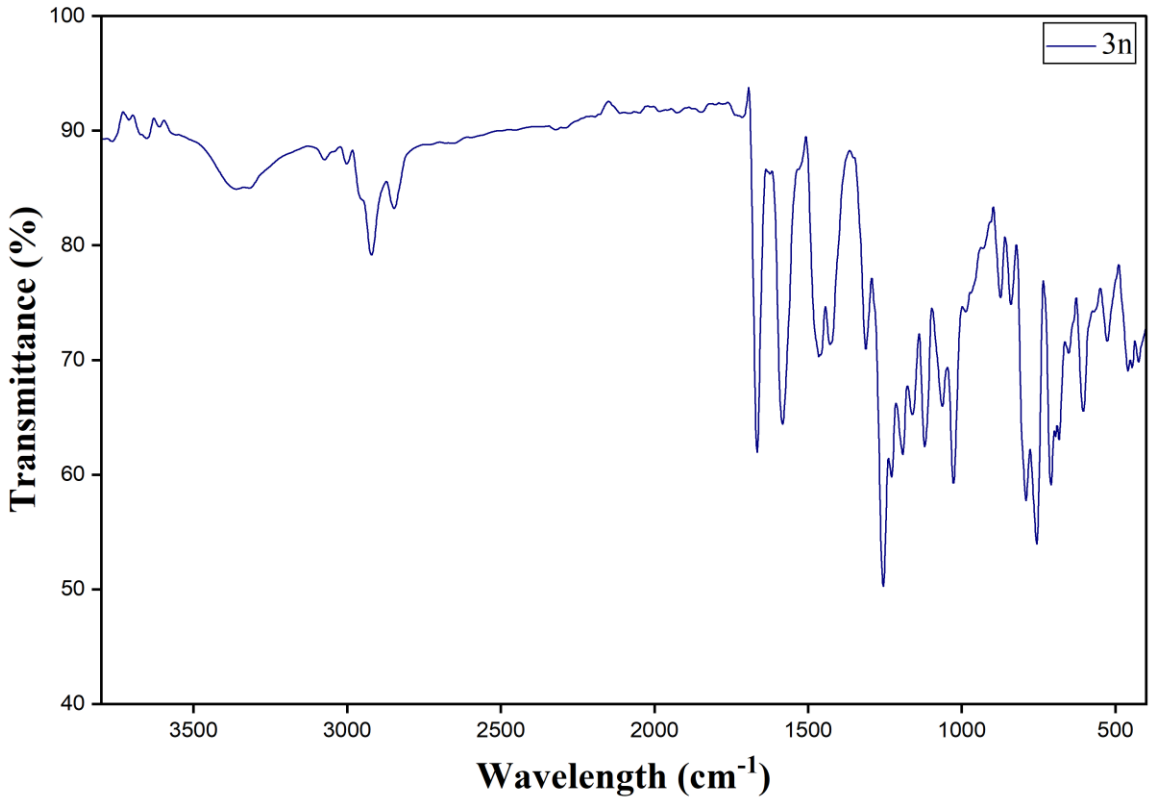
m/z	z	Abund	Formula	Ion
327.0035	1	20070.81	C17H12BrO2	(M+H)+
328.0067	1	3905.27	C17H12BrO2	(M+H)+
329.0019	1	19387.96	C17H12BrO2	(M+H)+
330.0055	1	3731.68	C17H12BrO2	(M+H)+
331.0089	1	899.03	C17H12BrO2	(M+H)+
332.0095	1	66.73	C17H12BrO2	(M+H)+
348.9812	1	914.41	C17H11BrNaO2	(M+Na)+
349.9818	1	284.85	C17H11BrNaO2	(M+Na)+

--- End Of Report ---

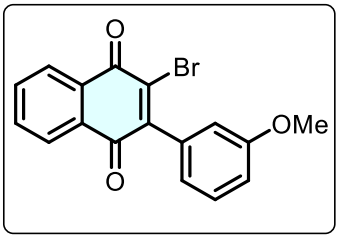
IR Spectra



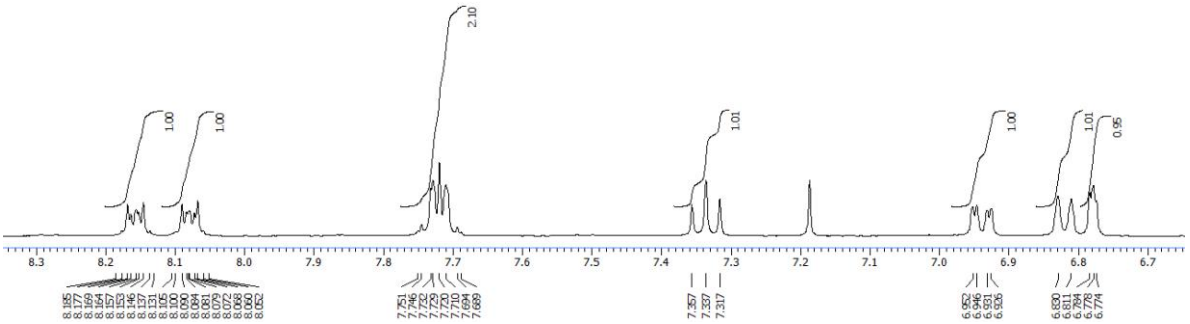
2-bromo-3-(3-methoxyphenyl)naphthalene-1,4-dione (3n)

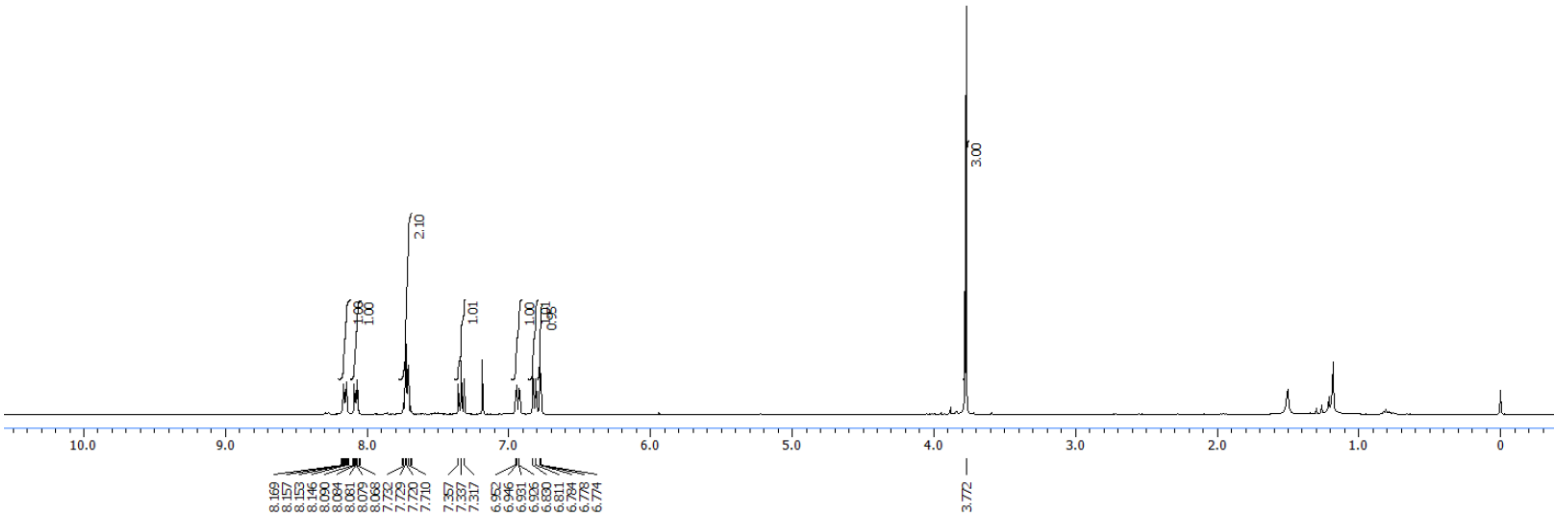


^{1}H NMR (400 MHz, $CDCl_3$)

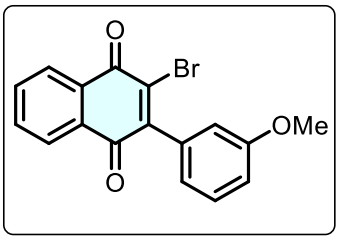


2-bromo-3-(3-methoxyphenyl)naphthalene-1,4-dione (3n).

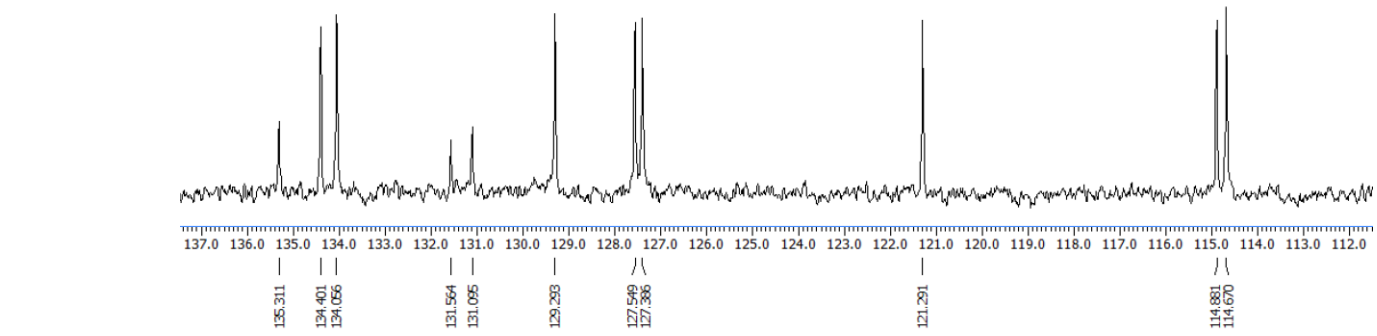


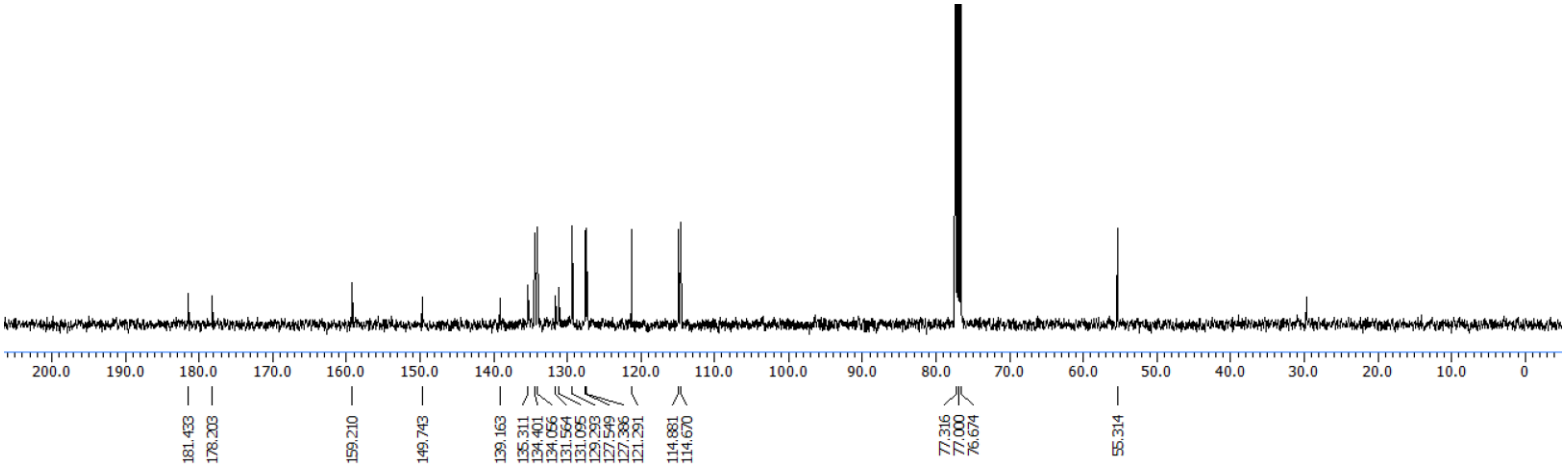


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

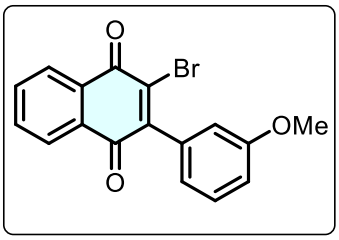


2-bromo-3-(3-methoxyphenyl)naphthalene-1,4-dione (3n).





$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-bromo-3-(3-methoxyphenyl)naphthalene-1,4-dione (3n).

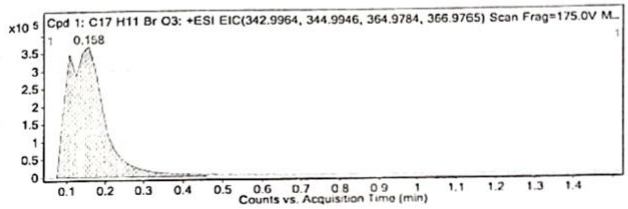
Qualitative Compound Report

Data File	MNS-300.d	Sample Name	MNS-300
Sample Type	Sample	Position	P1-A3
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	13-05-2024 14:16:22
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

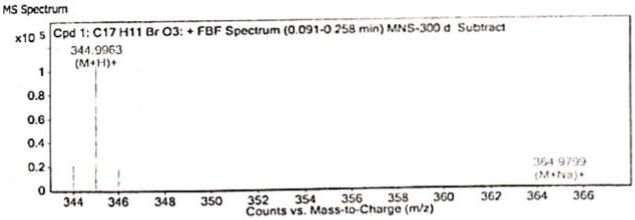
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H11 Br O3	0.158	341.991	105321	C17 H11 Br O3	341.9892	5.44	C17 H11 Br O3	C17 H11 Br O3

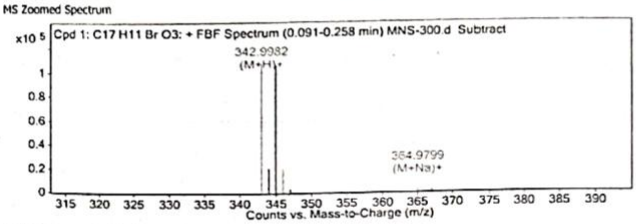
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H11 Br O3	342.9982	0.158	Find By Formula	341.991



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
342.9982	1	106321.27	C17H12BrO3	(M+H)+
344.0027	1	21468.66	C17H12BrO3	(M+H)+
344.9963	1	105363.95	C17H12BrO3	(M+H)+
345.9996	1	18958.19	C17H12BrO3	(M+H)+
347.003	1	2561.77	C17H12BrO3	(M+H)+
348.0029	1	187.86	C17H12BrO3	(M+H)+
364.9799	1	1568.85	C17H11BrNaO3	(M+Na)+
365.9823	1	326.81	C17H11BrNaO3	(M+Na)+
366.978	1	1550.11	C17H11BrNaO3	(M+Na)+
367.9867	1	314.61	C17H11BrNaO3	(M+Na)+

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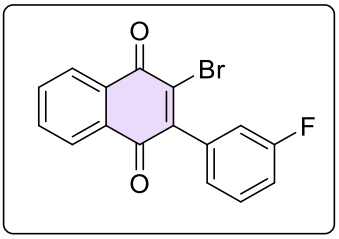
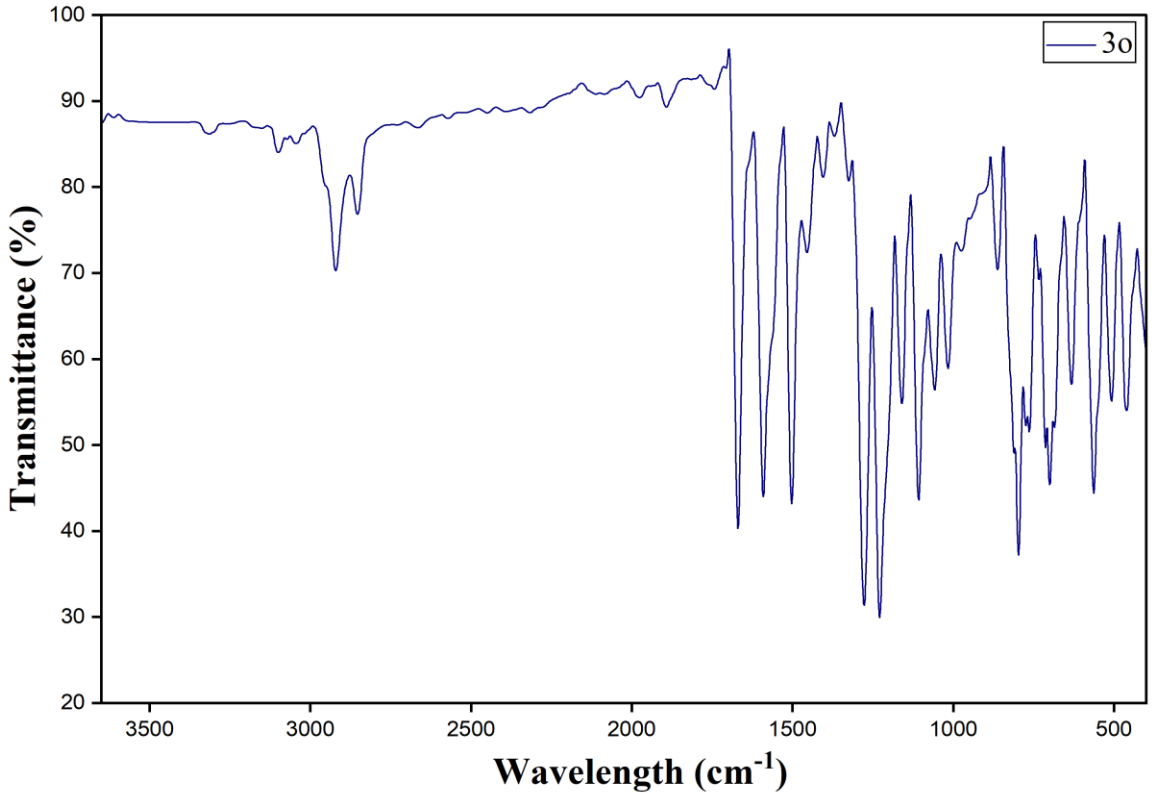
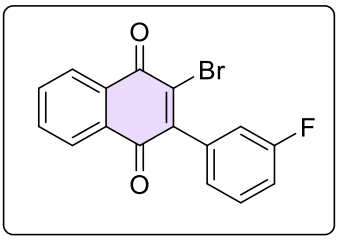
IR Spectra



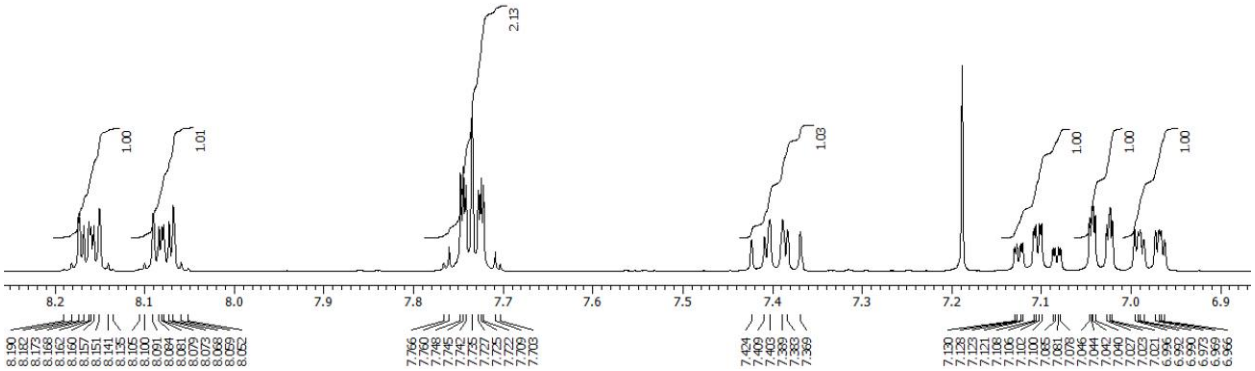
2-bromo-3-(3-fluorophenyl)naphthalene-1,4-dione (3o)

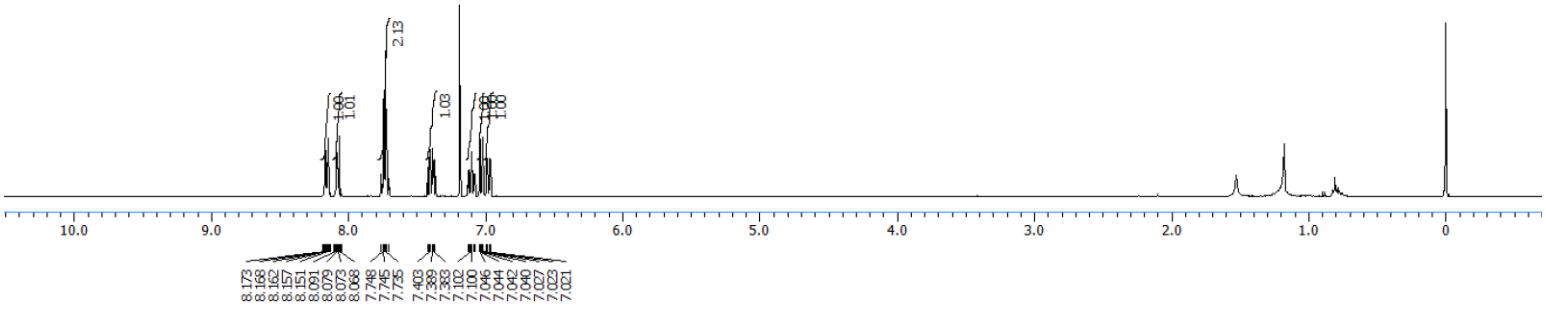


^{1}H NMR (400 MHz, $CDCl_3$)

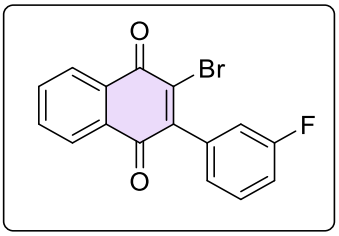


2-bromo-3-(3-fluorophenyl)naphthalene-1,4-dione (3o)

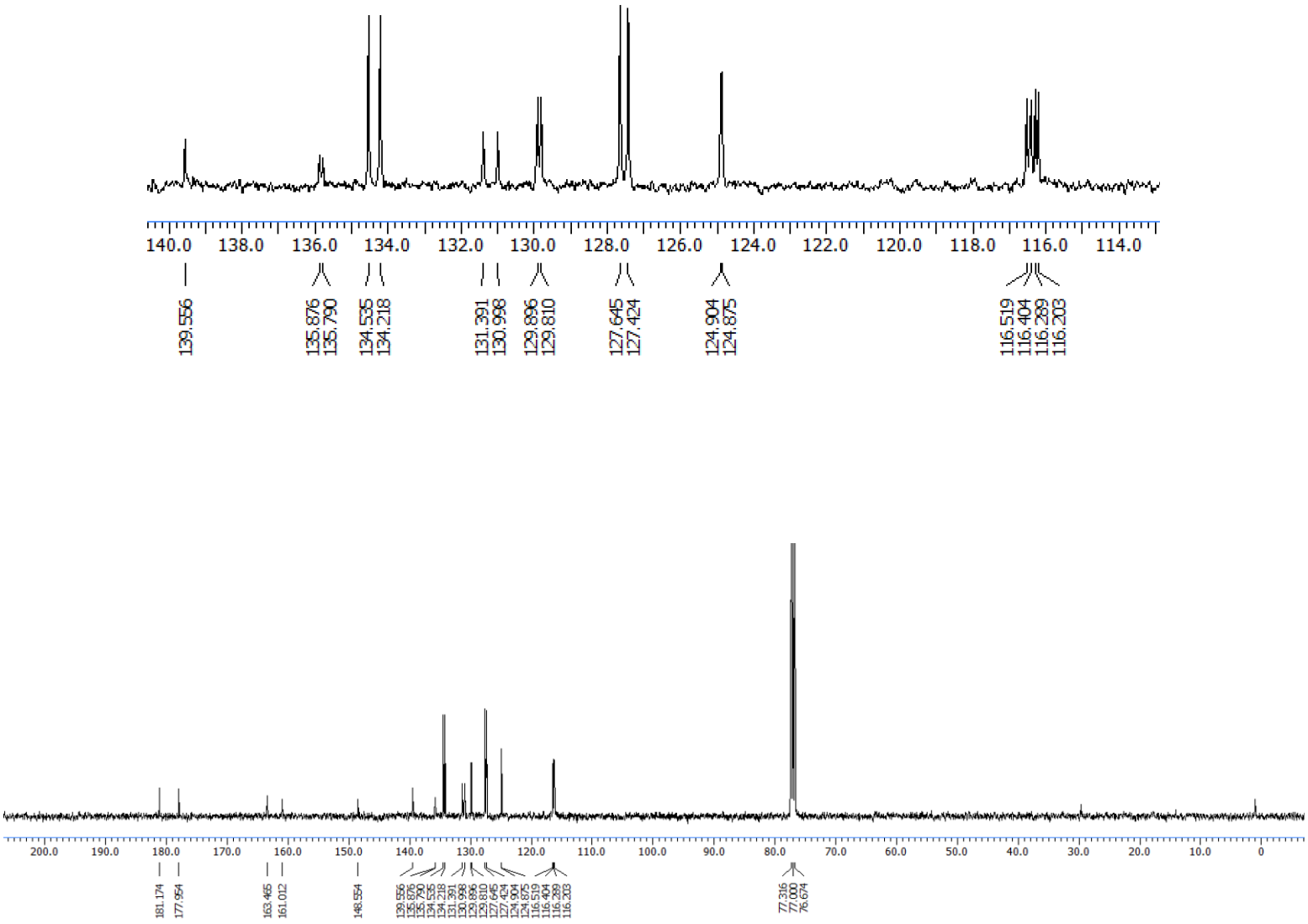




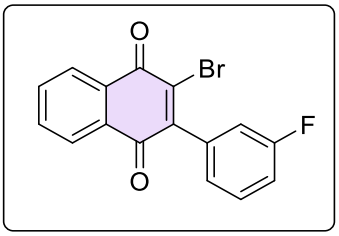
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



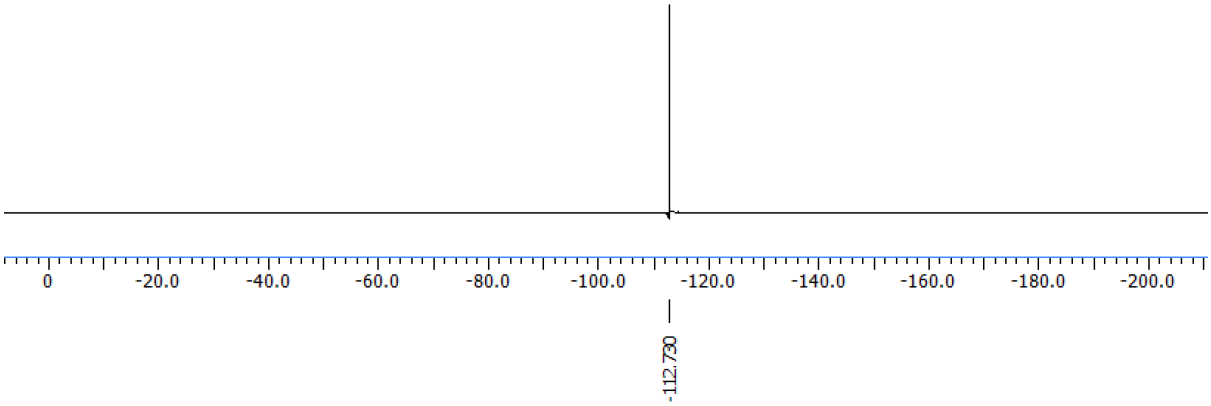
2-bromo-3-(3-fluorophenyl)naphthalene-1,4-dione (3o)



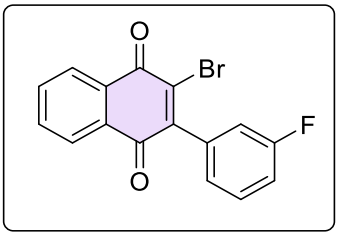
^{19}F NMR (376 MHz, $CDCl_3$)



2-bromo-3-(3-fluorophenyl)naphthalene-1,4-dione (3o)



HRMS



2-bromo-3-(3-fluorophenyl)naphthalene-1,4-dione (3o)

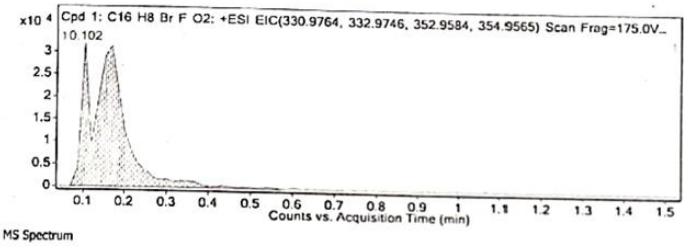
Qualitative Compound Report

Data File	MNS-302.d	Sample Name	MNS-302
Sample Type	Sample	Position	P1-A4
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	13-05-2024 14:20:15
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

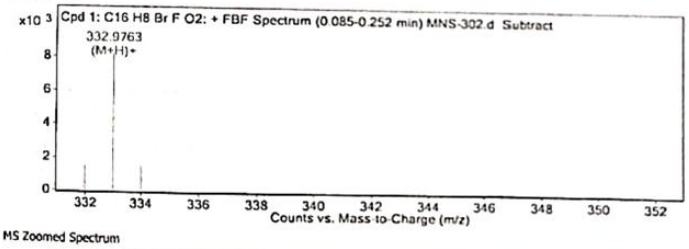
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C16 H8 Br F O2	0.102	329.9712	8267	C16 H8 Br F O2	329.9692	6.09	C16 H8 Br F O2	C16 H8 Br F O2

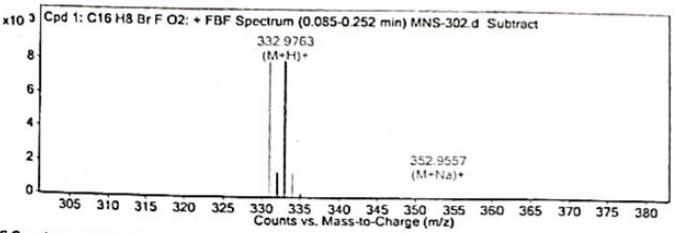
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C16 H8 Br F O2	332.9763	0.102	Find By Formula	329.9712



MS Spectrum



MS Zoomed Spectrum

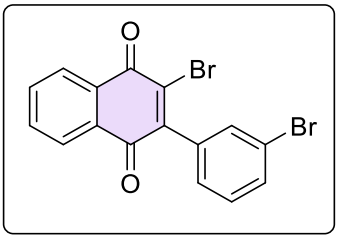


MS Spectrum Peak List

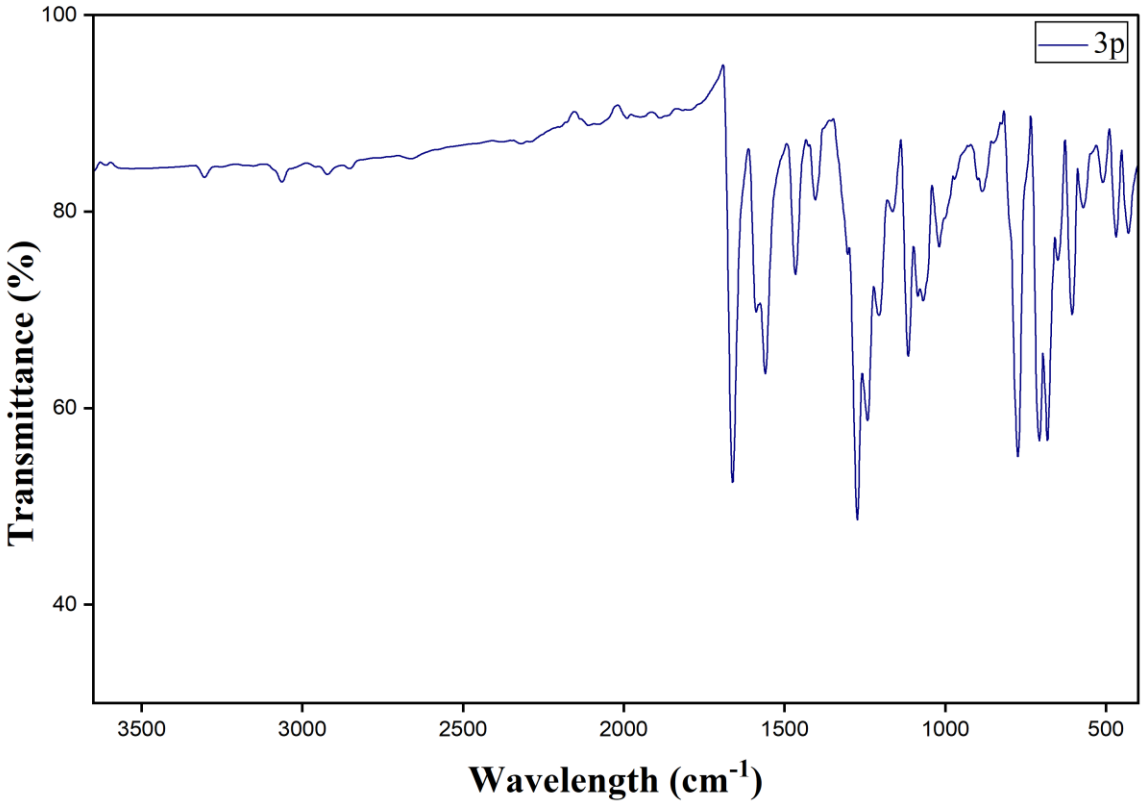
m/z	z	Abund	Formula	Ion
330.9785	1	7443.49	C16H9BrFO2	(M+H)+
331.9829	1	1502.41	C16H9BrFO2	(M+H)+
332.9763	1	8267.29	C16H9BrFO2	(M+H)+
333.9802	1	1465.49	C16H9BrFO2	(M+H)+
334.9861	1	220.44	C16H9BrFO2	(M+H)+
352.9557	1	61.64	C16H8BrFNaO2	(M+Na)+

--- End Of Report ---

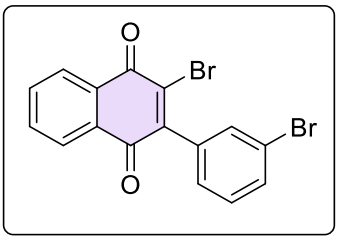
IR Spectra



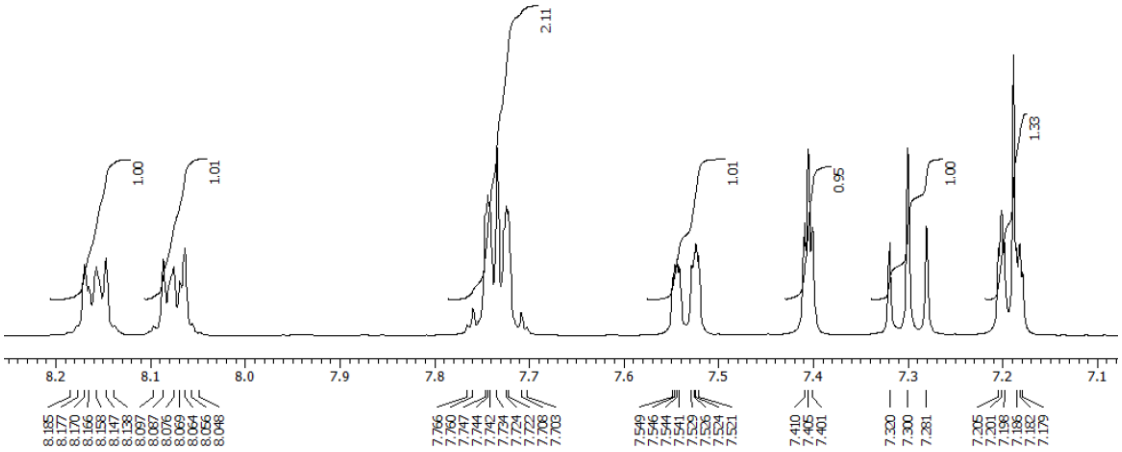
2-bromo-3-(3-bromophenyl)naphthalene-1,4-dione (3p)

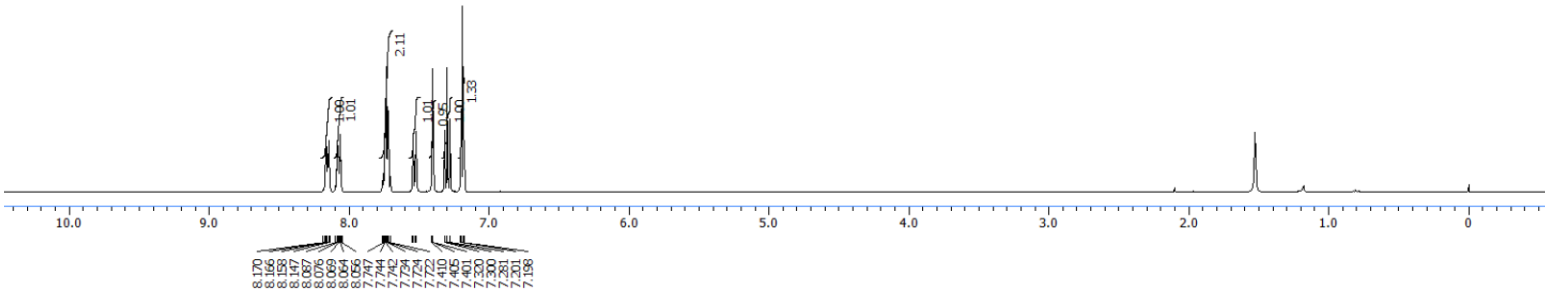


^{1}H NMR (400 MHz, $CDCl_3$)

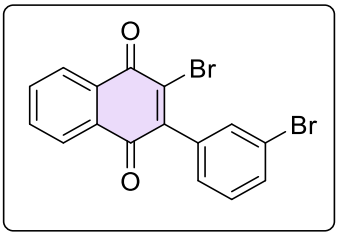


2-bromo-3-(3-bromophenyl)naphthalene-1,4-dione (3p)

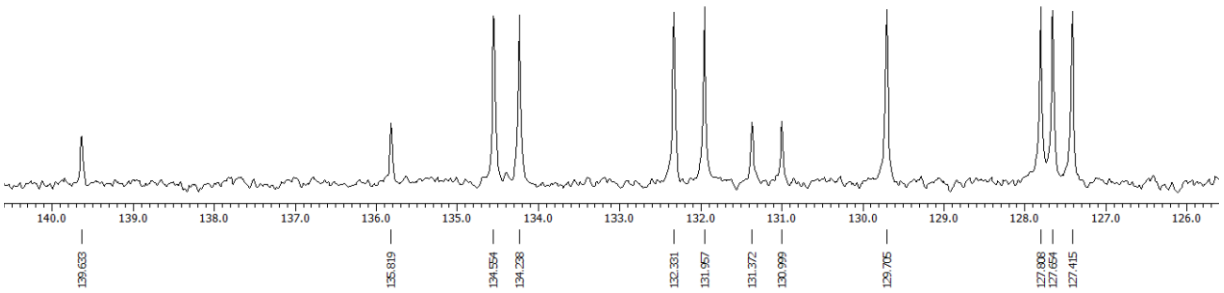


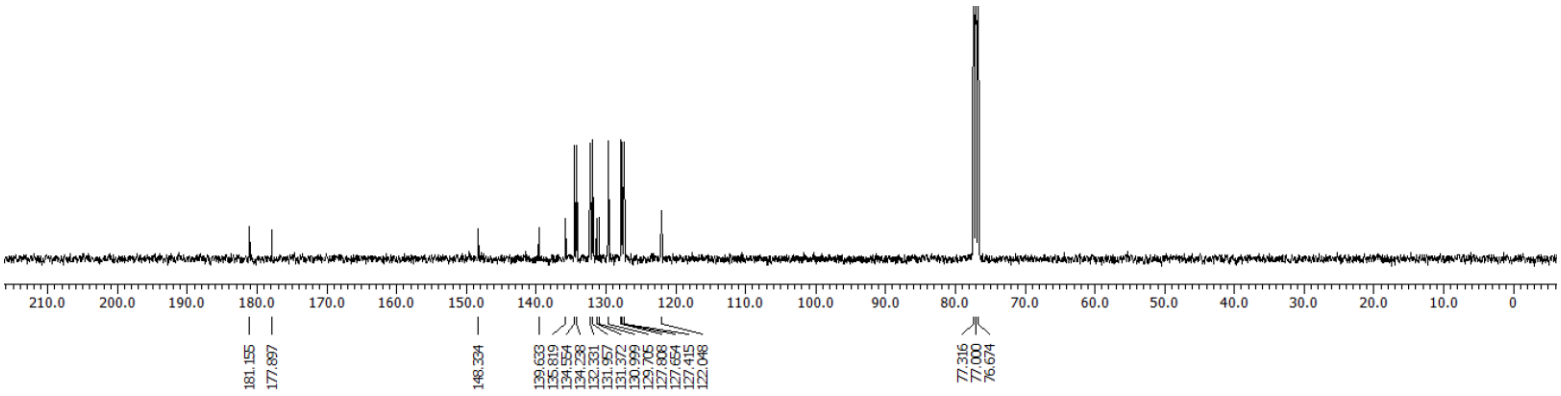


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

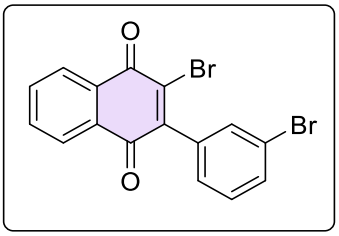


2-bromo-3-(3-bromophenyl)naphthalene-1,4-dione (3p)





$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-bromo-3-(3-bromophenyl)naphthalene-1,4-dione (3p)

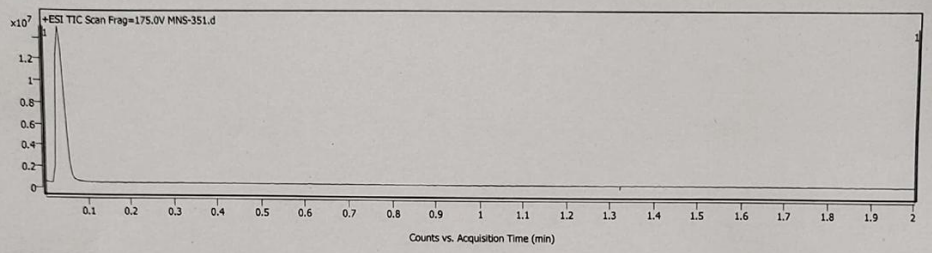
Compound Screening Report

Agilent

Sample Information

Sample Name	MNS-351	Data File Path	D:\Projects\demo & training\Data\MNS-351.d
Sample ID		Acq Time (Local)	01-08-2025 13:07:08 (UTC+05:30)
Instrument	BIO-QTOF	Acq Method Path	D:\Projects\demo & training\Methods\demo.m
MS Type	QTOF	Acq SW Version	6500 series Q-TOF (12.1.98.0)
Inj Vol (ul)	1	IRM Status	Success
Sample Position	P1-A4	DA Method Path	D:\Projects\Instrument_Verification\Methods\default.m
Plate Position		Target Source Path	
Acq Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Chromatograms



Compound Summary

Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
1		C16 H8 Br2 O2		0.042	389.8903	389.8891	3.16	67.25	FBF

Compound Details

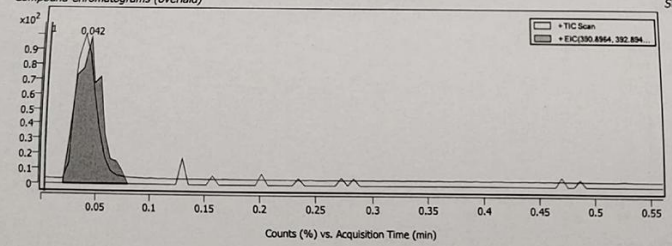
Cpd 1: C16 H8 Br2 O2

Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C16 H8 Br2 O2	0.042		389.8903	3.16		FBF	67.25	FBF

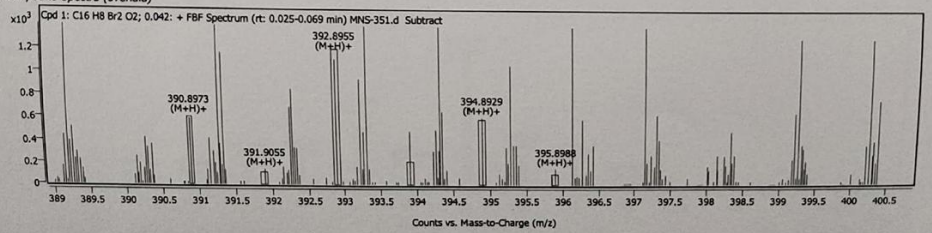
Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+H)+	390.8973	67.25				

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)

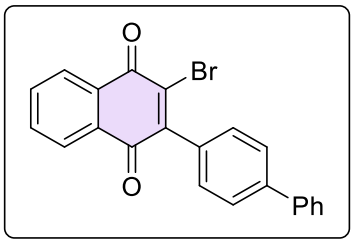


Compound ID Table

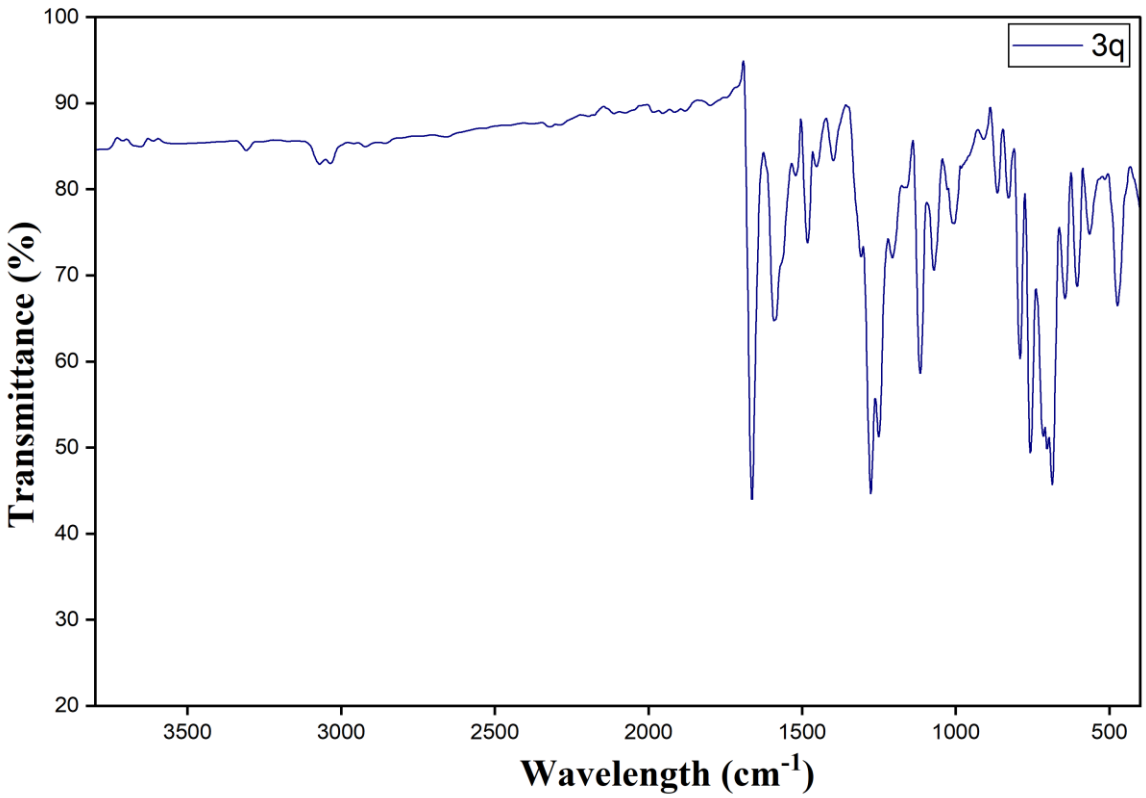
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C16 H8 Br2 O2	(M+H)+	0.042		389.8903		FBF	67.25		67.25

MassHunter Qual 12.0

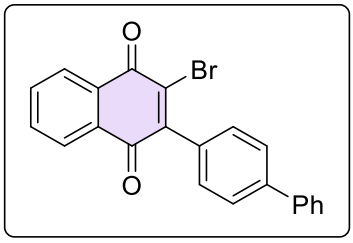
IR Spectra



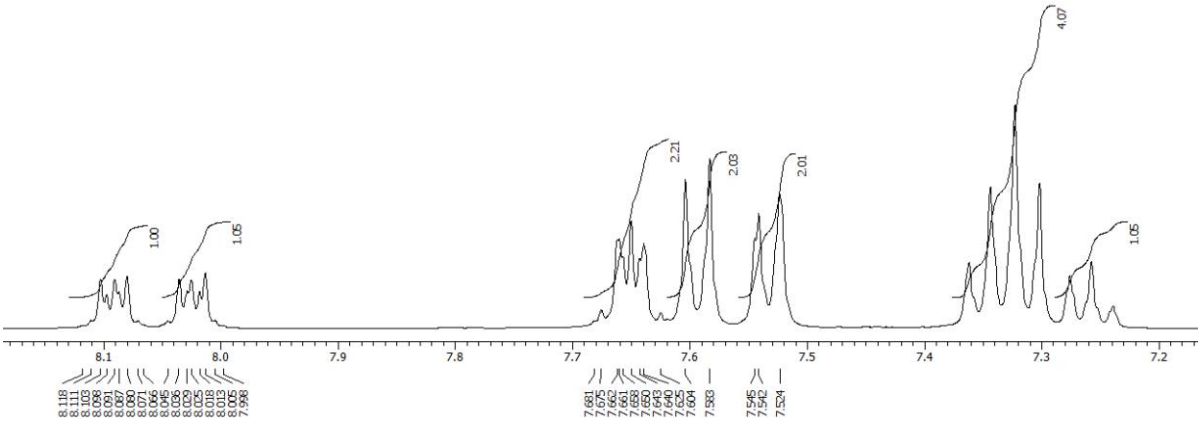
2-([1,1'-biphenyl]-4-yl)-3-bromonaphthalene-1,4-dione (3q)

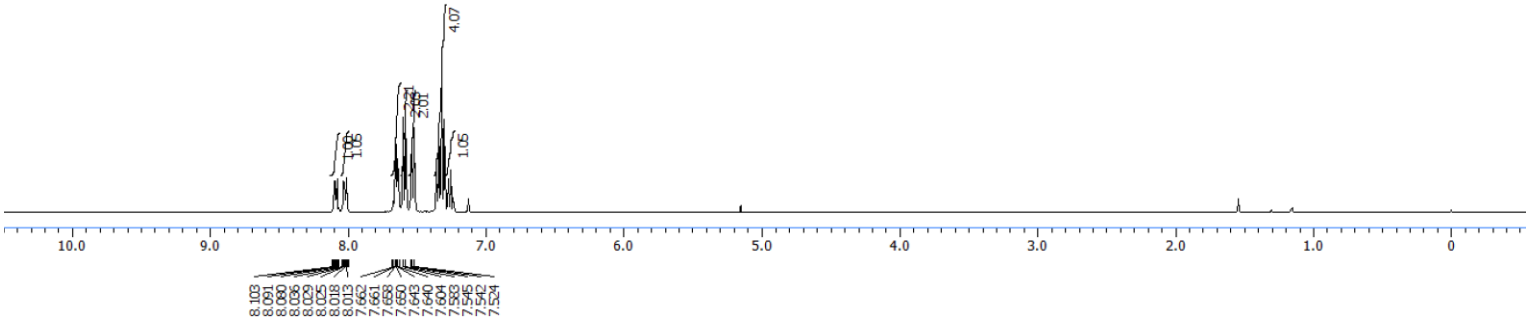


^{1}H NMR (400 MHz, $CDCl_3$)

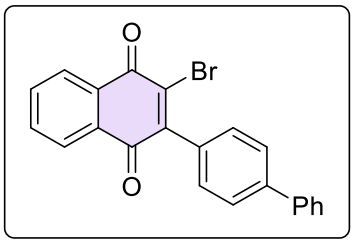


2-([1,1'-biphenyl]-4-yl)-3-bromonaphthalene-1,4-dione (3q)

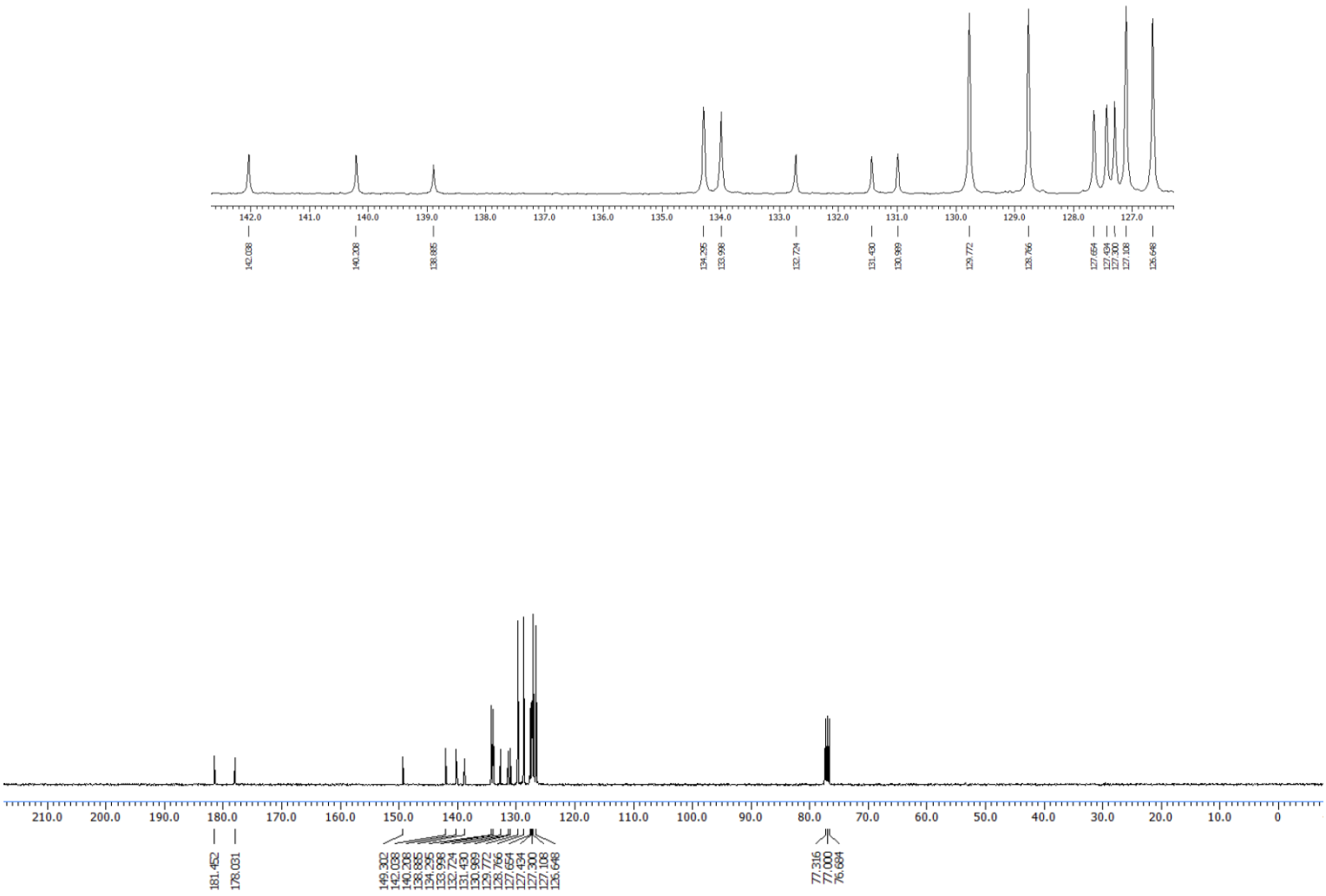




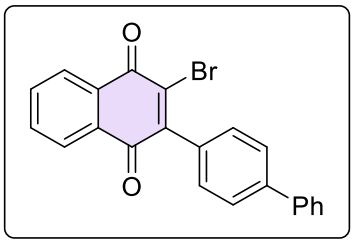
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-([1,1'-biphenyl]-4-yl)-3-bromonaphthalene-1,4-dione (3q)



HRMS



2-([1,1'-biphenyl]-4-yl)-3-bromonaphthalene-1,4-dione (3q)

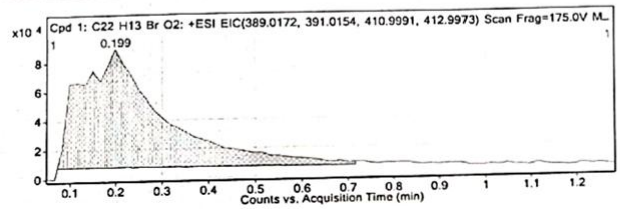
Qualitative Compound Report

Data File	MNS-350.d	Sample Name	MNS-350
Sample Type	Sample	Position	P1-D3
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-03-2025 15:00:01
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

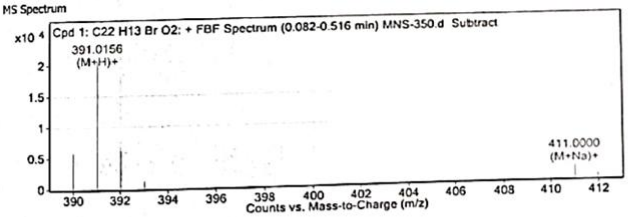
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C22 H13 Br O2	0.199	388.0101	20466	C22 H13 Br O2	388.0099	0.62	C22 H13 Br O2	C22 H13 Br O2

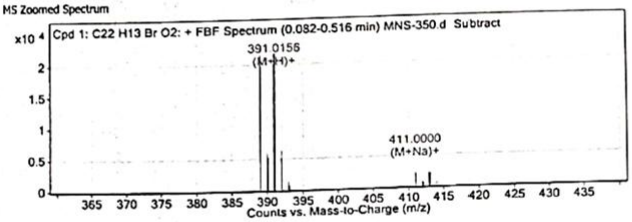
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C22 H13 Br O2	391.0156	0.199	Find By Formula	388.0101



MS Spectrum



MS Zoomed Spectrum

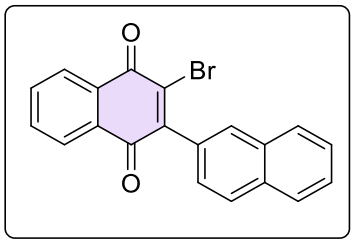


MS Spectrum Peak List

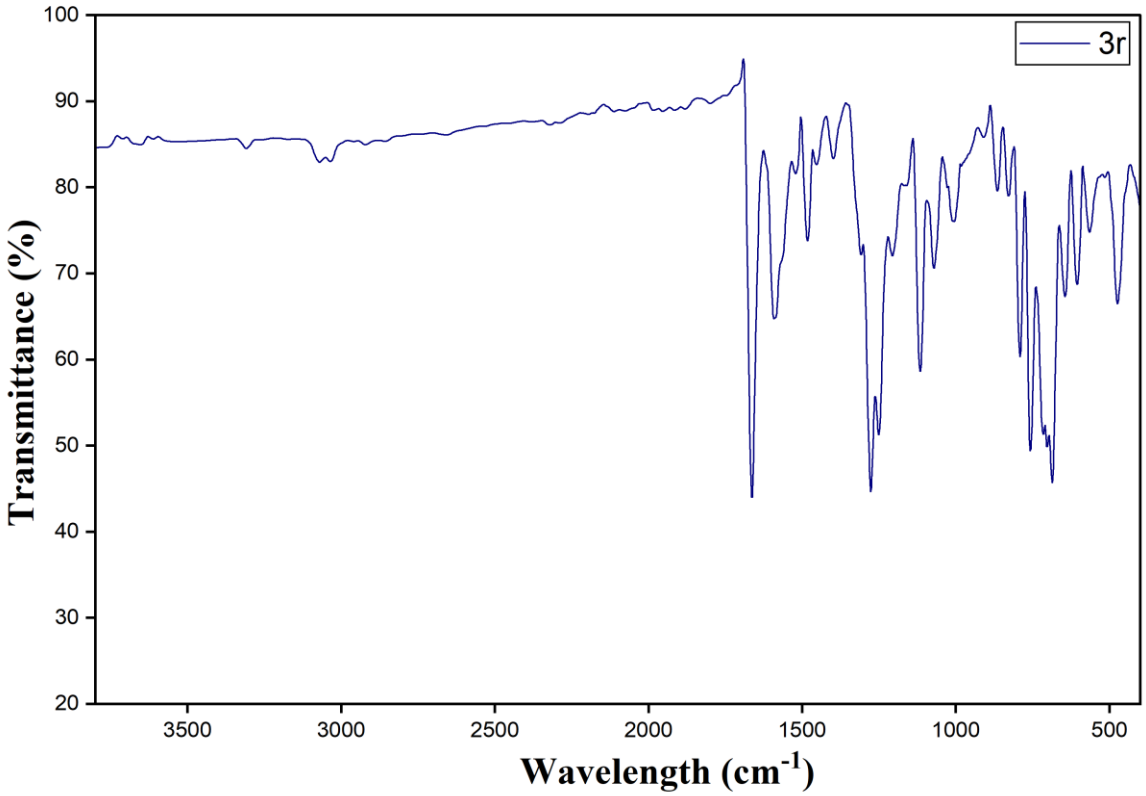
m/z	z	Abund	Formula	Ion
389.0171	1	20287.09	C22H14BrO2	(M+H)+
390.022	1	5892.73	C22H14BrO2	(M+H)+
391.0156	1	20466.24	C22H14BrO2	(M+H)+
392.0194	1	6250.45	C22H14BrO2	(M+H)+
393.0283	1	1262.03	C22H14BrO2	(M+H)+
411	1	2201.55	C22H13BrNaO2	(M+Na)+
411.9876	1	696.08	C22H13BrNaO2	(M+Na)+
412.9958	1	1644.31	C22H13BrNaO2	(M+Na)+

— End Of Report —

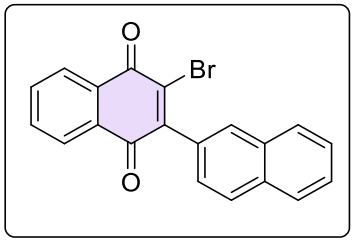
IR Spectra



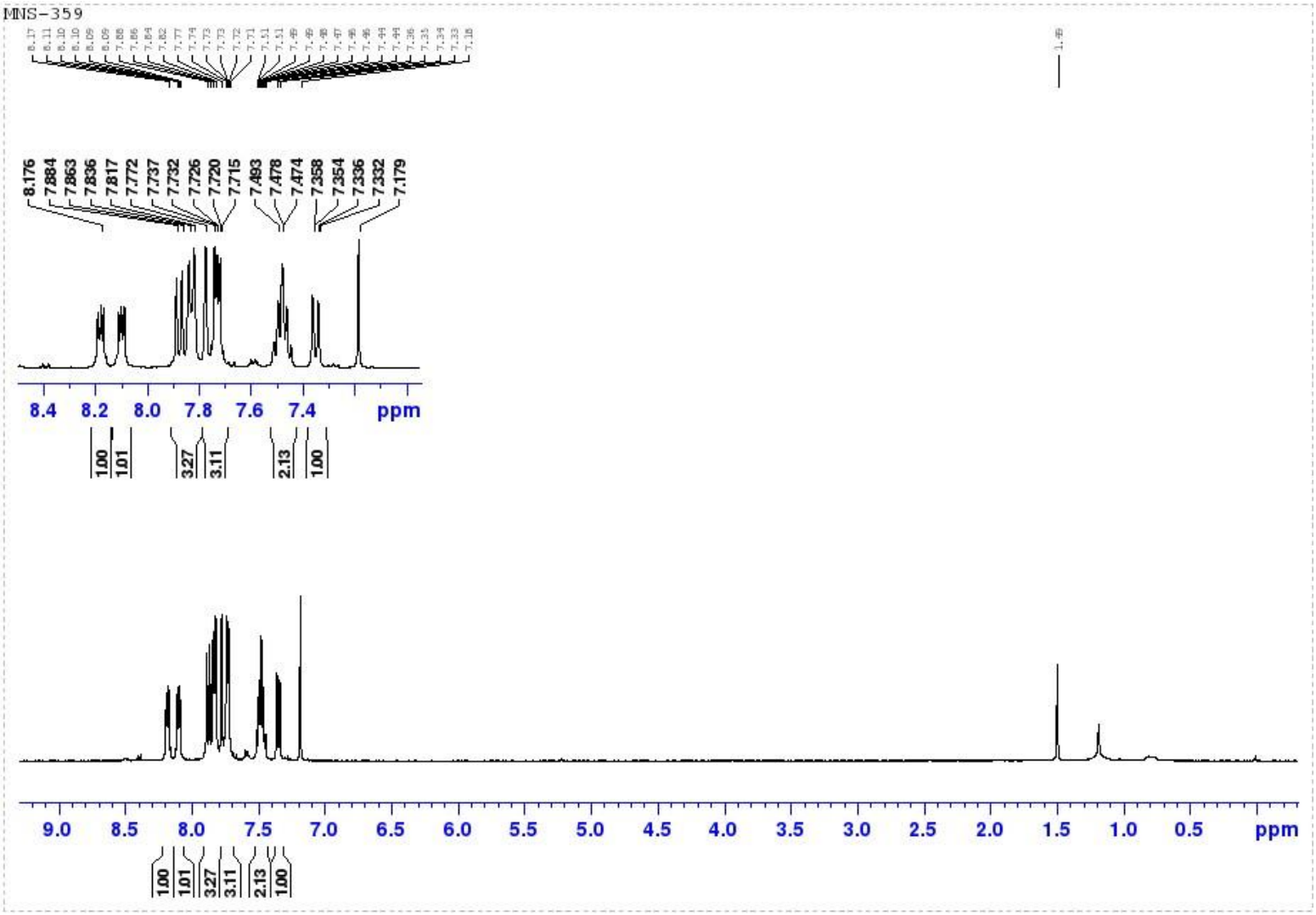
3-bromo-[2,2'-binaphthalene]-1,4-dione (3r)



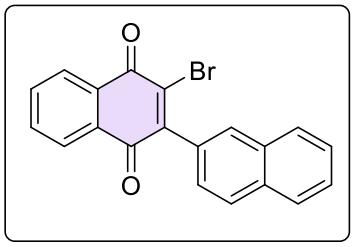
^{1}H NMR (400 MHz, $CDCl_3$)



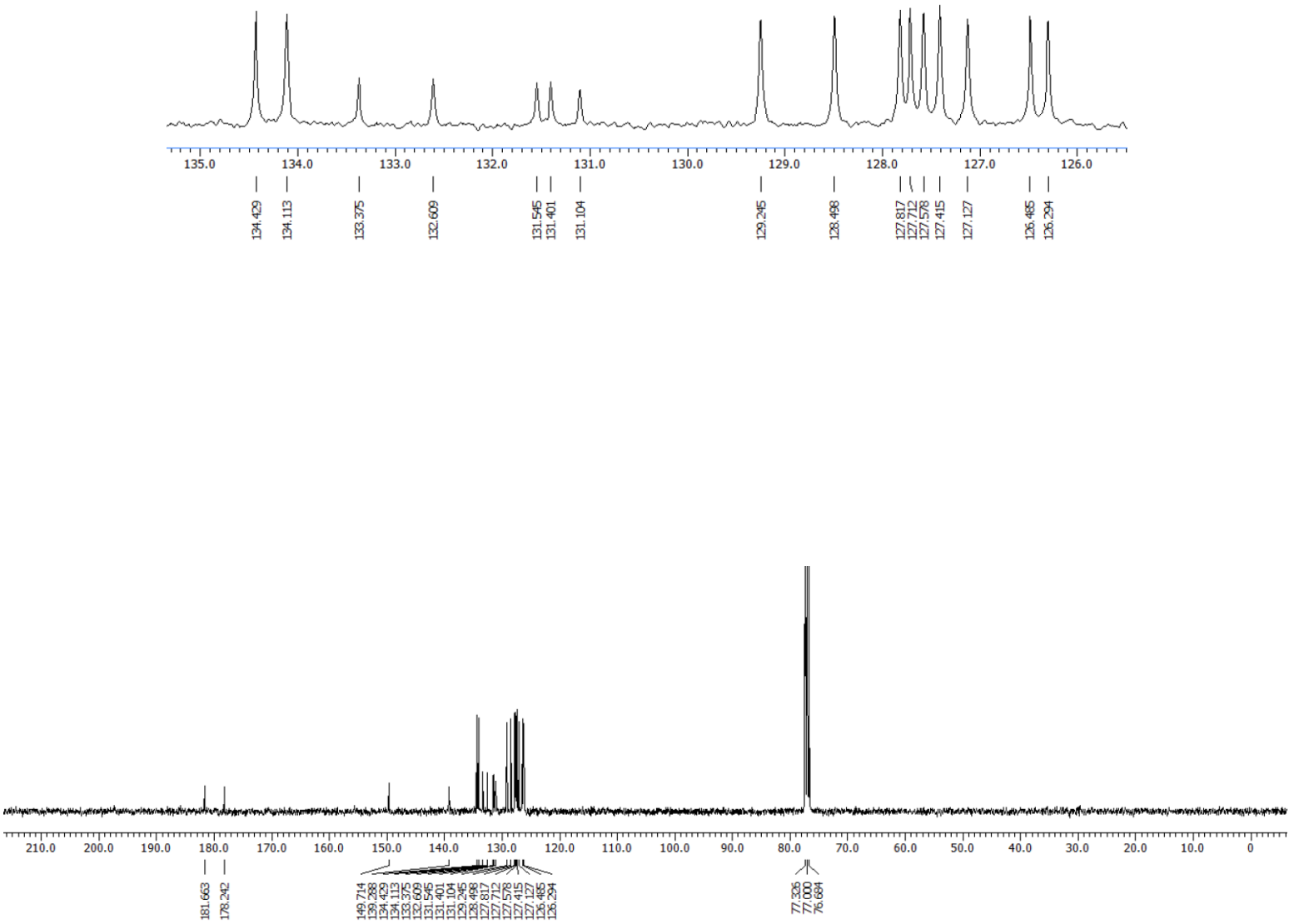
3-bromo-[2,2'-binaphthalene]-1,4-dione (3r)



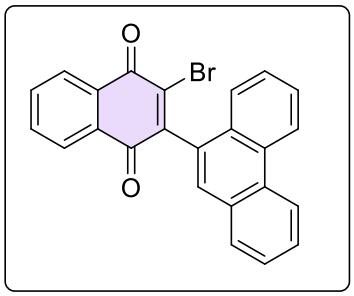
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



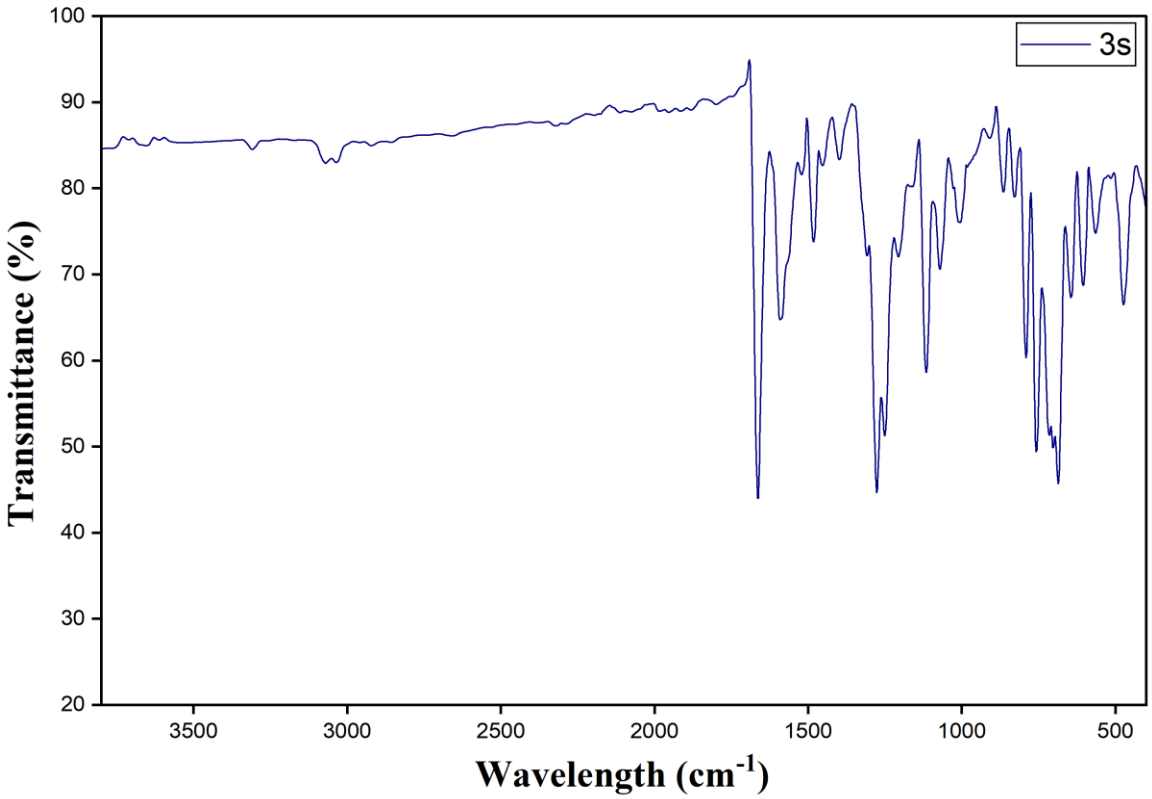
3-bromo-[2,2'-binaphthalene]-1,4-dione (3r)



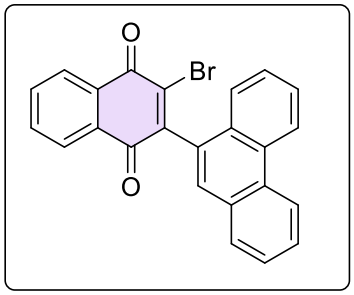
IR Spectra



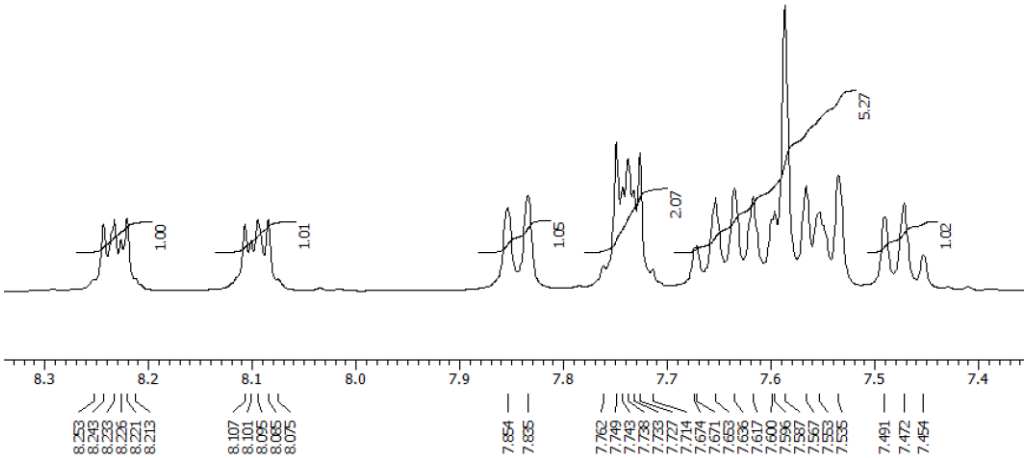
2-bromo-3-(phenanthren-9-yl)naphthalene-1,4-dione (3s)

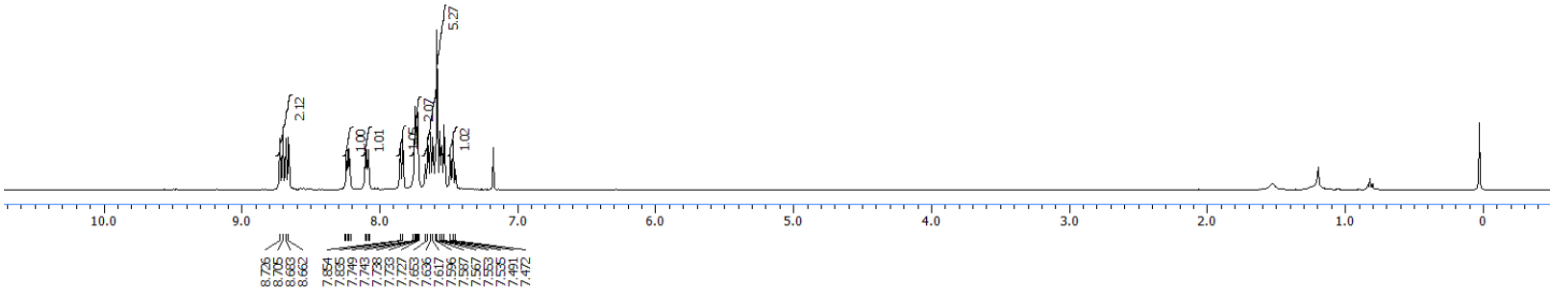


^{1}H NMR (400 MHz, $CDCl_3$)

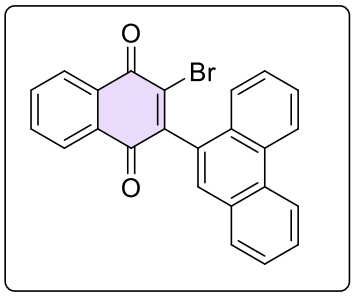


2-bromo-3-(phenanthren-9-yl)naphthalene-1,4-dione (3s)

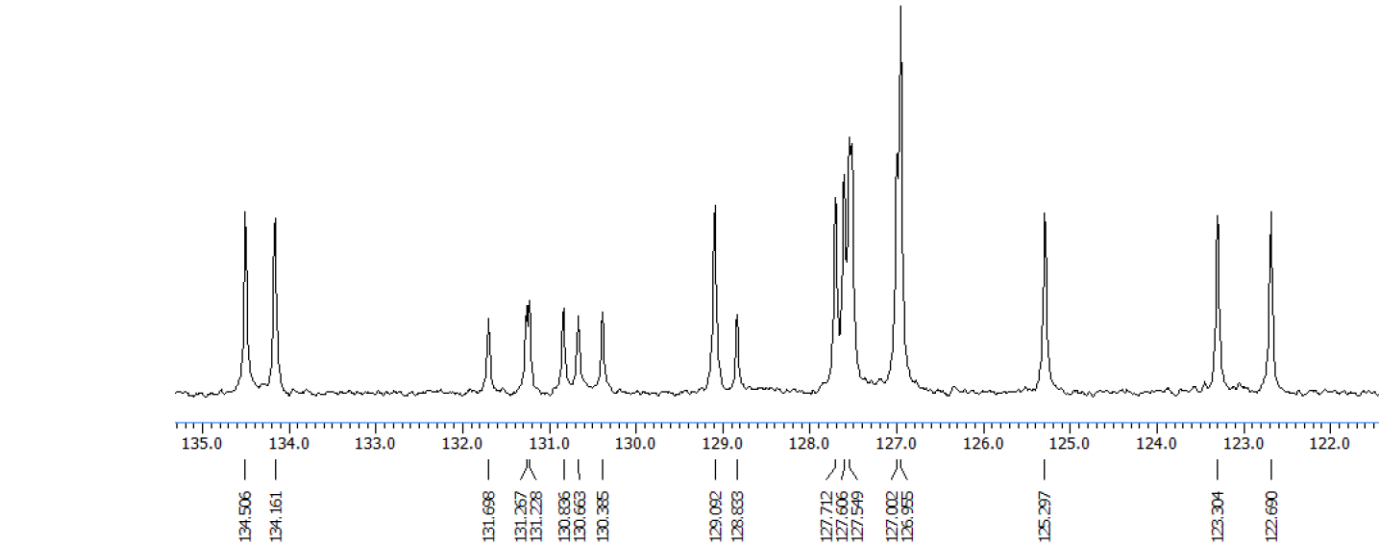


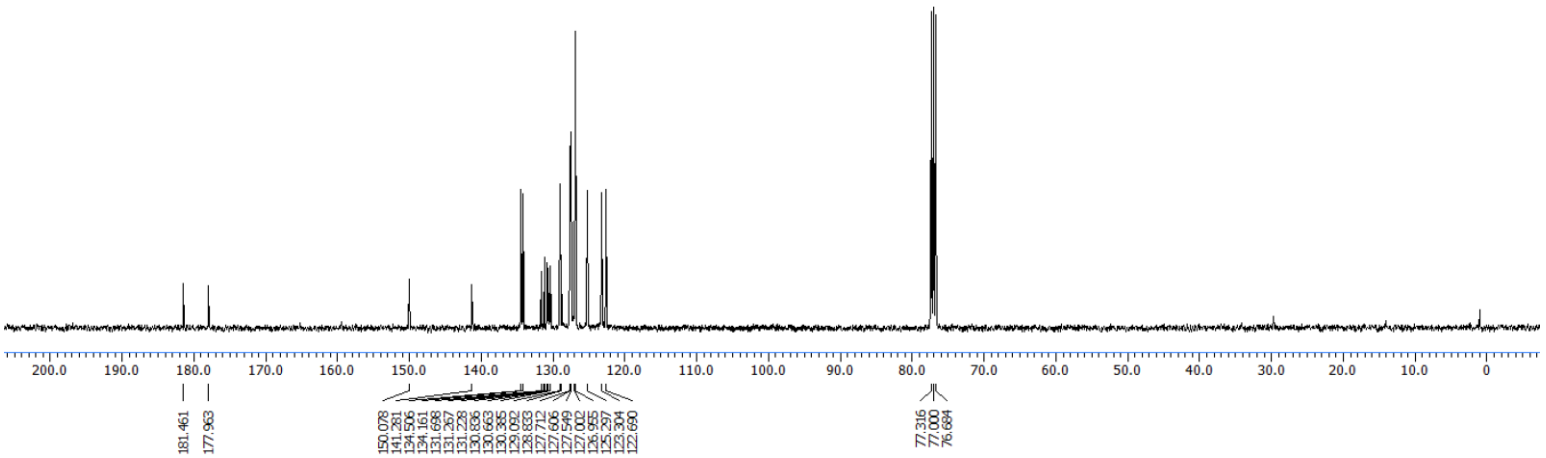


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

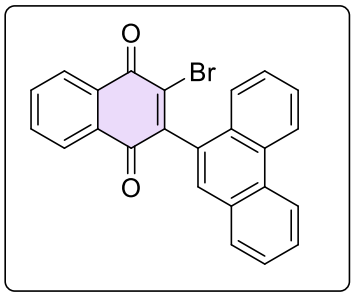


2-bromo-3-(phenanthren-9-yl)naphthalene-1,4-dione (3s)





HRMS



2-bromo-3-(phenanthren-9-yl)naphthalene-1,4-dione (3s)

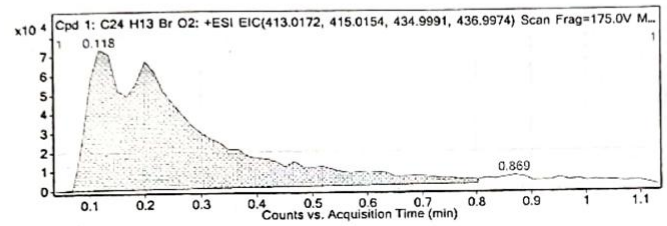
Qualitative Compound Report

Data File	MNS-353.d	Sample Name	MNS-353
Sample Type	Sample	Position	P1-B8
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	08-03-2025 12:42:04
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

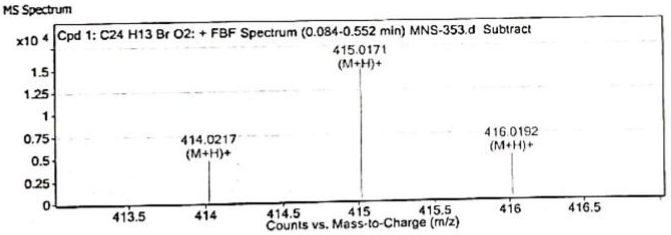
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C24 H13 Br O2	0.118	412.0113	15412	C24 H13 Br O2	412.0099	3.34	C24 H13 Br O2	C24 H13 Br O2

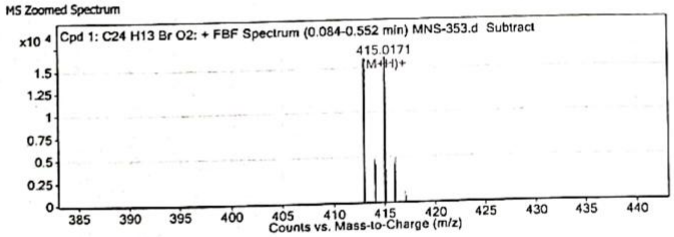
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C24 H13 Br O2	415.0171	0.118	Find By Formula	412.0113



MS Spectrum



MS Zoomed Spectrum

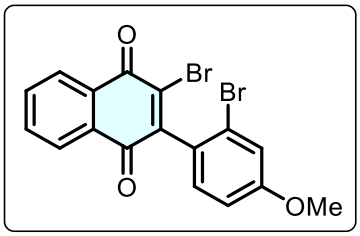


MS Spectrum Peak List

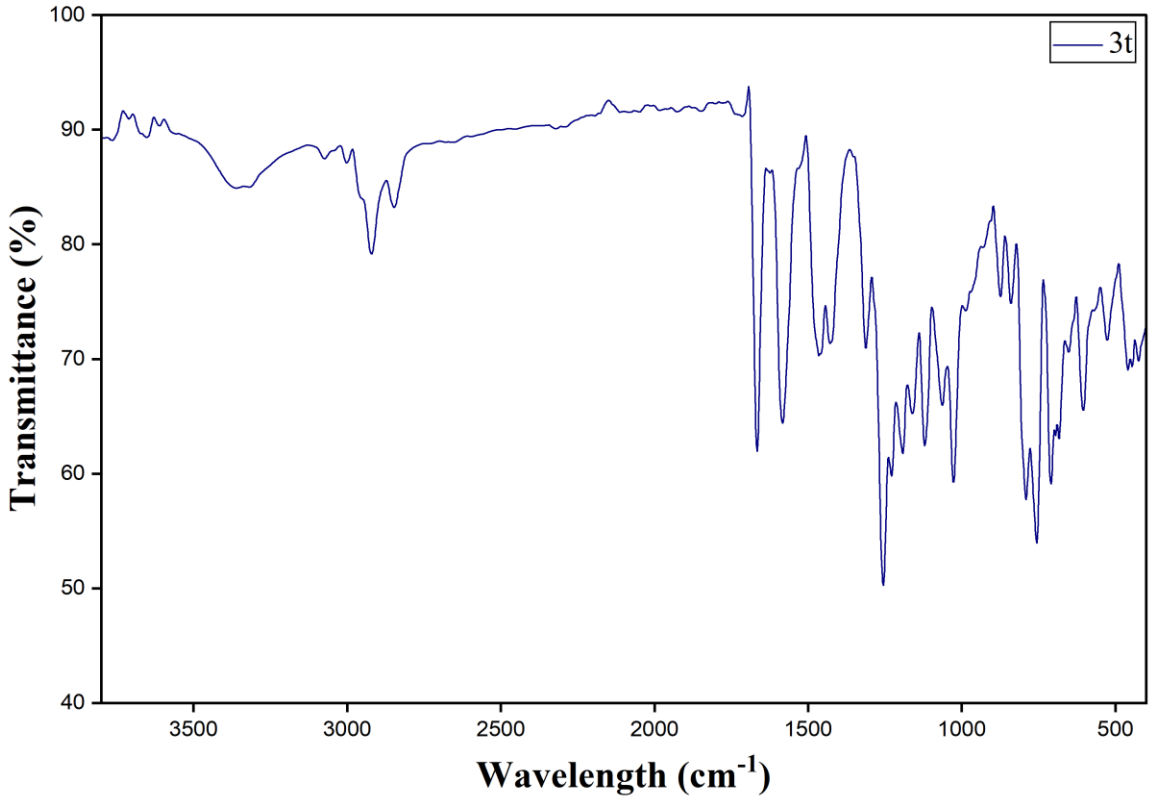
m/z	z	Abund	Formula	Ion
413.0184	1	14907.75	C24H14BrO2	(M+H)+
414.0217	1	4704.23	C24H14BrO2	(M+H)+
415.0171	1	15411.72	C24H14BrO2	(M+H)+
416.0192	1	4945.3	C24H14BrO2	(M+H)+
417.025	1	1116.52	C24H14BrO2	(M+H)+

--- End Of Report ---

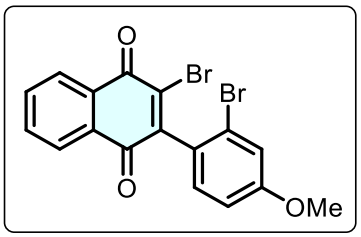
IR Spectra



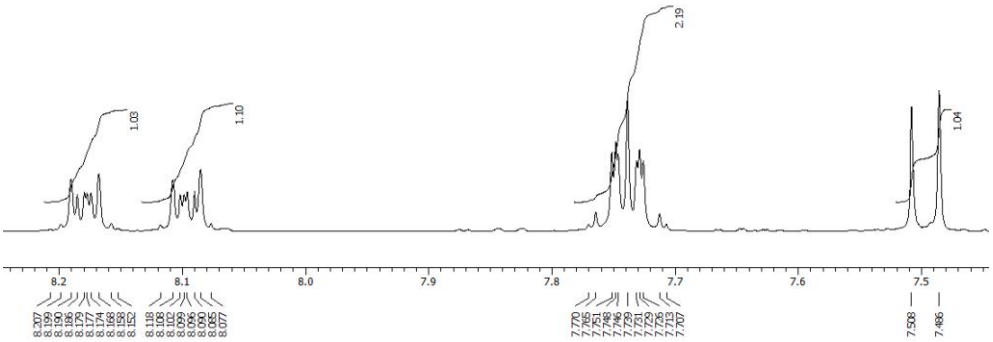
2-bromo-3-(2-bromo-4-methoxyphenyl)naphthalene-1,4-dione (3t)

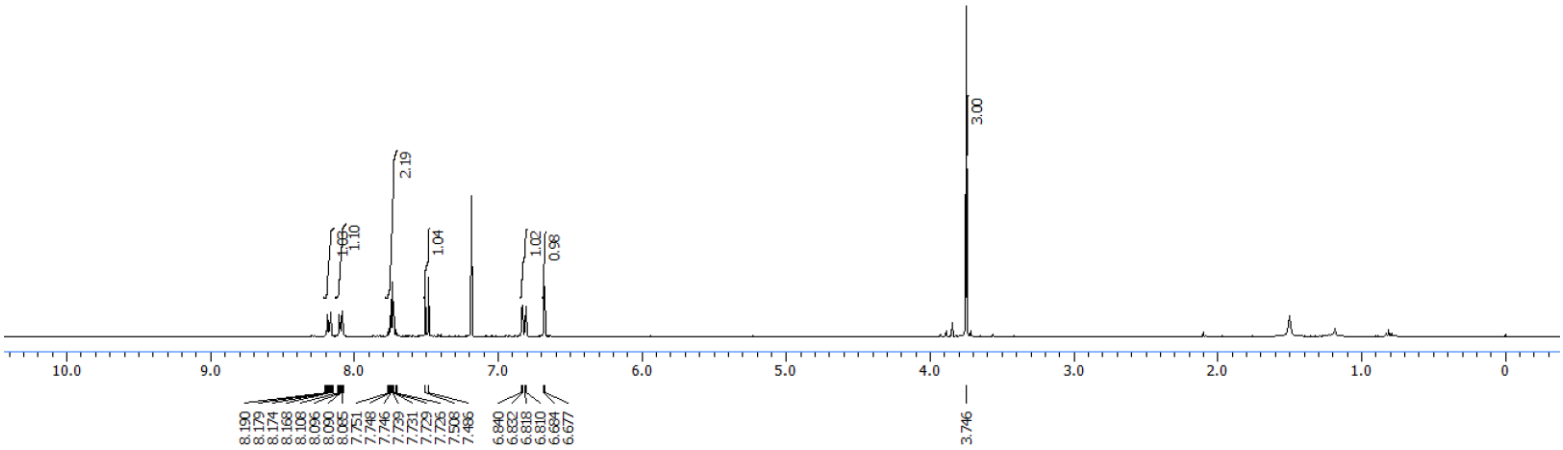


^{1}H NMR (400 MHz, $CDCl_3$)

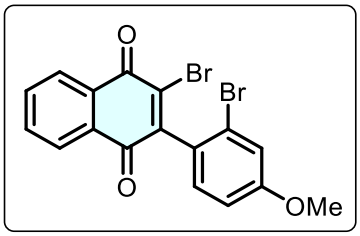


2-bromo-3-(2-bromo-4-methoxyphenyl)naphthalene-1,4-dione (3t)

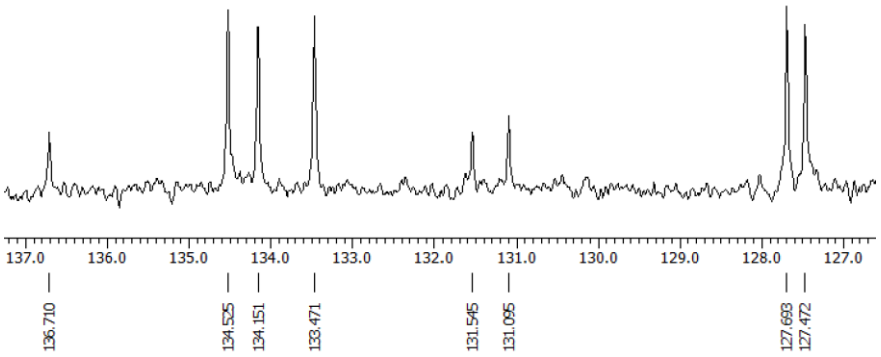


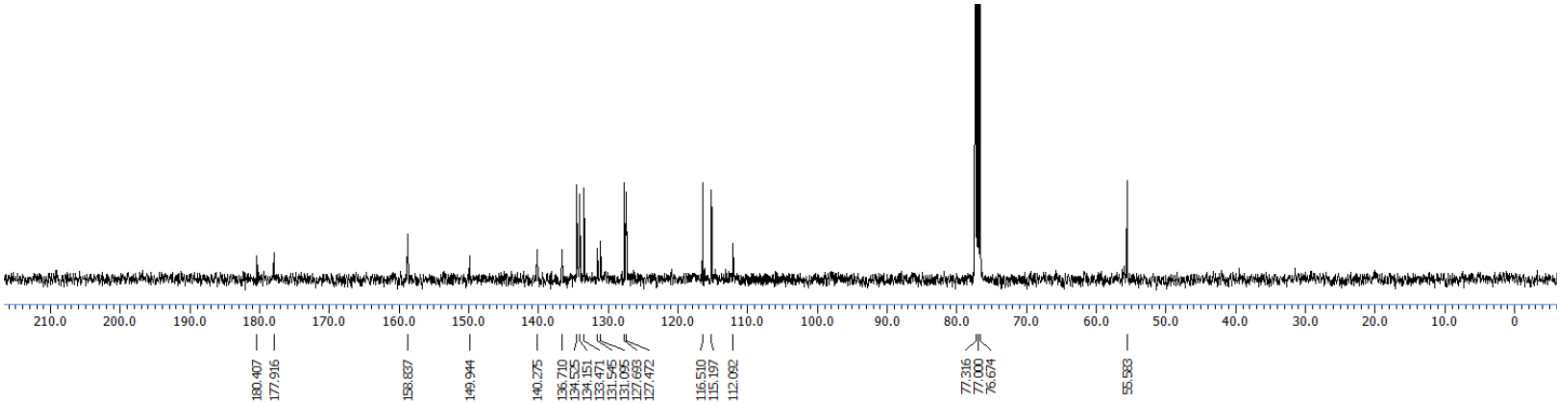


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

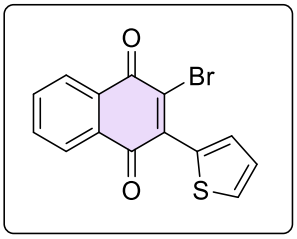


2-bromo-3-(2-bromo-4-methoxyphenyl)naphthalene-1,4-dione (3t)

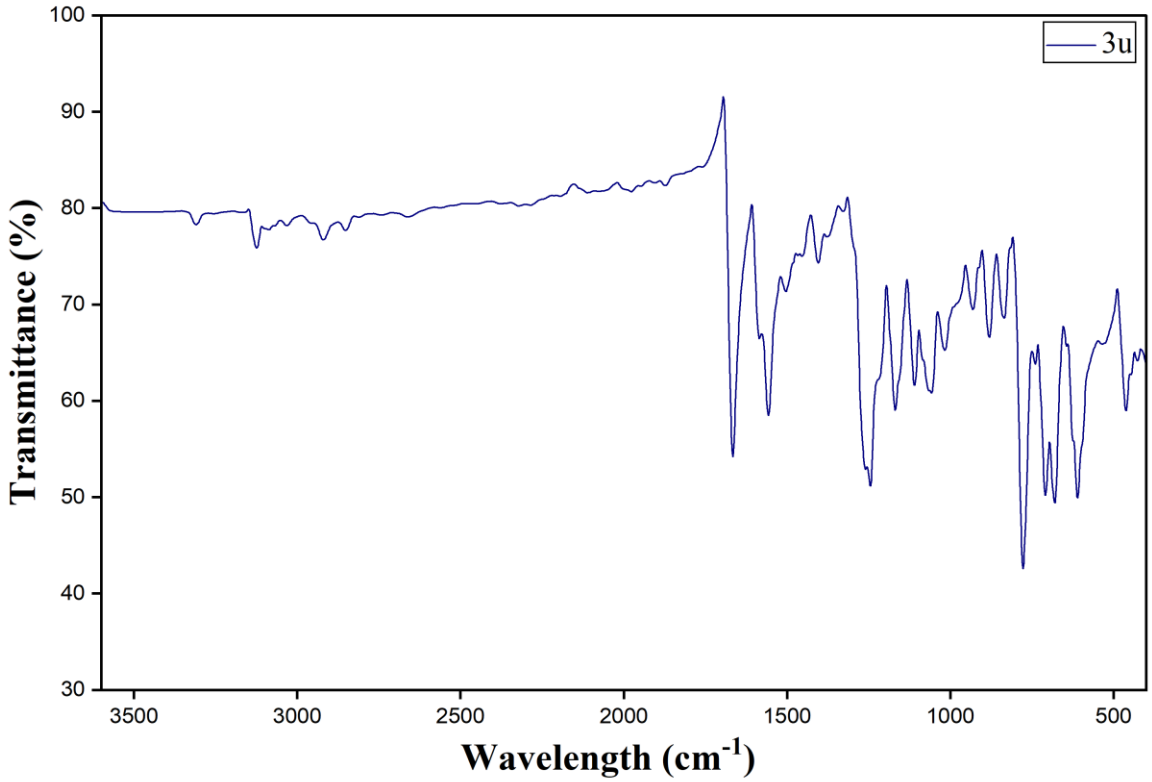




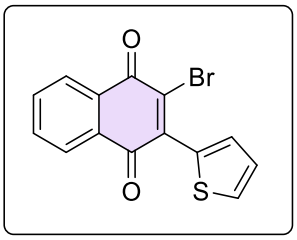
IR Spectra



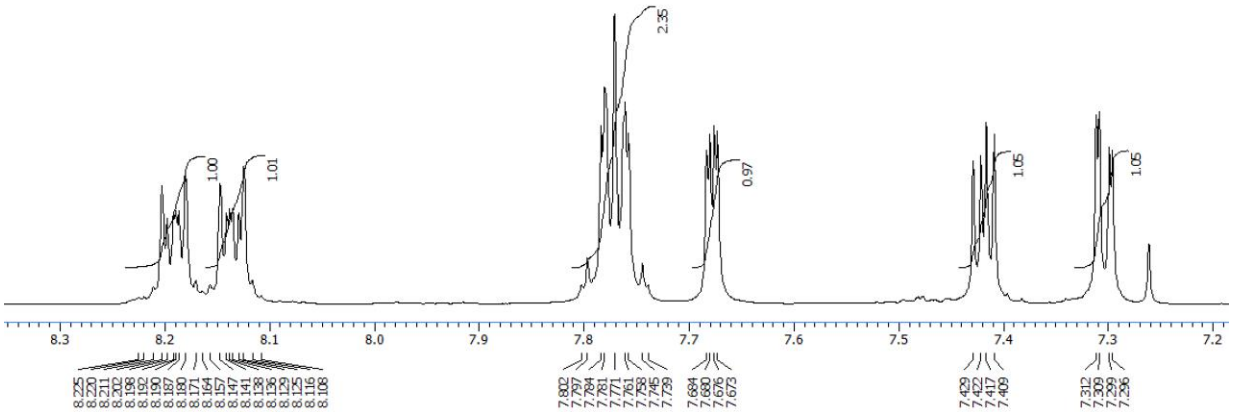
2-bromo-3-(thiophen-2-yl)naphthalene-1,4-dione (3u)

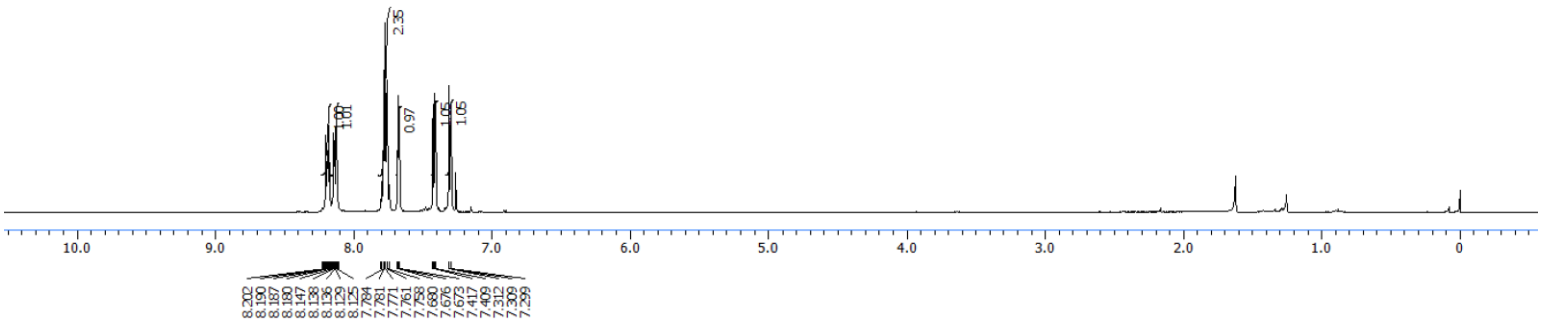


^{1}H NMR (400 MHz, $CDCl_3$)

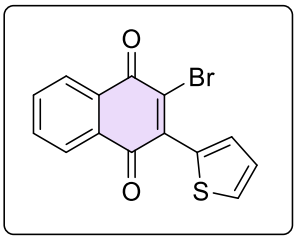


2-bromo-3-(thiophen-2-yl)naphthalene-1,4-dione (3u)

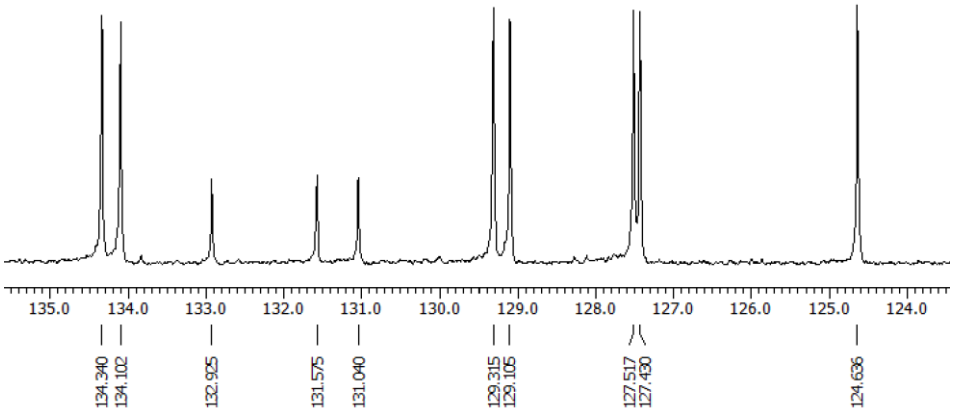


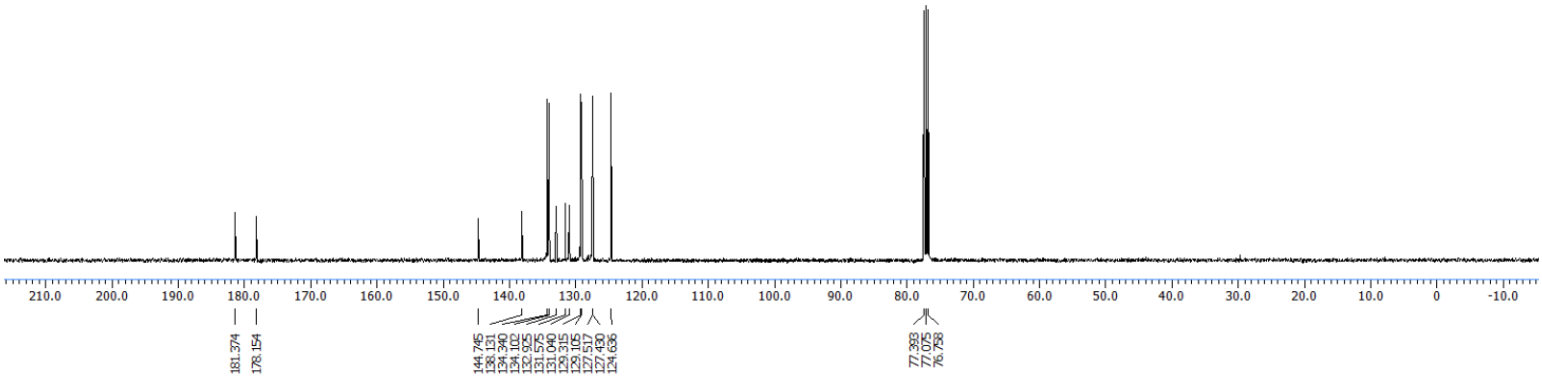


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

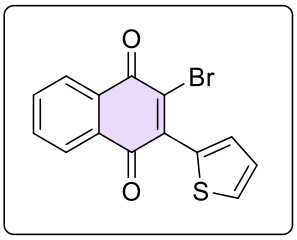


2-bromo-3-(thiophen-2-yl)naphthalene-1,4-dione (3u)





HRMS



2-bromo-3-(thiophen-2-yl)naphthalene-1,4-dione (3u)

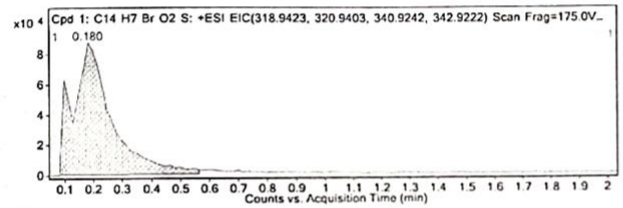
Qualitative Compound Report

Data File	MNS-312.d	Sample Name	MNS-312
Sample Type	Sample	Position	P1-A9
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	11-06-2024 13:20:27
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

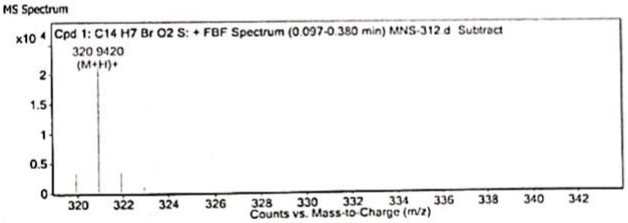
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C14 H7 Br O2 S	0.18	317.9368	21647	C14 H7 Br O2 S	317.935	5.7	C14 H7 Br O2 S	C14 H7 Br O2 S

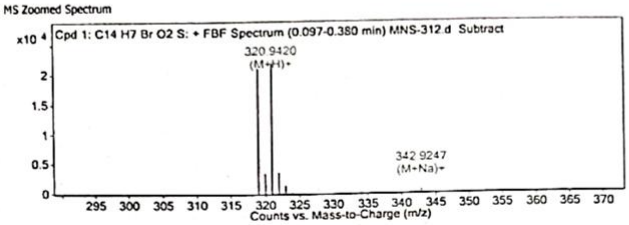
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C14 H7 Br O2 S	320.942	0.18	Find By Formula	317.9368



MS Spectrum



MS Zoomed Spectrum

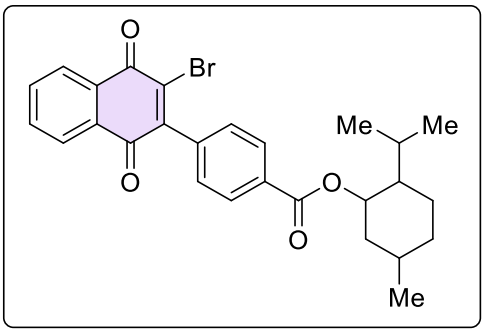


MS Spectrum Peak List

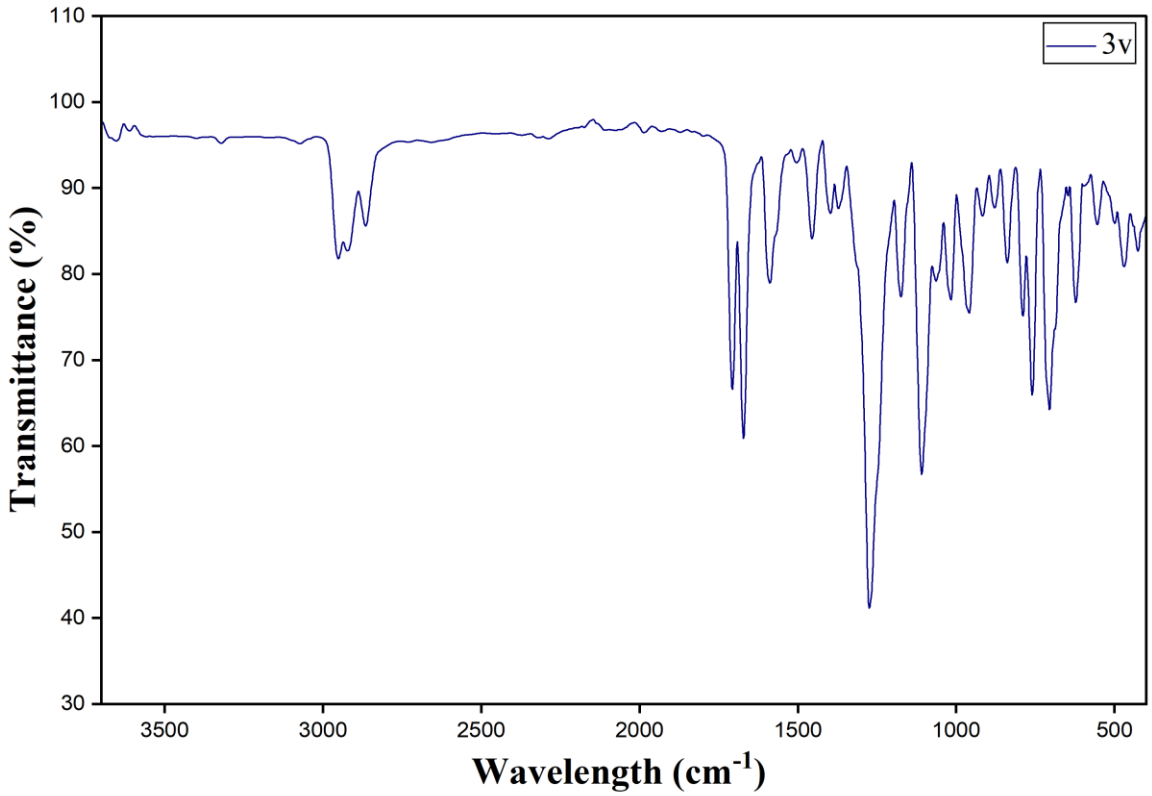
m/z	z	Abund	Formula	Ion
318.9441	1	21016.16	C14H8BrO2S	(M+H)+
319.9473	1	3464.53	C14H8BrO2S	(M+H)+
320.942	1	21647.11	C14H8BrO2S	(M+H)+
321.9456	1	3515.03	C14H8BrO2S	(M+H)+
322.941	1	1209.5	C14H8BrO2S	(M+H)+
323.9454	1	140.54	C14H8BrO2S	(M+H)+
342.9247	1	333.55	C14H7BrNaO2S	(M+Na)+
343.9211	1	62.64	C14H7BrNaO2S	(M+Na)+

--- End Of Report ---

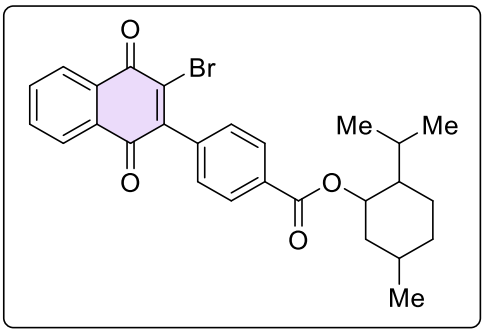
IR Spectra



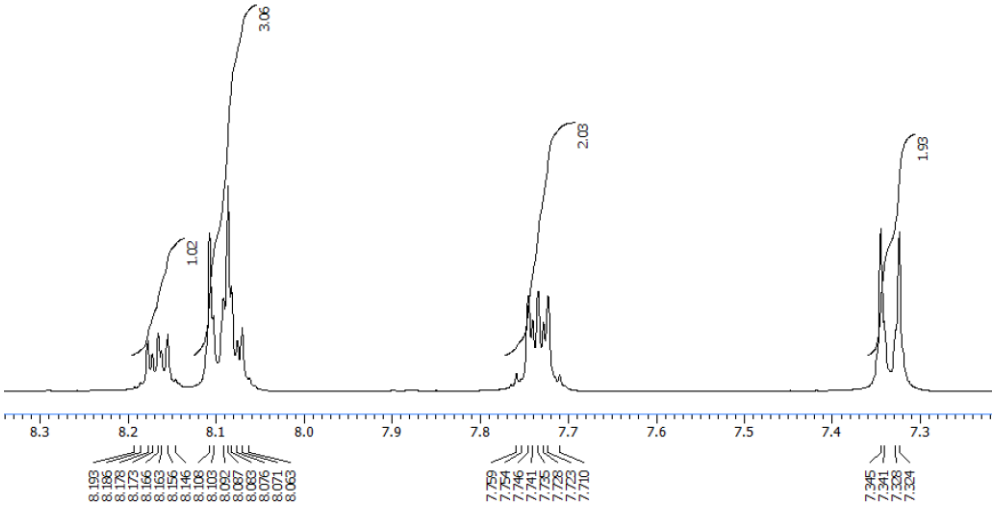
2-isopropyl-5-methylcyclohexyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate (3v)

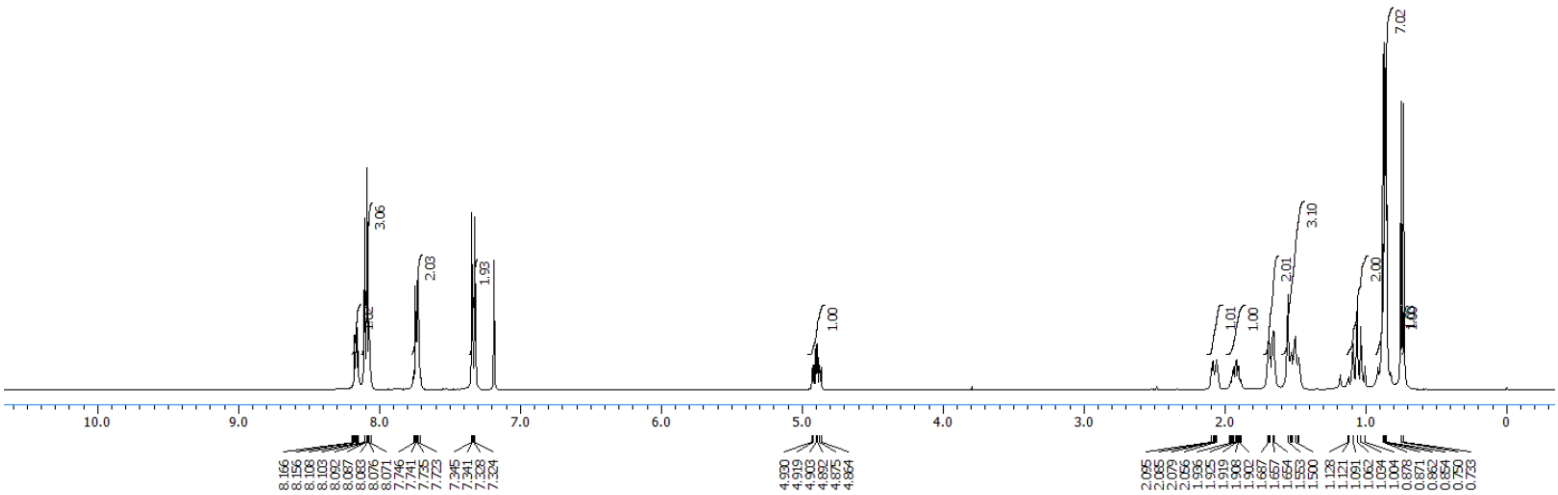


^{1}H NMR (400 MHz, $CDCl_3$)

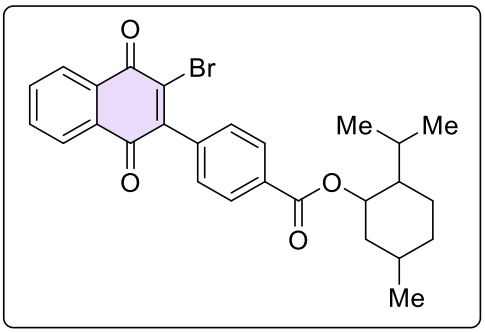


2-isopropyl-5-methylcyclohexyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate (3v)

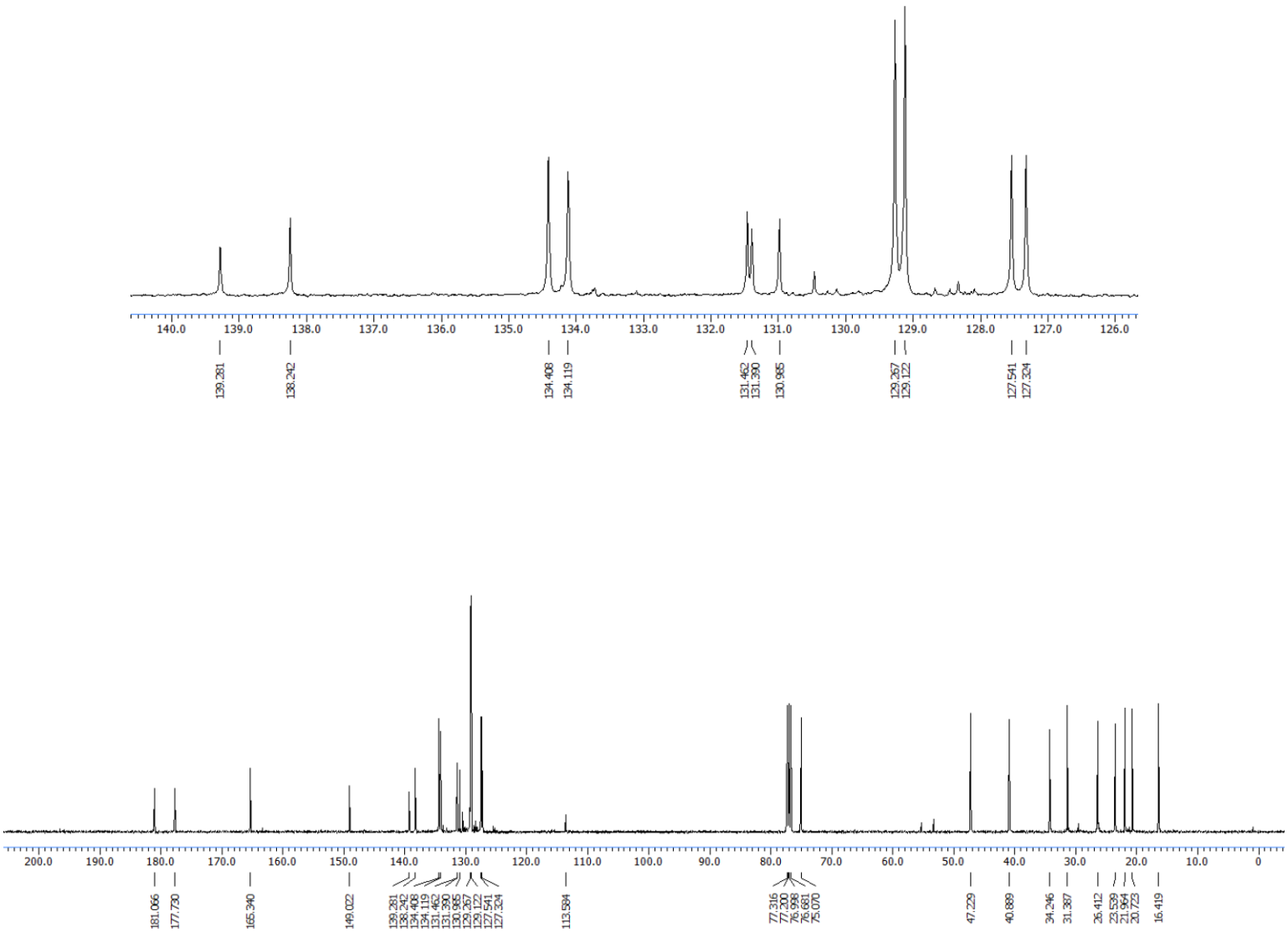




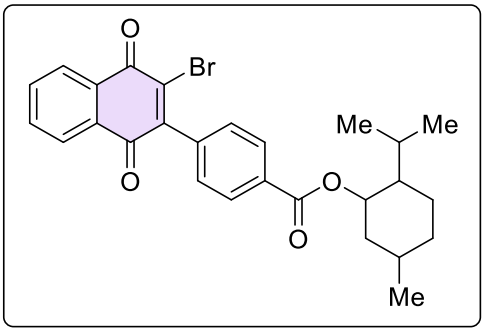
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-isopropyl-5-methylcyclohexyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate (3v)



HRMS



2-isopropyl-5-methylcyclohexyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate (3v)

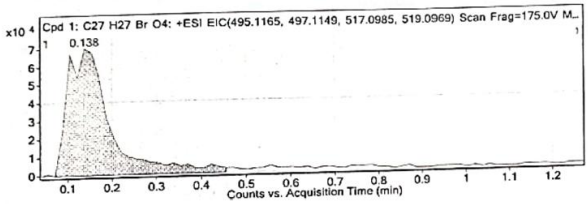
Qualitative Compound Report

Data File	MNS-ME.d	Sample Name	MNS-ME
Sample Type	Sample	Position	P1-C7
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-03-2025 14:50:34
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group	Info.	3	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

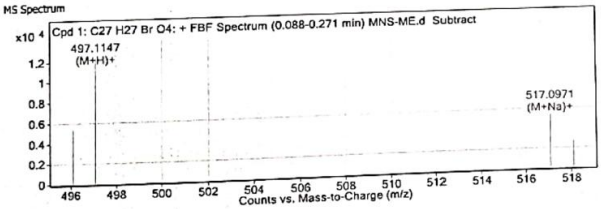
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C27 H27 Br O4	0.138	494.1095	12352	C27 H27 Br O4	494.1093	0.49	C27 H27 Br O4	C27 H27 Br O4

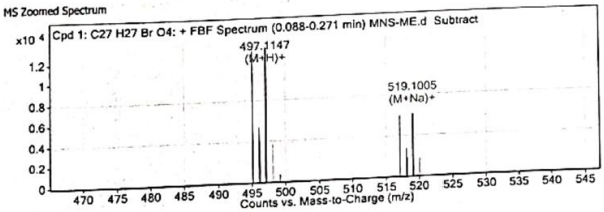
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C27 H27 Br O4	497.1147	0.138	Find By Formula	494.1095



MS Spectrum



MS Zoomed Spectrum

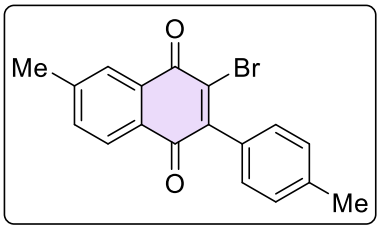


MS Spectrum Peak List

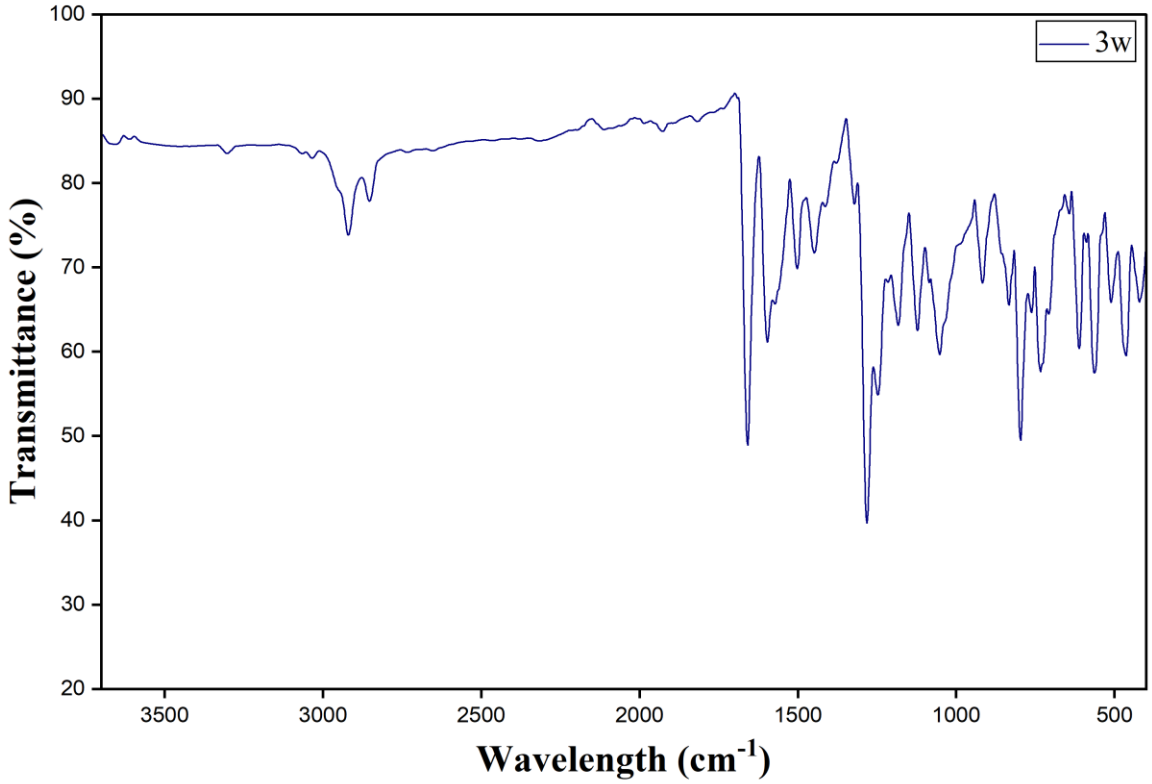
m/z	z	Abund	Formula	Ion
495.1165	1	12086.8	C27H28BrO4	(M+H)+
496.12	1	5300.8	C27H28BrO4	(M+H)+
497.1147	1	12351.86	C27H28BrO4	(M+H)+
517.0971	1	5347.51	C27H27BrNaO4	(M+Na)+
518.1022	1	2688.95	C27H27BrNaO4	(M+Na)+
519.1005	1	5638.95	C27H27BrNaO4	(M+Na)+

--- End Of Report ---

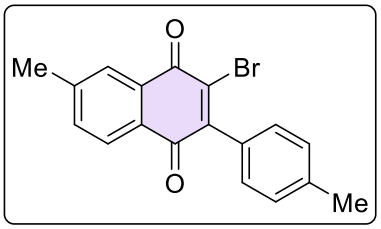
IR Spectra



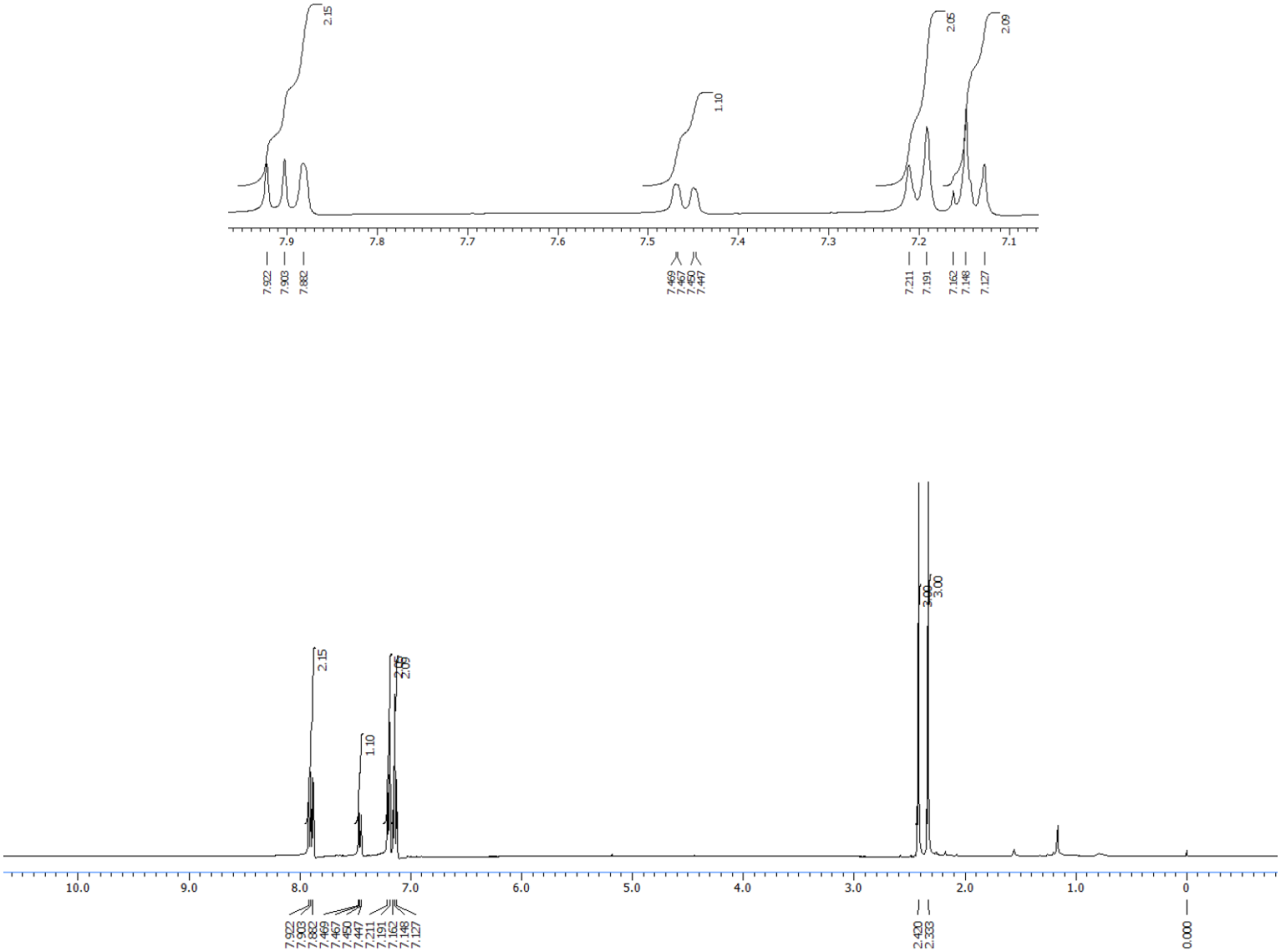
3-bromo-6-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3w)



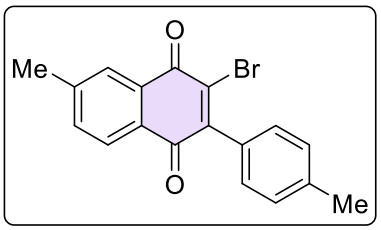
^{1}H NMR (400 MHz, $CDCl_3$)



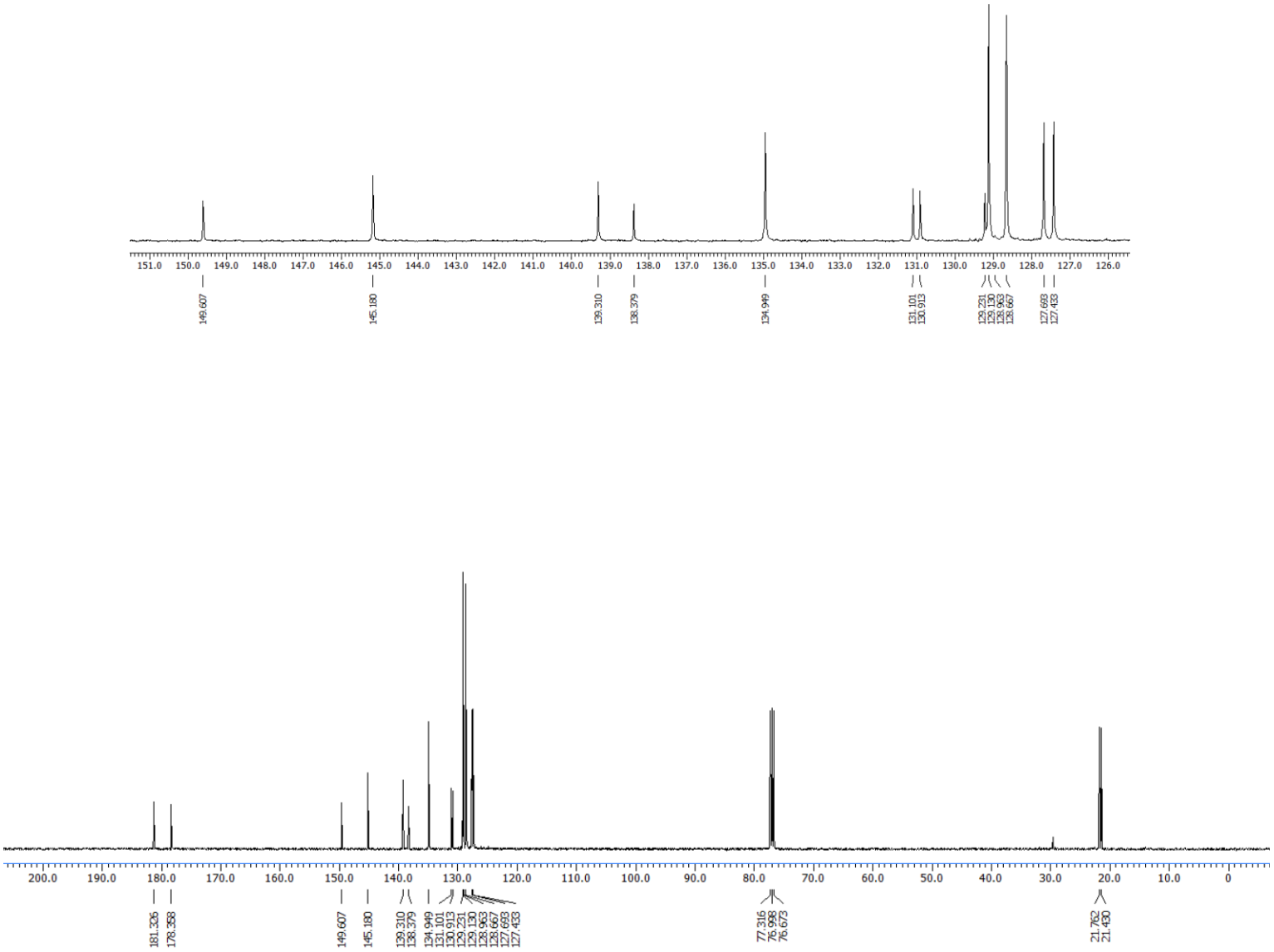
3-bromo-6-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3w)



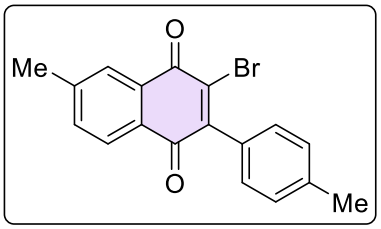
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



3-bromo-6-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3w)



HRMS



3-bromo-6-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3w)

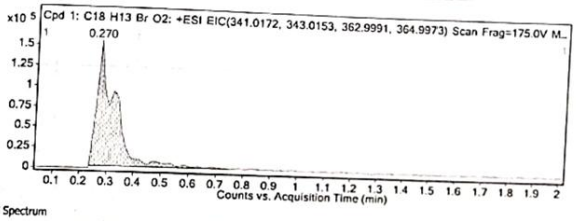
Qualitative Compound Report

Data File	MNS-307.d	Sample Name	MNS-307
Sample Type	Sample	Position	P1-B8
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-05-2024 14:07:25
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

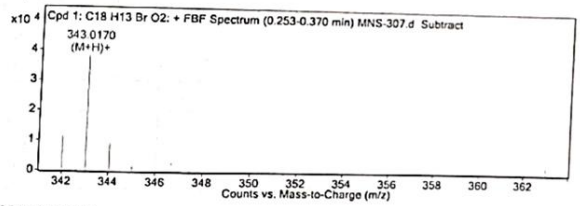
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C18 H13 Br O2	0.27	340.0112	40723	C18 H13 Br O2	340.0099	3.79	C18 H13 Br O2	C18 H13 Br O2

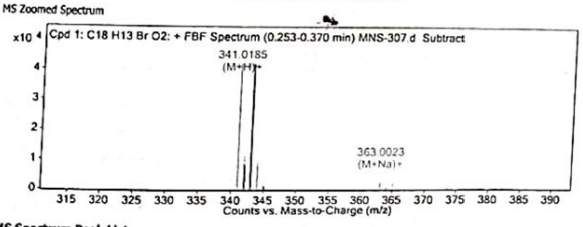
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H13 Br O2	341.0185	0.27	Find By Formula	340.0112



MS Spectrum



MS Zoomed Spectrum

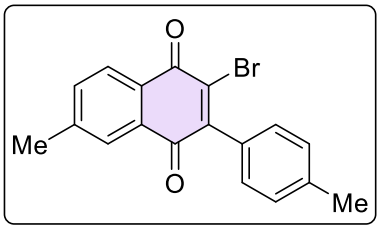


MS Spectrum Peak List

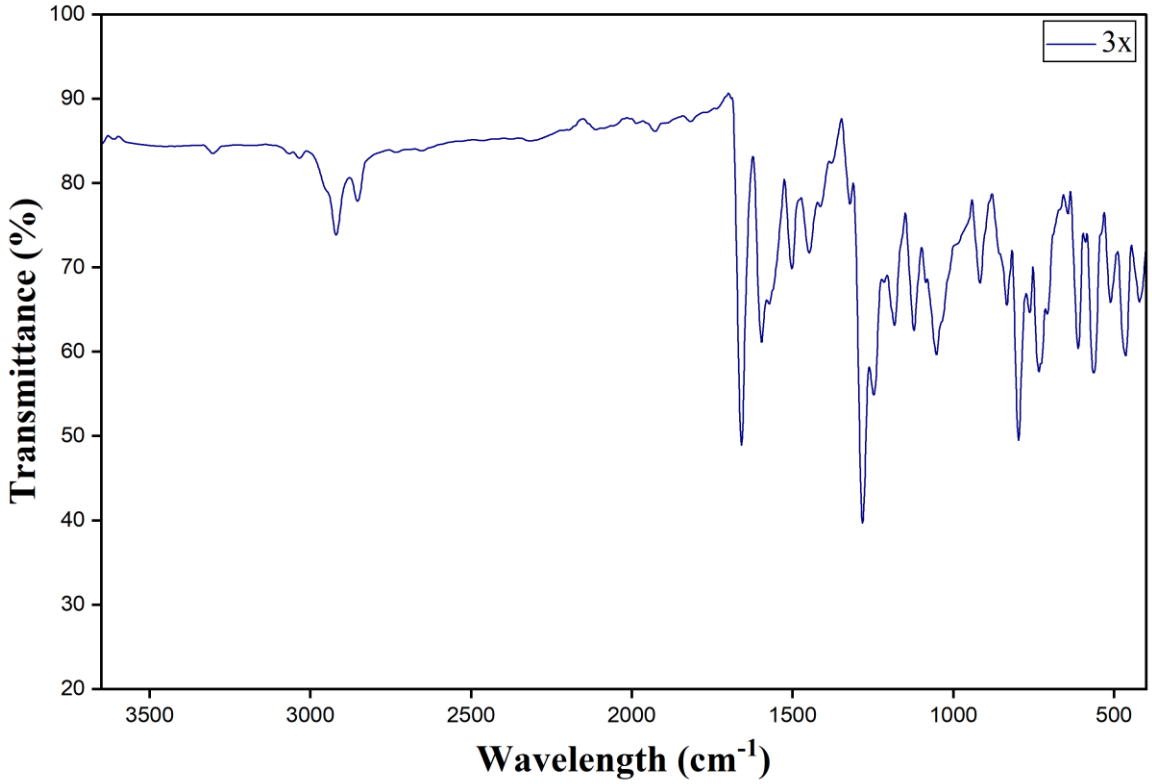
m/z	z	Abund	Formula	Ion
341.0185	1	40722.85	C18H14BrO2	(M+H)+
342.0182	1	11128.54	C18H14BrO2	(M+H)+
343.017	1	38246.57	C18H14BrO2	(M+H)+
344.0198	1	9322	C18H14BrO2	(M+H)+
345.0339	1	1677.25	C18H14BrO2	(M+H)+
363.0023	1	2096.13	C18H13BrNaO2	(M+Na)+
364.0069	1	507.7	C18H13BrNaO2	(M+Na)+

--- End Of Report ---

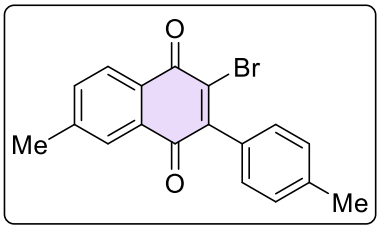
IR Spectra



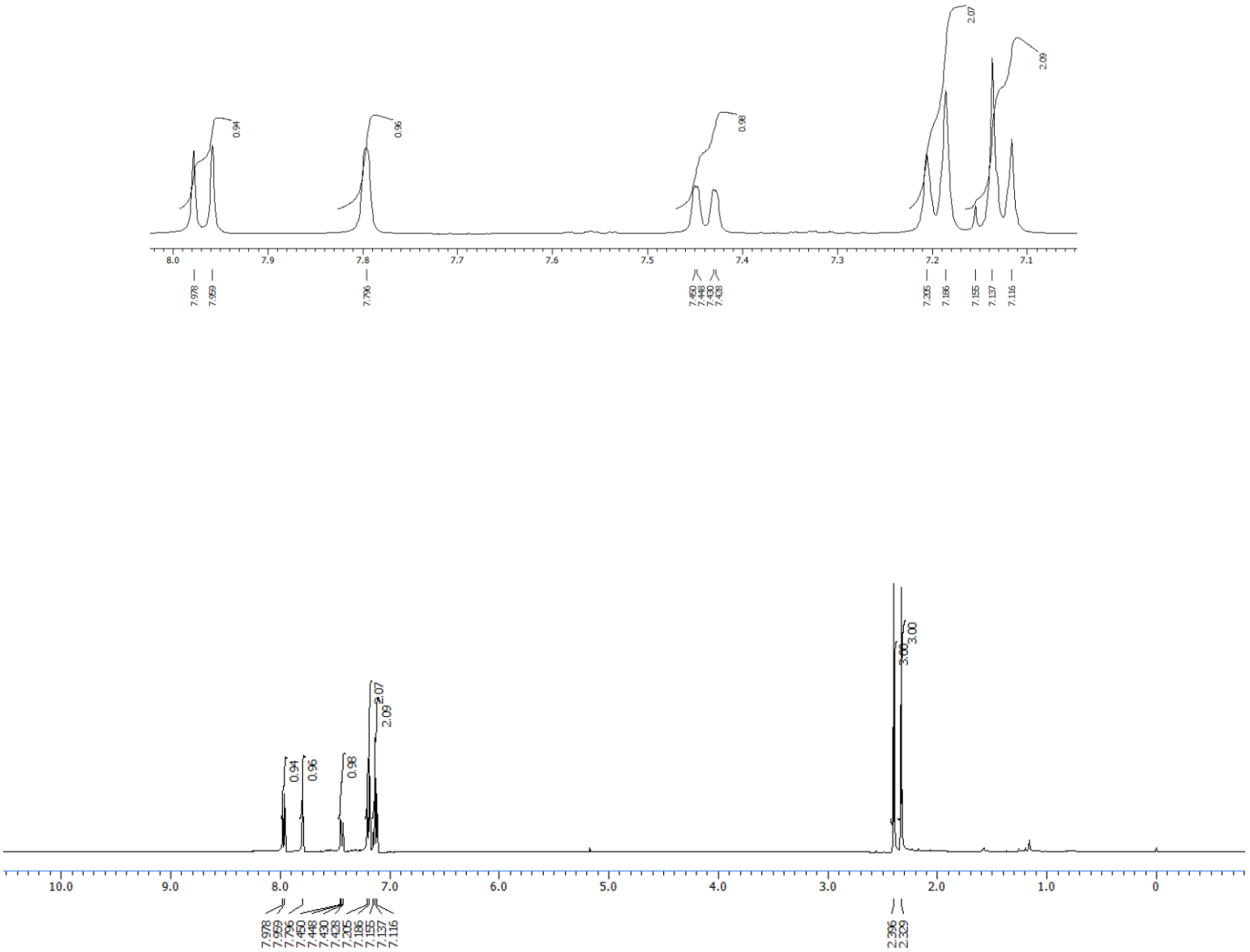
3-bromo-7-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3x)



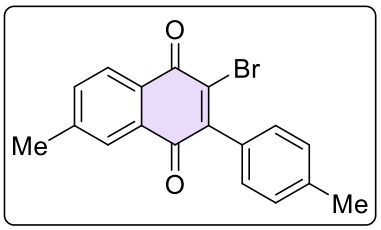
^{1}H NMR (400 MHz, $CDCl_3$)



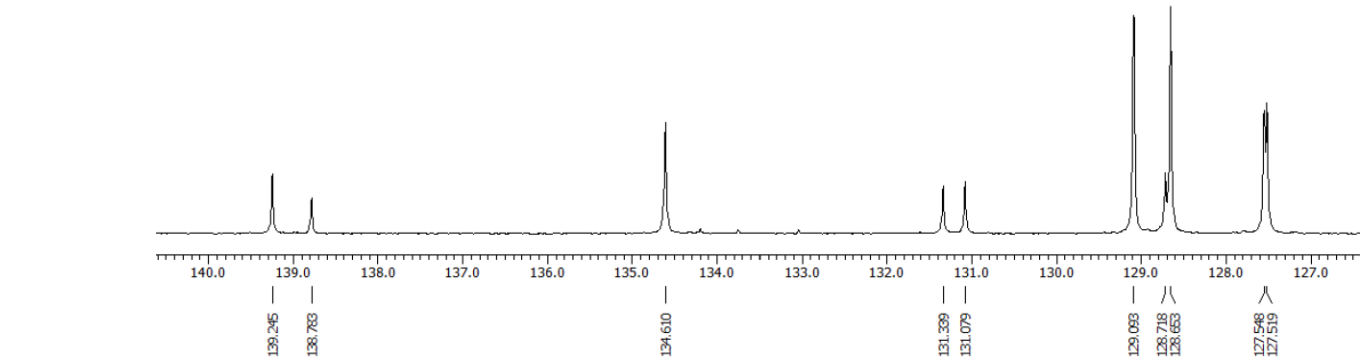
3-bromo-7-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3x)

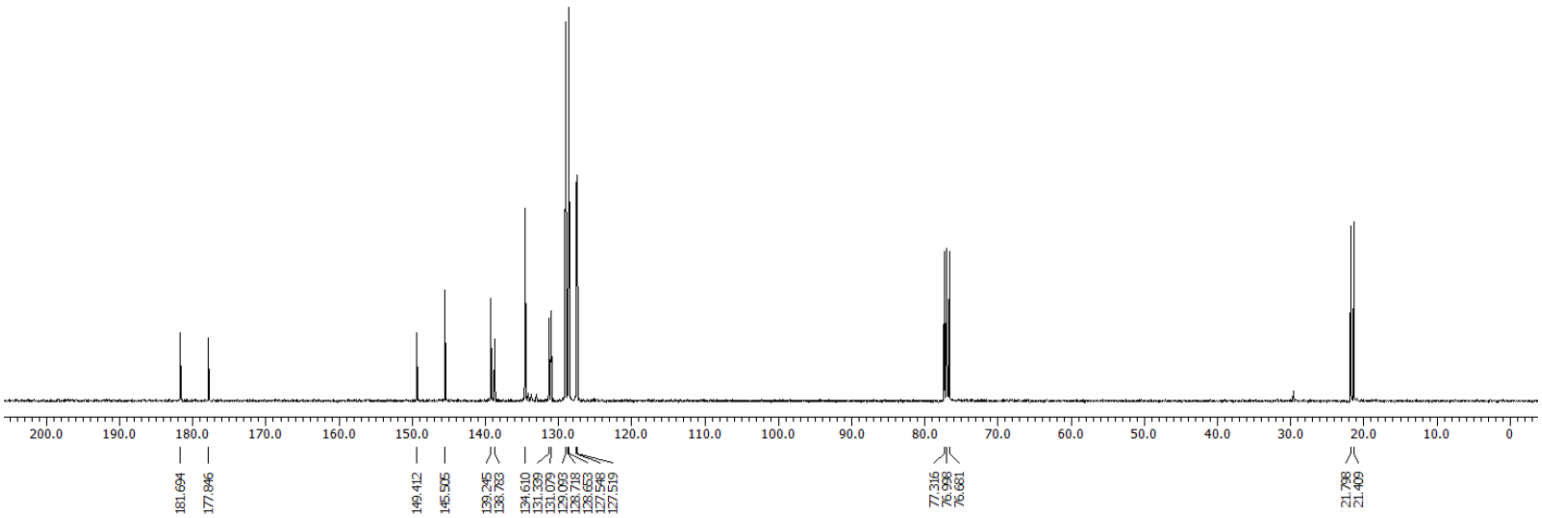


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

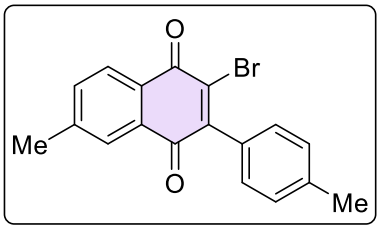


3-bromo-7-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3x)





HRMS



3-bromo-7-methyl-2-(*p*-tolyl)naphthalene-1,4-dione (3x)

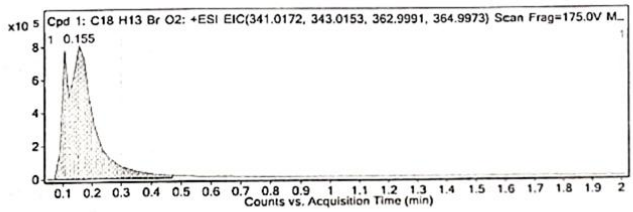
Qualitative Compound Report

Data File	MNS-308.d	**Sample Name**	MNS-308
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	11-06-2024 13:24:12
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

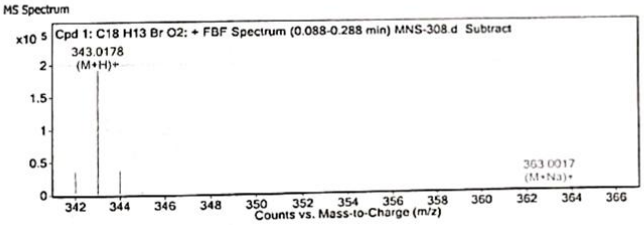
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C18 H13 Br O2	0.155	340.0123	198976	C18 H13 Br O2	340.0099	7.17	C18 H13 Br O2	C18 H13 Br O2

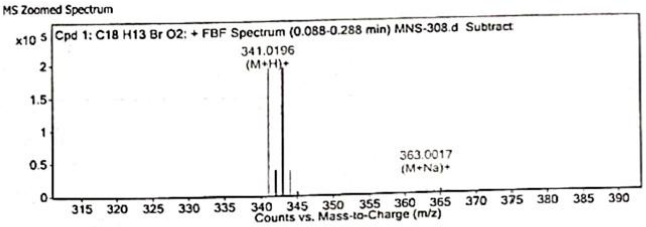
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H13 Br O2	341.0196	0.155	Find By Formula	340.0123



MS Spectrum



MS Zoomed Spectrum

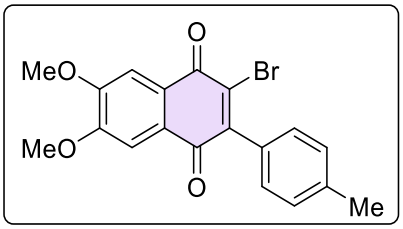


MS Spectrum Peak List

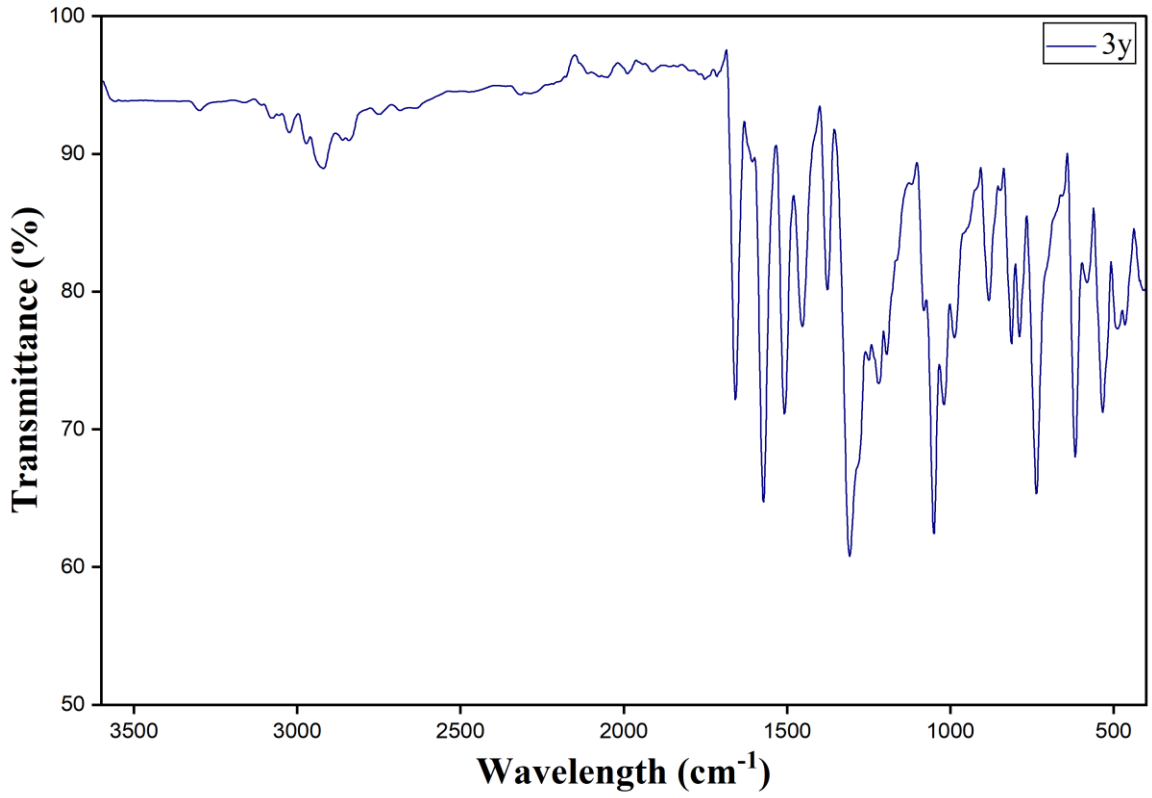
m/z	z	Abund	Formula	Ion
341.0196	1	198975.84	C18H14BrO2	(M+H)+
342.0229	1	36906.7	C18H14BrO2	(M+H)+
343.0178	1	192492.22	C18H14BrO2	(M+H)+
344.0209	1	35392.73	C18H14BrO2	(M+H)+
345.0239	1	4378.64	C18H14BrO2	(M+H)+
346.0271	1	309.46	C18H14BrO2	(M+H)+
363.0017	1	3811.13	C18H13BrNaO2	(M+Na)+
364.0053	1	752.79	C18H13BrNaO2	(M+Na)+
364.9998	1	3668.69	C18H13BrNaO2	(M+Na)+
366.0032	1	773.53	C18H13BrNaO2	(M+Na)+

--- End Of Report ---

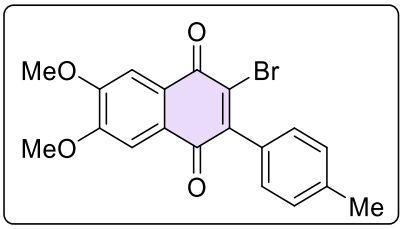
IR Spectra



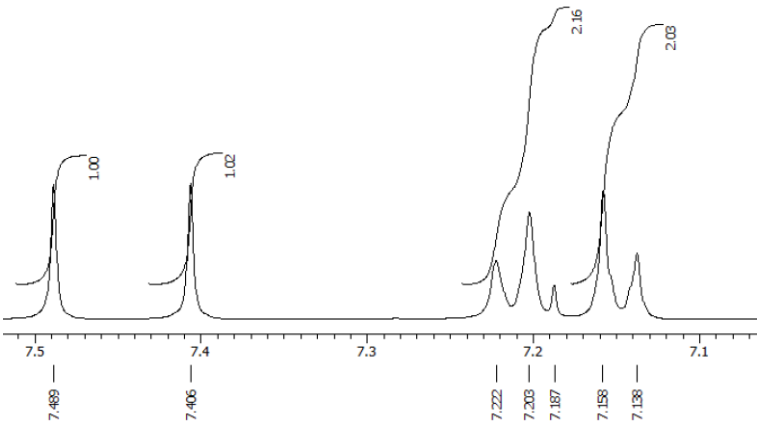
2-bromo-6,7-dimethoxy-3-(*p*-tolyl)naphthalene-1,4-dione (3y)

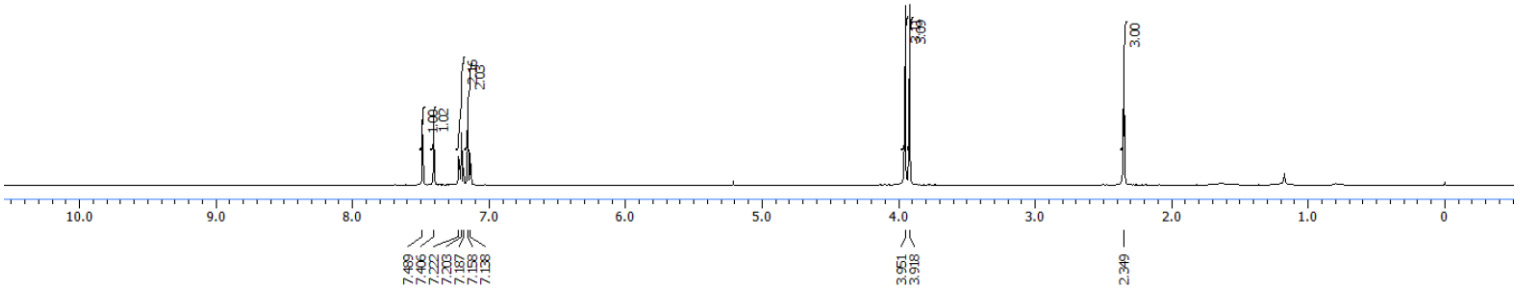


^{1}H NMR (400 MHz, $CDCl_3$)

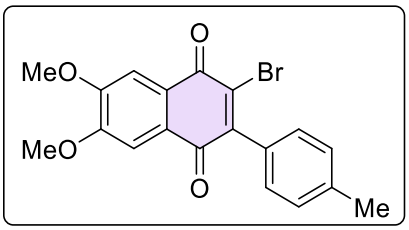


2-bromo-6,7-dimethoxy-3-(*p*-tolyl)naphthalene-1,4-dione (3y)

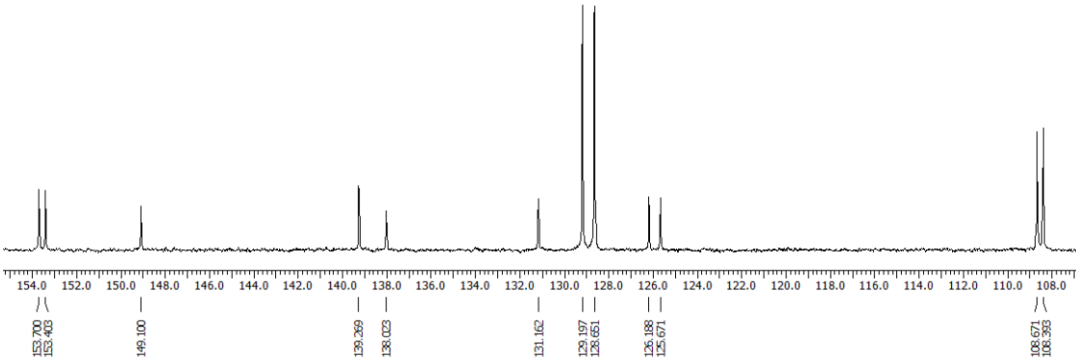


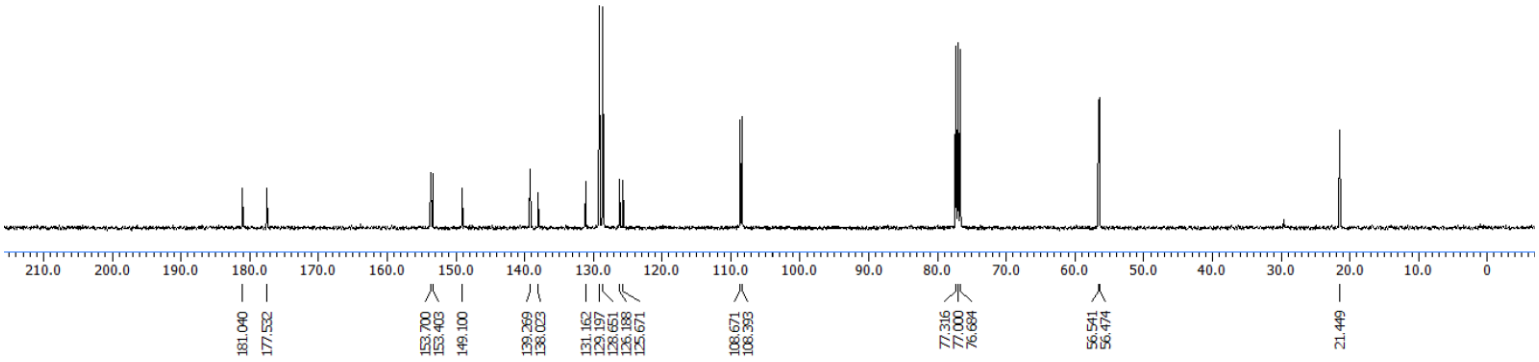


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

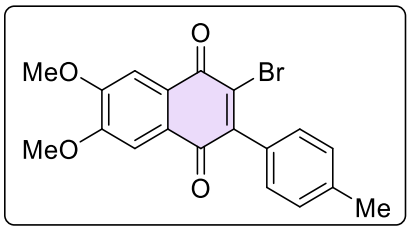


2-bromo-6,7-dimethoxy-3-(*p*-tolyl)naphthalene-1,4-dione (3y)





HRMS



2-bromo-6,7-dimethoxy-3-(*p*-tolyl)naphthalene-1,4-dione (3y)

Qualitative Compound Report

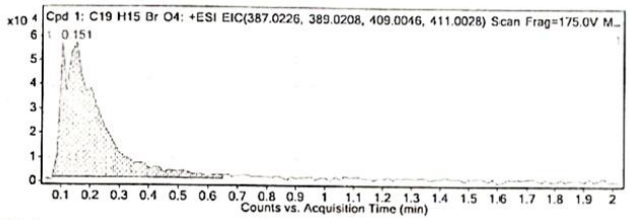
Data File	MNS-326.d	**Sample Name**	MNS-326
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	HP-PC\Admin
Acq Method	MS Scan.m	**Acquired Time**	31-01-2025 15:14:10
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

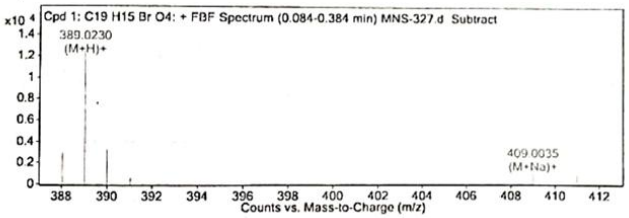
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C19 H15 Br O4	0.151	386.0183	12551	C19 H15 Br O4	386.0154	7.49	C19 H15 Br O4	C19 H15 Br O4

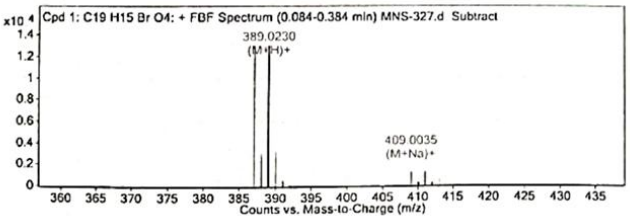
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H15 Br O4	389.023	0.151	Find By Formula	386.0183



MS Spectrum



MS Zoomed Spectrum

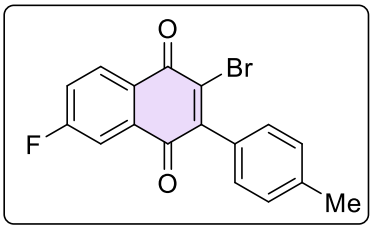


MS Spectrum Peak List

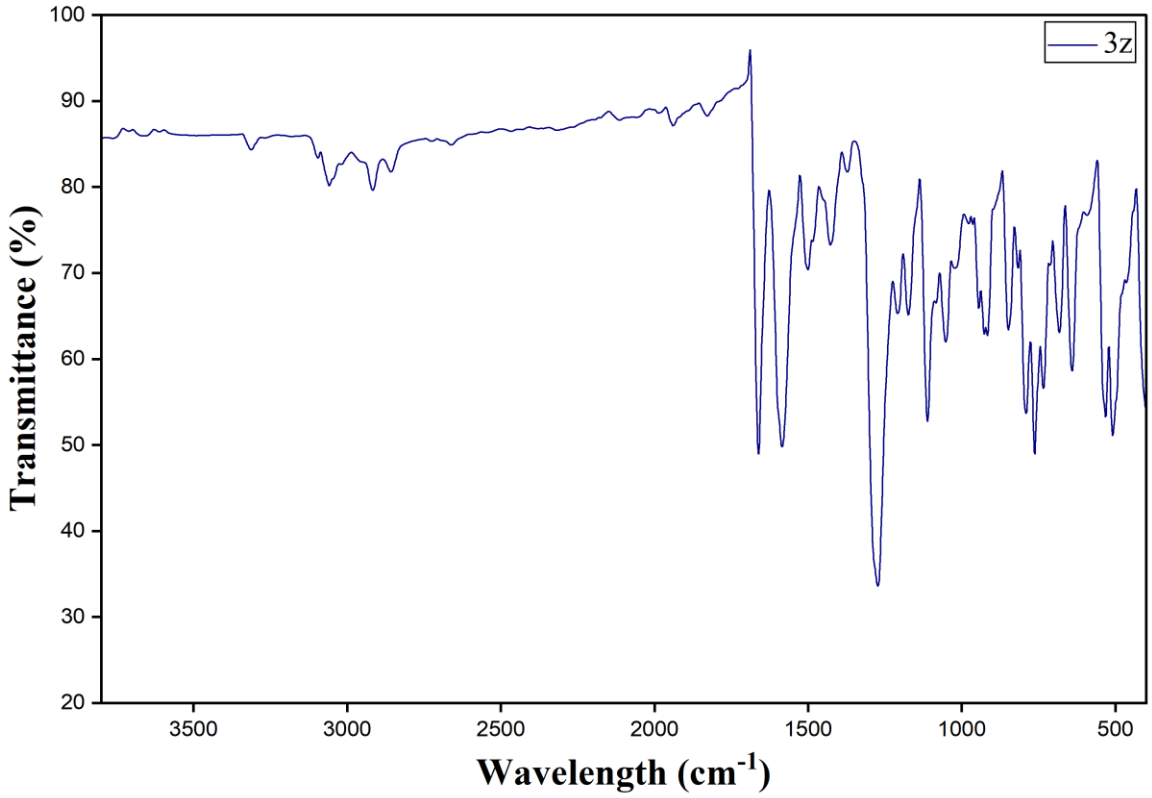
m/z	z	Abund	Formula	Ion
387.0252	1	12527.12	C19H16BrO4	(M+H)+
388.0291	1	3009.36	C19H16BrO4	(M+H)+
389.023	1	12550.58	C19H16BrO4	(M+H)+
390.0277	1	3206.66	C19H16BrO4	(M+H)+
391.0329	1	569.2	C19H16BrO4	(M+H)+
409.0035	1	914.87	C19H15BrNaO4	(M+Na)+
410.0098	1	224.33	C19H15BrNaO4	(M+Na)+
411.01	1	898.98	C19H15BrNaO4	(M+Na)+
412.0176	1	239.31	C19H15BrNaO4	(M+Na)+
413.025	1	567.53	C19H15BrNaO4	(M+Na)+

--- End Of Report ---

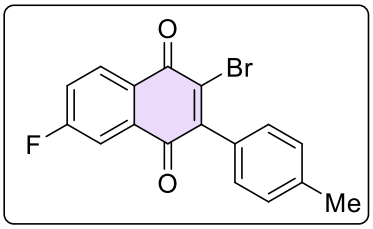
IR Spectra



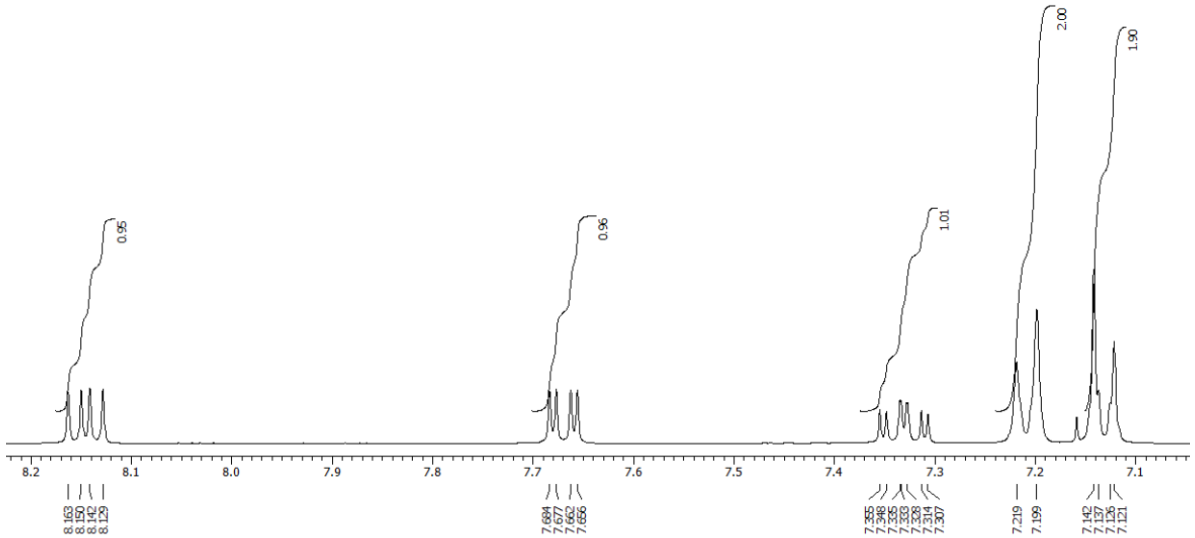
2-bromo-6-fluoro-3-(*p*-tolyl)naphthalene-1,4-dione (3z)

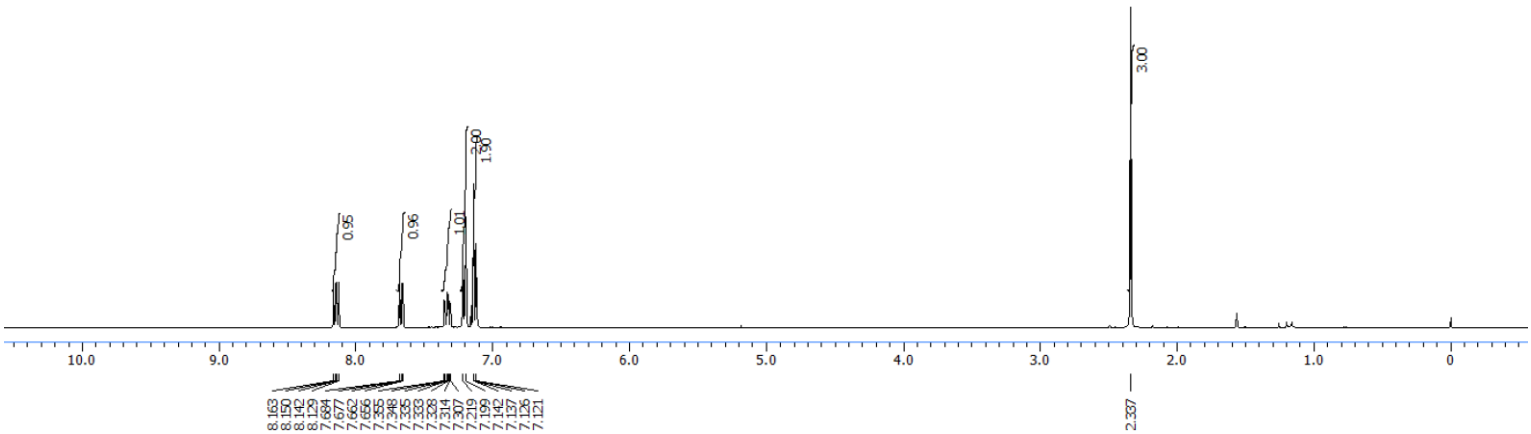


^{1}H NMR (400 MHz, $CDCl_3$)

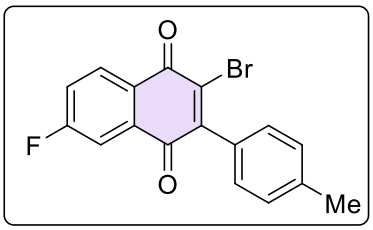


2-bromo-6-fluoro-3-(*p*-tolyl)naphthalene-1,4-dione (3z)

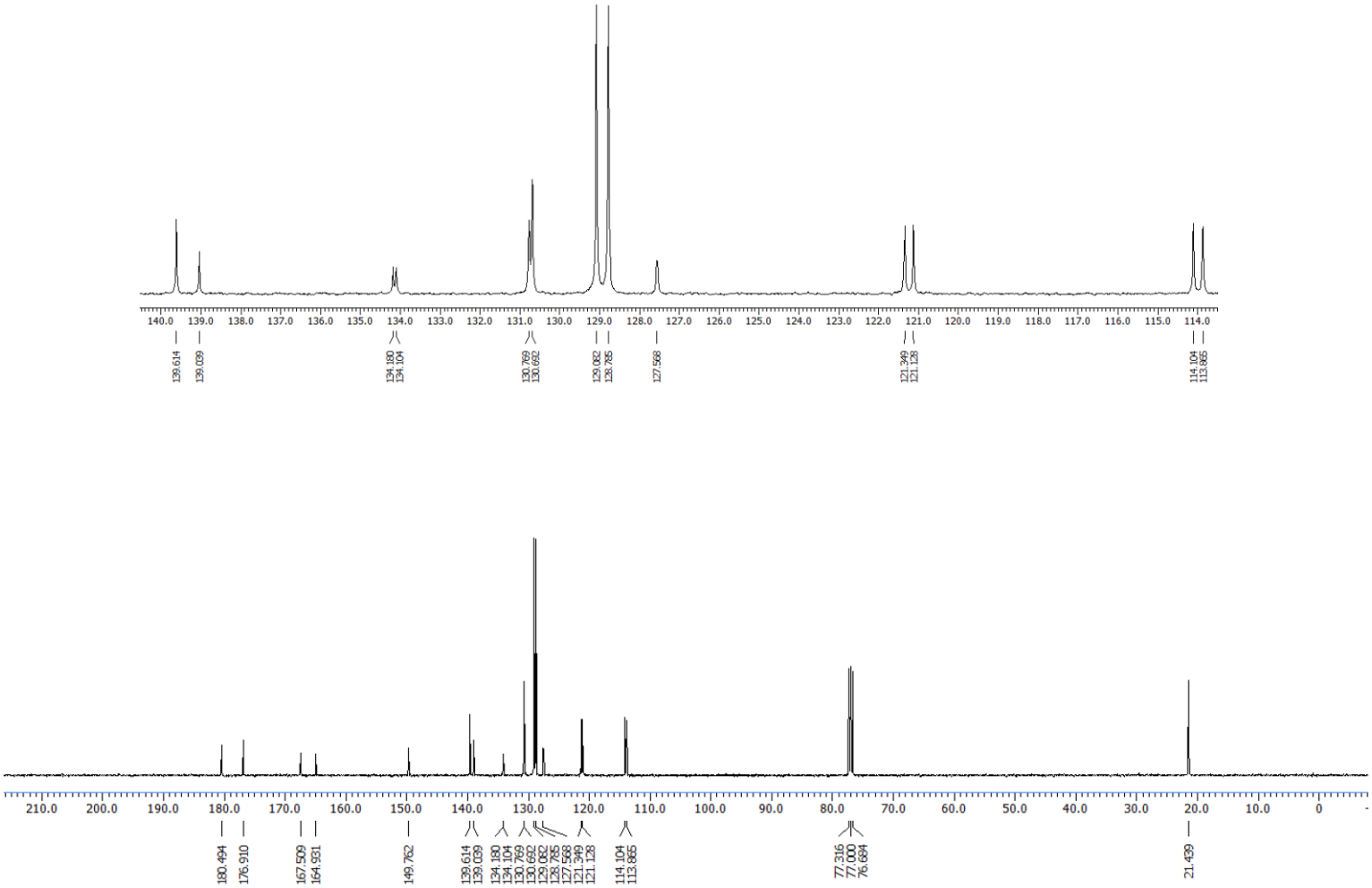




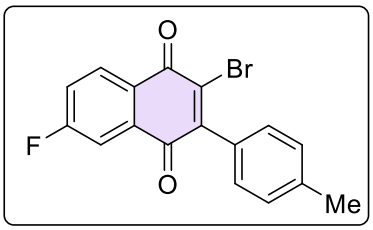
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



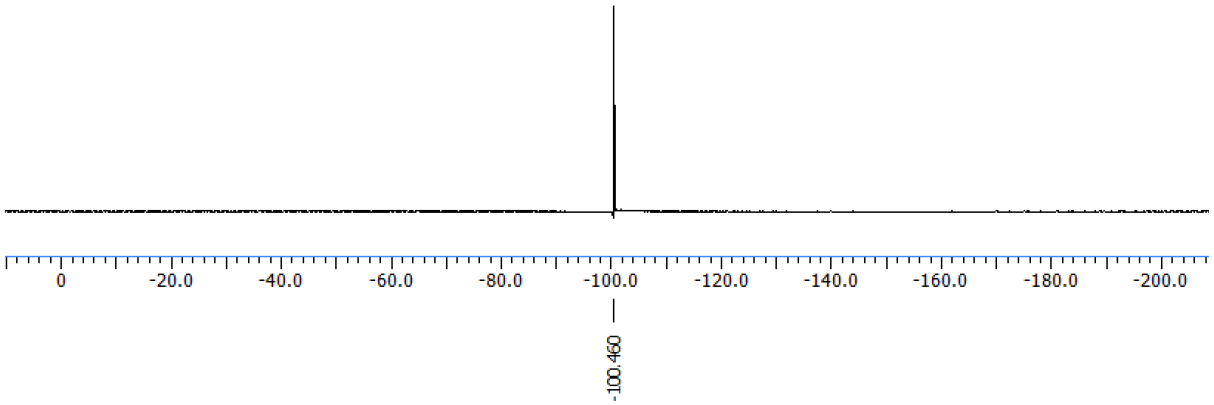
2-bromo-6-fluoro-3-(*p*-tolyl)naphthalene-1,4-dione (3z)



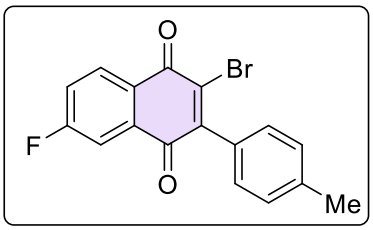
^{19}F NMR (376 MHz, $CDCl_3$)



2-bromo-6-fluoro-3-(*p*-tolyl)naphthalene-1,4-dione (3z)



HRMS



2-bromo-6-fluoro-3-(*p*-tolyl)naphthalene-1,4-dione (3z)

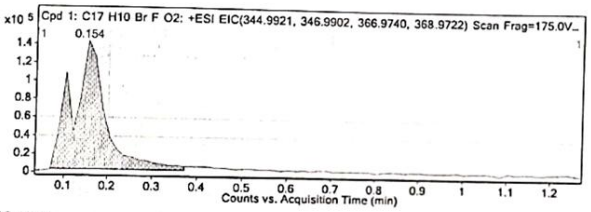
Qualitative Compound Report

Data File	MNS-343.d	Sample Name	MNS-343
Sample Type	Sample	Position	P1-C9
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-03-2025 14:53:37
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

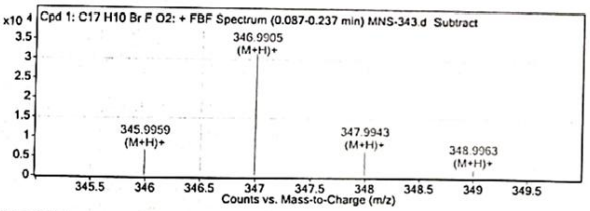
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H10 Br F O2	0.154	343.9851	32198	C17 H10 Br F O2	343.9848	0.91	C17 H10 Br F O2	C17 H10 Br F O2

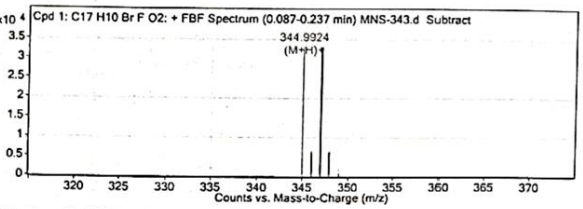
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H10 Br F O2	344.9924	0.154	Find By Formula	343.9851



MS Spectrum



MS Zoomed Spectrum

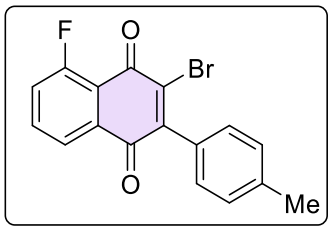


MS Spectrum Peak List

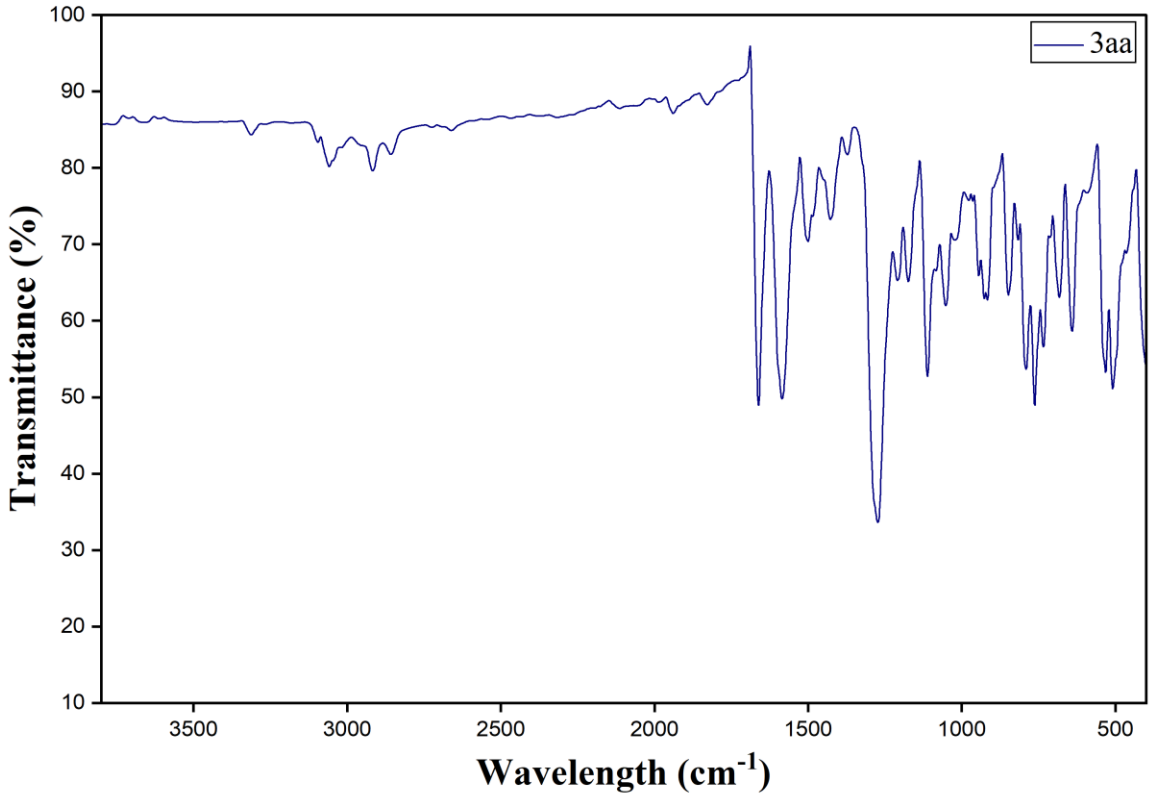
m/z	z	Abund	Formula	Ion
344.9924	1	32197.95	C17H11BrFO2	(M+H)+
345.9959	1	6764.91	C17H11BrFO2	(M+H)+
346.9905	1	31816.02	C17H11BrFO2	(M+H)+
347.9943	1	6577.36	C17H11BrFO2	(M+H)+
348.9963	1	2117.14	C17H11BrFO2	(M+H)+
349.9919	1	78.84	C17H11BrFO2	(M+H)+

--- End Of Report ---

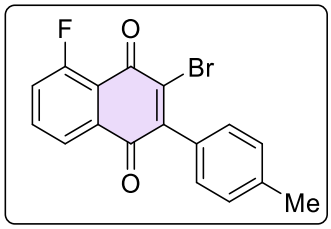
IR Spectra



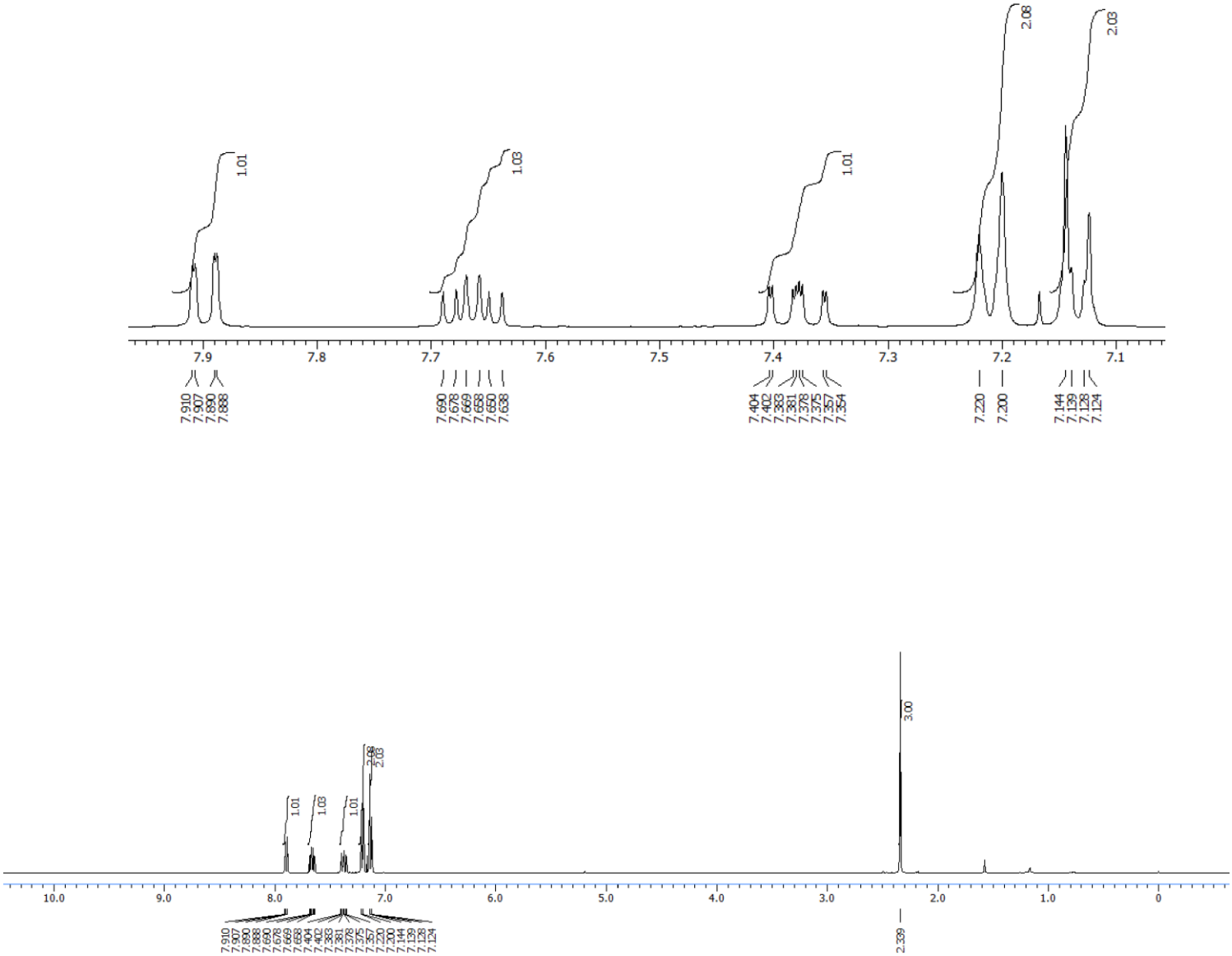
3-bromo-5-fluoro-2-(p-tolyl)naphthalene-1,4-dione (3aa)



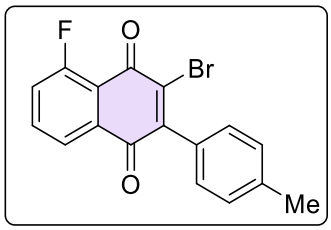
^{1}H NMR (400 MHz, $CDCl_3$)



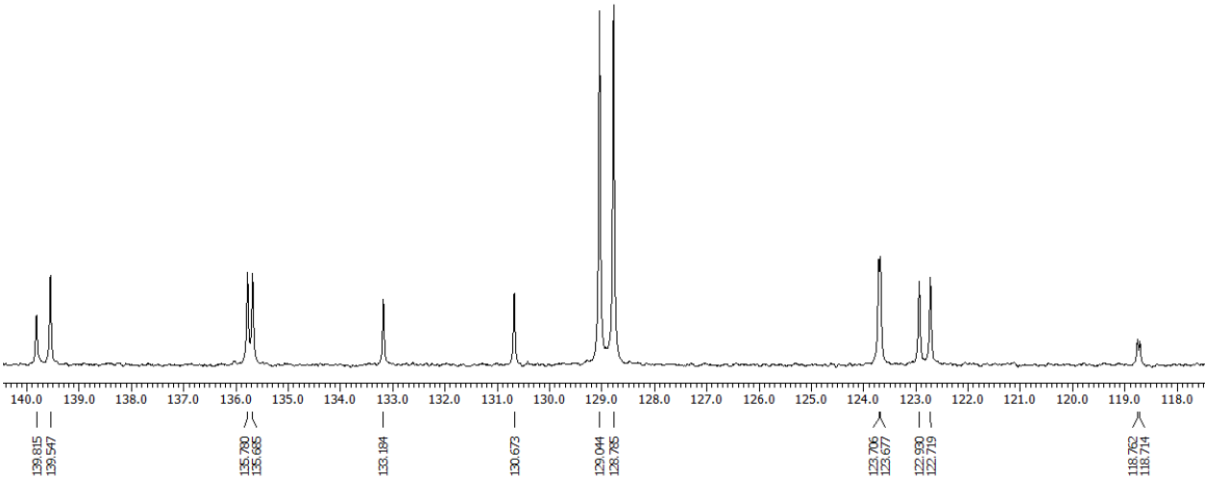
3-bromo-5-fluoro-2-(p-tolyl)naphthalene-1,4-dione (3aa)

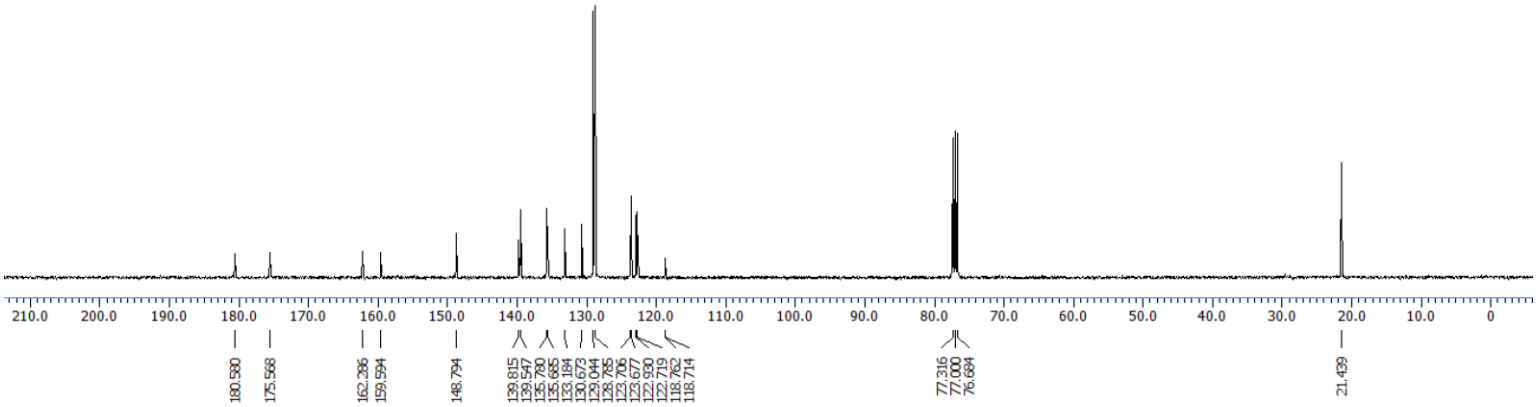


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

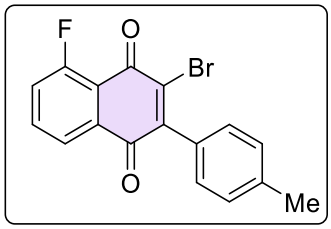


3-bromo-5-fluoro-2-(*p*-tolyl)naphthalene-1,4-dione (3aa)

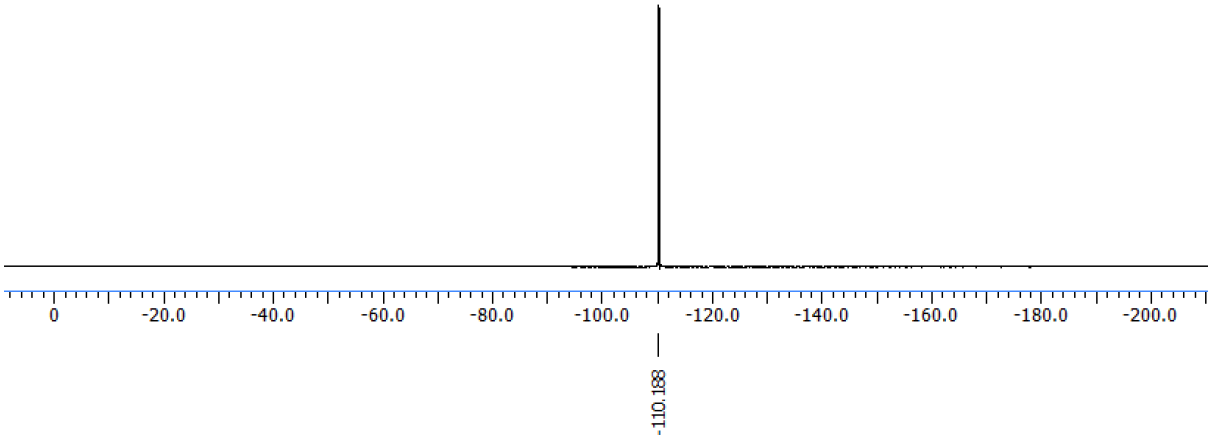




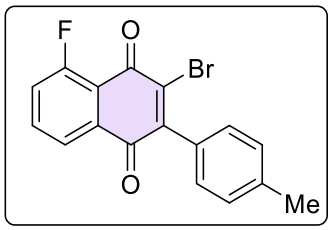
^{19}F NMR (376 MHz, $CDCl_3$)



3-bromo-5-fluoro-2-(p-tolyl)naphthalene-1,4-dione (3aa)



HRMS



3-bromo-5-fluoro-2-(p-tolyl)naphthalene-1,4-dione (3aa)

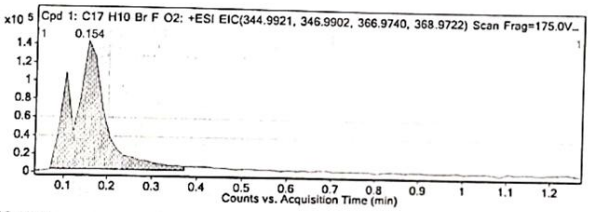
Qualitative Compound Report

Data File	MNS-343.d	Sample Name	MNS-343
Sample Type	Sample	Position	P1-C9
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-03-2025 14:53:37
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

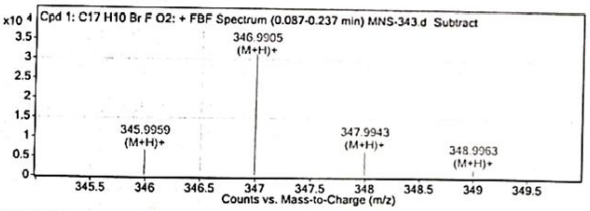
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H10 Br F O2	0.154	343.9851	32198	C17 H10 Br F O2	343.9848	0.91	C17 H10 Br F O2	C17 H10 Br F O2

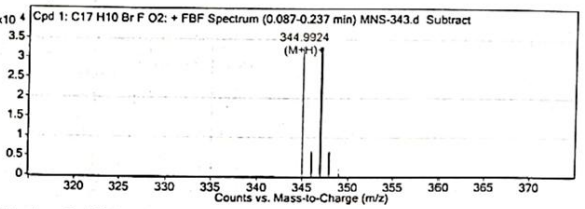
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H10 Br F O2	344.9924	0.154	Find By Formula	343.9851



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
344.9924	1	32197.95	C17H11BrFO2	(M+H)+
345.9959	1	6764.91	C17H11BrFO2	(M+H)+
346.9905	1	31816.02	C17H11BrFO2	(M+H)+
347.9943	1	6577.36	C17H11BrFO2	(M+H)+
348.9963	1	2117.14	C17H11BrFO2	(M+H)+
349.9919	1	78.84	C17H11BrFO2	(M+H)+

--- End Of Report ---

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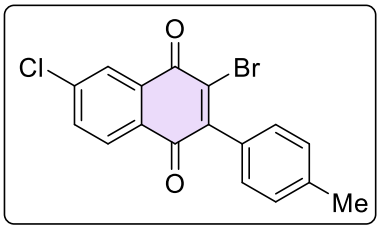
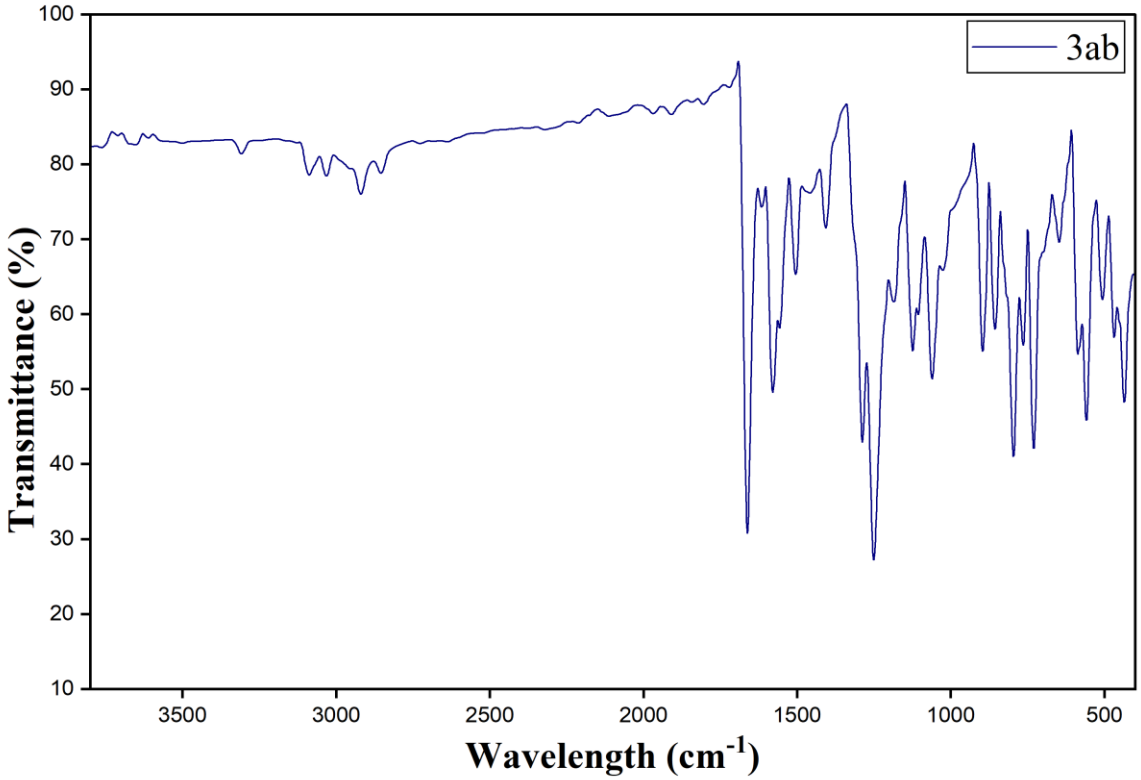
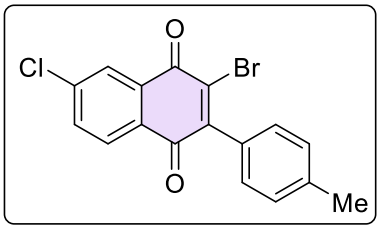
IR Spectra



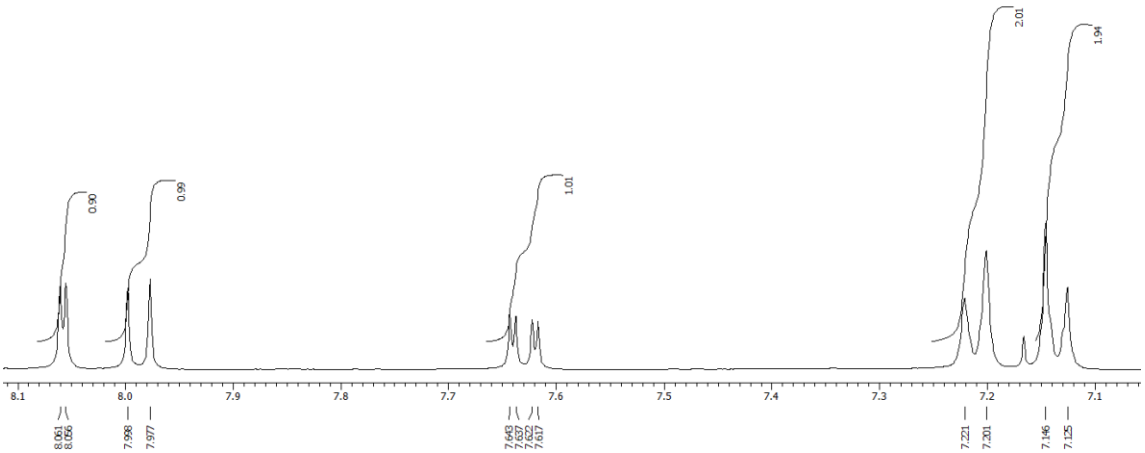
3-bromo-6-chloro-2-(*p*-tolyl)naphthalene-1,4-dione (3ab)

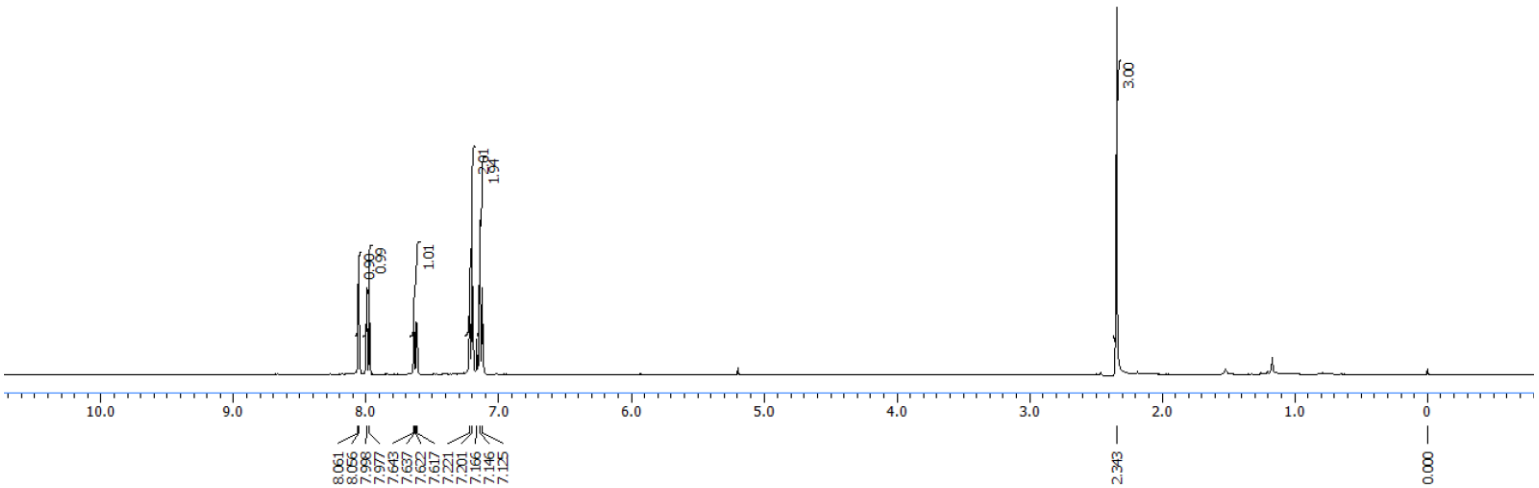


^{1}H NMR (400 MHz, $CDCl_3$)

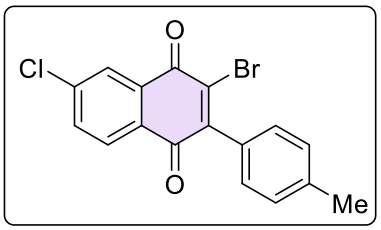


3-bromo-6-chloro-2-(*p*-tolyl)naphthalene-1,4-dione (3ab)

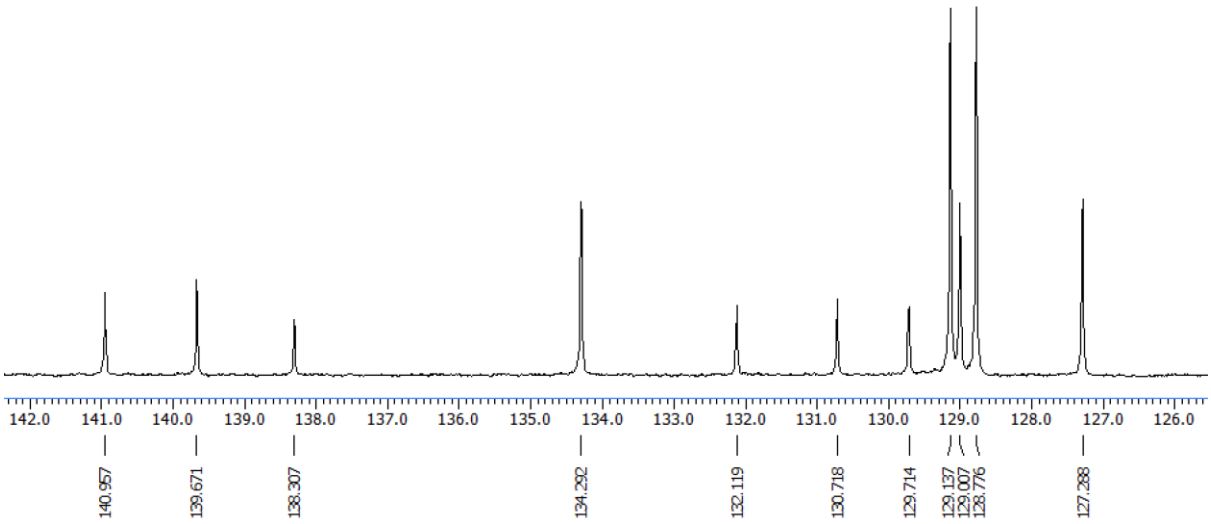


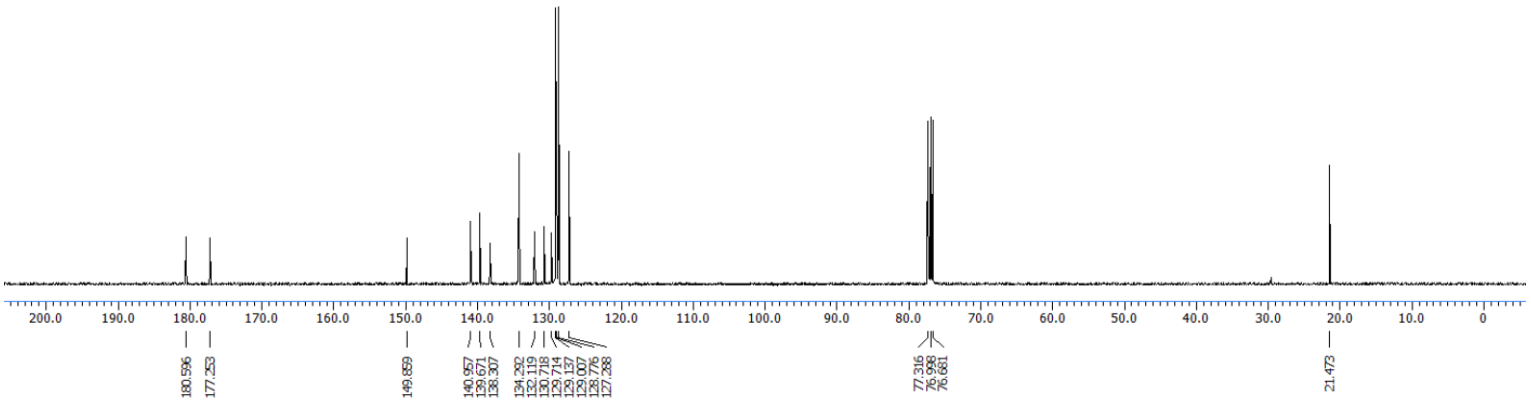


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

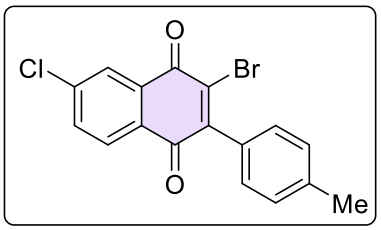


3-bromo-6-chloro-2-(*p*-tolyl)naphthalene-1,4-dione (3ab)





HRMS



3-bromo-6-chloro-2-(*p*-tolyl)naphthalene-1,4-dione (3ab)

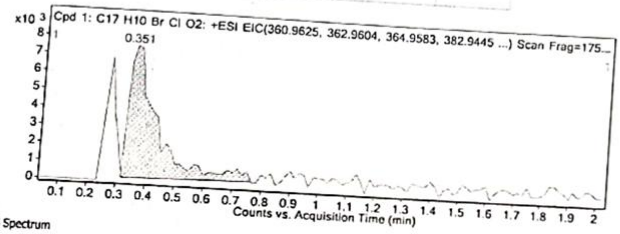
Qualitative Compound Report

Data File	MNS-305.d	Sample Name	MNS-305
Sample Type	Sample	Position	P1-B6
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-05-2024 14:01:35
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group			
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)	Info.	3

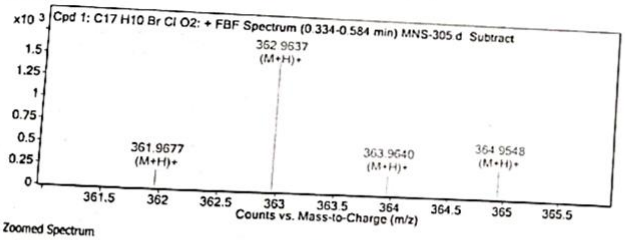
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H10 Br Cl O2	0.351	359.9568	1511	C17 H10 Br Cl O2	359.9553	4.27	C17 H10 Br Cl O2	C17 H10 Br Cl O2

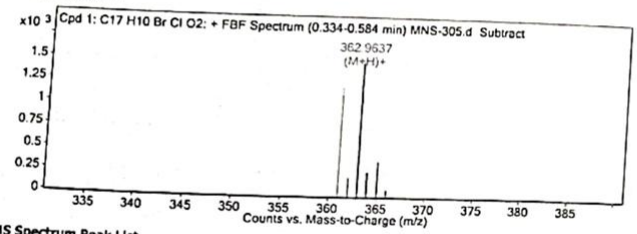
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H10 Br Cl O2	362.9637	0.351	Find By Formula	359.9568



MS Spectrum



MS Zoomed Spectrum

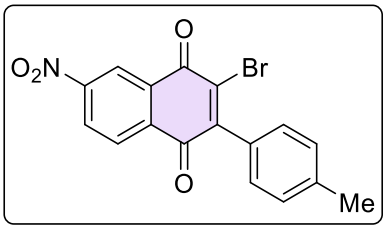


MS Spectrum Peak List

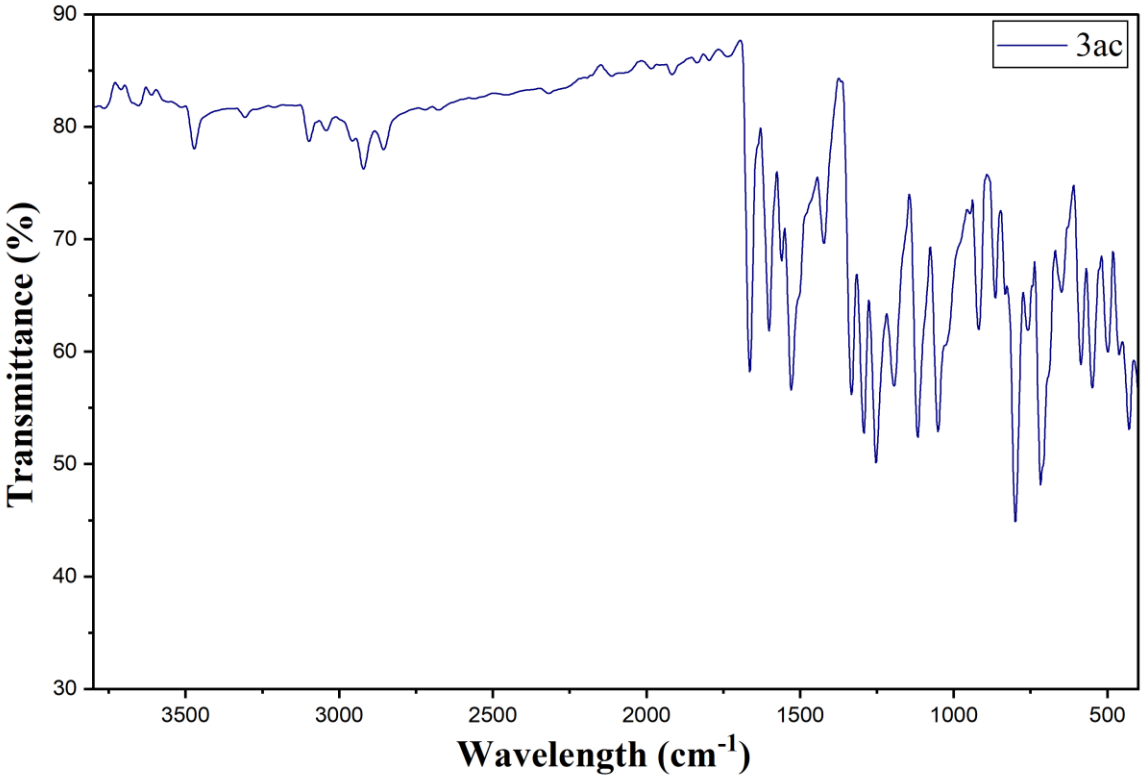
m/z	z	Abund	Formula	Ion
360.9635	1	1234.87	C17H11BrClO2	(M+H)+
361.9677	1	209.45	C17H11BrClO2	(M+H)+
362.9637	1	1511.33	C17H11BrClO2	(M+H)+
363.964	1	247.96	C17H11BrClO2	(M+H)+
364.9548	1	337.53	C17H11BrClO2	(M+H)+
365.9613	1	24.17	C17H11BrClO2	(M+H)+

--- End Of Report ---

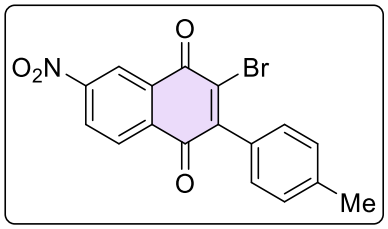
IR Spectra



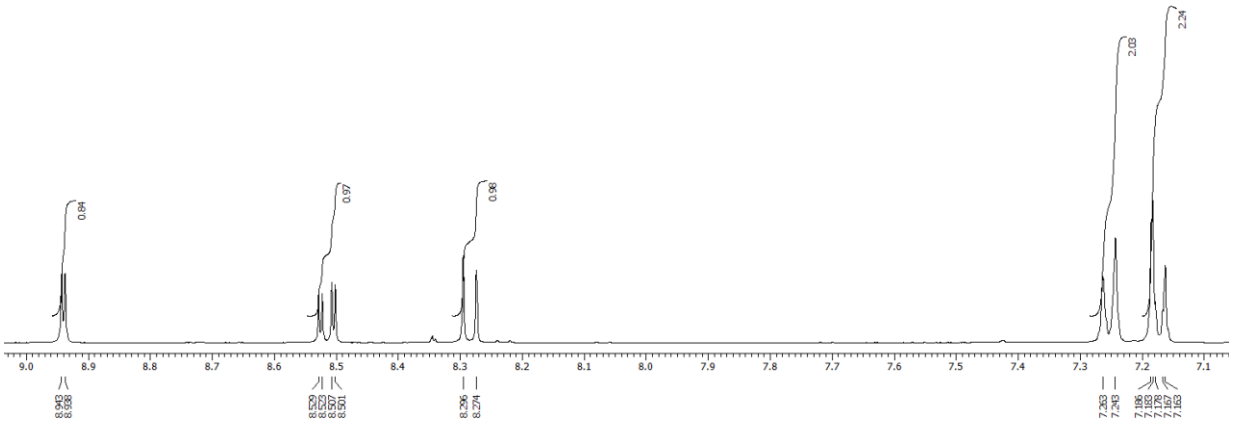
3-bromo-6-nitro-2-(*p*-tolyl)naphthalene-1,4-dione (3ac)

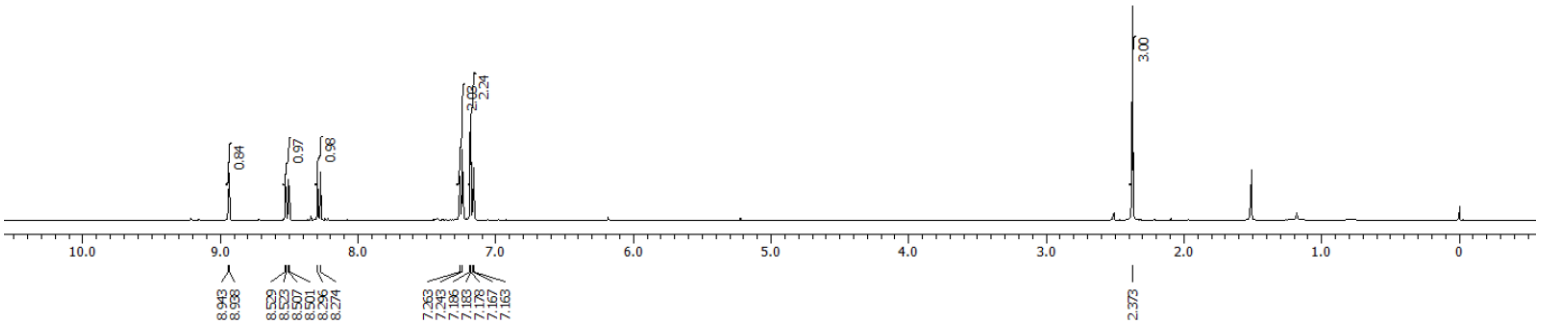


^{1}H NMR (400 MHz, $CDCl_3$)

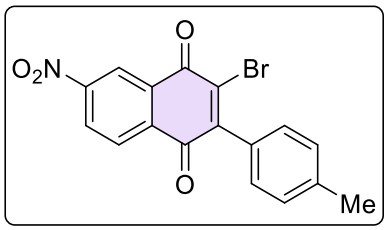


3-bromo-6-nitro-2-(*p*-tolyl)naphthalene-1,4-dione (3ac)

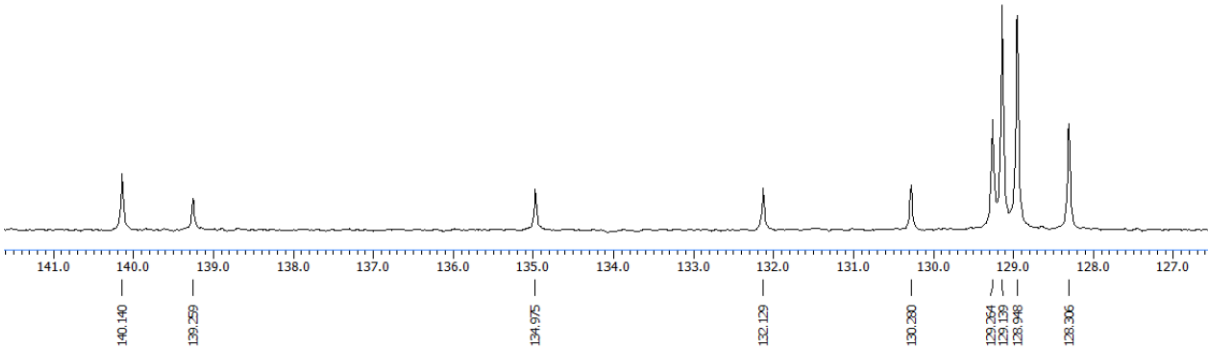


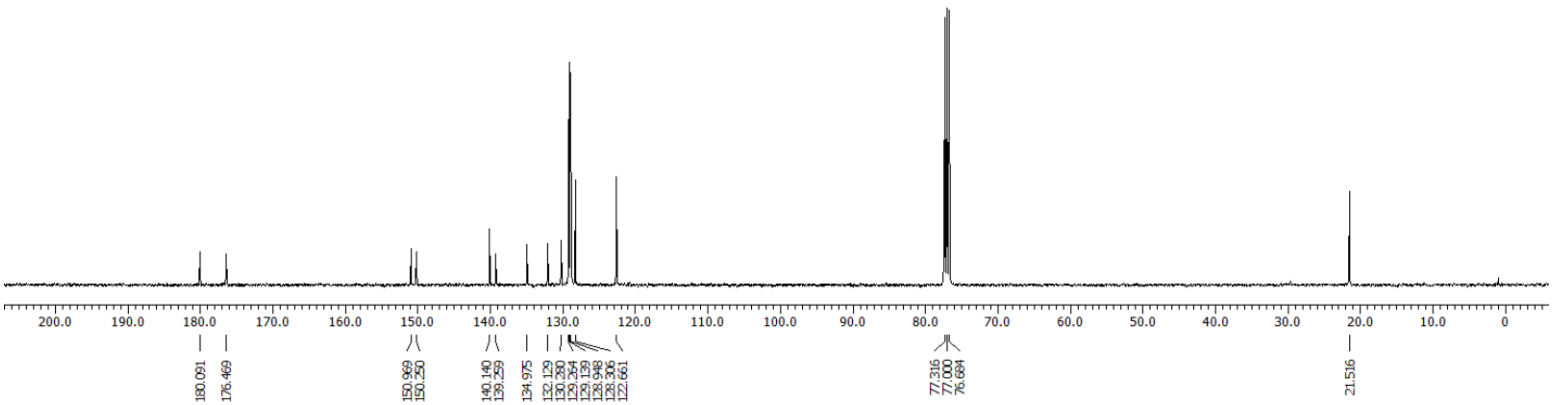


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

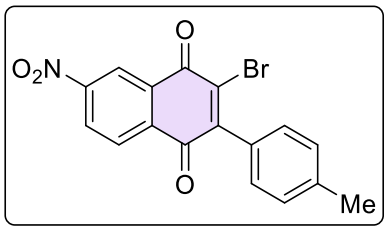


3-bromo-6-nitro-2-(*p*-tolyl)naphthalene-1,4-dione (3ac)





HRMS



3-bromo-6-nitro-2-(*p*-tolyl)naphthalene-1,4-dione (3ac)

Qualitative Compound Report

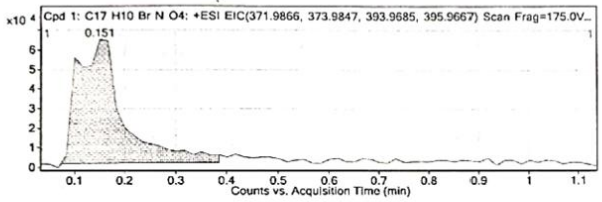
Data File	MNS-352.d	**Sample Name**	MNS-352
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	08-03-2025 12:45:09
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group		**Info.**	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

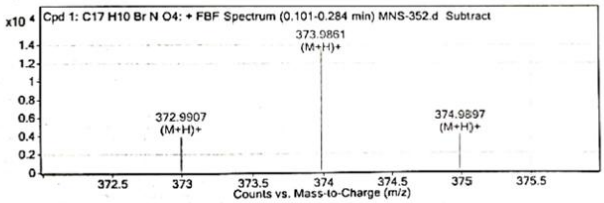
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H10 Br N O4	0.151	370.9807	13881	C17 H10 Br N O4	370.9793	3.77	C17 H10 Br N O4	C17 H10 Br N O4

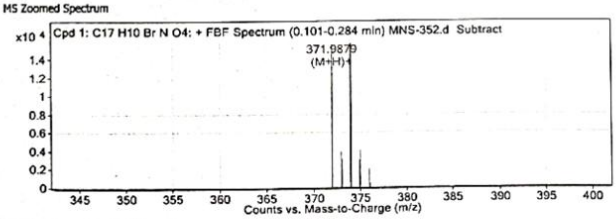
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C17 H10 Br N O4	371.9879	0.151	Find By Formula	370.9807



MS Spectrum



MS Zoomed Spectrum

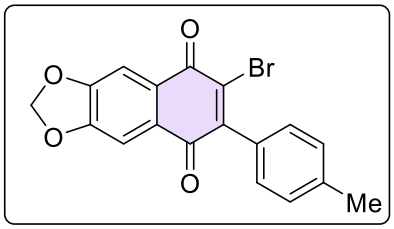


MS Spectrum Peak List

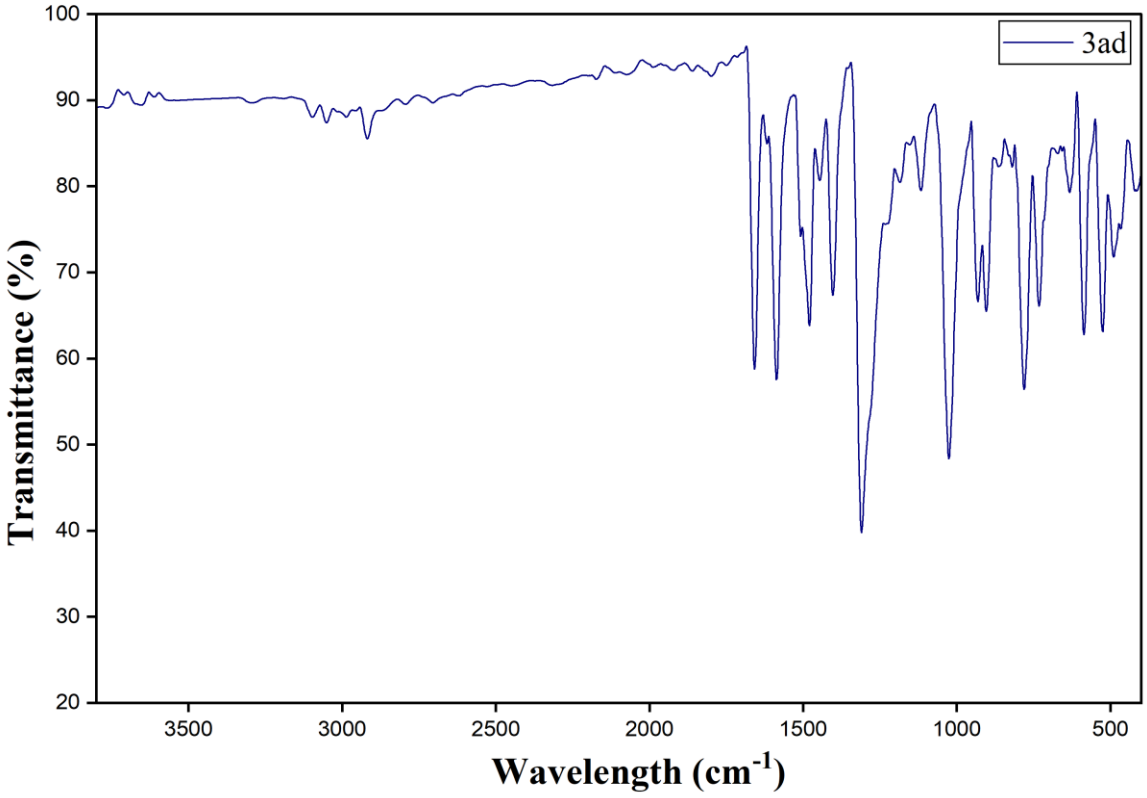
m/z	z	Abund	Formula	Ion
371.9879	1	13881.47	C17H11BrNO4	(M+H)+
372.9907	1	3959.85	C17H11BrNO4	(M+H)+
373.9861	1	13668.22	C17H11BrNO4	(M+H)+
374.9897	1	4041.41	C17H11BrNO4	(M+H)+
375.9928	1	2034.66	C17H11BrNO4	(M+H)+

--- End Of Report ---

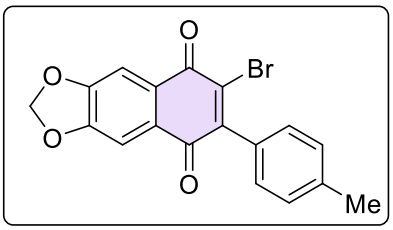
IR Spectra



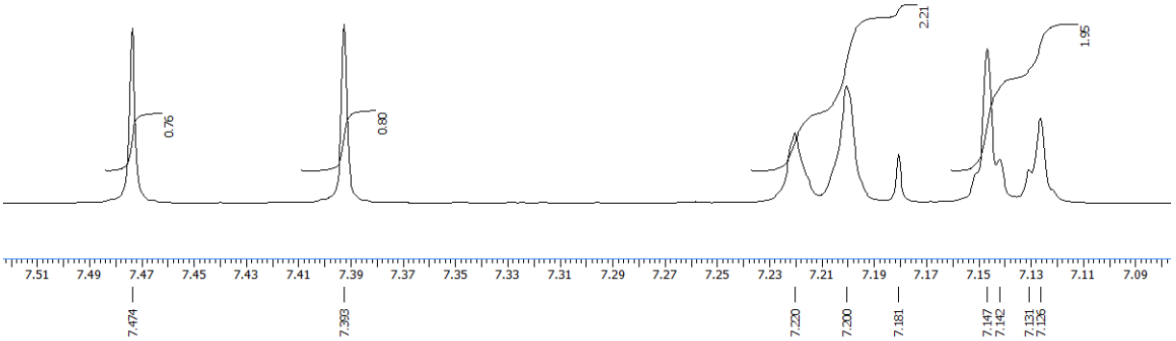
6-bromo-7-(*p*-tolyl)naphtho[2,3-d][1,3]dioxole-5,8-dione (3ad)

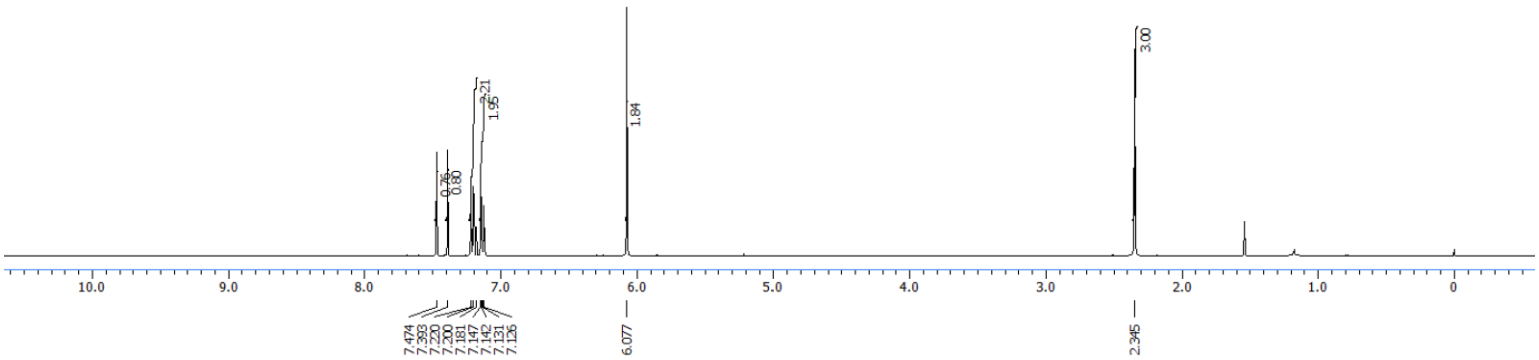


^{1}H NMR (400 MHz, $CDCl_3$)

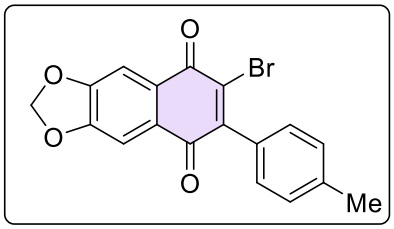


6-bromo-7-(*p*-tolyl)naphtho[2,3-d][1,3]dioxole-5,8-dione (3ad)

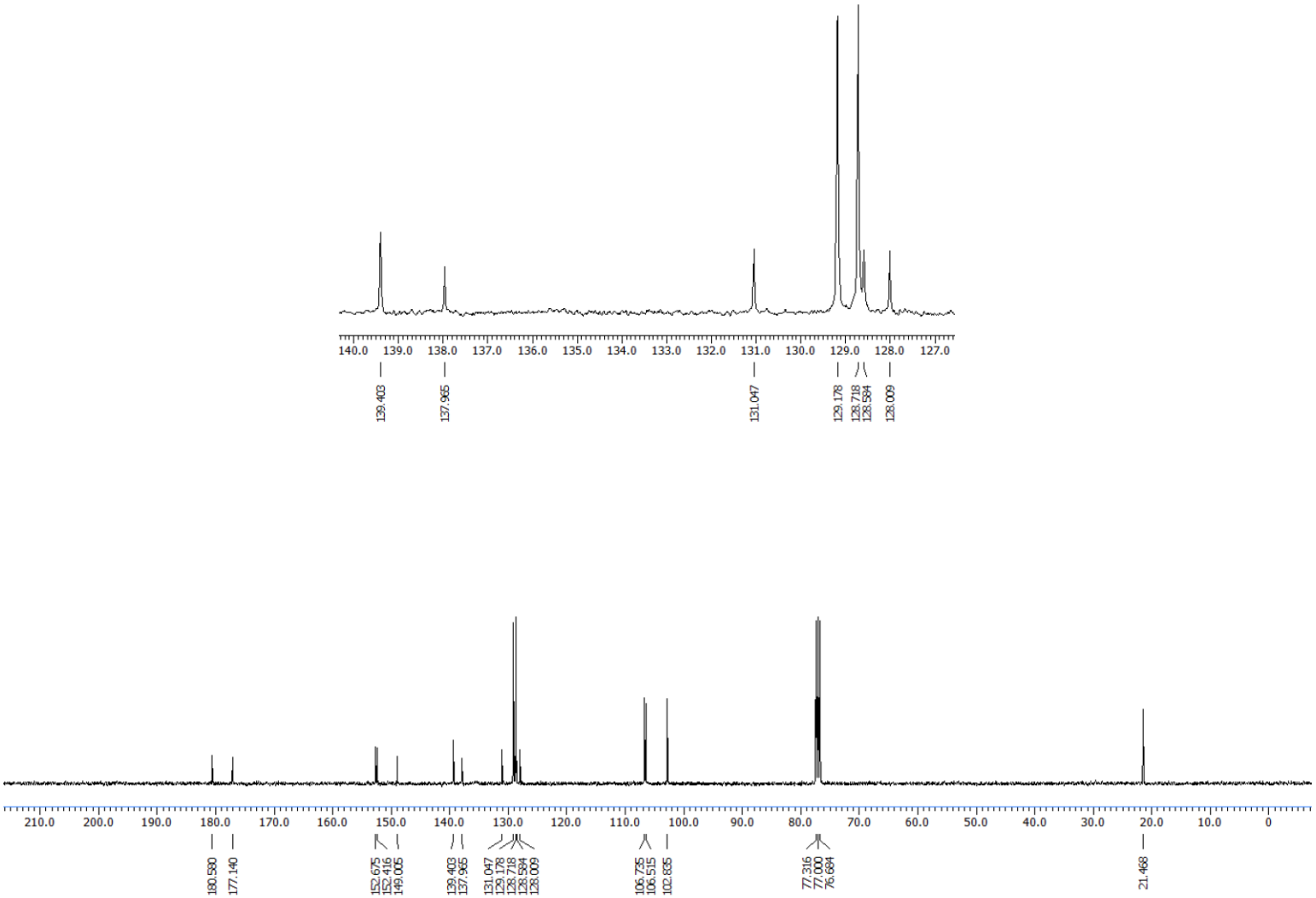




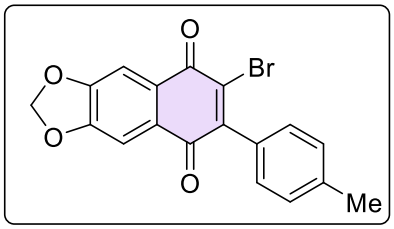
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



6-bromo-7-(*p*-tolyl)naphtho[2,3-d][1,3]dioxole-5,8-dione (3ad)



HRMS



6-bromo-7-(*p*-tolyl)naphtho[2,3-d][1,3]dioxole-5,8-dione (3ad)

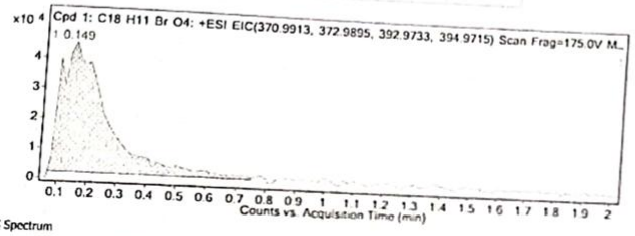
Qualitative Compound Report

Data File	MNS-345.d	Sample Name	MNS-345
Sample Type	Sample	Position	P1-A2
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	31-01-2025 15:23:20
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group			
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (85125)	Info.	3

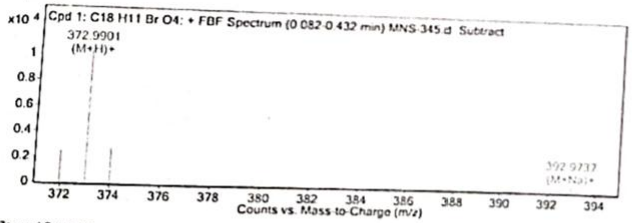
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C18 H11 Br O4	0.149	369.9845	10298	C18 H11 Br O4	369.9841	1.13	C18 H11 Br O4	C18 H11 Br O4

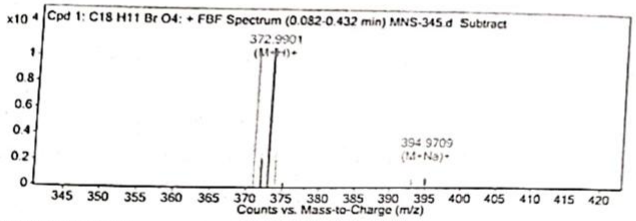
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C18 H11 Br O4	372.9901	0.149	Find By Formula	369.9845



MS Spectrum



MS Zoomed Spectrum

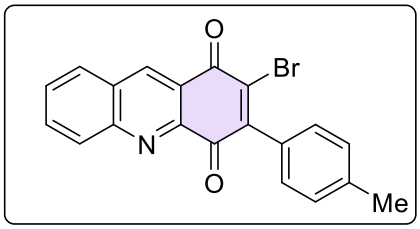


MS Spectrum Peak List

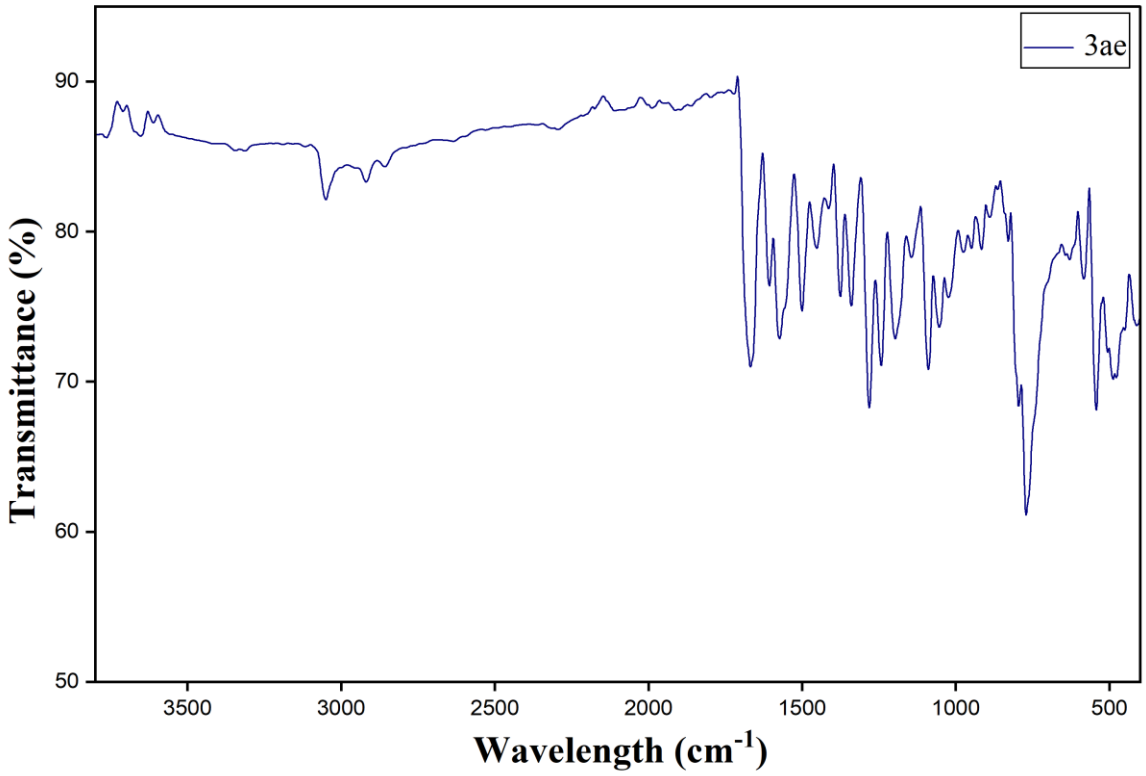
m/z	z	Abund	Formula	Ion
370.9918	1	10201.53	C18H12BrO4	(M+H)+
371.9955	1	2545.42	C18H12BrO4	(M+H)+
372.9901	1	10297.83	C18H12BrO4	(M+H)+
373.9929	1	2623.86	C18H12BrO4	(M+H)+
374.9921	1	301.27	C18H12BrO4	(M+H)+
392.9737	1	529.89	C18H11BrNaO4	(M+Na)+
393.9757	1	68.17	C18H11BrNaO4	(M+Na)+
394.9709	1	795.11	C18H11BrNaO4	(M+Na)+

— End Of Report —

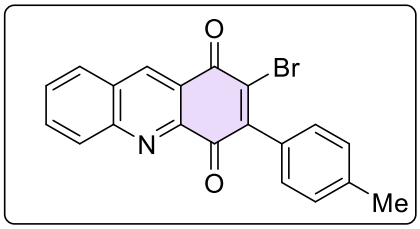
IR Spectra



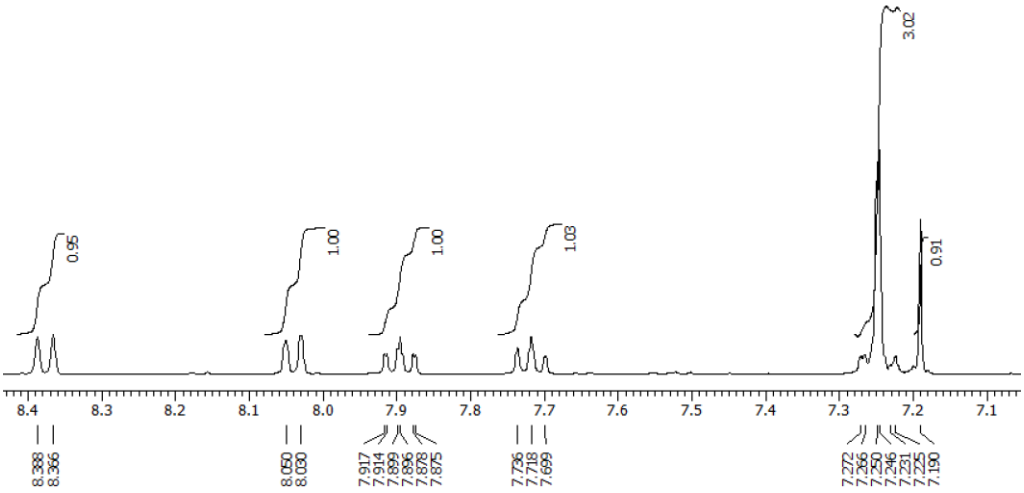
2-bromo-3-(*p*-tolyl)acridine-1,4-dione (3ae)

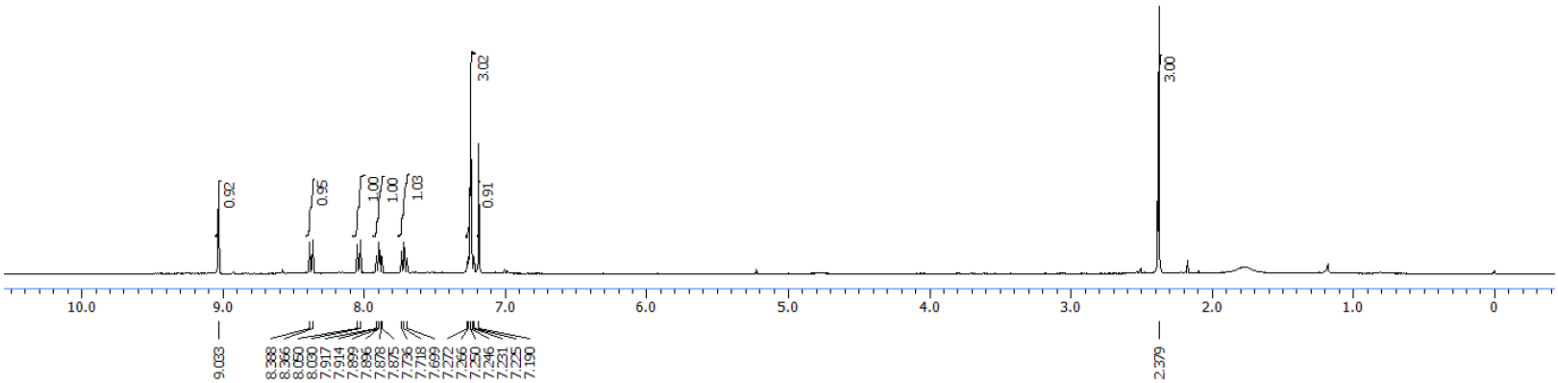


^{1}H NMR (400 MHz, $CDCl_3$)

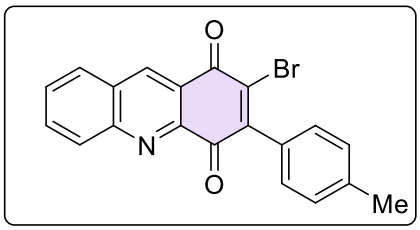


2-bromo-3-(*p*-tolyl)acridine-1,4-dione (3ae)

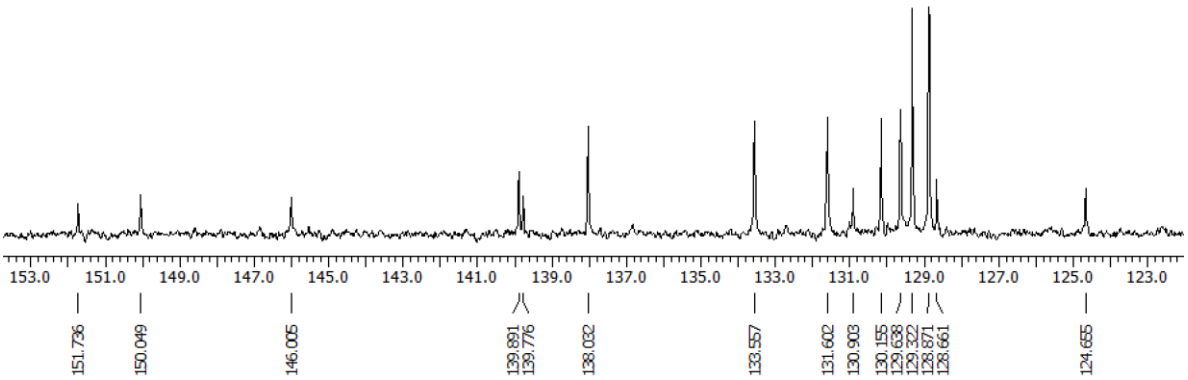


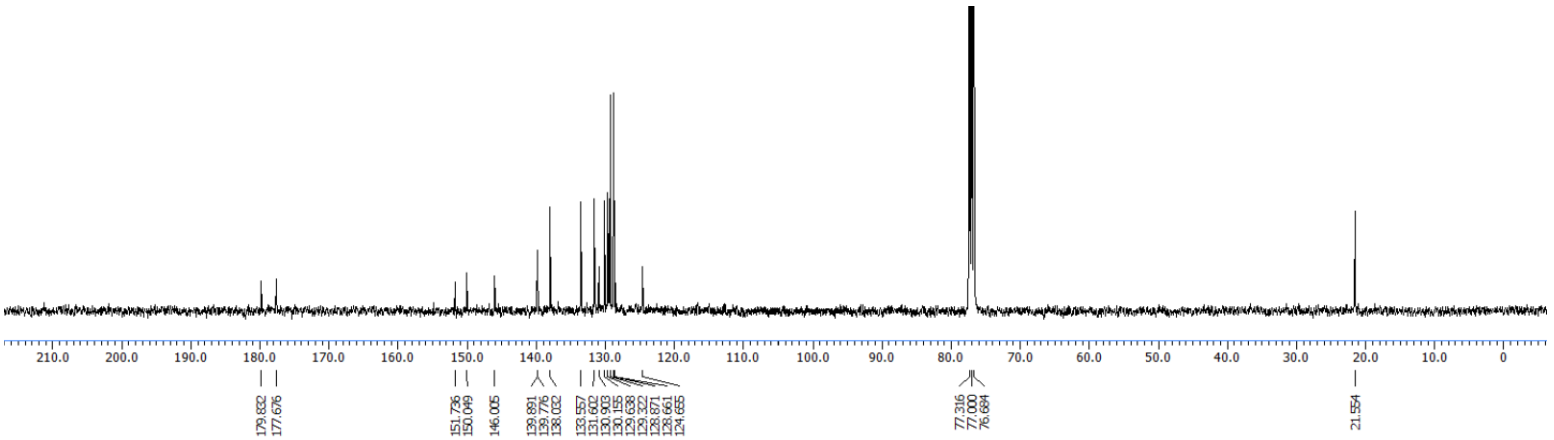


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

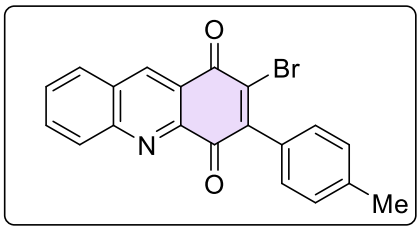


2-bromo-3-(*p*-tolyl)acridine-1,4-dione (3ae)





HRMS



2-bromo-3-(*p*-tolyl)acridine-1,4-dione (3ae)

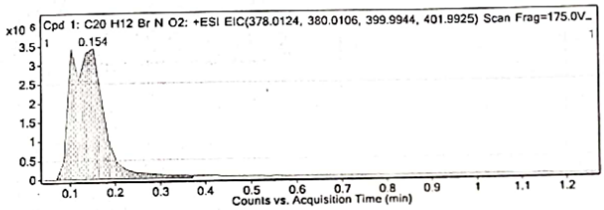
Qualitative Compound Report

Data File	MNS-349.d	Sample Name	MNS-349
Sample Type	Sample	Position	P1-C8
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	20-03-2025 14:51:29
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group	Info.	3	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

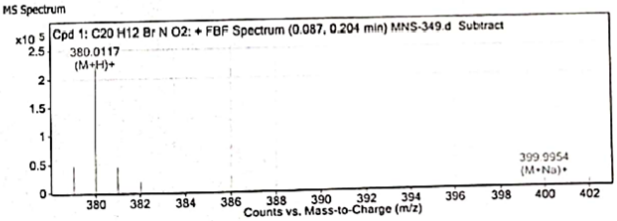
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C20 H12 Br N O2	0.154	377.0061	224193	C20 H12 Br N O2	377.0051	2.65	C20 H12 Br N O2	C20 H12 Br N O2

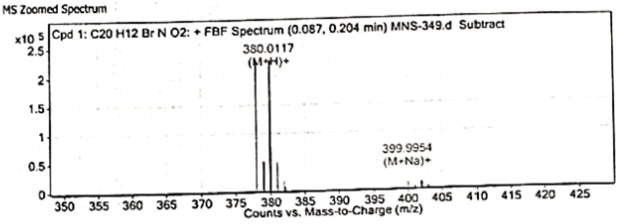
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H12 Br N O2	380.0117	0.154	Find By Formula	377.0061



MS Spectrum



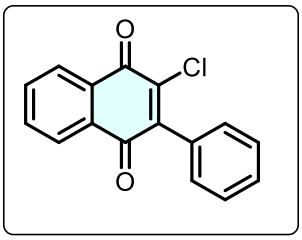
MS Zoomed Spectrum



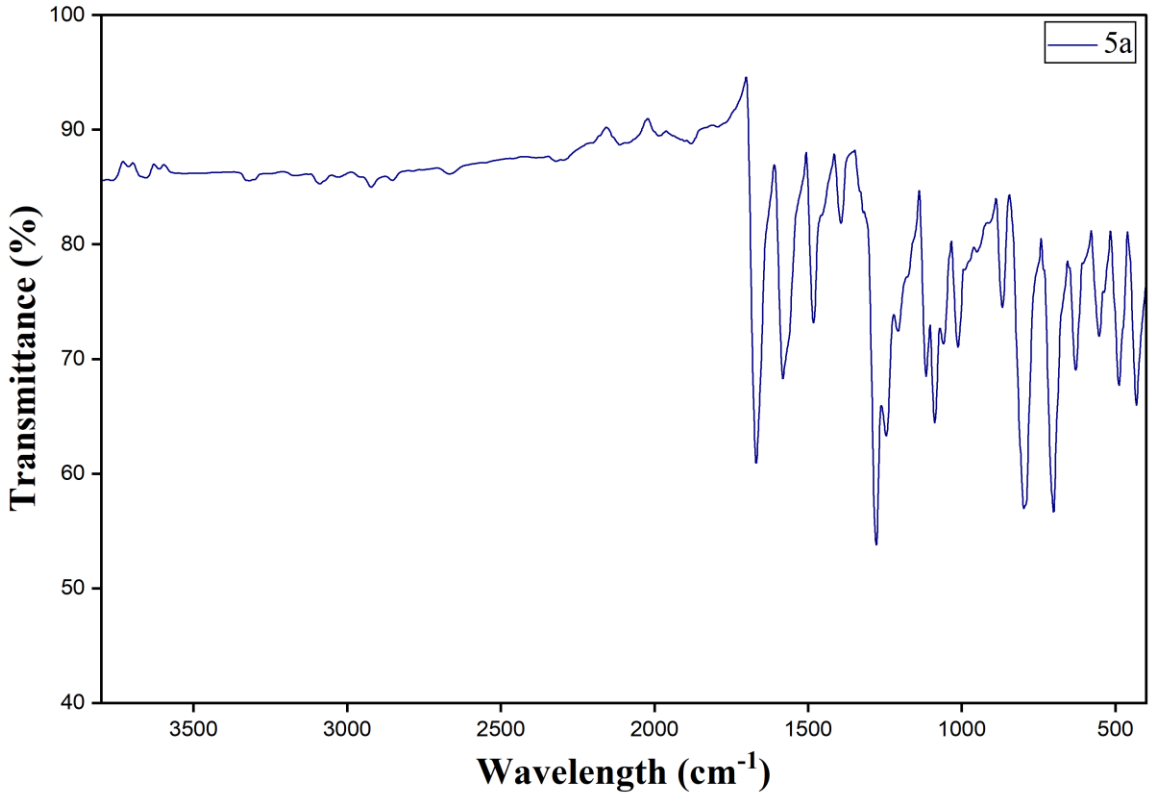
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
378.0129	1	223393.84	C20H13BrNO2	(M+H)+
379.0161	1	46849.85	C20H13BrNO2	(M+H)+
380.0117	1	224193.06	C20H13BrNO2	(M+H)+
381.0149	1	45882.78	C20H13BrNO2	(M+H)+
382.0237	1	18065.91	C20H13BrNO2	(M+H)+
383.0275	1	3640.91	C20H13BrNO2	(M+H)+
399.9954	1	10184.73	C20H12BrNNaO2	(M+Na)+
400.9956	1	3208.83	C20H12BrNNaO2	(M+Na)+
401.9933	1	9868.73	C20H12BrNNaO2	(M+Na)+
402.9919	1	3348.97	C20H12BrNNaO2	(M+Na)+

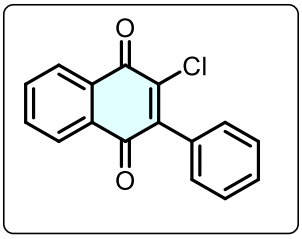
IR Spectra



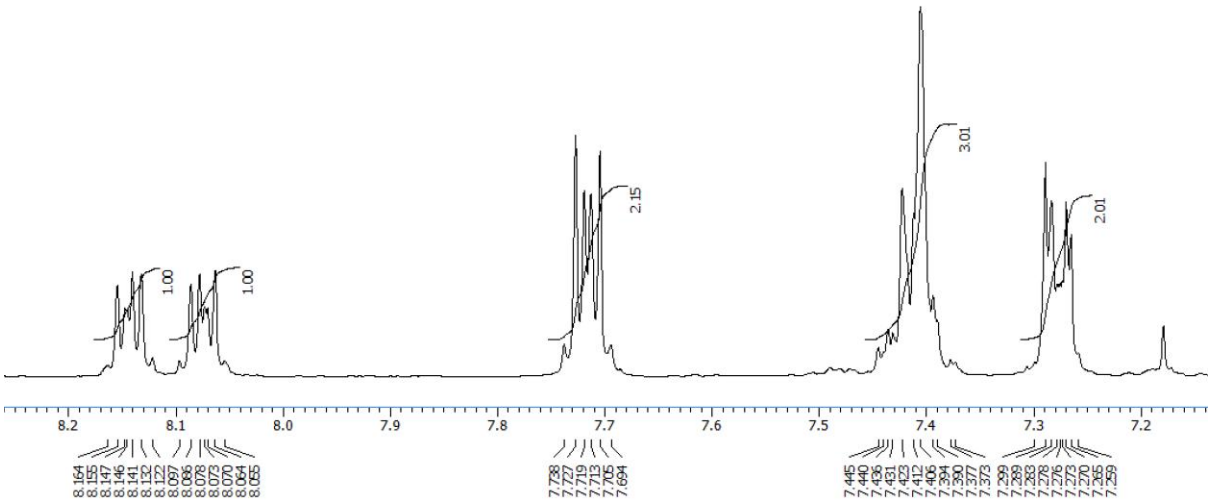
2-Chloro-3-phenylnaphthalene-1,4-dione (5a)

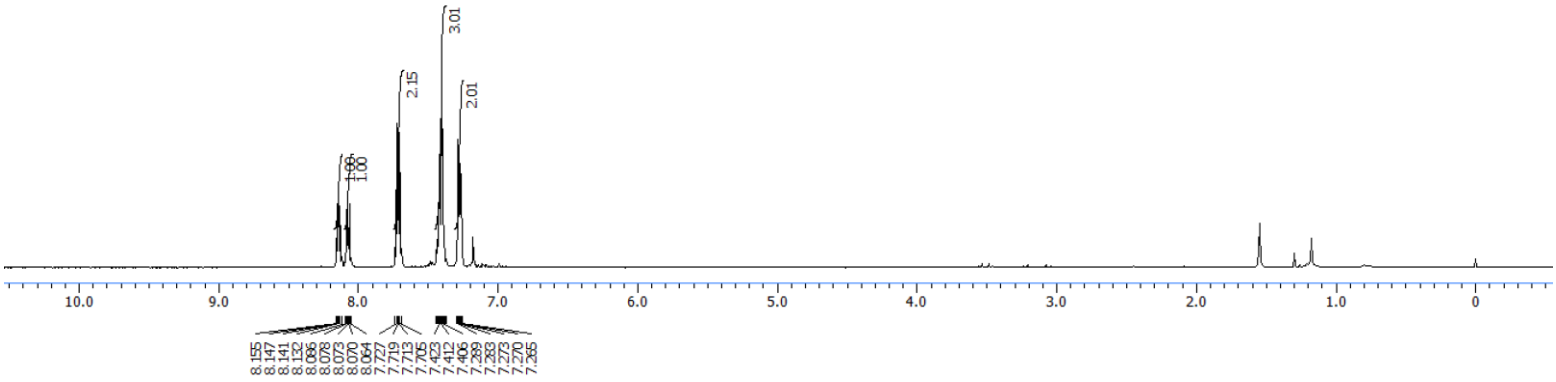


^{1}H NMR (400 MHz, $CDCl_3$)

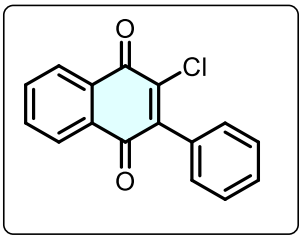


2-Chloro-3-phenylnaphthalene-1,4-dione (5a)

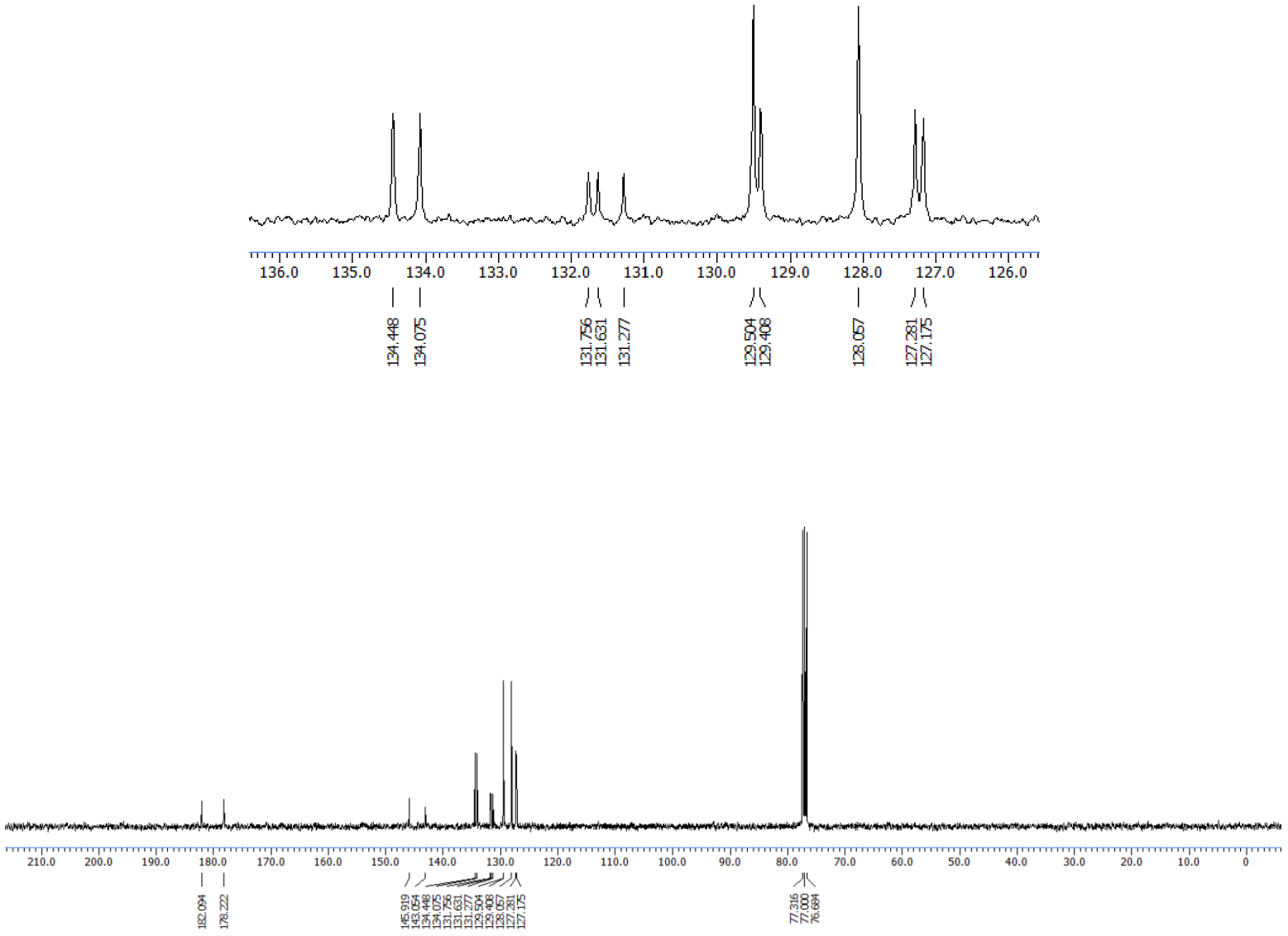




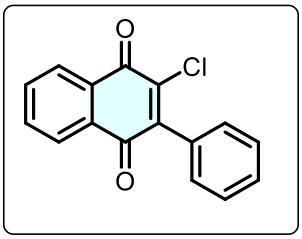
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



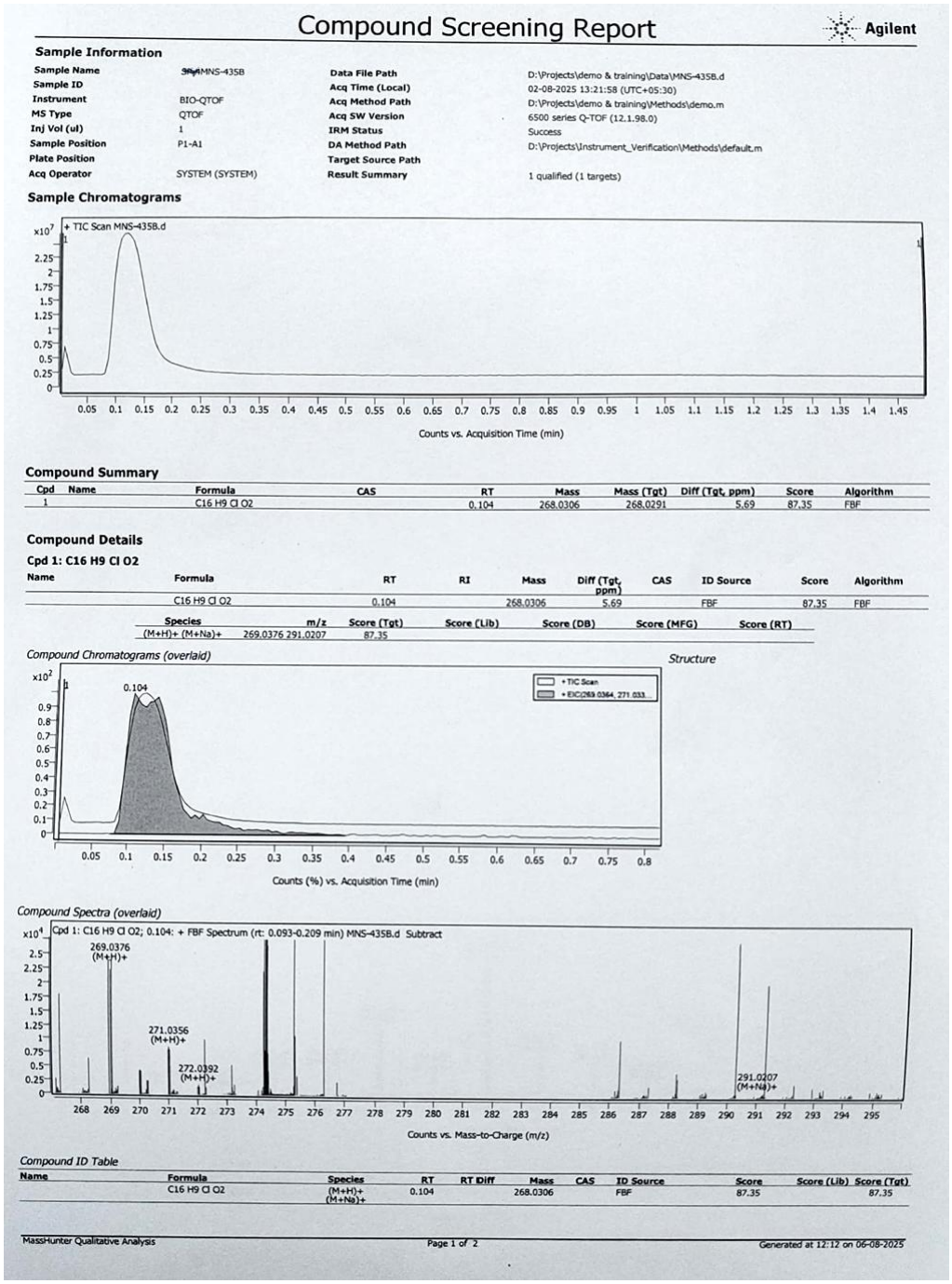
2-Chloro-3-phenylnaphthalene-1,4-dione (5a)



HRMS



2-Chloro-3-phenylnaphthalene-1,4-dione (5a)



Compound Screening Report

Agilent

Sample Information

Sample Name	MNS-435B	Data File Path	D:\Projects\demo & training\Data\MNS-435B.d
Sample ID		Acq Time (Local)	02-08-2025 13:21:58 (UTC+05:30)
Instrument	BIO-QTOF	Acq Method Path	D:\Projects\demo & training\Methods\demo.m
MS Type	QTOF	Acq SW Version	6500 series Q-TOF (12.1.98.0)
Inj Vol (ul)	1	IRM Status	Success
Sample Position	P1-A1	DA Method Path	D:\Projects\Instrument_Verification\Methods\default.m
Plate Position		Target Source Path	
Acq Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Chromatograms

+ TIC Scan MNS-435B.d

Counts vs. Acquisition Time (min)

Compound Summary

Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
1		C16 H9 Cl O2		0.104	268.0306	268.0291	5.69	87.35	FBF

Compound Details

Cpd 1: C16 H9 Cl O2

Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C16 H9 Cl O2	0.104		268.0306	5.69		FBF	87.35	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	269.0376 291.0207	87.35				

Compound Chromatograms (overlaid)

Structure

+ TIC Scan
+ EIC(269.0364, 271.033...

Counts (%) vs. Acquisition Time (min)

Compound Spectra (overlaid)

Cpd 1: C16 H9 Cl O2; 0.104: + FBF Spectrum (rt: 0.093-0.209 min) MNS-435B.d Subtract

269.0376 (M+H)+
271.0356 (M+H)+
272.0392 (M+H)+
291.0207 (M+Na)+

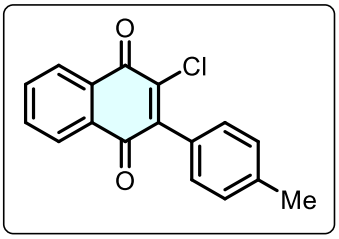
Counts vs. Mass-to-Charge (m/z)

Compound ID Table

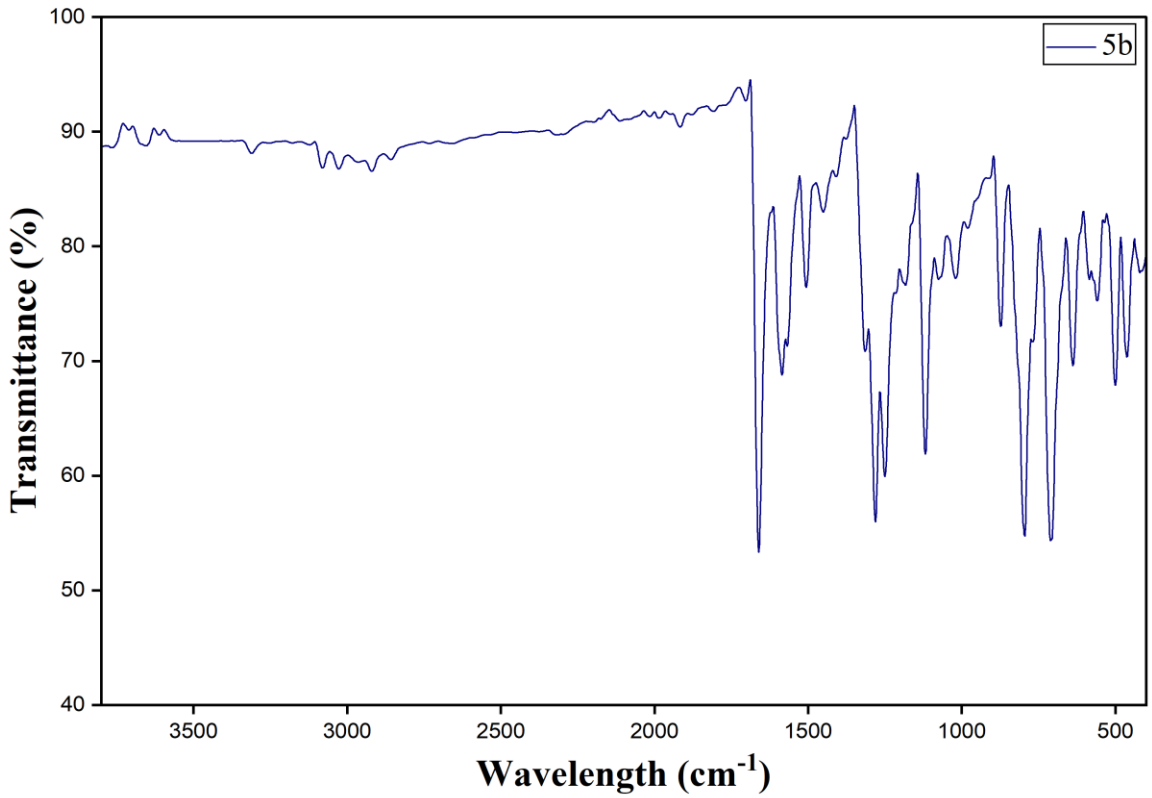
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C16 H9 Cl O2	(M+H)+ (M+Na)+	0.104		268.0306		FBF	87.35		87.35

MassHunter Qualitative Analysis — Page 1 of 2 — Generated at 12:12 on 06-08-2025

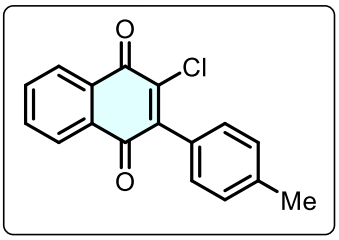
IR Spectra



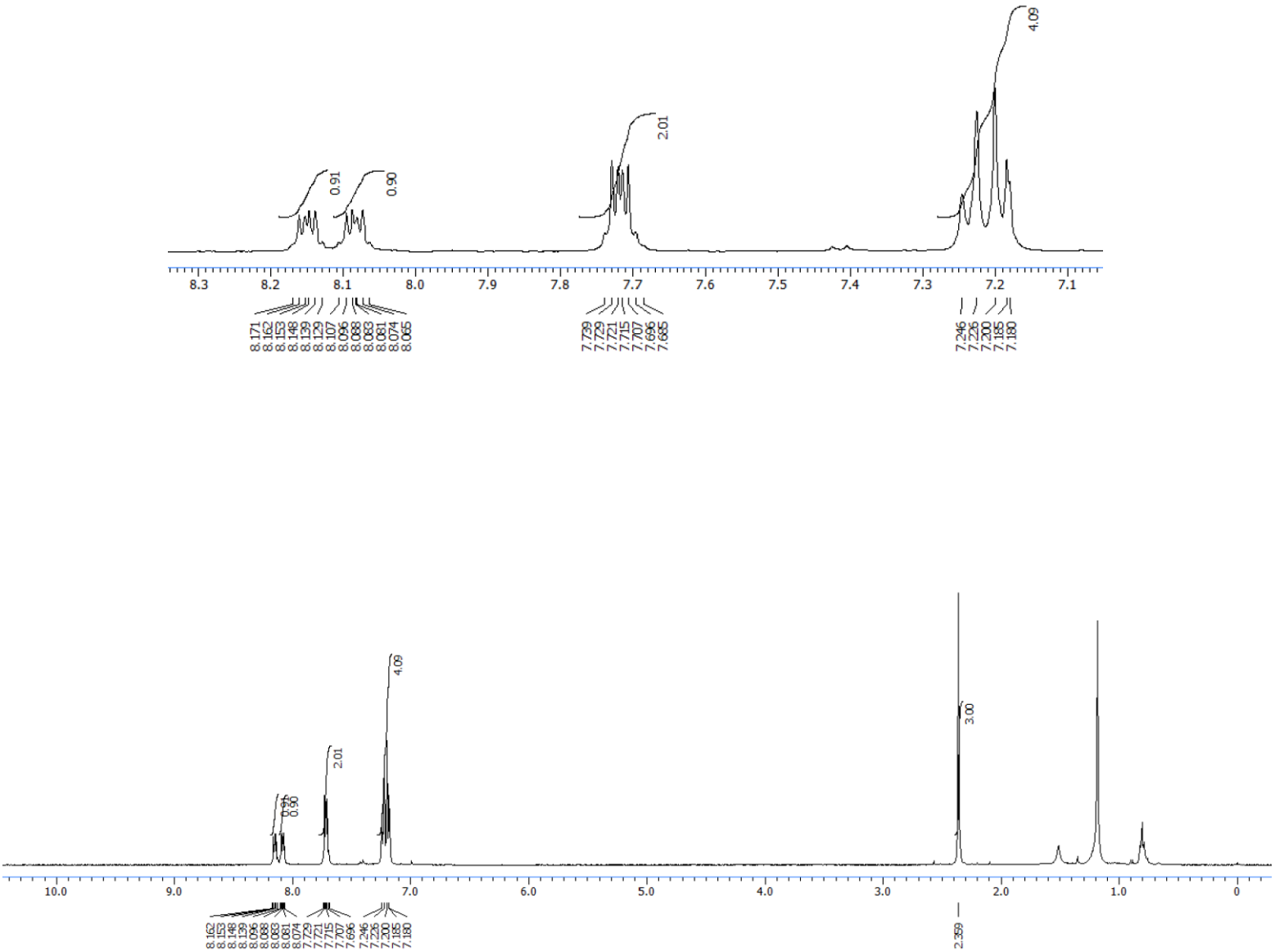
2-chloro-3-(p-tolyl)naphthalene-1,4-dione (5b).



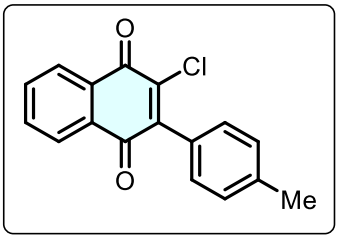
^{1}H NMR (400 MHz, $CDCl_3$)



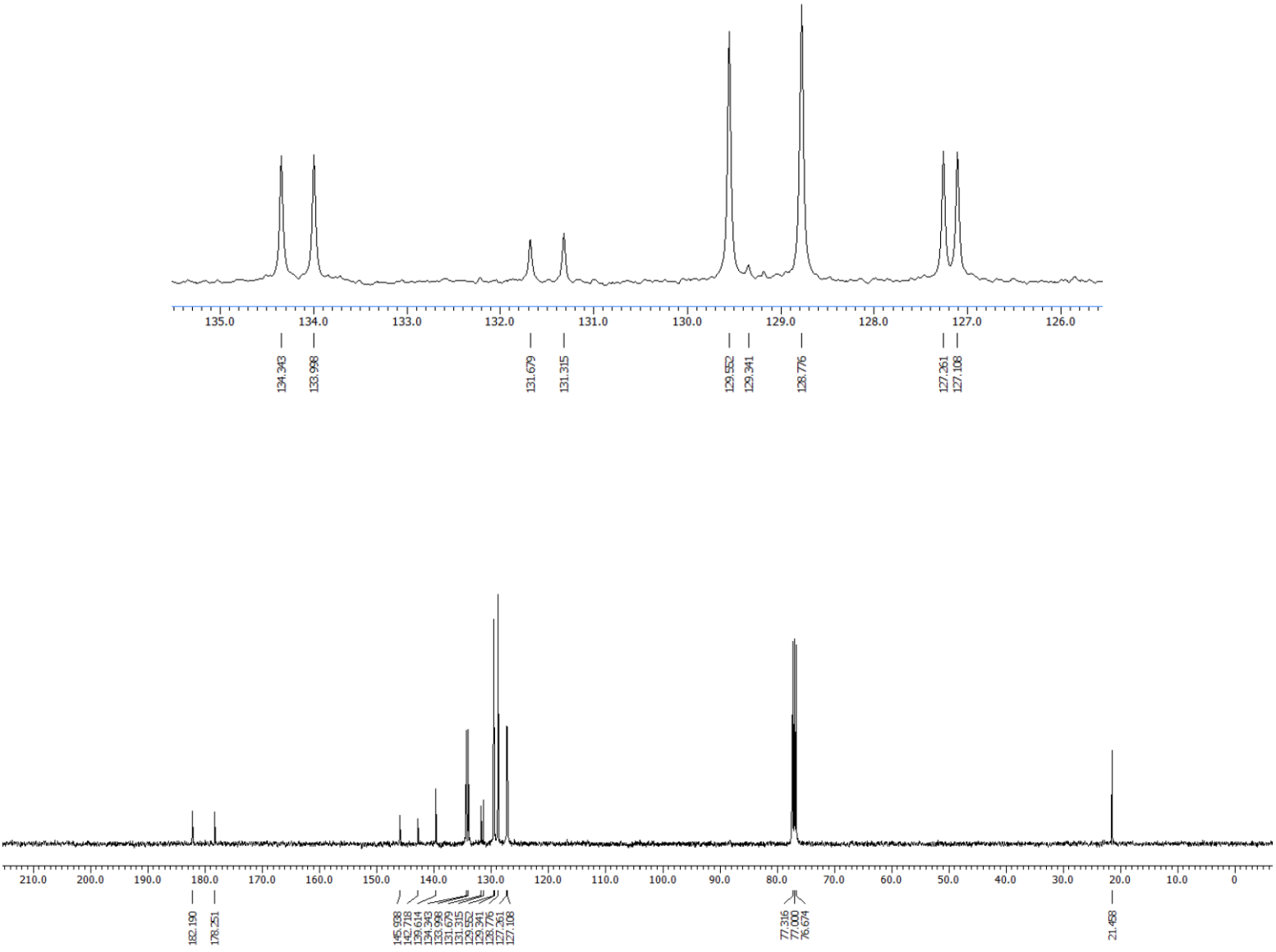
2-chloro-3-(p-tolyl)naphthalene-1,4-dione (5b).



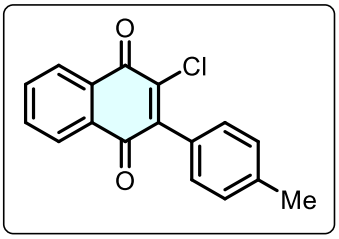
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-chloro-3-(p-tolyl)naphthalene-1,4-dione (5b).



HRMS



2-chloro-3-(p-tolyl)naphthalene-1,4-dione (5b).

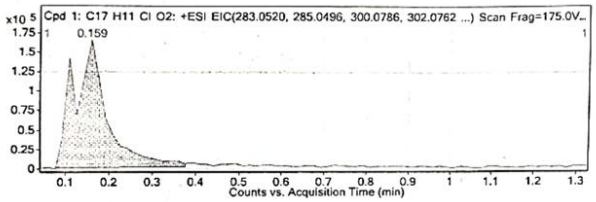
Qualitative Compound Report

Data File	MNS-398.d	**Sample Name**	MNS-398
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	20-05-2025 13:06:17
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

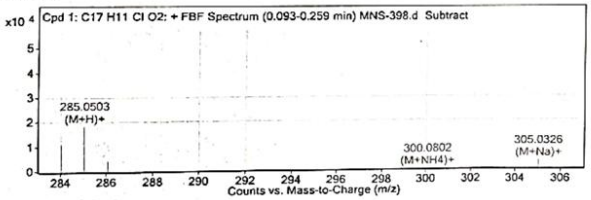
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H11 Cl O2	0.159	282.0453	50150	C17 H11 Cl O2	282.0448	1.82	C17 H11 Cl O2	C17 H11 Cl O2

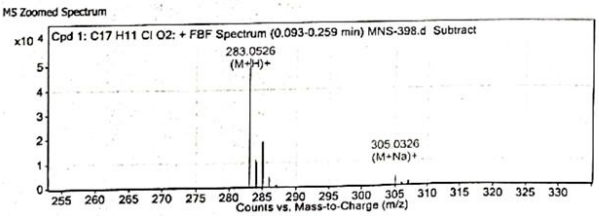
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C17 H11 Cl O2	283.0526	0.159	Find By Formula	282.0453



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
283.0526	1	50149.84	C17H12ClO2	(M+H)+
284.0565	1	11052.92	C17H12ClO2	(M+H)+
285.0503	1	18559.03	C17H12ClO2	(M+H)+
286.0526	1	3790.17	C17H12ClO2	(M+H)+
287.0621	1	501.44	C17H12ClO2	(M+H)+
300.0802	1	130.44	C17H15ClNO2	(M+NH4)+
305.0326	1	3377.94	C17H11ClNaO2	(M+Na)+
306.0315	1	901.04	C17H11ClNaO2	(M+Na)+
307.0333	1	1012.36	C17H11ClNaO2	(M+Na)+

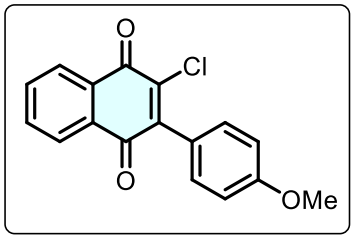
--- End Of Report ---

Agilent Technologies

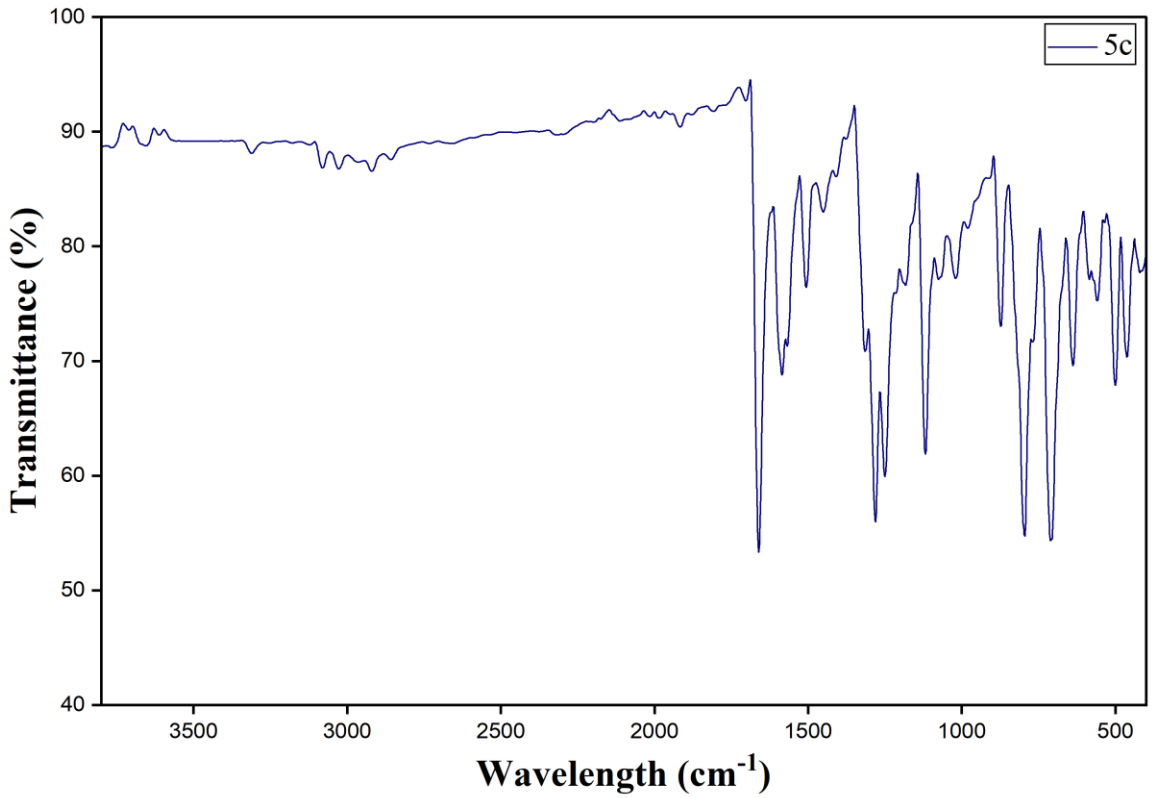
Page 1 of 1

Printed at: 10:54 on:21-05-2025

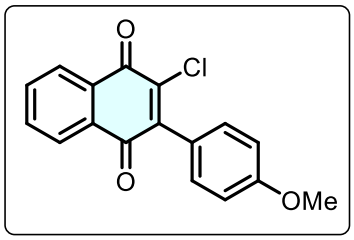
IR Spectra



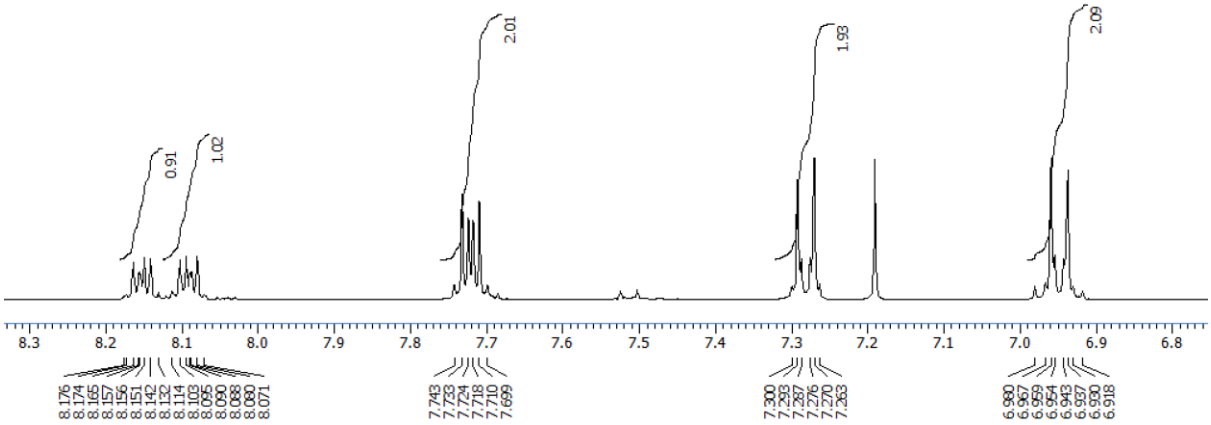
2-chloro-3-(4-methoxyphenyl)naphthalene-1,4-dione (5c).

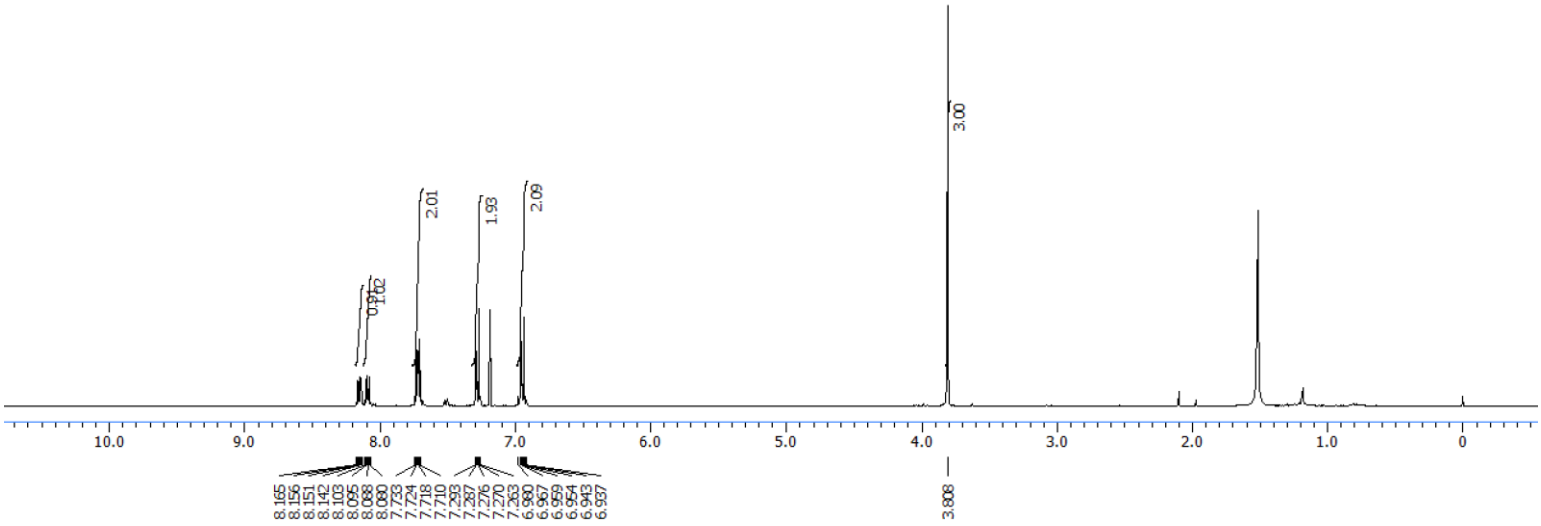


^{1}H NMR (400 MHz, $CDCl_3$)

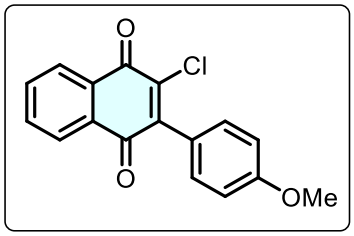


2-chloro-3-(4-methoxyphenyl)naphthalene-1,4-dione (5c).

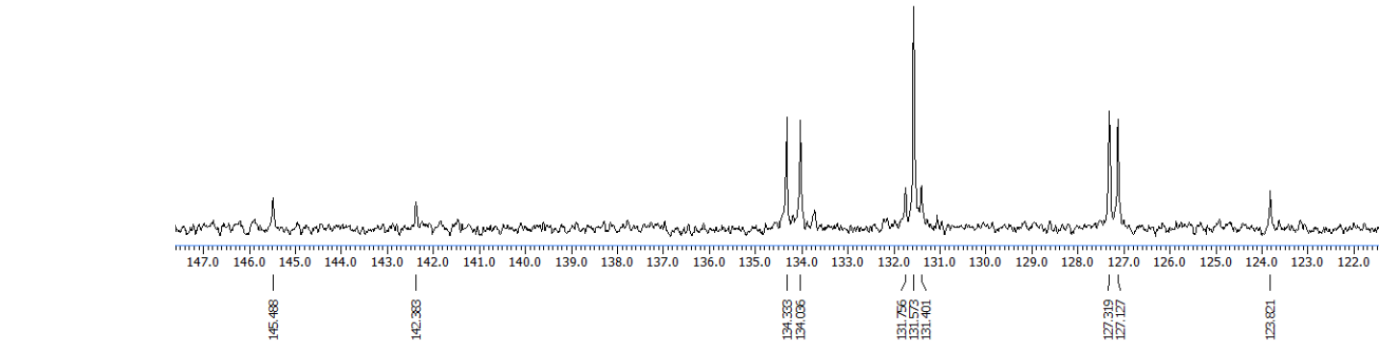


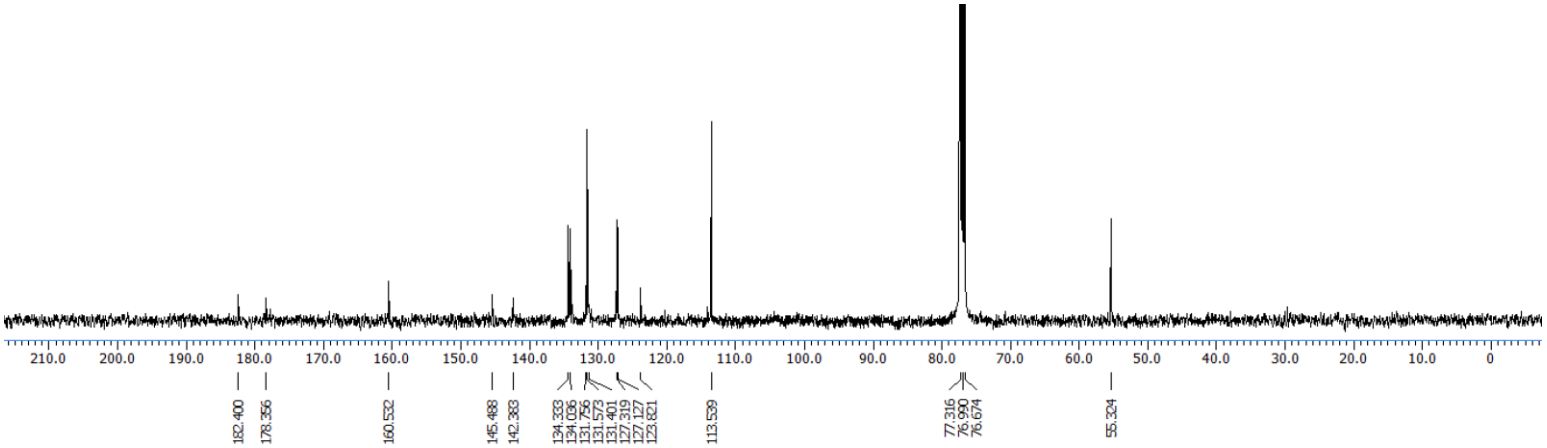


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

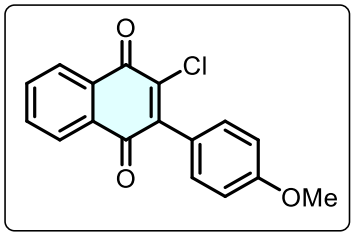


2-chloro-3-(4-methoxyphenyl)naphthalene-1,4-dione (5c).

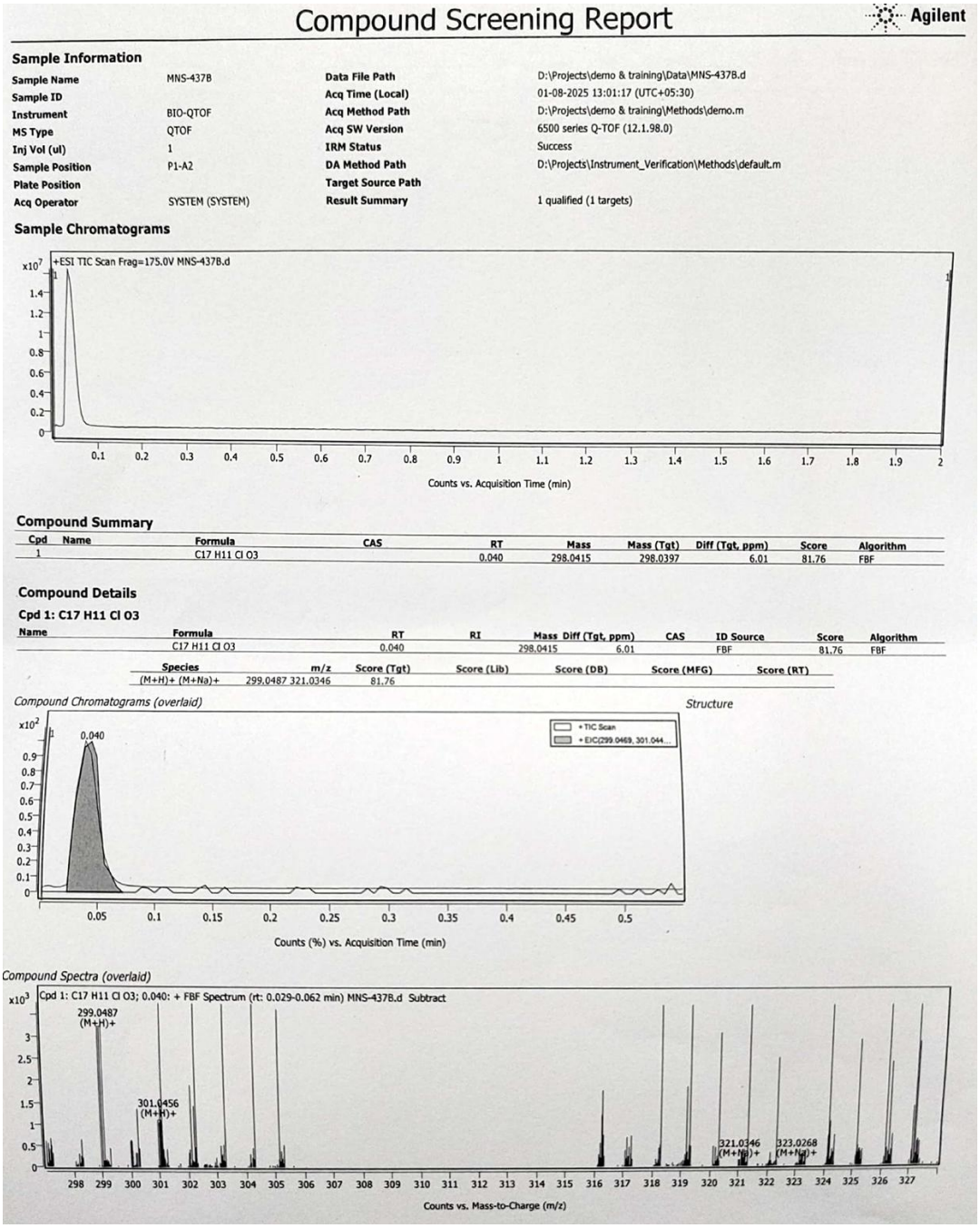




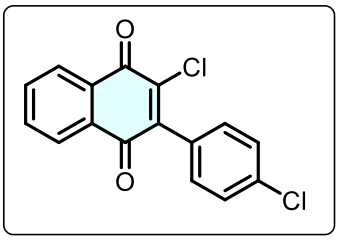
HRMS



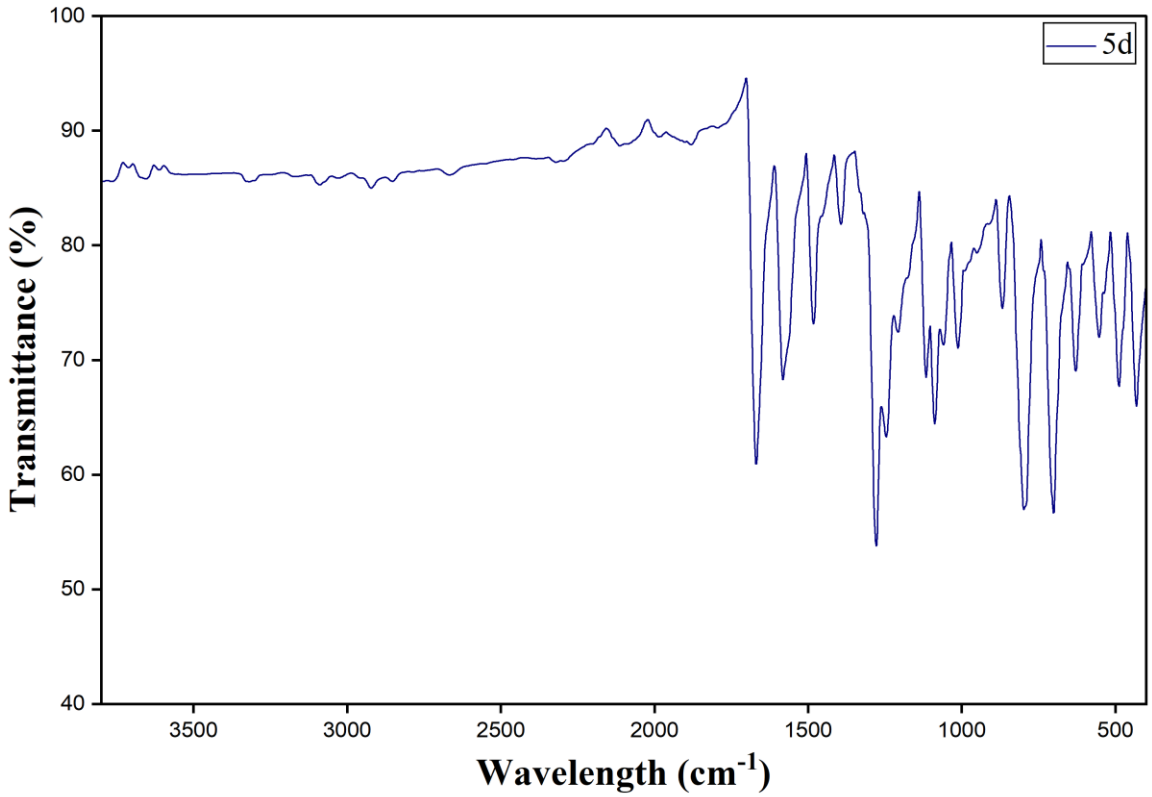
2-chloro-3-(4-methoxyphenyl)naphthalene-1,4-dione (5c).



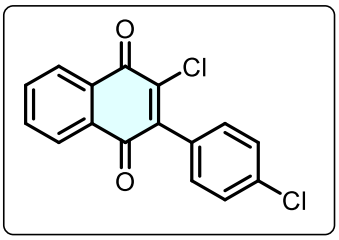
^{1}H NMR (400 MHz, $CDCl_3$)



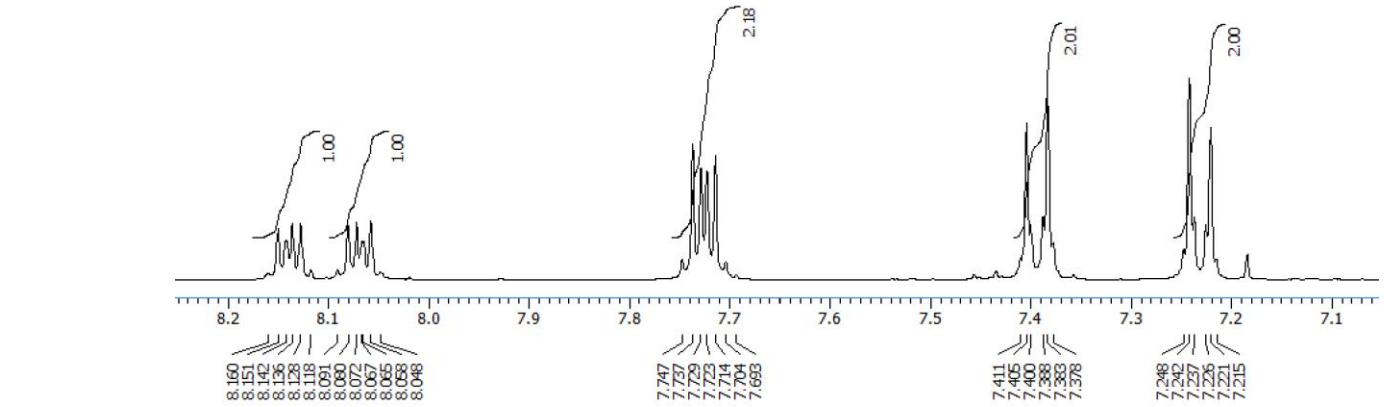
2-chloro-3-(4-chlorophenyl)naphthalene-1,4-dione (5d).

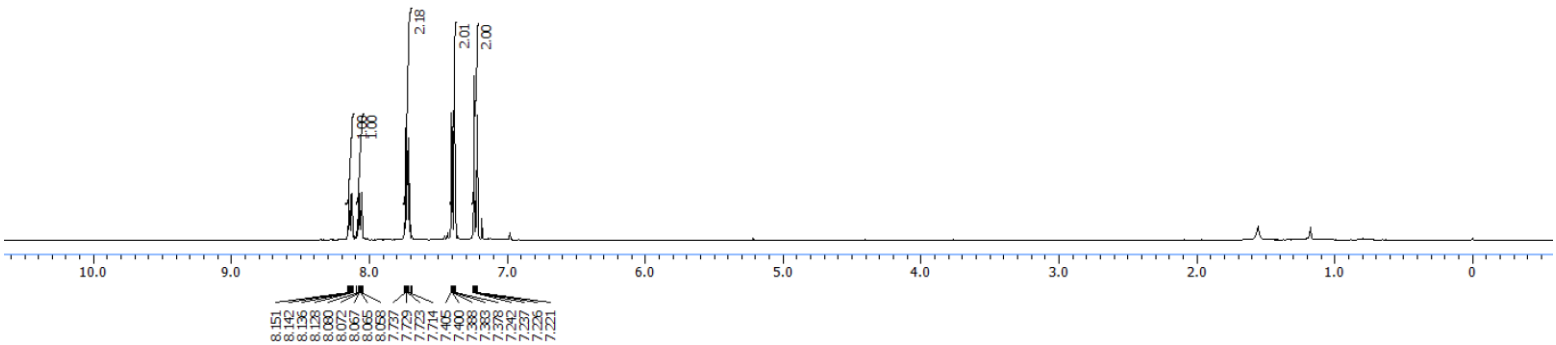


^{1}H NMR (400 MHz, $CDCl_3$)

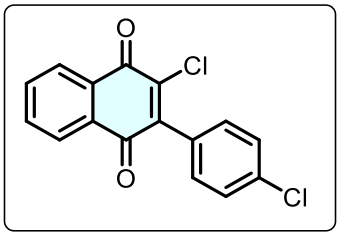


2-chloro-3-(4-chlorophenyl)naphthalene-1,4-dione (5d).

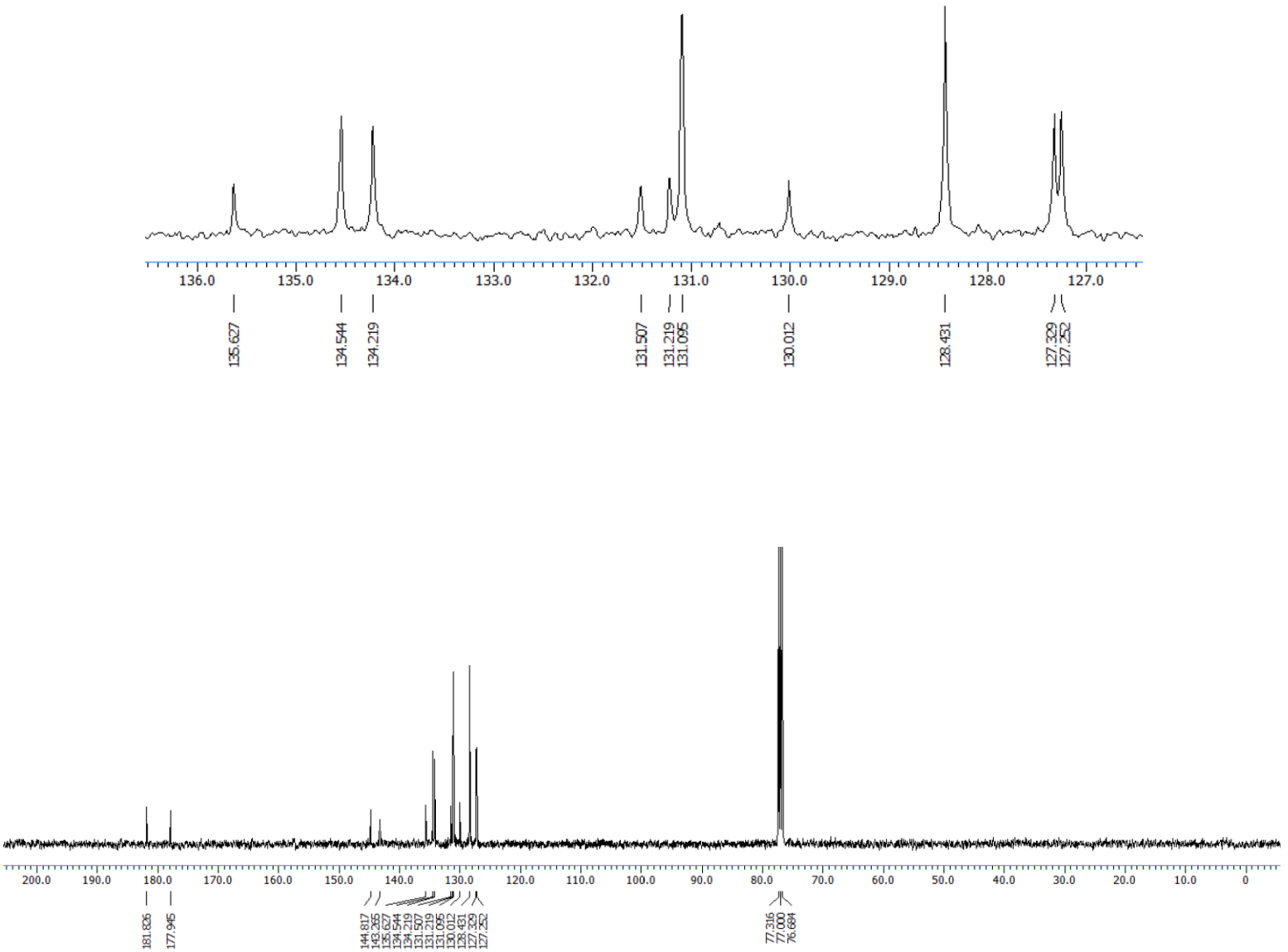




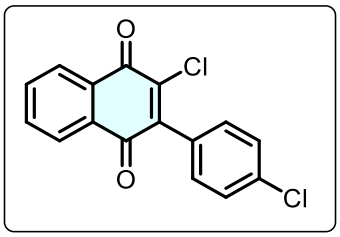
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



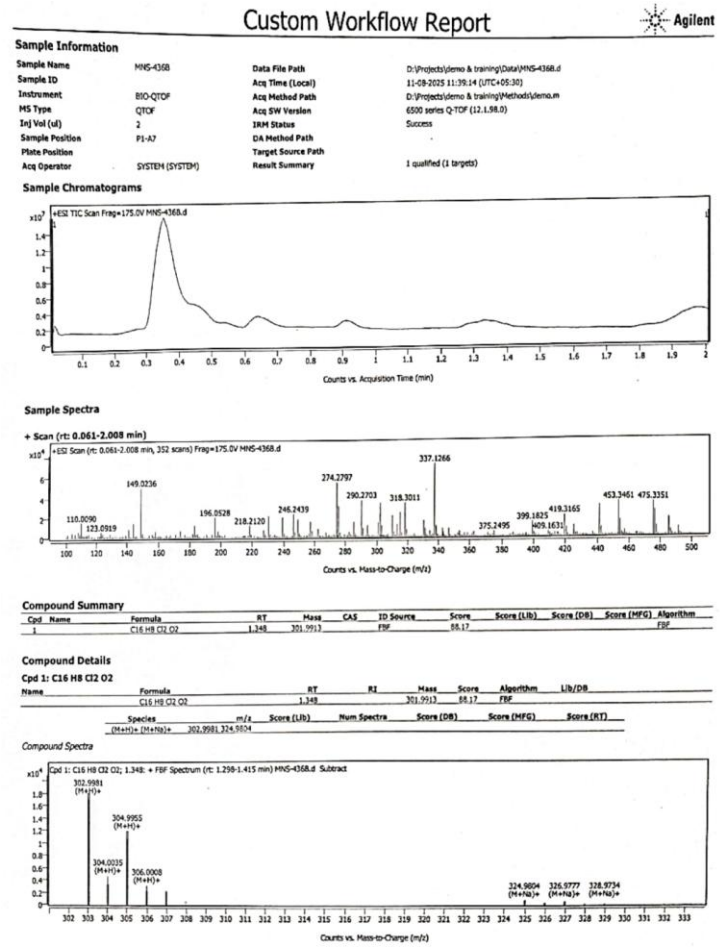
2-chloro-3-(4-chlorophenyl)naphthalene-1,4-dione (5d).

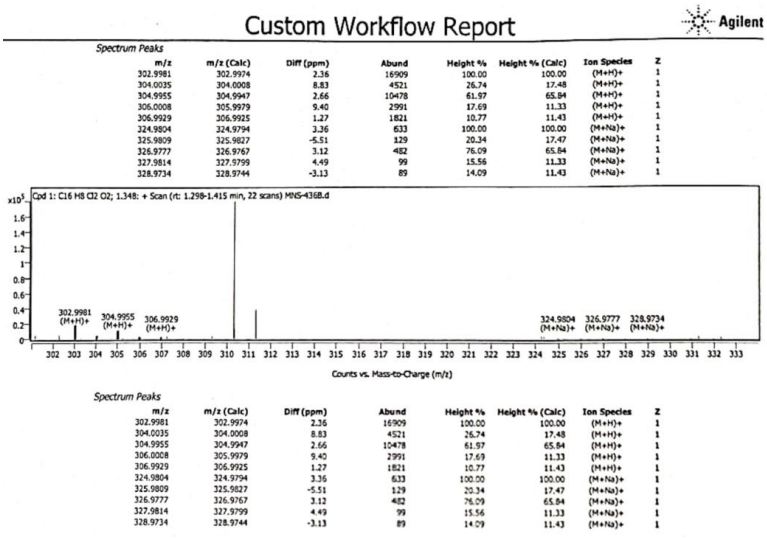


HRMS

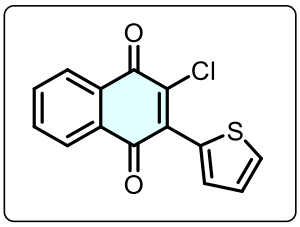


2-chloro-3-(4-chlorophenyl)naphthalene-1,4-dione (5d).

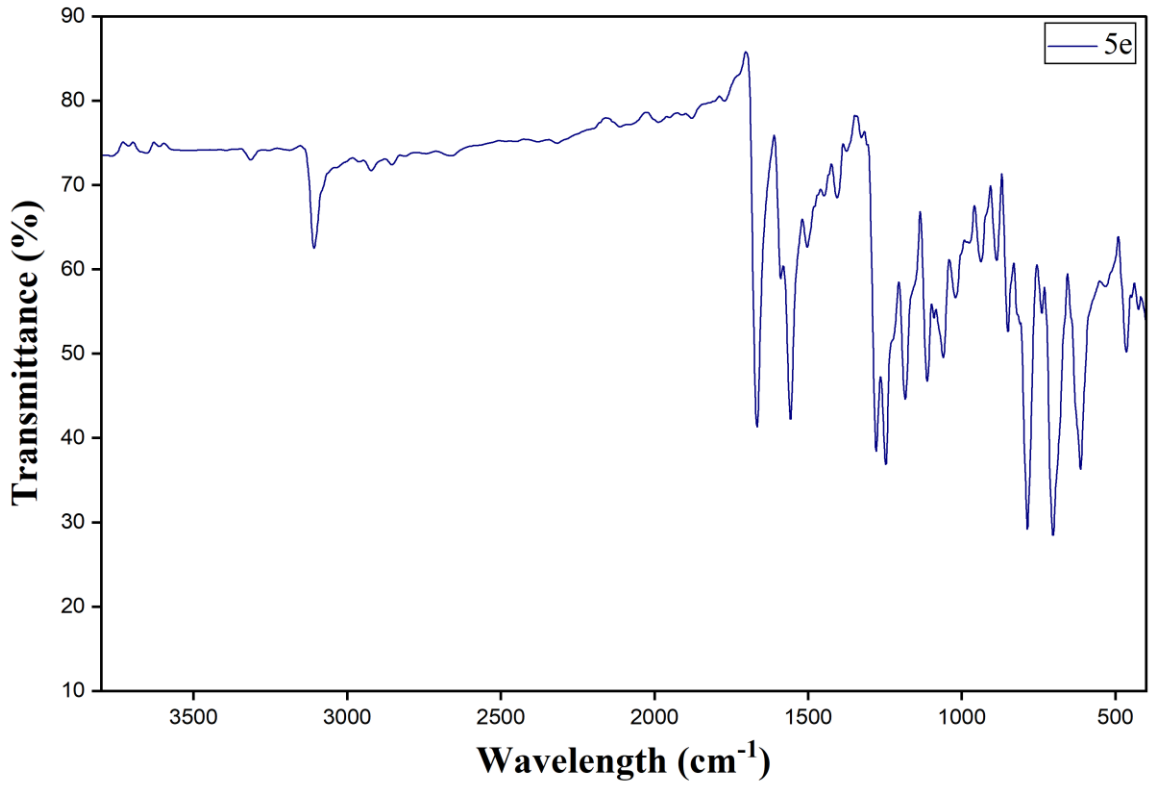




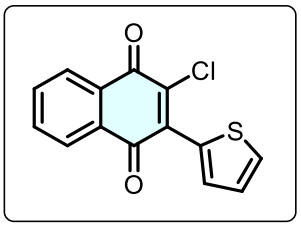
^{1}H NMR (400 MHz, $CDCl_3$)



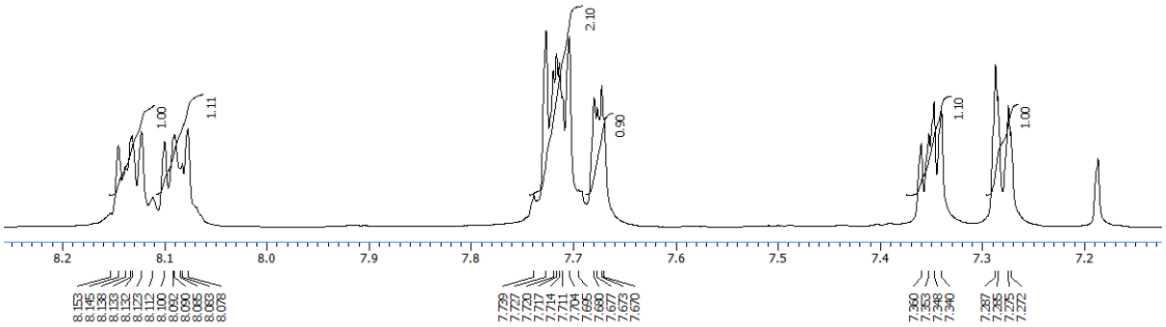
2-Chloro-3-(thiophen-2-yl)naphthalene-1,4-dione (5e).

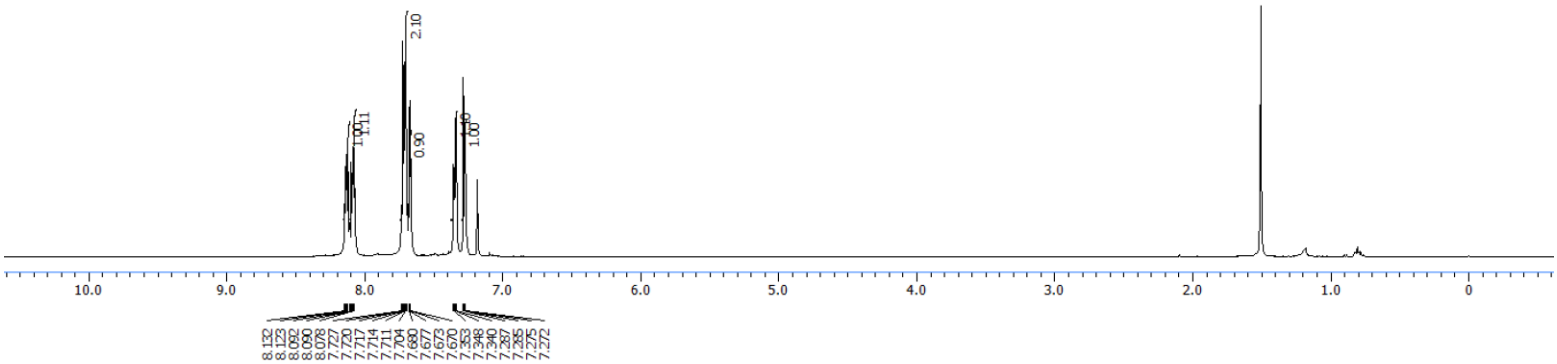


^{1}H NMR (400 MHz, $CDCl_3$)

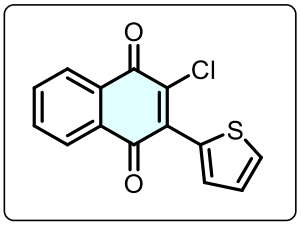


2-Chloro-3-(thiophen-2-yl)naphthalene-1,4-dione (5e).

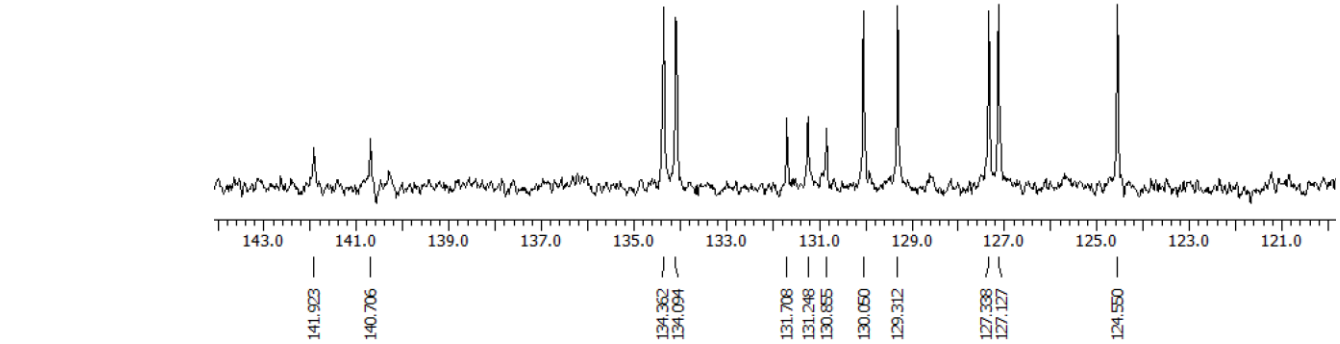


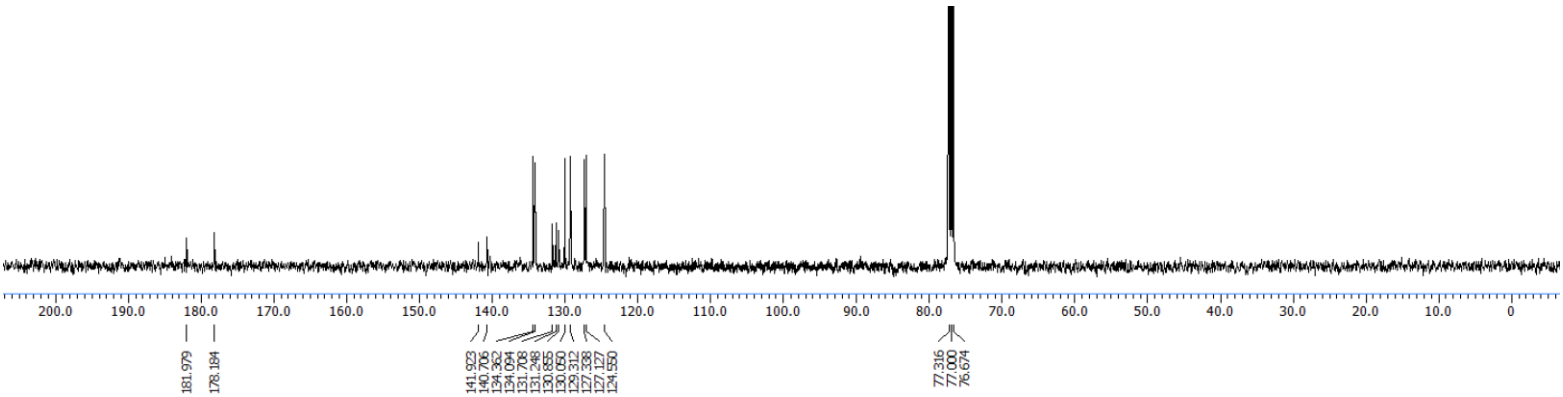


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

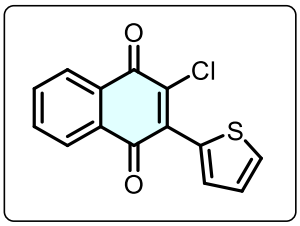


2-Chloro-3-(thiophen-2-yl)naphthalene-1,4-dione (5e).





HRMS



2-Chloro-3-(thiophen-2-yl)naphthalene-1,4-dione (5e).

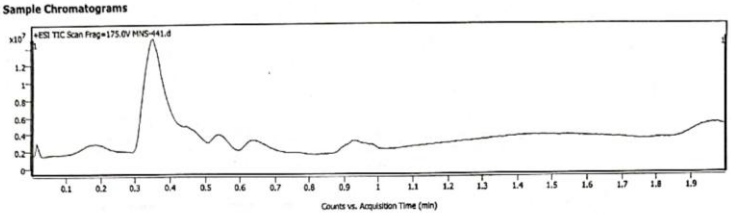
Custom Workflow Report

Agilent

Sample Information

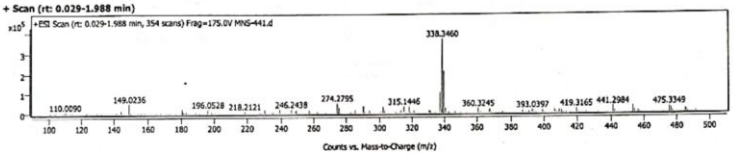
Sample Name	MNS-441	Data File Path	D:\Projects\demo & training\Data\MNS-441.d
Sample ID		Acq Time (Local)	11-08-2025 11:36:22 (UTC+05:30)
Instrument	80-QTOF	Acq Method Path	D:\Projects\demo & training\Methods\demo.m
MS Type	QTOF	Acq SW Version	6500 series Q-TOF (12.1.98.0)
Inj Vol (ul)	2	IRM Status	Success
Sample Position	P1-A6	DA Method Path	
Plate Position		Target Source Path	
Acq Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Chromatograms



Sample Spectra

+ Scan (rt: 0.029-1.988 min)



Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
1		C14 H7 Cl O2 S	0.950	273.9867		FBF	90.95				FBF

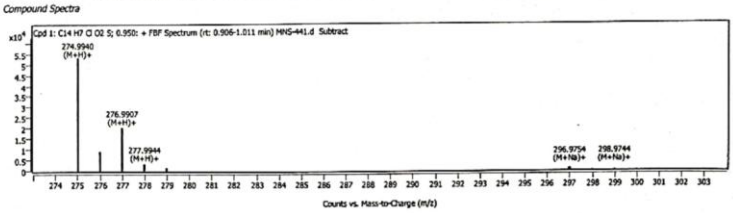
Compound Details

Cpd 1: C14 H7 Cl O2 S

Name	Formula	RT	RI	Mass	Score	Algorithm	Lib/DB
	C14 H7 Cl O2 S	0.950		273.9867	90.95	FBF	

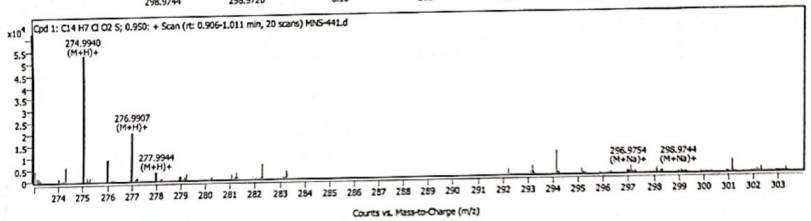
Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Score (MFG)	Score (RT)
(M+H)+ (M+Na)+	274.9940 296.9754					

Compound Spectra



Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Abund	Height %	Height % (Calc)	Ion Species	Z
274.9940	274.9928	4.44	53256	100.00	100.00	(M+H)+	1
275.9974	275.9960	5.12	7936	14.90	16.10	(M+H)+	1
276.9907	276.9901	2.33	16729	31.41	38.09	(M+H)+	1
277.9944	277.9931	4.78	2656	4.99	5.96	(M+H)+	1
278.9901	278.9886	5.61	970	1.82	2.04	(M+H)+	1
296.9754	296.9747	2.30	545	100.00	100.00	(M+Na)+	1
297.9812	297.9779	10.82	81	14.86	16.09	(M+Na)+	1
298.9744	298.9720	8.10	202	37.00	38.09	(M+Na)+	1



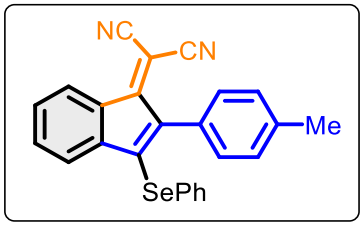
Spectrum Peaks

m/z	m/z (Calc)	Diff (ppm)	Abund	Height %	Height % (Calc)	Ion Species	Z
274.9940	274.9928	4.44	53256	100.00	100.00	(M+H)+	1
275.9974	275.9960	5.12	7936	14.90	16.10	(M+H)+	1
276.9907	276.9901	2.33	16729	31.41	38.09	(M+H)+	1
277.9944	277.9931	4.78	2656	4.99	5.96	(M+H)+	1
278.9901	278.9886	5.61	970	1.82	2.04	(M+H)+	1
296.9754	296.9747	2.30	545	100.00	100.00	(M+Na)+	1
297.9812	297.9779	10.82	81	14.86	16.09	(M+Na)+	1
298.9744	298.9720	8.10	202	37.00	38.09	(M+Na)+	1

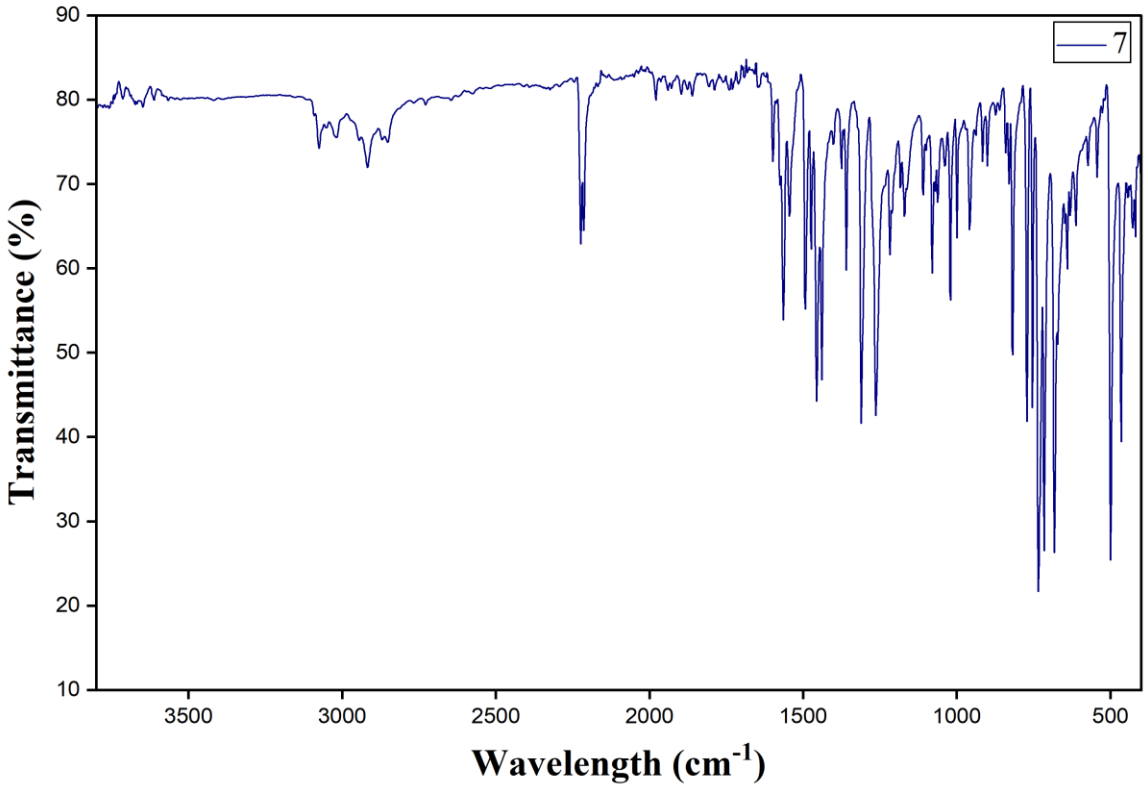
MassHunter Qual 12.0

(End of Report)

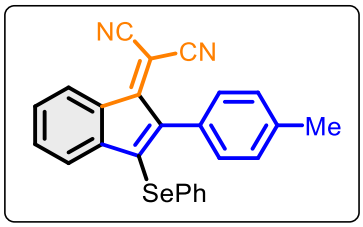
IR Spectra



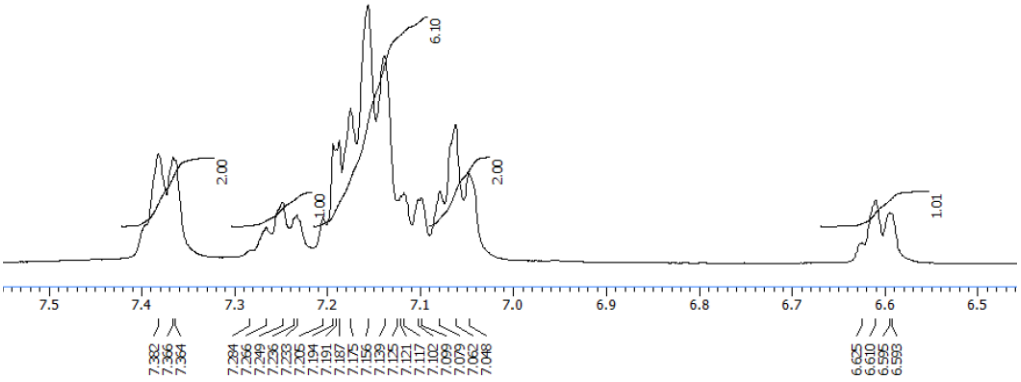
2-(3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-ylidene)malononitrile (7).

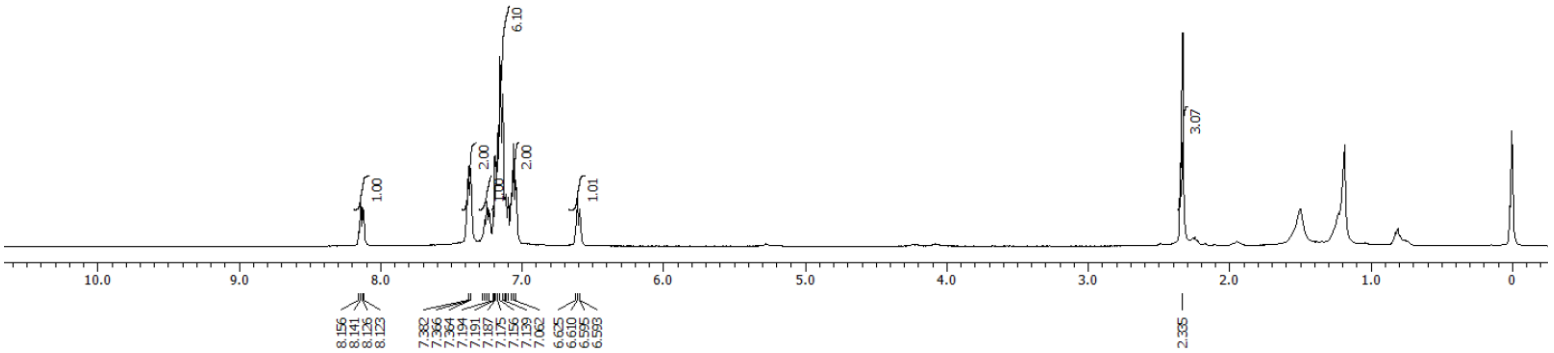


^{1}H NMR (400 MHz, $CDCl_3$)

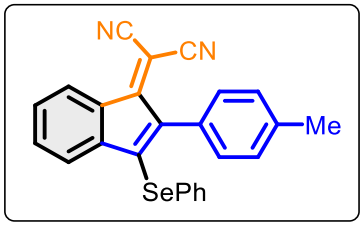


2-(3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-ylidene)malononitrile (7).

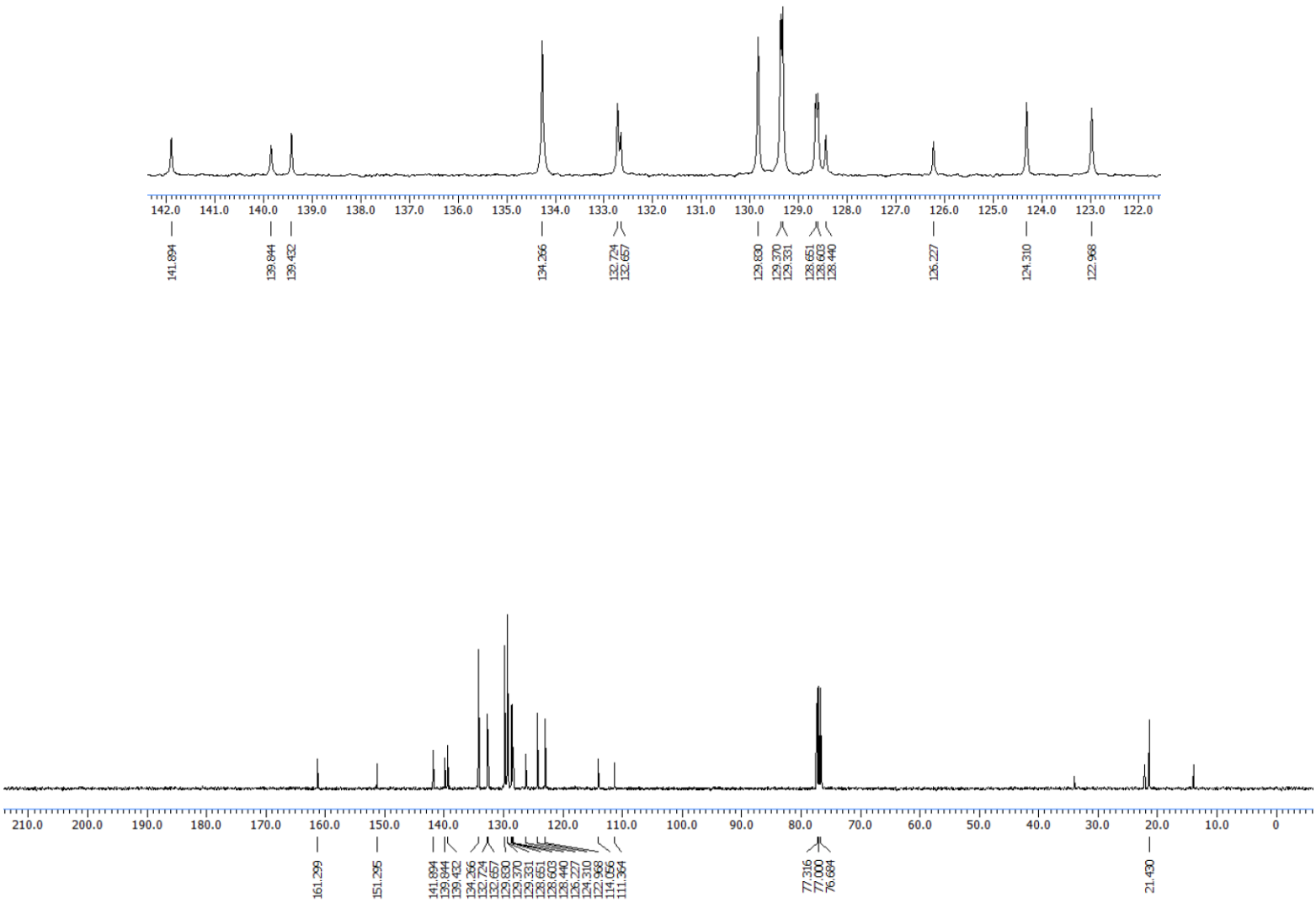




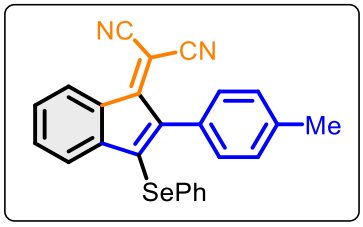
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



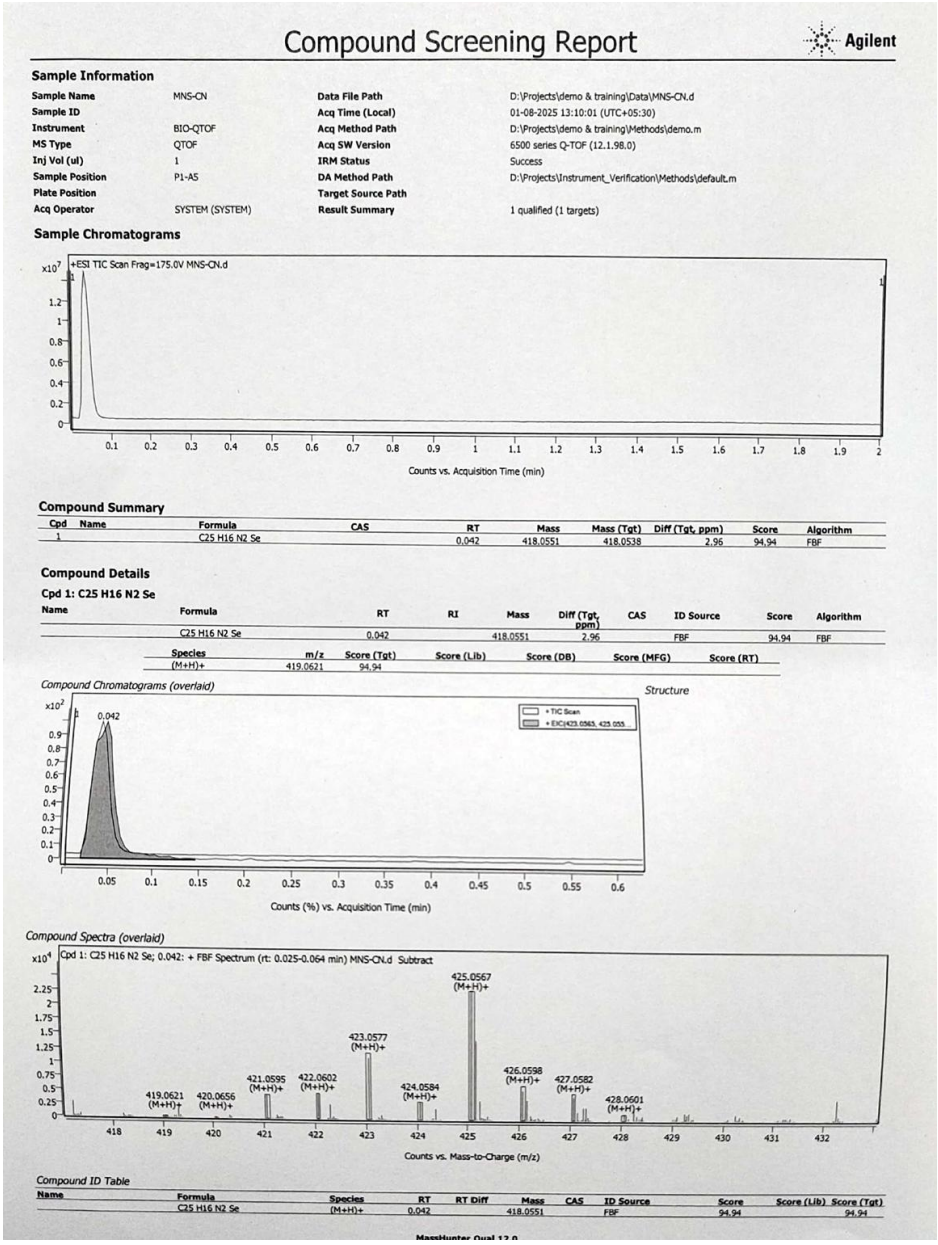
2-(3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-ylidene)malononitrile (7).



HRMS



2-(3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-ylidene)malononitrile (7).



Compound Screening Report

Agilent

Sample Information

Sample Name	MNS-CN	Data File Path	D:\Projects\demo & training\Data\MNS-CN.d
Sample ID		Acq Time (Local)	01-08-2025 13:10:01 (UTC+05:30)
Instrument	BIO-QTOF	Acq Method Path	D:\Projects\demo & training\Methods\demo.m
MS Type	QTOF	Acq SW Version	6500 series Q-TOF (12.1.98.0)
Inj Vol (ul)	1	IRM Status	Success
Sample Position	P1-A5	DA Method Path	D:\Projects\Instrument_Verification\Methods\default.m
Plate Position		Target Source Path	
Acq Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Chromatograms

+ESI TIC Scan Frag=175.0V MNS-CN.d

Counts vs. Acquisition Time (min)

Compound Summary

Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
1		C25 H16 N2 Se		0.042	418.0551	418.0538	2.96	94.94	FBF

Compound Details

Cpd 1: C25 H16 N2 Se

Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C25 H16 N2 Se	0.042		418.0551	2.96		FBF	94.94	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+H)+	419.0621	94.94				

Compound Chromatograms (overlaid)

Structure

Counts (%) vs. Acquisition Time (min)

Compound Spectra (overlaid)

Cpd 1: C25 H16 N2 Se; 0.042: + FBF Spectrum (rt: 0.025-0.064 min) MNS-CN.d Subtract

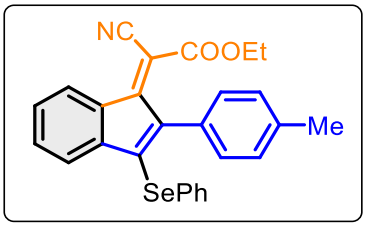
Counts vs. Mass-to-Charge (m/z)

Compound ID Table

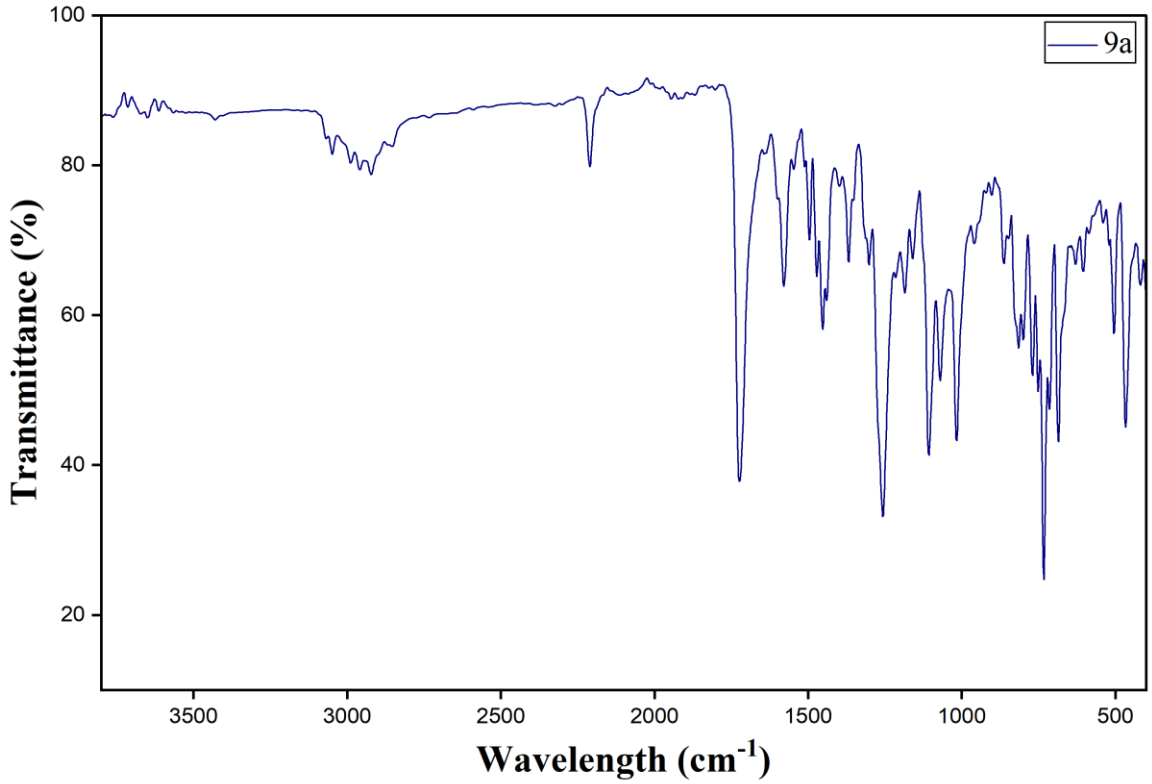
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C25 H16 N2 Se	(M+H)+	0.042		418.0551		FBF	94.94		94.94

MassHunter Qual 12.0

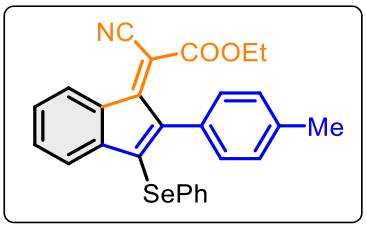
IR Spectra



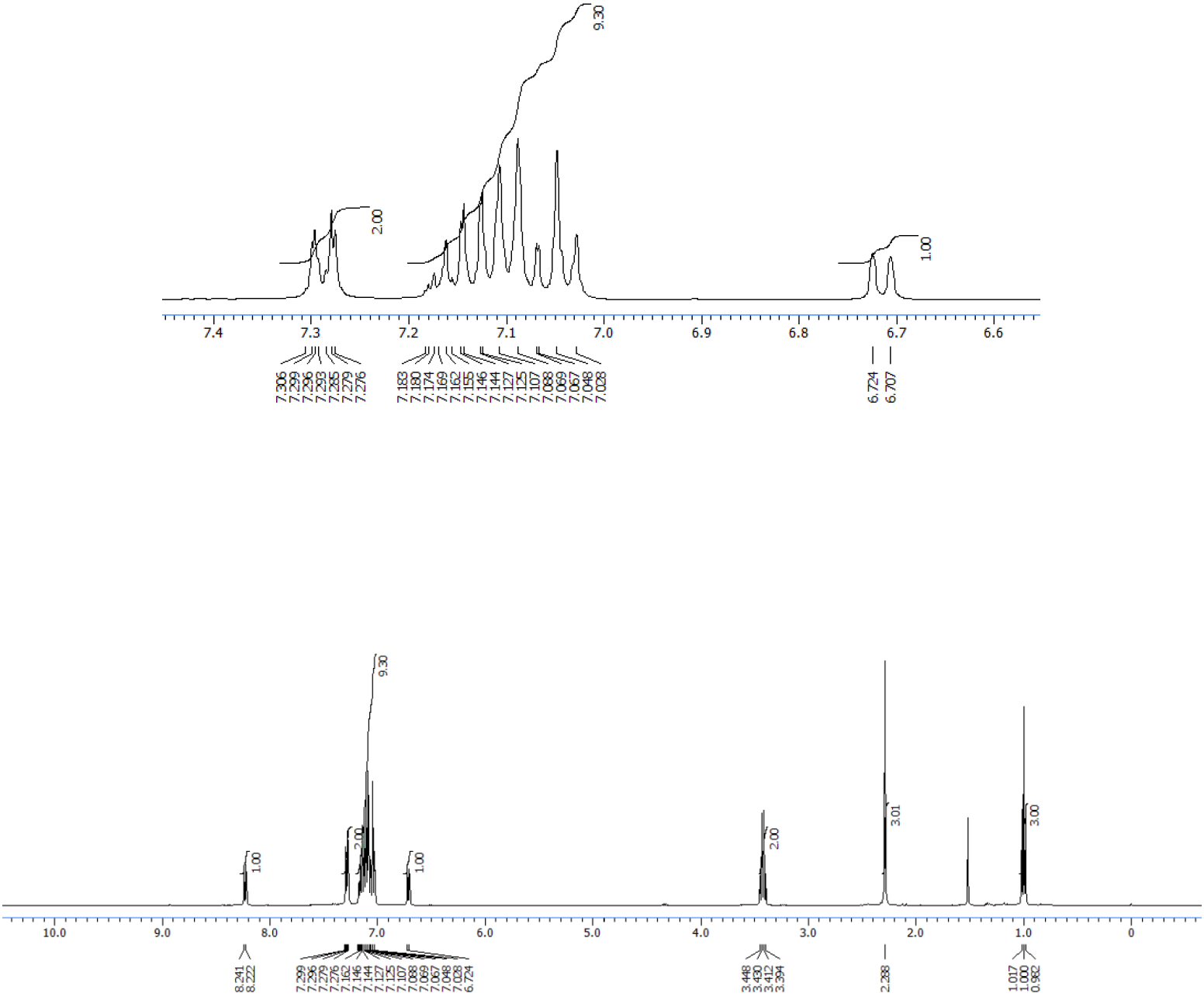
Ethyl (Z)-2-cyano-2-(3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-ylidene)acetate (9a).



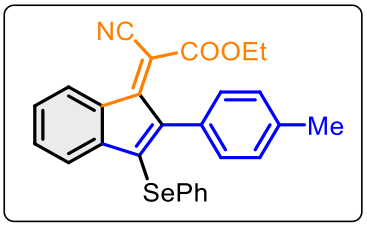
^{1}H NMR (400 MHz, $CDCl_3$)



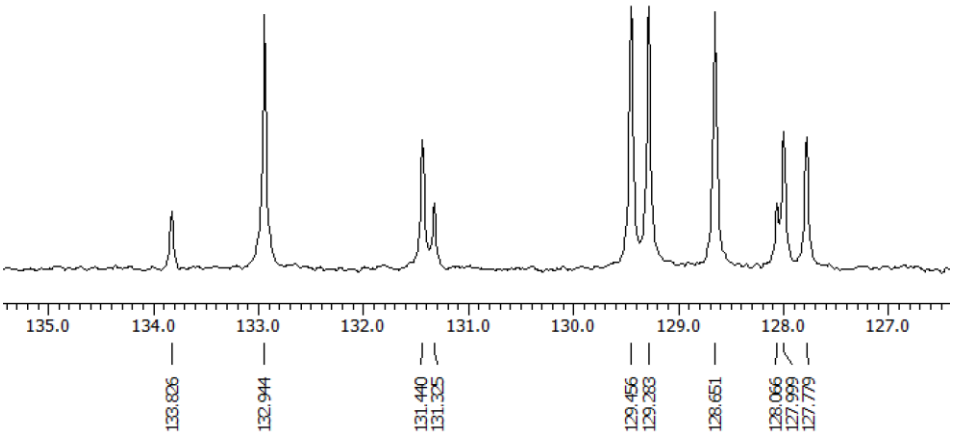
Ethyl (Z)-2-cyano-2-(3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-ylidene)acetate (9a).

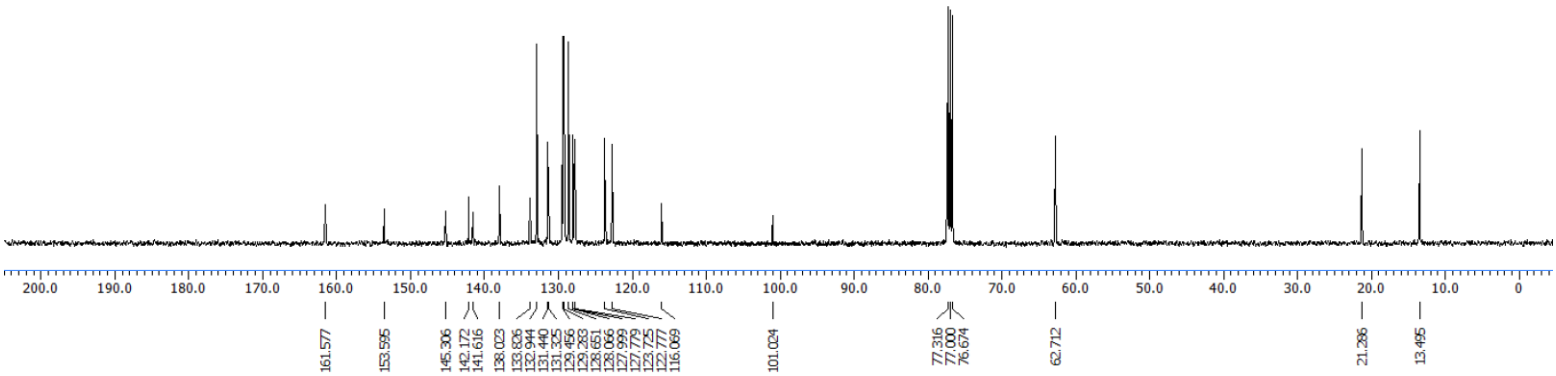


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

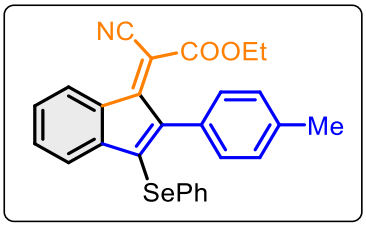


Ethyl (Z)-2-cyano-2-(3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-ylidene)acetate (9a).

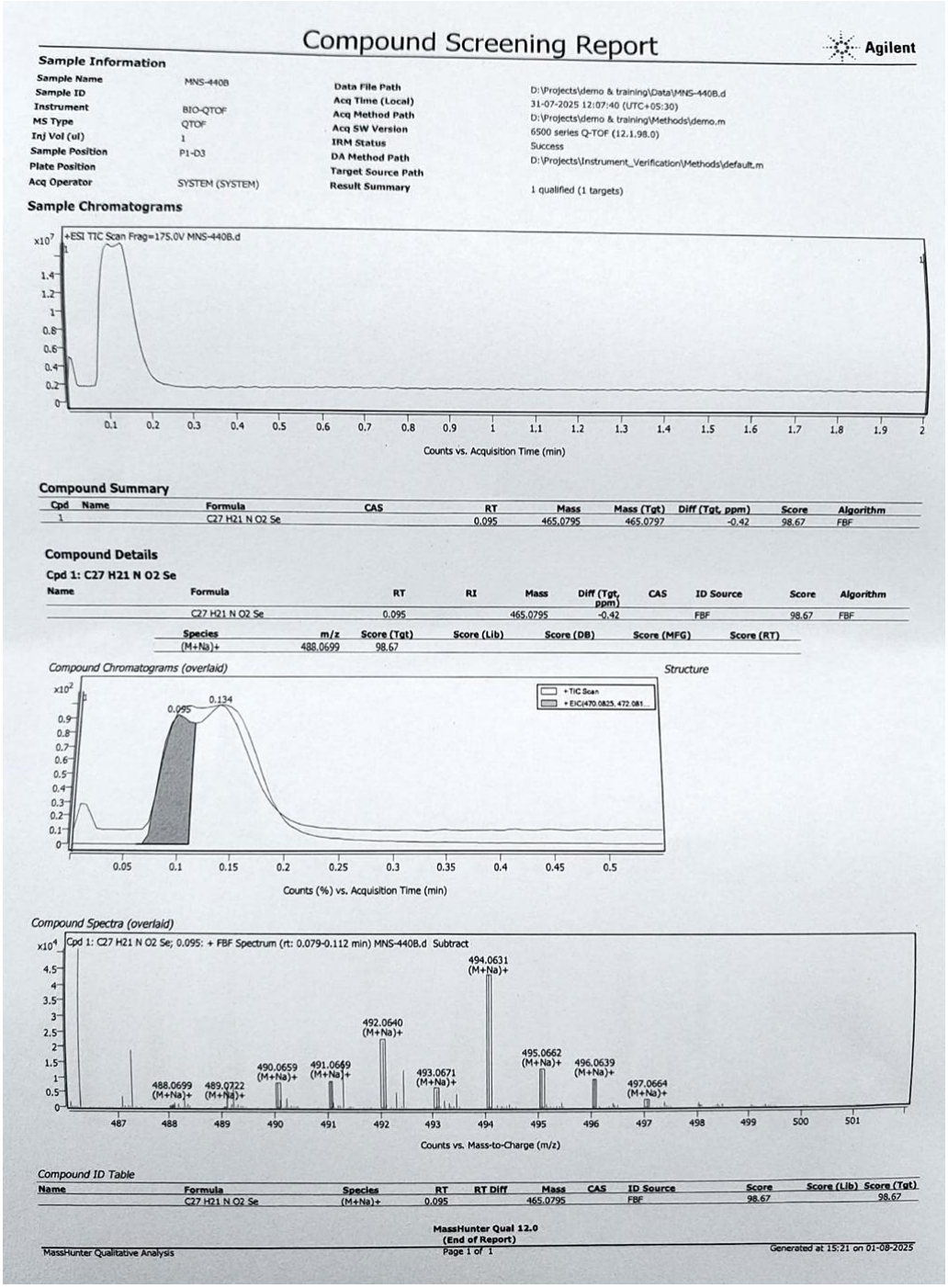




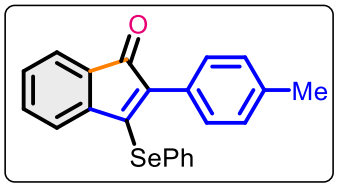
HRMS



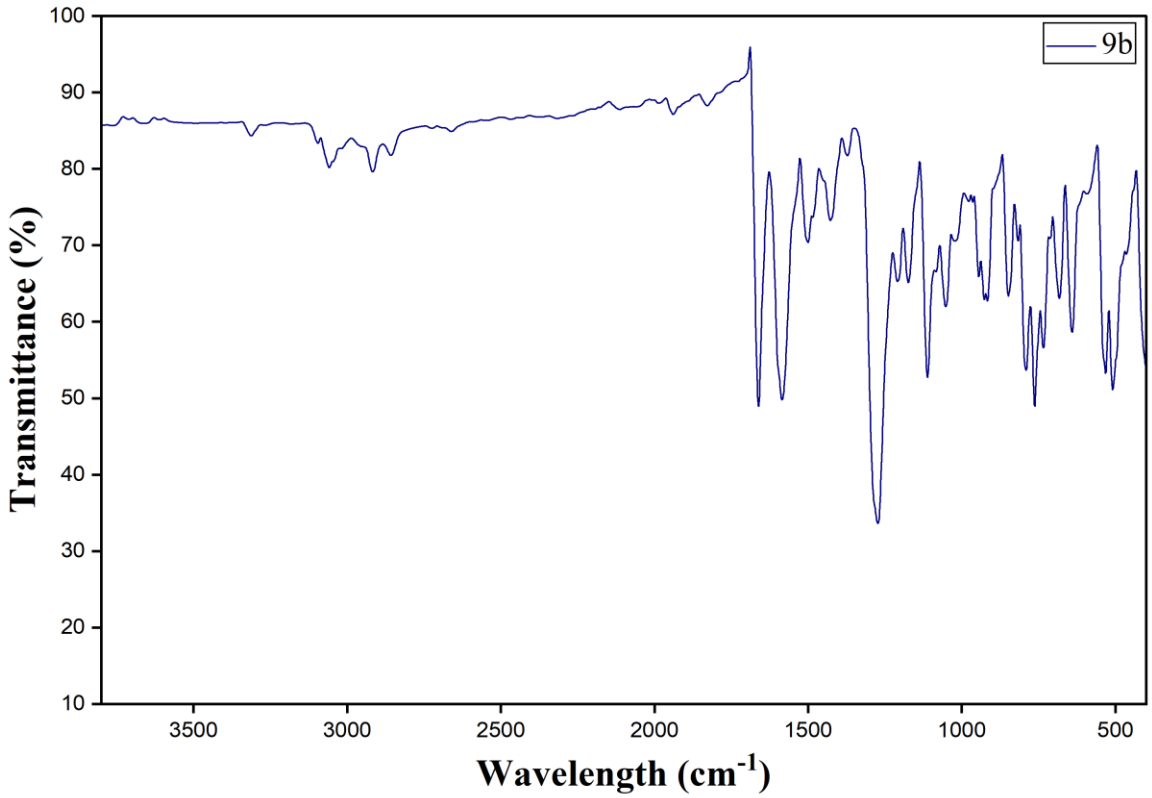
Ethyl (Z)-2-cyano-2-(3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-ylidene)acetate (9a).



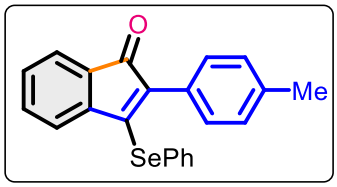
IR Spectra



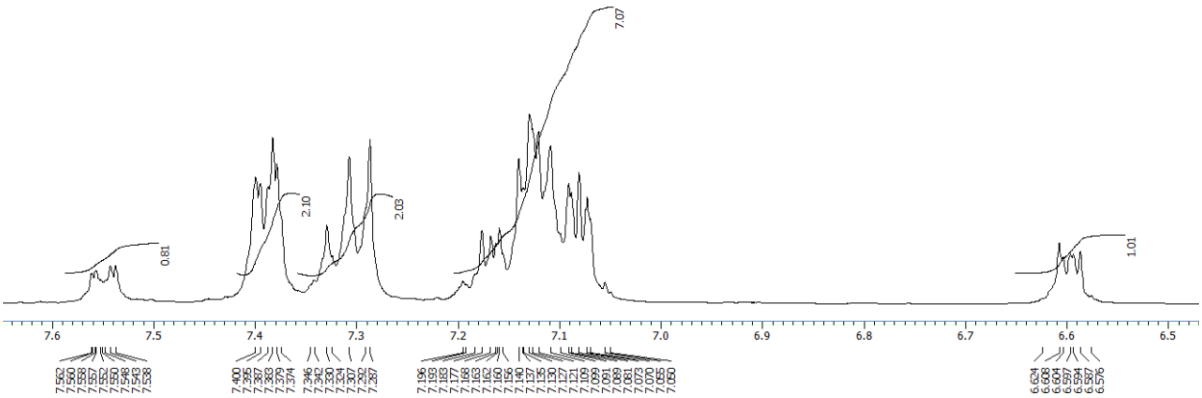
3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-one (9b).

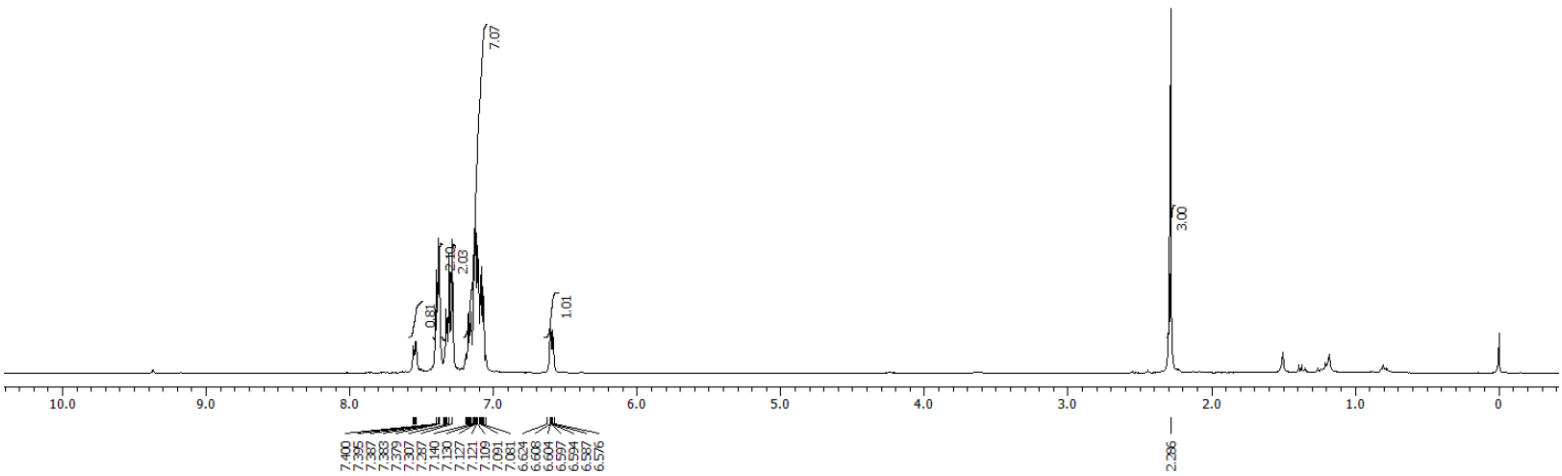


^{1}H NMR (400 MHz, $CDCl_3$)

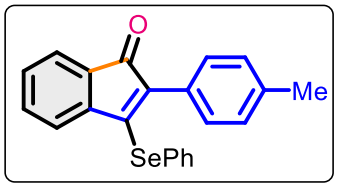


3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-one (9b).

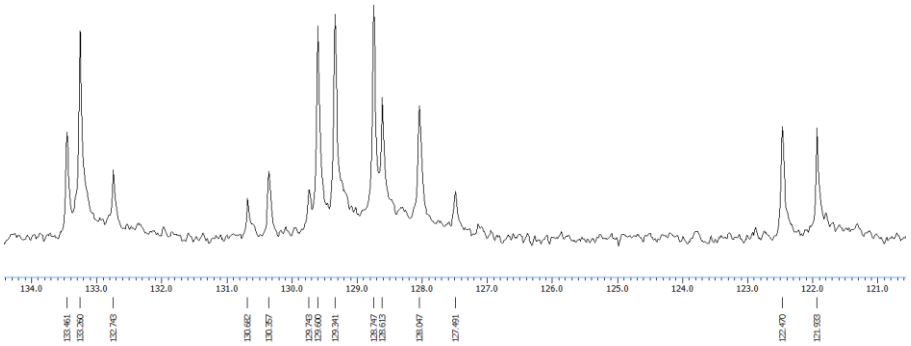


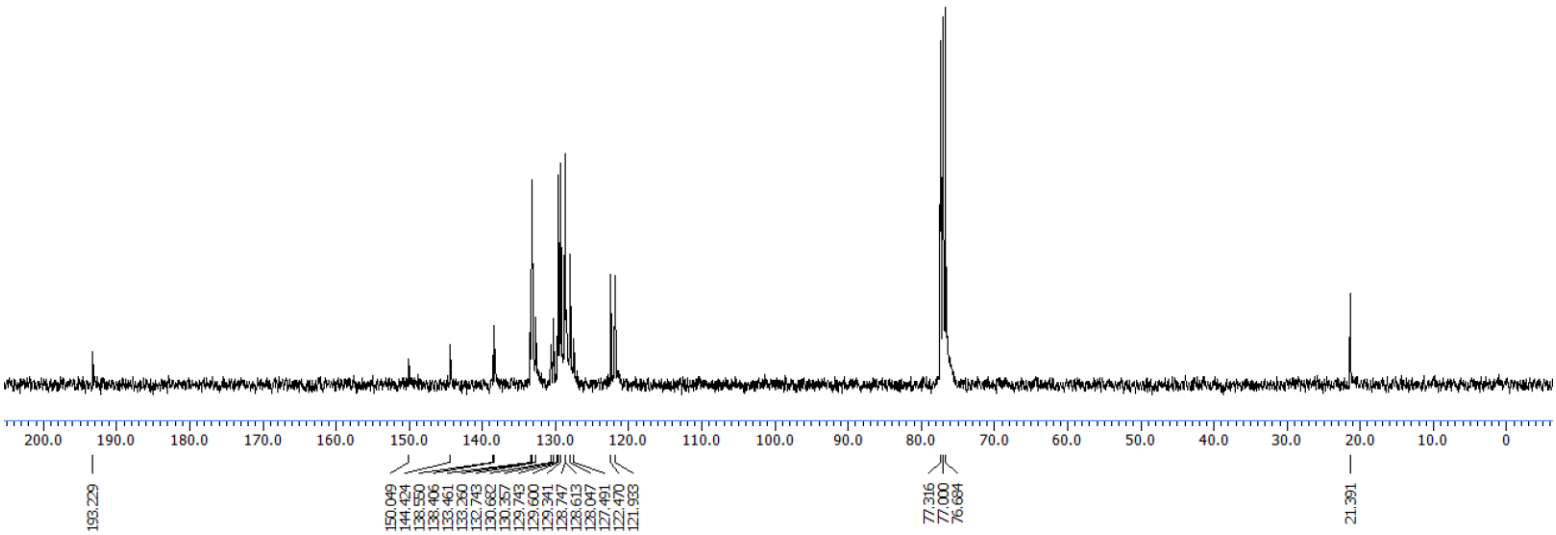


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

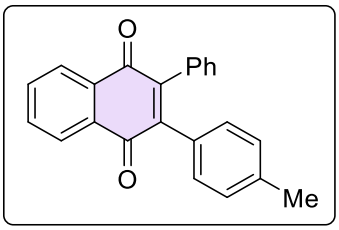


3-(phenylselanyl)-2-(p-tolyl)-1H-inden-1-one (9b).

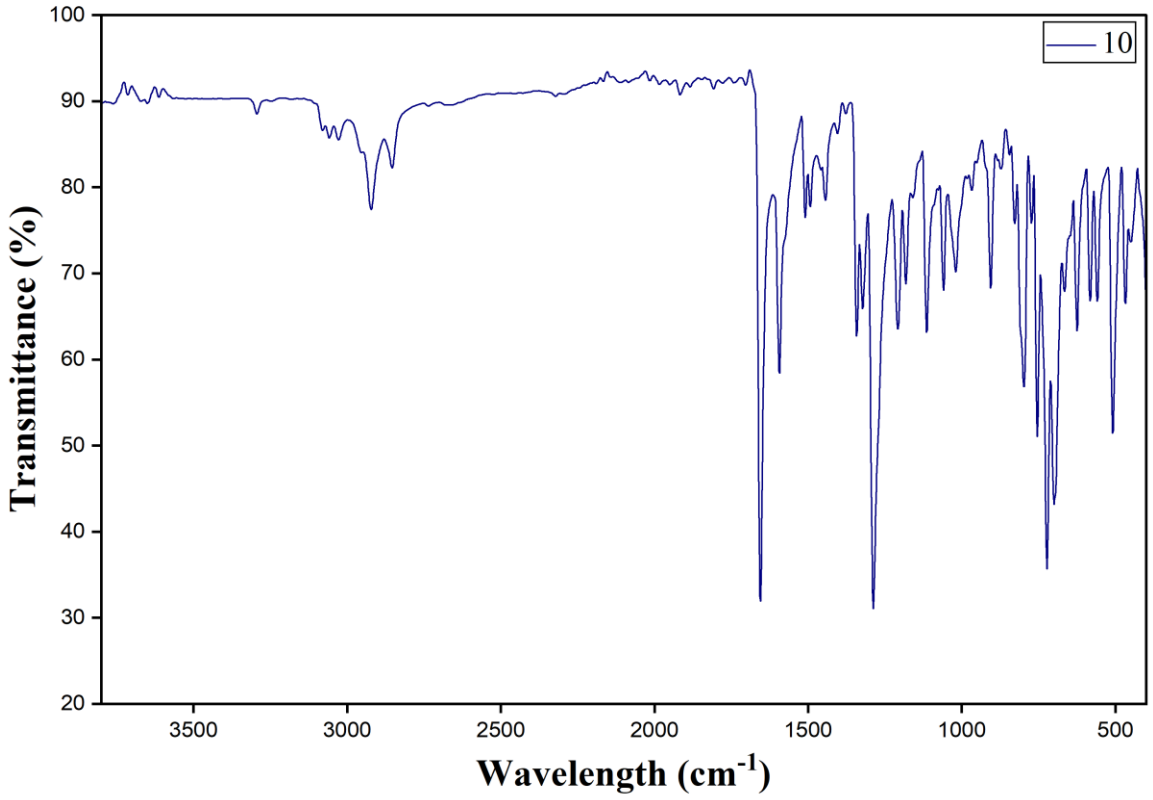




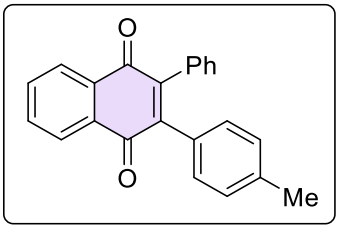
IR Spectra



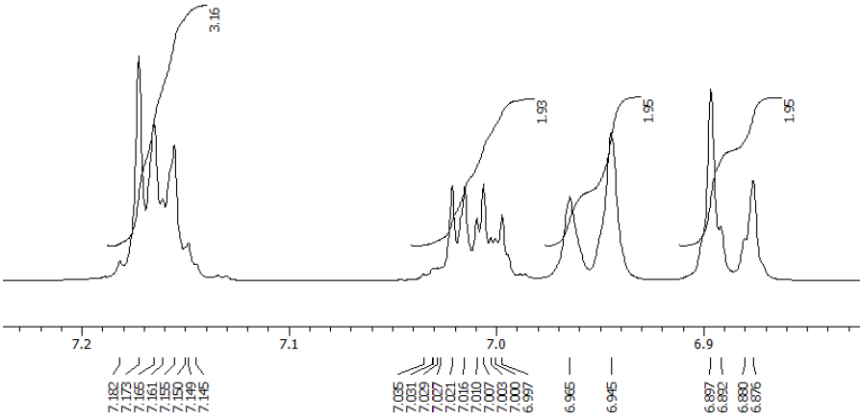
2-phenyl-3-(*p*-tolyl)naphthalene-1,4-dione (10)

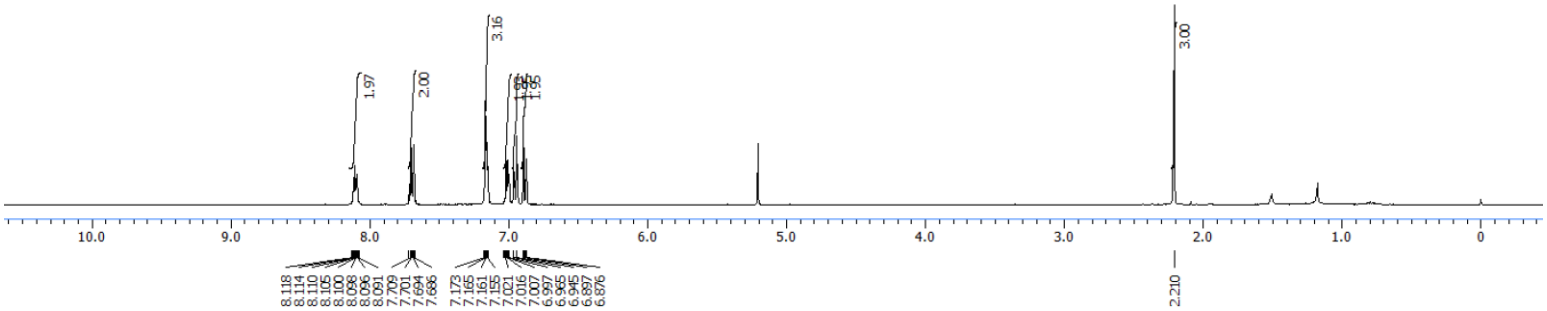


^{1}H NMR (400 MHz, $CDCl_3$)

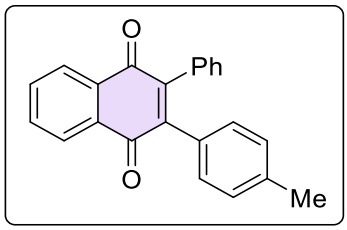


2-phenyl-3-(*p*-tolyl)naphthalene-1,4-dione (10)

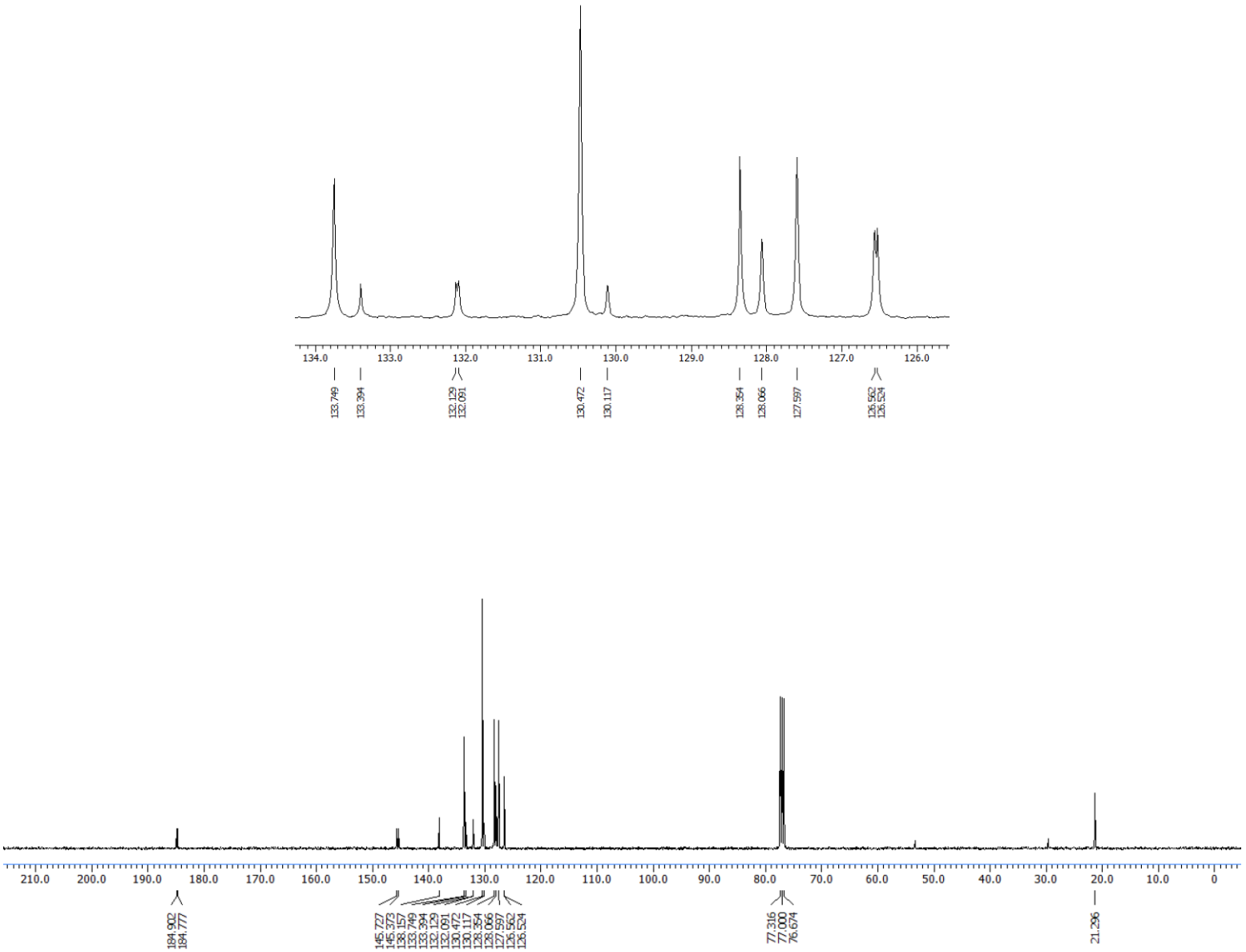




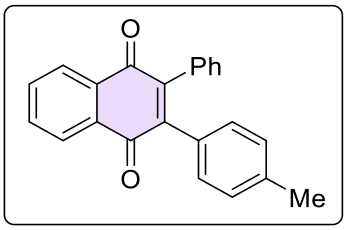
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-phenyl-3-(*p*-tolyl)naphthalene-1,4-dione (10)



HRMS



2-phenyl-3-(*p*-tolyl)naphthalene-1,4-dione (10)

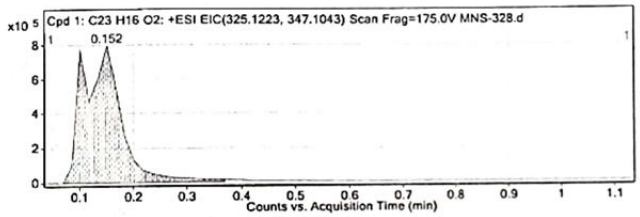
Qualitative Compound Report

Data File	MNS-328.d	**Sample Name**	MNS-328
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	08-03-2025 12:46:04
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Sample Group		**Info.**	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

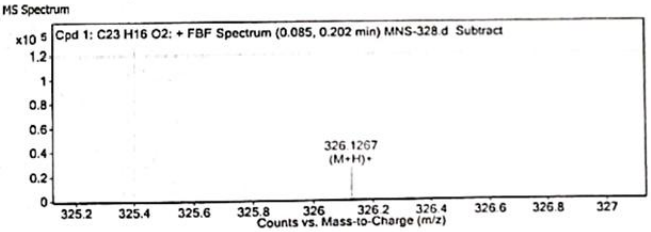
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C23 H16 O2	0.152	324.1162	110550	C23 H16 O2	324.115	3.68	C23 H16 O2	C23 H16 O2

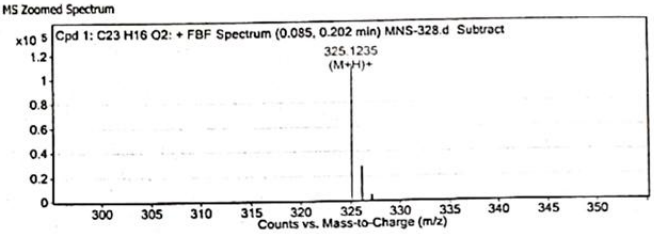
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H16 O2	325.1235	0.152	Find By Formula	324.1162



MS Spectrum



MS Zoomed Spectrum

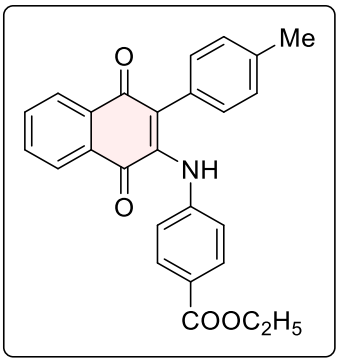


MS Spectrum Peak List

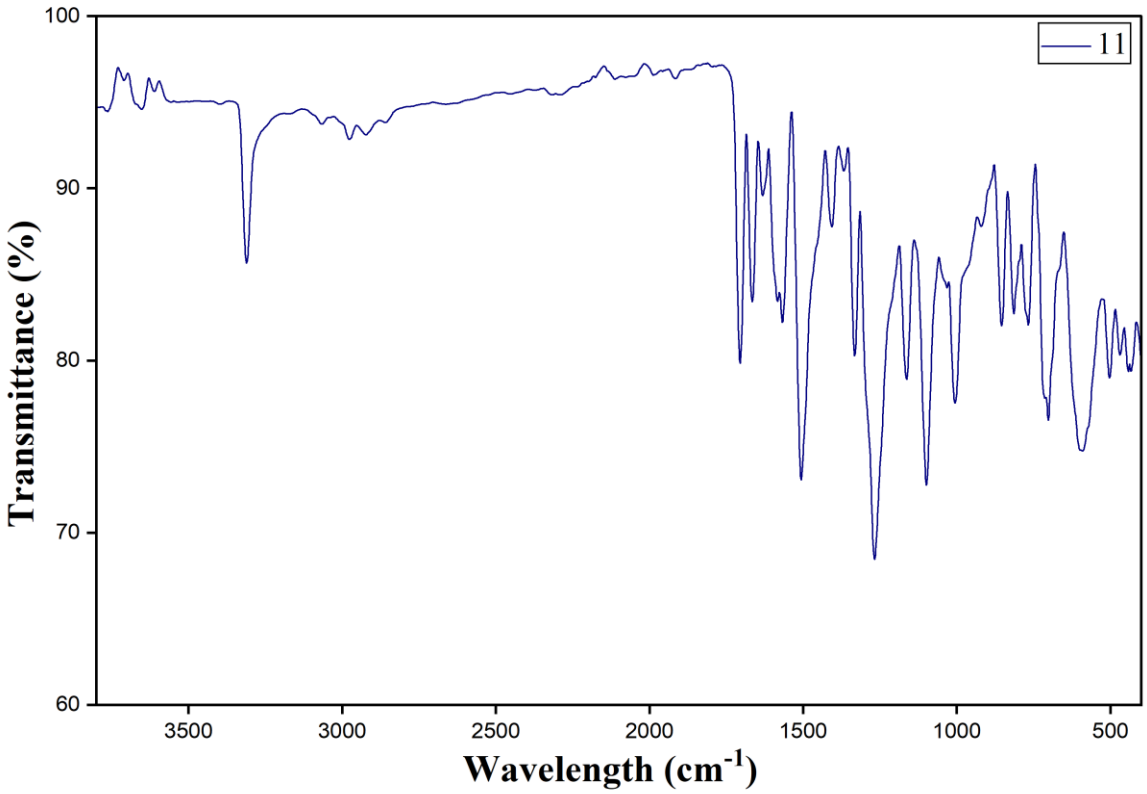
m/z	z	Abund	Formula	Ion
325.1235	1	110550.06	C23H17O2	(M+H)+
326.1267	1	26070.9	C23H17O2	(M+H)+
327.131	1	3960.02	C23H17O2	(M+H)+

--- End Of Report ---

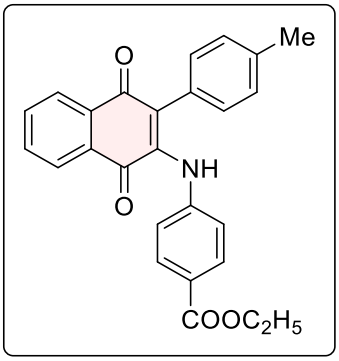
IR Spectra



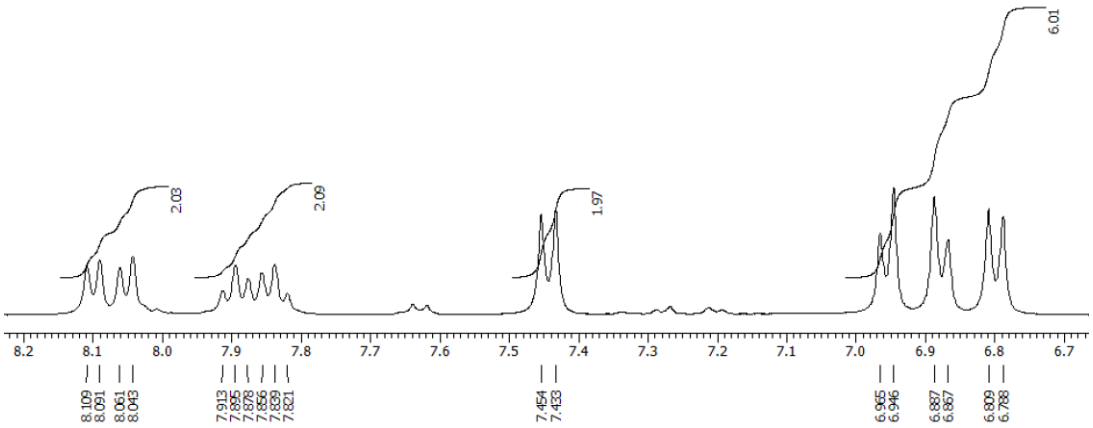
ethyl 4-((1,4-dioxo-3-(*p*-tolyl)-1,4-dihydronaphthalen-2-yl)amino)benzoate (11)

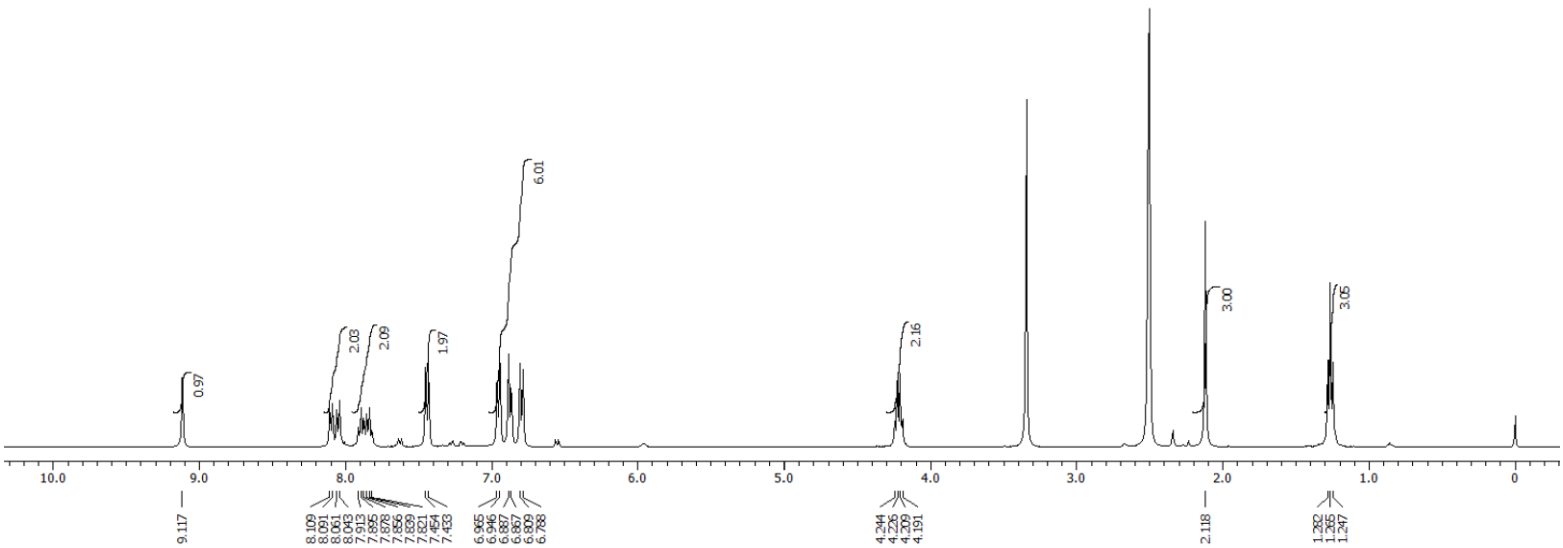


^{1}H NMR (400 MHz, $CDCl_3$)

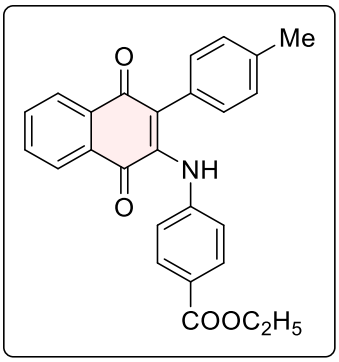


ethyl 4-((1,4-dioxo-3-(*p*-tolyl)-1,4-dihydronaphthalen-2-yl)amino)benzoate (11)

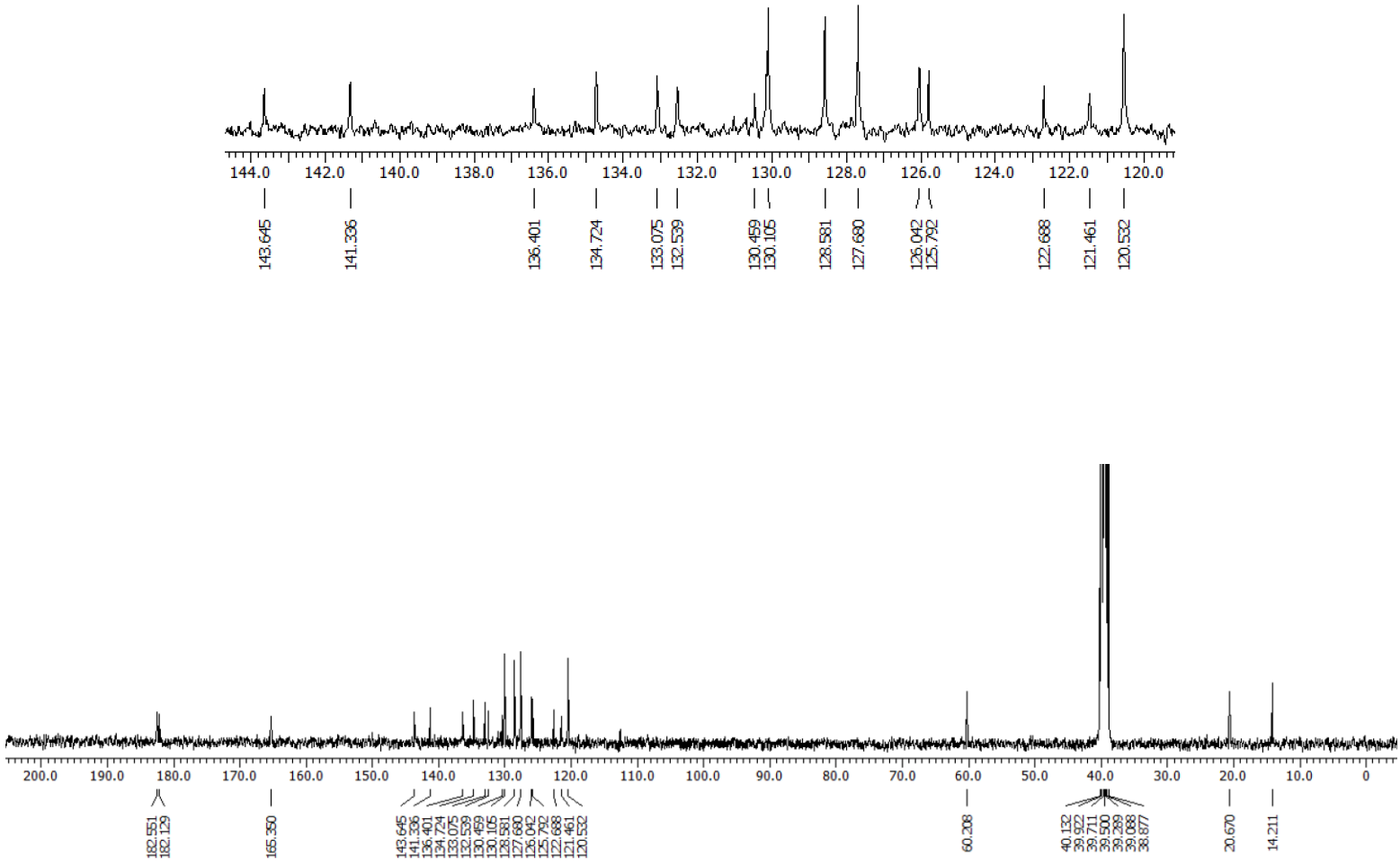




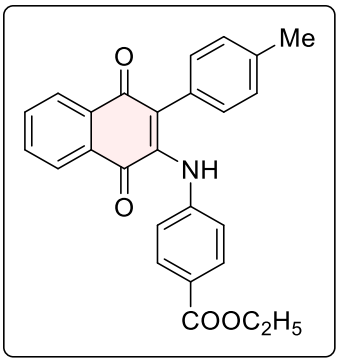
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



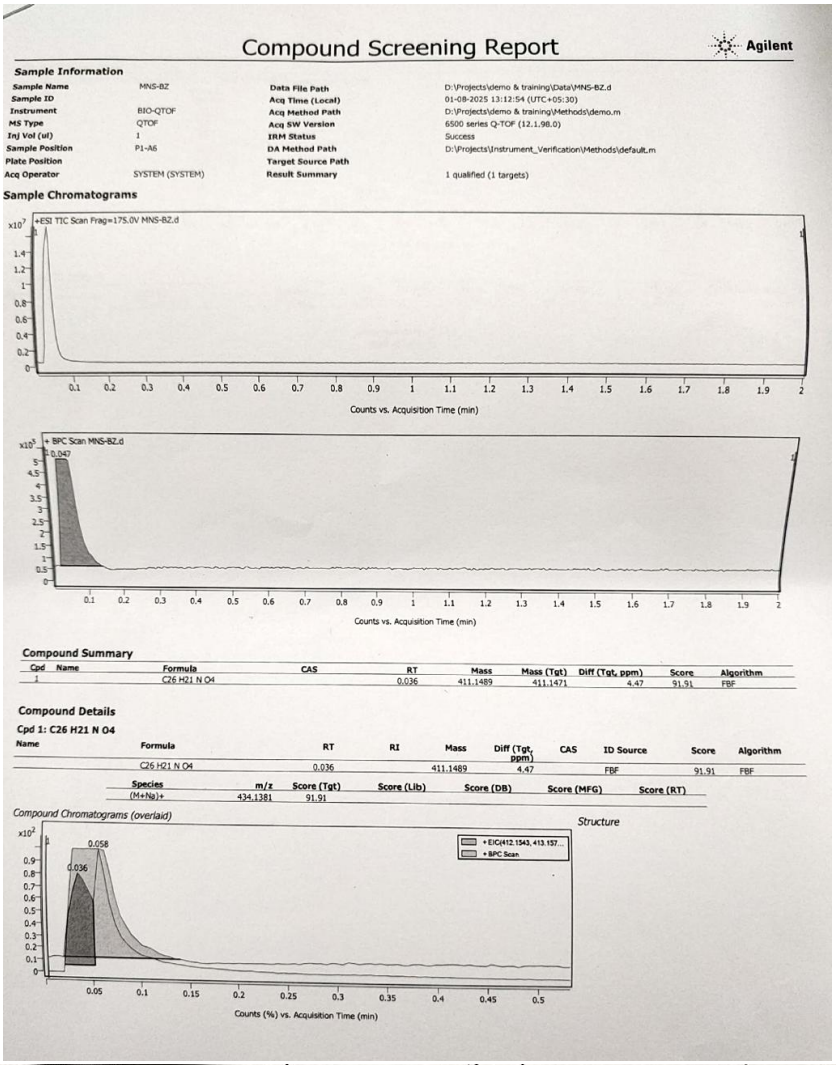
ethyl 4-((1,4-dioxo-3-(*p*-tolyl)-1,4-dihydronaphthalen-2-yl)amino)benzoate (11)



HRMS



ethyl 4-((1,4-dioxo-3-(*p*-tolyl)-1,4-dihydronaphthalen-2-yl)amino)benzoate (11)



Compound Screening Report — Agilent

Sample Information

Sample Name	MNS-BZ	Data File Path	D:\Projects\demo & training\Data\MNS-BZ.d
Sample ID		Acq Time (Local)	01-08-2025 13:12:54 (UTC+05:30)
Instrument	BIO-QTOF	Acq Method Path	D:\Projects\demo & training\Methods\demo.m
MS Type	QTOF	Acq SW Version	6500 series Q-TOF (12.1.98.0)
Inj Vol (ul)	1	IRM Status	Success
Sample Position	P1-A6	DA Method Path	D:\Projects\Instrument_Verification\Methods\default.m
Plate Position		Target Source Path	
Acq Operator	SYSTEM (SYSTEM)	Result Summary	1 qualified (1 targets)

Sample Chromatograms

Compound Summary

Cpd	Name	Formula	CAS	RT	Mass	Mass (Tgt)	Diff (Tgt, ppm)	Score	Algorithm
1		C26 H21 N O4		0.036	411.1489	411.1471	4.47	91.91	FBF

Compound Details

Cpd 1: C26 H21 N O4

Name	Formula	RT	RI	Mass	Diff (Tgt, ppm)	CAS	ID Source	Score	Algorithm
	C26 H21 N O4	0.036		411.1489	4.47		FBF	91.91	FBF

Species	m/z	Score (Tgt)	Score (Lib)	Score (DB)	Score (MFG)	Score (RT)
(M+Na)+	434.1381	91.91				

Compound Chromatograms (overlaid)

Structure

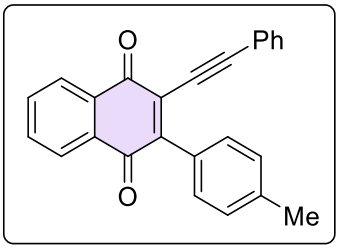
Compound Spectra (overlaid)

Compound ID Table

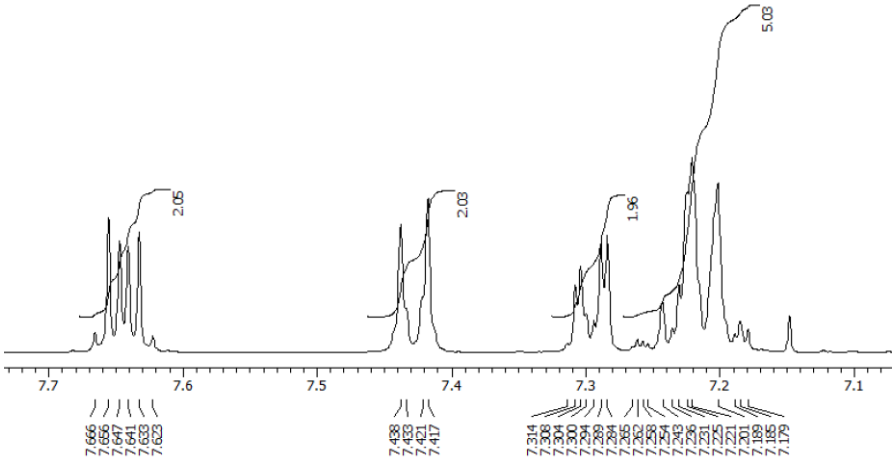
Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C26 H21 N O4	(M+Na)+	0.036		411.1489		FBF	91.91		91.91

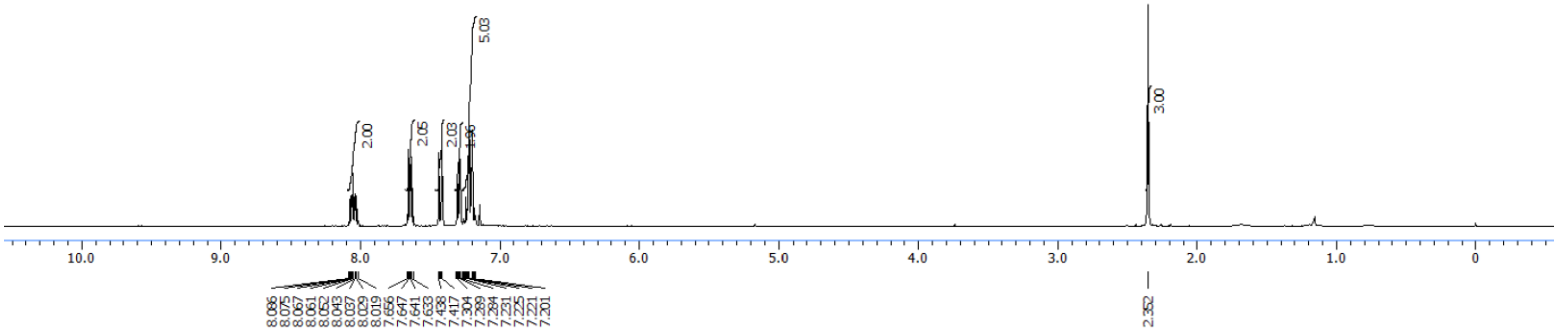
MassHunter Qual 12.0
(End of Report)

^{1}H NMR (400 MHz, $CDCl_3$)

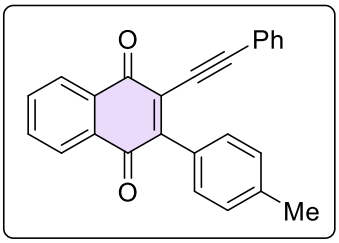


2-(phenylethynyl)-3-(*p*-tolyl)naphthalene-1,4-dione (12)

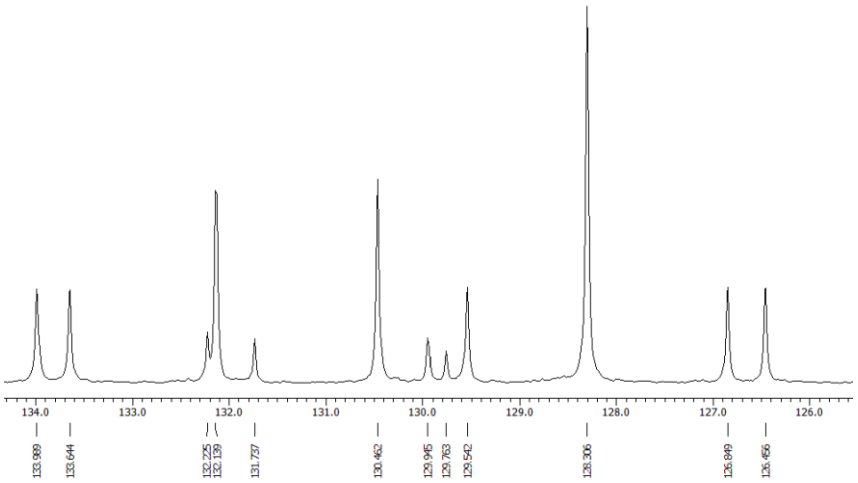


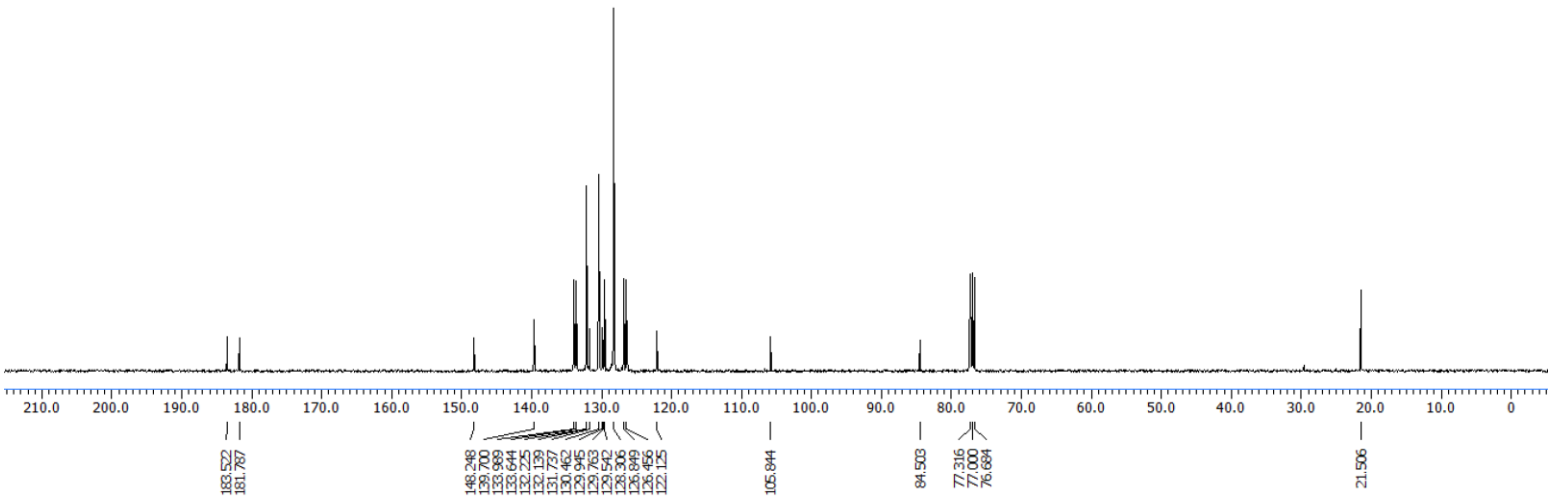


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

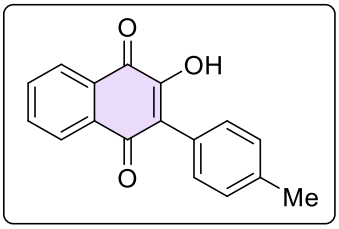


2-(phenylethynyl)-3-(*p*-tolyl)naphthalene-1,4-dione (12)

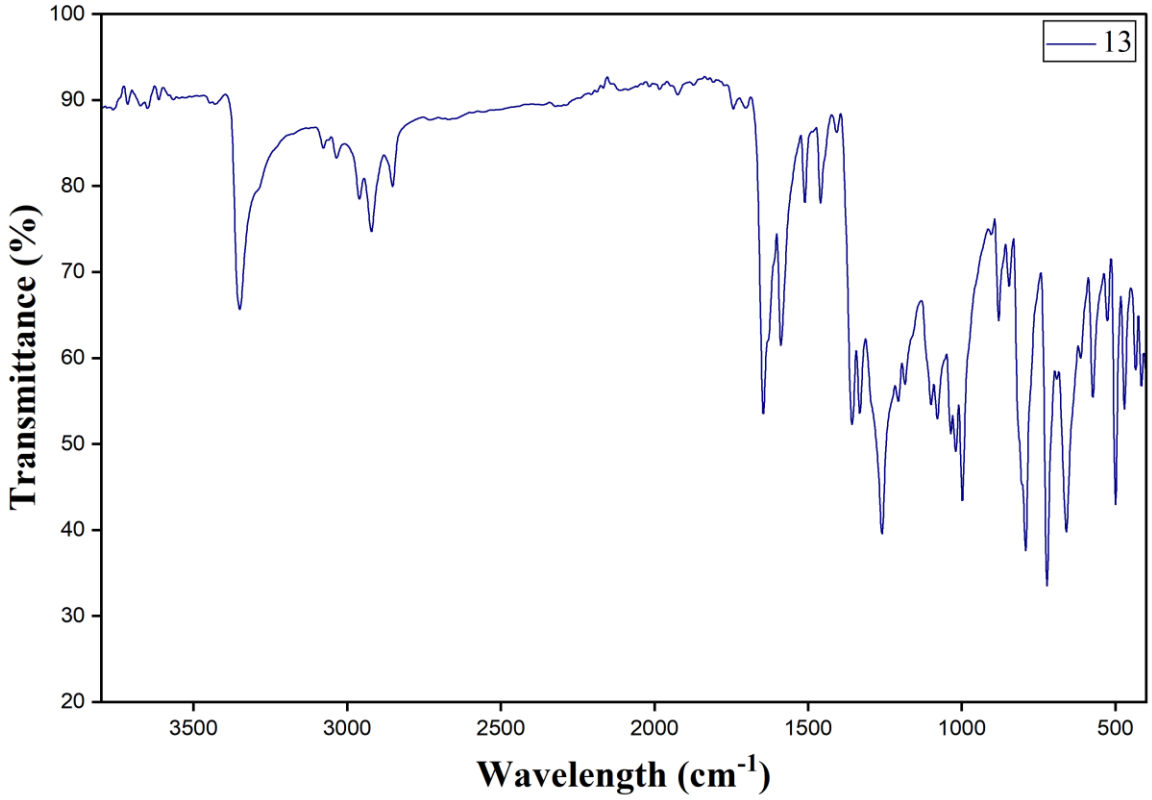




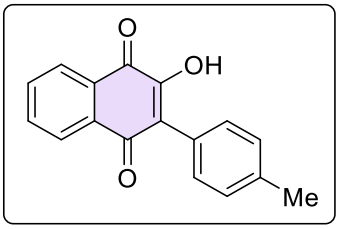
^{1}H NMR (400 MHz, $CDCl_3$)



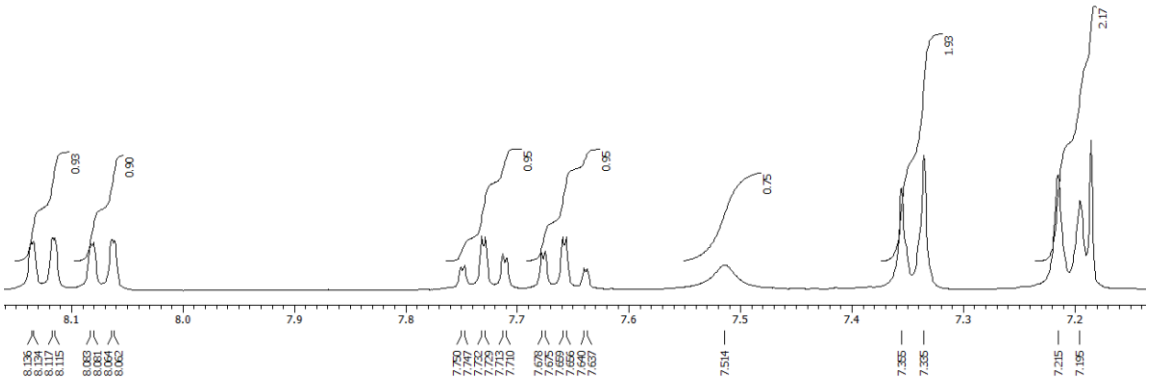
2-hydroxy-3-(*p*-tolyl)naphthalene-1,4-dione (13)

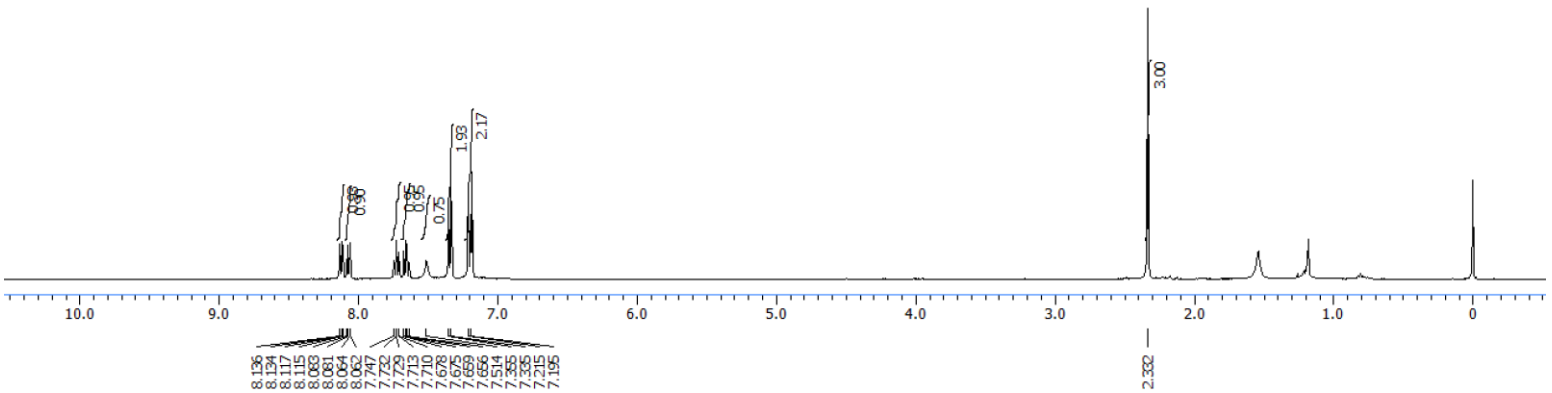


^{1}H NMR (400 MHz, $CDCl_3$)

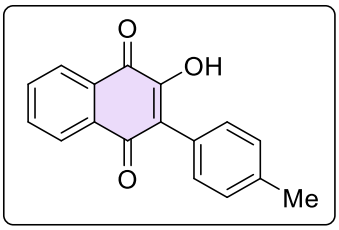


2-hydroxy-3-(*p*-tolyl)naphthalene-1,4-dione (13)

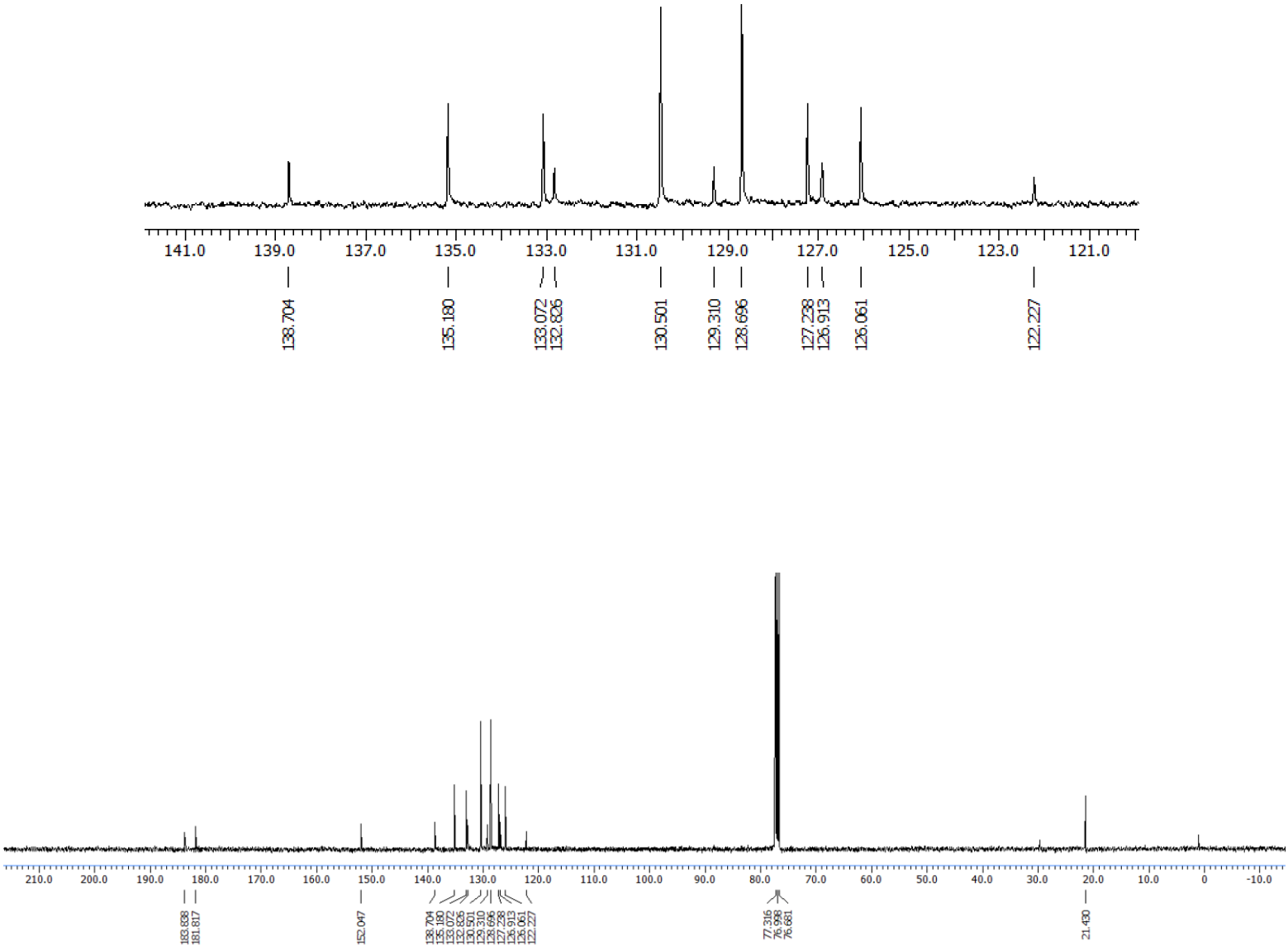




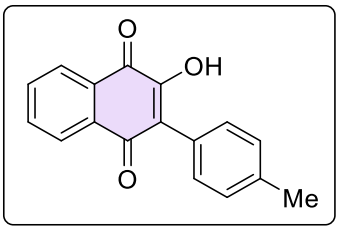
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



2-hydroxy-3-(*p*-tolyl)naphthalene-1,4-dione (13)



HRMS



2-hydroxy-3-(*p*-tolyl)naphthalene-1,4-dione (13)

Qualitative Compound Report

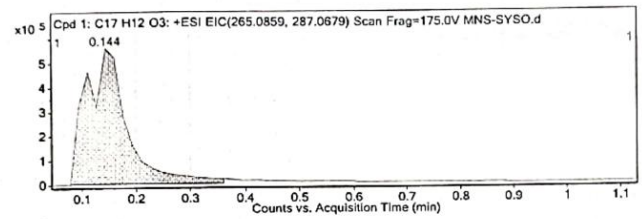
Data File	MNS-SYSO.d	Sample Name	MNS-SYSO
Sample Type	Sample	Position	P1-C2
Instrument Name	Instrument 1	User Name	
Acq Method	MS Scan.m	Acquired Time	08-03-2025 12:48:02
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

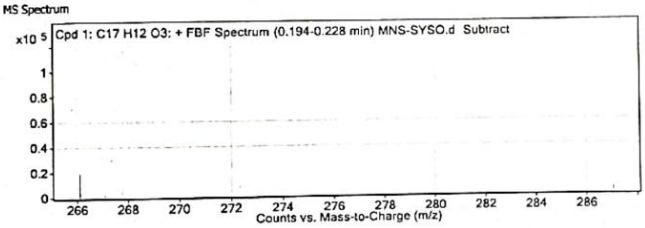
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C17 H12 O3	0.144	264.0799	104627	C17 H12 O3	264.0786	4.6	C17 H12 O3	C17 H12 O3

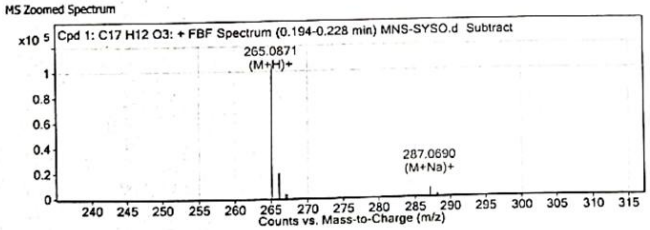
Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C17 H12 O3	265.0871	0.144	Find By Formula	264.0799



MS Spectrum



MS Zoomed Spectrum

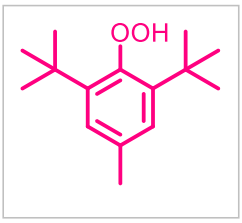


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
265.0871	1	104626.56	C17H13O3	(M+H)+
266.0905	1	19418.01	C17H13O3	(M+H)+
267.096	1	2525.97	C17H13O3	(M+H)+
287.069	1	4962.73	C17H12NaO3	(M+Na)+
288.0728	1	2094.22	C17H12NaO3	(M+Na)+

--- End Of Report ---

HRMS of BHT adduct



1,3-di-*tert*-butyl-2-hydroperoxy-5-methylbenzene

Qualitative Compound Report

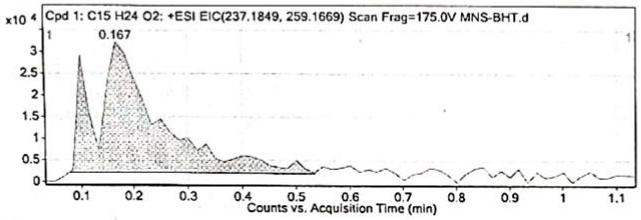
Data File	MNS-BHT.d	**Sample Name**	MNS-BHT
Sample Type	Sample	**Position**	P1-F9
Instrument Name	Instrument 1	**User Name**	
Acq Method	MS Scan.m	**Acquired Time**	21-05-2025 15:17:37
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group		**Info.**	3
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

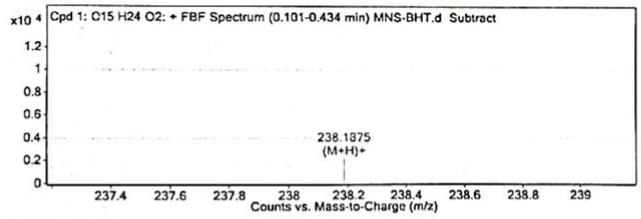
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C15 H24 O2	0.167	236.1773	11709	C15 H24 O2	236.1776	-1.28	C15 H24 O2	C15 H24 O2

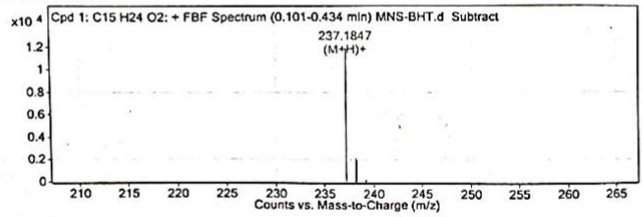
Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C15 H24 O2	237.1847	0.167	Find By Formula	236.1773



MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
237.1847	1	11709.03	C15H25O2	(M+H)+
238.1875	1	2192.14	C15H25O2	(M+H)+
239.1879	1	71.03	C15H25O2	(M+H)+

--- End Of Report ---