

Synthesis of Tetrahydrochromenes and Dihydronaphthofurans via Cascade Process of [3+3] and [3+2] Annulation Reactions: Mechanistic Insight for 6-endo-trig and 5-exo-trig Cyclisation

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Supporting Information

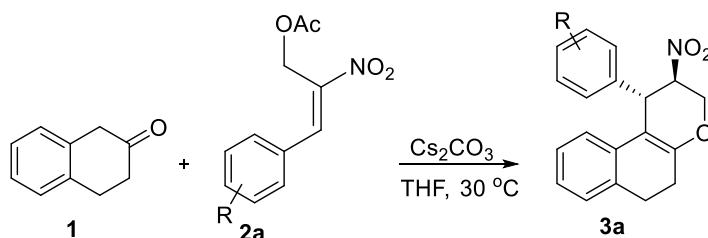
| | |
|-----------------------------------|----------------|
| Contents | S1 |
| Experimental Section | S2- S5 |
| Compounds Characterisation | S5-S13 |
| NMR Spectra | S14-S48 |
| Crystal Data | S49-S51 |
| DFT | S52-S97 |

Experimental Section

General

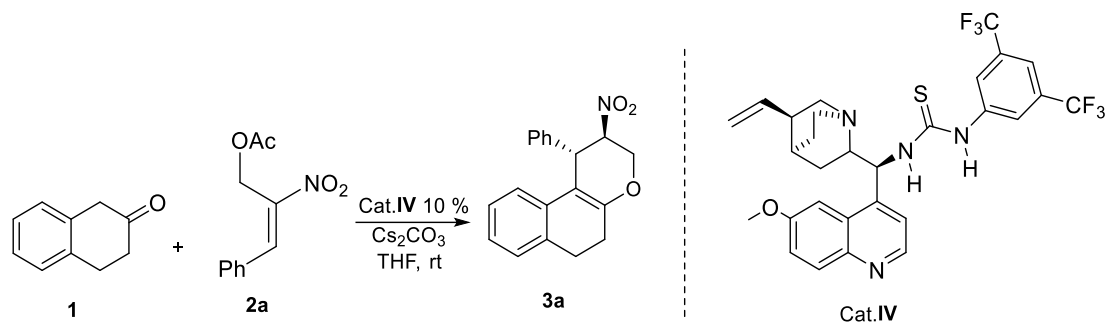
All reactions were carried out with dry, freshly distilled solvents in anhydrous conditions. Thin-layer chromatography (TLC) was performed on silica gel plates (60F-254) using UV-light (254 and 365 nm). Flash chromatography was performed on silica gel (230–400 mesh). NMR (400 MHz for ^1H NMR, and ^{13}C NMR) spectra were recorded in CDCl_3 with TMS as the internal standard. Chemical shifts are reported in ppm and coupling constants are given in Hz. Data for ^1H NMR are recorded as follows: chemical shift (ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet, coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (δ , ppm). High-resolution mass spectra (HRMS) were recorded on micro mass ESI-TOF MS. Melting points were determined in a Hanon auto melting point system (MP 450). IR was recorded on FTIR Bruker Technologies. HPLC chromatogram was recorded on Shimadzu LC-20AT using chiral cell OD-H column.

General procedure for the synthesis tetrahydrochromene 3a:



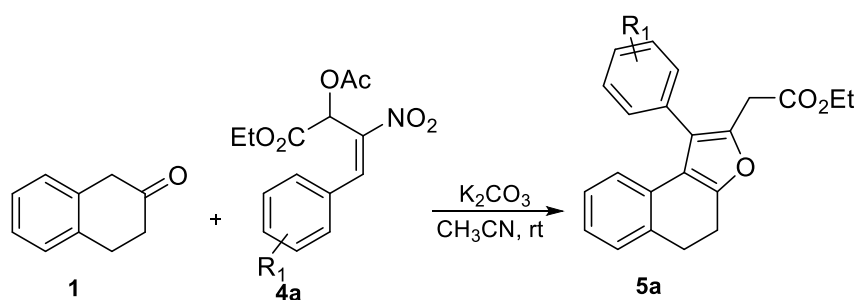
To a solution of β -tetralone **1** (200 mg, 1.36 mmol, 1.0 equiv.) with nitro allylic primary acetate **2** (300 mg, 1.36 mmol, 1.0 equiv.) and Cs_2CO_3 (886 mg, 2.72 mmol, 2.0 equiv.) in THF (3 mL). The reaction mixture was stirred at room temperature till the completion reaction. After the completion of the reaction, the organic layer was extracted with ethyl acetate, washed with brine solution and dried over Na_2SO_4 , and concentrated under reduced pressure. The resulted crude was subjected to flash column chromatography on silica gel (200-400) by eluting ethyl acetate in hexane (4:96) to afford the desired products **3a**.

General procedure for the synthesis of tetrahydrochromene 3a using catalyst:



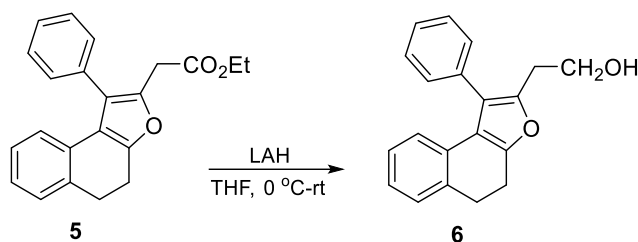
To a solution of β -tetralone **1** (50 mg, 0.34 mmol, 1.0 equiv.) with nitro allylic primary acetate **2a** (75 mg, 0.34 mmol, 1.0 equiv.) and Cs_2CO_3 (221 mg, 0.68 mmol, 2.0 equiv.) and catalyst **VI** (20 mg) in THF (2 mL). The reaction mixture was stirred at room temperature till the completion reaction. After the completion of the reaction, the organic layer was extracted with ethyl acetate, washed with brine solution and dried over Na_2SO_4 , and concentrated under reduced pressure. The resulted crude was subjected to flash column chromatography on silica gel (200-400) by eluting ethyl acetate in hexane (4:96) to afford the desired products **3a**. We have performed HPLC chromatogram by using chiral cell OD-H column to furnished **3a** as 49% of enantiomeric excess.

General procedure for the synthesis dihydronaphthofuran 5a:



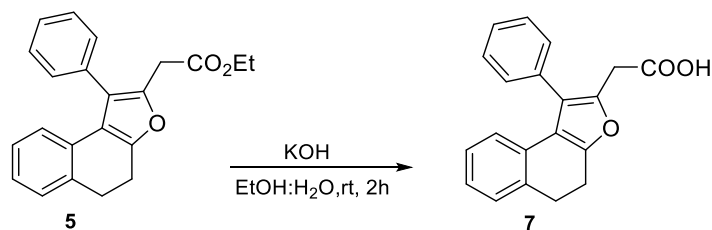
To a solution of β -tetralone **1** (200 mg, 1.36 mmol, 1.0 equiv.) with nitro allylic secondary acetate **4** (401 mg, 1.36 mmol, 1.0 equiv.) and K_2CO_3 (375 mg, 2.72 mmol, 2.0 equiv.) in CH_3CN (3 mL). The reaction mixture was stirred at room temperature till the completion reaction. After the completion of the reaction, the organic layer was extracted with ethyl acetate, washed with brine solution and dried over Na_2SO_4 , and concentrated under reduced pressure. The crude was subjected to flash column chromatography on silica gel (200-400) by eluting ethyl acetate in hexane (4:96) to afford the desired products **5**.

Procedure for preparation of compound 6:



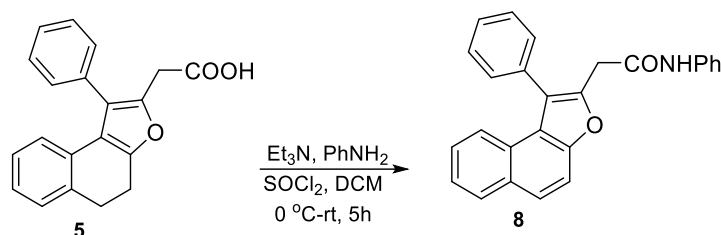
To a solution of **5** (200 mg, 0.30 mmol, 1 equiv.), lithium aluminium hydride (45 mg 1.20 mmol, 2 equiv.) in THF (4 mL), at 0 °C in nitrogen condition. After the completion of addition, the reaction mixture was allowed to stir at 30 °C till the completion of reaction. The reaction mixture was extracted with ethyl acetate and dried over NaSO₄, concentrated under reduced pressure to get the crude compound. The crude was subjected to column chromatography on silica gel by eluting ethyl acetate in hexane (5:95) to afford the desired product **6**

Procedure for preparation of compound 7:



To a stirred solution of dihydronaphthofuran **5** (80mg, 0.24 mmol, 1 equiv.) in EtOH/H₂O (2:0.2 ml), was added KOH (17mg, 0.31 mmol, 1.3 equiv.) drop wise at room temperature. The stirring was continued still the starting material completely disappeared (2-3 h) in the reaction mixture. Then 5N HCl was added and the reaction mixture was stirred for 30 min in order to neutralise the excess of KOH. After that the reaction mixture was filtered through filter paper by using vacuum pump to afford a desired product **7** in white solid, which was used directly used in the next step without further purification.

Procedure for preparation of compound 8:

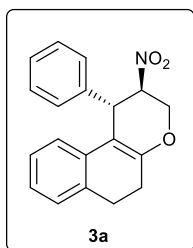


To a solution of **5** (50 mg, 0.16 mmol, 1 equiv.), aniline was added (20 μl , 0.16 mmol, 1 equiv.) and Et_3N (45 μl , 0.328 mmol, 2 equiv.) as a base in DCM (3 mL). SOCl_2 (23 μl , 0.328 mmol, 2 equiv.) was added drop wise at 0 $^{\circ}\text{C}$. After the completion of addition, the reaction mixture was allowed to stir at 30 $^{\circ}\text{C}$ till the completion of reaction using TLC. The reaction mixture was extracted with ethyl acetate and dried over NaSO_4 , concentrated under reduced pressure to get the crude compound. The crude was subjected to column chromatography on silica gel by eluting ethyl acetate in hexane (7:93) to afford the desired product **8** as light yellow solid.

Compounds Characterisation

2-nitro-1-phenyl-2,3,5,6-tetrahydro-1H-benzo[f]chromene (3a):

Compound **3a** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **2a** (300 mg, 1.36 mmol, 1.0 equiv.), Cs_2CO_3 (886 mg, 2.72 mmol, 2.0 equiv.) in THF (3 mL).



Yellow solid; Yield: 77% (316.0 mg, 1.02 mmol); mp 183-185 $^{\circ}\text{C}$

IR (neat, cm^{-1}) 2933, 2856, 1624, 1540, 1492, 1226, 889, 817, 740.

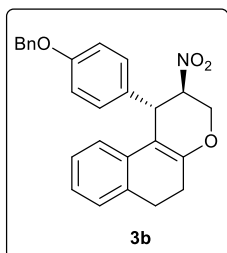
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.35-7.25 (m, 5H), 7.09-7.06 (m, 1H), 6.97-6.95 (m, 2H), 6.73-6.71 (m, 1H), 4.76-4.67 (m, 3H), 4.18 (dd, $J = 13.2, 3.2$ Hz, 1H), 2.94 (t, $J = 8.0$ Hz, 2H), 2.55-2.50 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 153.6, 140.4, 133.9, 133.1, 129.2, 128.3, 127.8, 127.2, 126.4, 124.9, 122.2, 102.5, 84.3, 61.5, 39.8, 28.3, 26.6.

HRMS calcd. $\text{C}_{19}\text{H}_{18}\text{NO}_3$, 308.12867; found 308.12814 [$\text{M} + \text{H}$]

1-(4-(benzyloxy)phenyl)-2-nitro-2,3,5,6-tetrahydro-1H-benzo[f]chromene (3b):

Compound **3b** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **2b** (447 mg, 1.36 mmol, 1.0 equiv.), Cs₂CO₃ (886 mg, 2.72 mmol, 2.0 equiv.) in THF (3 mL).



Yellow gummy liquid Yield: 76% (429.0 mg, 1.03 mmol).

IR (neat, cm⁻¹) 2971, 1656, 1601, 1564, 1441, 1301, 1224, 1022, 847, 803, 791.

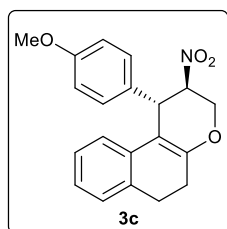
¹H NMR (400 MHz, CDCl₃); δ 7.42-7.25 (m, 6H), 7.22 (d, *J* = 5.6 Hz, 1H), 7.06-7.05 (m, 1H), 6.96-6.91 (m, 3H), 6.83 (d, *J* = 8.4 Hz, 1H), 6.73 (t, *J* = 4.8 Hz, 1H), 4.99 (s, 2H), 4.68-4.66 (m, 3H), 4.14 (d, *J* = 10.0 Hz, 1H), 2.91 (t, *J* = 8.0 Hz, 2H), 2.48 (t, *J* = 4.8 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃); δ 158.9, 136.5, 136.4, 134.9, 128.7, 128.6, 128.5, 128.3, 127.9, 127.4, 125.9, 125.2, 124.4, 120.1, 115.2, 89.1, 70.0, 65.6, 36.5, 28.1, 26.1.

HRMS calcd. C₂₆H₂₄NO₄, 414.17053; found 414.17146 [M + H]

1-(4-methoxyphenyl)-2-nitro-2,3,5,6-tetrahydro-1H-benzo[f]chromene (3c):

Compound **3c** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **2c** (343 mg, 1.36 mmol, 1 equiv.), Cs₂CO₃ (886 mg, 1.36 mmol, 2.0 equiv.) in THF (3 mL).



Yellow gummy liquid Yield: 68% (312.0 mg, 0.92 mmol).

IR (neat, cm⁻¹) 2960, 1621, 1536, 1464, 1536, 1267, 1175, 1031, 860, 807, 767.

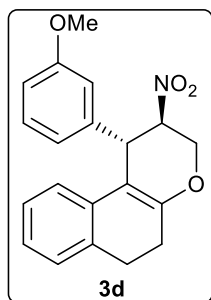
¹H NMR (400 MHz, CDCl₃); δ 7.28-7.24 (m, 1H), 7.08-7.06 (m, 1H), 6.97-6.93 (m, 3H), 6.89 (s, 1H), 6.82-6.79 (m, 1H), 6.76-6.74 (m, 1H), 4.72-4.67 (m, 3H), 4.21 (dd, *J* = 13.2, 2.8, Hz, 1H), 3.78 (s, 3H), 2.93 (t, *J* = 8.0, Hz, 2H), 2.52 (t, *J* = 4.0, Hz, 2H).

¹³C NMR (100 MHz, CDCl₃); δ 160.2, 153.6, 142.1, 133.9, 133.0, 130.3, 127.2, 126.4, 124.9, 122.1, 120.6, 114.5, 112.6, 102.5, 61.6, 55.2, 39.8, 28.3, 26.6.

HRMS calcd. C₂₀H₂₀NO₄, 338.13923; found 338.13960 [M + H]

1-(3-methoxyphenyl)-2-nitro-2,3,5,6-tetrahydro-1H-benzo[f]chromene (3d):

Compound **3d** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **2d** (343 mg, 1.36 mmol, 1 equiv.), Cs₂CO₃ (886 mg, 1.36 mmol, 2.0 equiv.) in THF (3 mL).



Yellow gummy liquid; Yield: 71% (327.4 mg, 0.97 mmol)

IR (neat, cm⁻¹) 2967, 1619, 1529, 1460, 1531, 1267, 1175, 1031, 861, 817, 757.

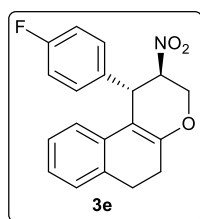
¹H NMR (400 MHz, CDCl₃); δ 7.26-7.24 (m, 2H), 7.08-7.06 (m, 1H), 6.97-6.95 (m, 2H), 6.87-6.83 (m, 2H), 6.75-6.72 (m, 1H), 4.69-4.66 (m, 3H), 4.18 (dd, *J* = 12.8, 3.2 Hz, 1H), 3.81 (s, 3H), 2.93 (t, *J* = 8.0 Hz, 2H), 2.53-2.49 (m, 2H),

¹³C NMR (CDCl₃, 100 MHz) δ 159.1, 153.4, 134.0, 133.1, 132.2, 129.3, 127.3, 127.2, 126.4, 124.9, 122.2, 114.6, 114.3, 113.8, 102.8, 61.5, 55.2, 39.1, 28.3, 26.6.

HRMS calcd. C₂₀H₂₀NO₄, 338.13923; found 338.13960 [M + H]

1-(4-fluorophenyl)-2-nitro-2,3,5,6-tetrahydro-1H-benzo[f]chromene (3e):

Compound **3e** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **2e** (325 mg, 1.36 mmol, 1 equiv.), Cs₂CO₃ (886 mg, 2.72 mmol, 2.0 equiv.) in THF (3 mL). 13



Yellow gummy liquid Yield: 72% (320.0 mg, 0.98 mmol).

IR (neat, cm⁻¹) 2927, 1621, 1546, 1508, 1321, 1227, 1158, 1071, 810, 831, 734, 767.

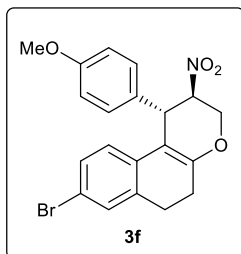
¹H NMR (400 MHz, CDCl₃); δ 7.51-7.37 (m, 2H), 7.37-7.24 (m, 1H), 7.20-7.12 (m, 2H), 7.10-7.06 (m, 1H), 6.96-6.92 (m, 2H), 6.73-6.71 (m, 1H), 5.18 (d, *J* = 2.0 Hz, 1H), 4.78 (s, 1H), 4.64 (d, *J* = 12.8 Hz, 1H), 4.06 (q, *J* = 1.6 Hz, 1H), 3.01 (t, *J* = 6.4 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H)

¹³C NMR (100 MHz, CDCl₃); δ 162.6, 162.0, (d, *J*_{C-F} = 240 Hz) 153.3, 138.8, 136.3, 133.7, 132.9, 132.7, 131.8, 131.5, 131.2, 130.9, 130.8, 130.7, 130.6, 128.3, 127.2, 126.2, 124.6, 121.5, 83.3, 37.4, 27.6, 26.1.

HRMS calcd. C₁₉H₁₇FNO₃, 326.11925; found 326.11760 [M + H]

8-bromo-1-(4-methoxyphenyl)-2-nitro-2,3,5,6-tetrahydro-1H-benzo[f]chromene (3f):

Compound **3f** was synthesized according to the general procedure by taking **1b** (200 mg, 0.88 mmol, 1.0 equiv.), **2e** (223 mg, 0.88 mmol, 1 equiv.), Cs₂CO₃ (577 mg, 1.77 mmol, 2.0 equiv.) in THF (3 mL).



Yellow gummy liquid Yield: 68% (312.0 mg, 0.92 mmol).

IR (neat, cm⁻¹) 2926, 1624, 1549, 1507, 1329, 1226, 1158, 1072, 817, 832, 737, 765.

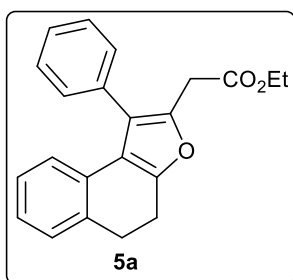
¹H NMR (400 MHz, CDCl₃); δ 7.28-7.06 (m, 1H), 6.98-6.96 (m, 2H), 6.95-6.81 (m, 2H), 6.80-6.74 (m, 2H), 4.72-4.23 (m, 3H), 4.23-4.19 (m, 1H), 3.78 (s, 3H), 2.93 (t, *J* = 9.6 Hz, 2H), 2.53 (t, *J* = 6.4 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃); δ 159.1, 153.4, 134.2, 133.1, 132.2, 129.3, 127.3, 127.2, 126.4, 122.2, 114.6, 114.3, 113.8, 102.8, 84.4, 61.5, 55.2, 39.1, 28.3, 26.6.

HRMS calcd. C₂₀H₁₉BrNO₄, 416.04975; found 416.04969 [M + H].

Ethyl 2-(1-phenyl-4,5-dihydronaphtho[2,1-b]furan-2-yl) acetate (5a):

Compound **5a** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **4a** (401 mg, 1.36 mmol, 1.0 equiv.), K₂CO₃ (378 mg, 2.73 mmol, 2.0 equiv.) in CH₃CN (3 mL).



Yellow gummy liquid; Yield: 72% (331.0 mg, 0.99 mmol).

IR (neat, cm⁻¹) 2934, 2283, 1735, 1597, 1457, 1281, 1180, 1029, 737.

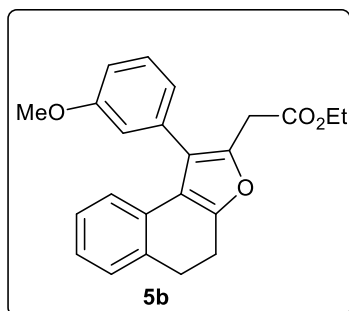
¹H NMR (400 MHz, CDCl₃); δ 7.44-7.35 (m, 5H), 7.28-7.21 (m, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.01 (t, *J* = 6.8 Hz, 1H), 6.92 (t, *J* = 7.2 Hz, 1H), 4.17 (q, *J* = 6.8 Hz, 2H), 3.59 (s, 2H), 3.08 (t, *J* = 8.0 Hz, 2H), 2.89 (t, *J* = 8.0 Hz, 2H), 1.24 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (400 MHz, CDCl₃); δ 169.8, 152.7, 143.7, 133.7, 133.1, 131.2, 129.8, 128.7, 128.4, 127.9, 127.4, 126.3, 125.4, 122.6, 122.2, 117.7, 61.1, 32.6, 29.7, 22.1, 14.1.

HRMS calcd. C₂₂H₂₁O₃, 333.14907; found 333.14901 [M + H]

Ethyl 2-(1-(3-methoxyphenyl)-4,5-dihydronaphtho[2,1-b]furan-2-yl)acetate(5b):

Compound **5b** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **4b** (439 mg, 1.36 mmol, 2.0 equiv.), K₂CO₃ (378 mg, 2.73 mmol, 2.0 equiv.) in CH₃CN (3 mL).



Gummy liquid; Yield: 67% (332.0 mg, 0.91 mmol).

IR (neat, cm⁻¹) 2933, 2271, 1735, 1607, 1492, 1281, 1184, 1026, 740.

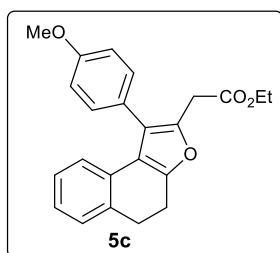
¹H NMR (400 MHz, CDCl₃); δ 7.84 (d, *J* = 8.8 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 1H), 7.03-6.92 (m, 4H), 6.86 (d, *J* = 7.6 Hz, 1H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 3.57 (s, 2H), 3.08 (t, *J* = 7.6 Hz, 2H), 2.88 (t, *J* = 8.4 Hz, 2H), 1.26 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (400 MHz, CDCl₃); δ 169.9, 158.9, 152.6, 143.5, 133.7, 133.7, 131.9, 131.4, 130.9, 127.9, 126.3, 125.3, 125.2, 122.5, 121.8, 117.8, 114.3, 113.9, 61.1, 55.2, 32.6, 29.7, 22.1, 14.1.

HRMS calcd. C₂₃H₂₃O₄, 363.15963; found 363.15938 [M + H]

Ethyl 2-(1-(4-methoxyphenyl)-4,5-dihydronaphtho[2,1-b]furan-2-yl)acetate(5c):

Compound **5c** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **4c** (439 mg, 1.36 mmol, 1.0 equiv.), K₂CO₃ (378 mg, 2.73 mmol, 2.0 equiv.) in CH₃CN (3 mL).



Gummy liquid; Yield: 62% (310.0 mg, 0.85 mmol).

IR (neat, cm⁻¹) 2940, 2268, 1742, 1619, 1499, 1297, 1180, 1021, 737.

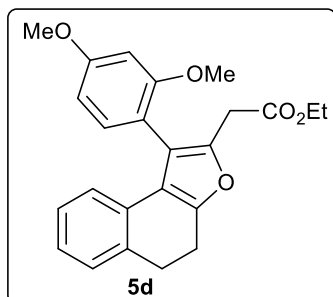
¹H NMR (400 MHz, CDCl₃); δ 7.45 (d, *J* = 6.4 Hz, 1H), 7.40-7.31 (m, 1H), 7.20-7.14 (m, 2H), 7.03-7.00 (m, 2H), 6.96-6.87 (m, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.80 (s, 3H), 3.60 (s, 2H), 3.09 (t, *J* = 8.0 Hz, 2H), 2.89 (t, *J* = 8.4 Hz, 2H), 1.28 (t, *J* = 3.6 Hz, 3H).

¹³C NMR (400 MHz, CDCl₃); δ 168.9, 158.9, 152.6, 145.5, 132.7, 131.9, 131.4, 130.9, 127.9, 126.3, 125.3, 125.2, 122.5, 121.8, 117.8, 114.3, 113.9, 61.2, 54.2, 31.6, 29.7, 22.1, 14.1.

HRMS calcd. C₂₃H₂₃O₄, 363.15963; found 363.15938 [M + H]

Ethyl 2-(1-(2,4-dimethoxyphenyl)-4,5-dihydronaphtho[2,1-b]furan-2-yl)acetate (5d):

Compound **5d** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **4d** (483 mg, 1.36 mmol, 1.0 equiv.), K₂CO₃ (378 mg, 2.73 mmol, 2.0 equiv.) in CH₃CN (3 mL).



Gummy liquid; Yield: 60% (326.0 mg, 0.83 mmol)

IR (neat, cm⁻¹) 2997, 2264, 1731, 1606, 1498, 1281, 1176, 1026, 791, 750.

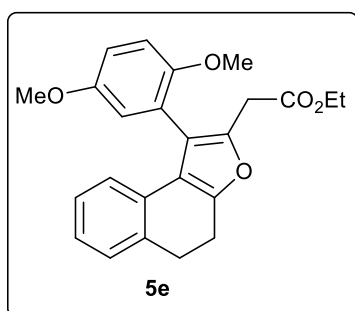
¹H NMR (400 MHz, CDCl₃); δ 7.21 (d, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 7.2 Hz, 1H), 7.01-6.97 (m, 1H), 6.92 (t, *J* = 6.8 Hz, 1H), 6.77 (d, *J* = 7.6 Hz, 1H), 6.56-6.53 (m, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 3.66 (s, 3H), 3.55 (s, 2H), 3.08 (t, *J* = 8.0 Hz, 2H), 2.90 (t, *J* = 8.0 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (400 MHz, CDCl₃); δ 169.9, 160.7, 158.3, 152.2, 144.0, 133.4, 132.3, 131.9, 127.6, 126.2, 125.1, 122.0, 118.4, 117.6, 114.3, 104.3, 98.8, 60.9, 55.4, 55.3, 32.8, 29.6, 22.2, 14.1.

HRMS calcd. C₂₄H₂₅O₅, 393.17020; found 393.16912 [M + H]

Ethyl 2-(1-(2,5-dimethoxyphenyl)-4,5-dihydronaphtho[2,1-b]furan-2-yl)acetate (5e):

Compound **5e** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **4e** (483 mg, 1.36 mmol, 1.0 equiv.), K₂CO₃ (378 mg, 2.73 mmol, 2.0 equiv.) in CH₃CN (3 mL).



Gummy liquid; Yield: 58% (315.0 mg, 0.80 mmol)

IR (neat, cm⁻¹) 3013, 2246, 1717, 1619, 1401, 1267, 1129, 1036, 781.

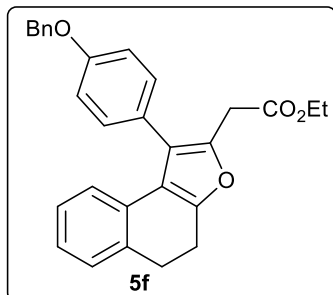
¹H NMR (400 MHz, CDCl₃); δ 7.23 (d, *J* = 5.2 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.12-6.97 (m, 1H), 6.92 (t, *J* = 6.8 Hz, 1H), 6.77 (d, *J* = 7.6 Hz, 1H), 6.55-6.53 (m, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 3.85 (s, 3H), 3.63 (s, 3H), 3.53 (s, 2H), 3.08 (t, *J* = 8.0 Hz, 2H), 2.90 (t, *J* = 8.0 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (400 MHz, CDCl₃); δ 168.9, 166.7, 157.3, 154.2, 145.0, 133.4, 132.3, 131.9, 127.6, 126.2, 125.1, 122.0, 118.4, 117.6, 114.3, 104.3, 98.8, 60.9, 55.4, 55.3, 32.8, 29.6, 22.2, 14.1.

HRMS calcd. C₂₄H₂₅O₅, 393.17020; found 393.16912 [M + H]

Ethyl 2-(1-(4-(benzyloxy)phenyl)-4,5-dihydronaphtho[2,1-b]furan-2-yl)acetate (**5f**):

Compound **5f** was synthesized according to the general procedure by taking **1a** (200 mg, 1.36 mmol, 1.0 equiv.), **4f** (542 mg, 1.36 mmol, 1.0 equiv.), K₂CO₃ (378 mg, 2.73 mmol, 2.0 equiv.) in CH₃CN (3 mL).



Gummy liquid; Yield: 70% (419.0 mg, 0.95 mmol).

IR (neat, cm⁻¹) 3016, 2286, 1713, 1621, 1407, 1269, 1137, 1041, 779.

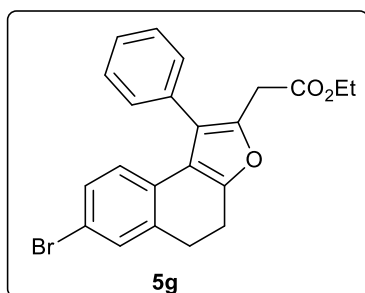
¹H NMR (400 MHz, CDCl₃); δ 7.84 (d, *J* = 8.8 Hz, 1H), 7.48 (d, *J* = 7.2 Hz, 2H), 7.43-7.39 (m, 3H), 7.36-7.31 (m, 3H), 7.16 (d, *J* = 7.2 Hz, 1H), 7.09-6.95 (m, 3H), 5.11 (s, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.58 (s, 2H), 3.08 (t, *J* = 7.6 Hz, 2H), 2.88 (t, *J* = 8.0 Hz, 2H), 1.26 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (400 MHz, CDCl₃); δ 169.9, 158.2, 152.6, 143.5, 136.9, 133.7, 131.9, 131.3, 130.9, 128.7, 128.5, 128.3, 120.0, 127.9, 127.5, 127.4, 126.3, 125.5, 125.3, 122.5, 121.7, 117.8, 115.1, 114.8, 70.0, 61.1, 32.6, 29.7, 22.1, 14.1.

HRMS calcd. C₂₉H₂₇O₄, 439.19093; found 439.19049 [M + H]

ethyl 2-(7-bromo-1-phenyl-4,5-dihydronaphtho[2,1-b]furan-2-yl)acetate (**5g**):

Compound **5g** was synthesized according to the general procedure by taking **1b** (200 mg, 0.88 mmol, 1.0 equiv.), **4a** (196 mg, 0.88 mmol, 1.0 equiv.), K₂CO₃ (241 mg, 1.77 mmol, 2.0 equiv.) in CH₃CN (3 mL).



Gummy liquid; Yield: 60% (326.0 mg, 0.83 mmol).

IR (neat, cm⁻¹) 3015, 2287, 1710, 1625, 1404, 1270, 1134, 1042, 774.

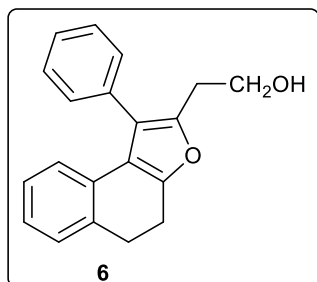
¹H NMR (400 MHz, CDCl₃); δ 7.44-7.35 (m, 4H), 7.28-7.02 (m, 1H), 7.02-6.99 (m, 1H), 6.94-6.91 (m, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 4.17 (q, *J* = 6.4 Hz, 2H), 3.59 (s, 2H), 3.08 (t, *J* = 12.0 Hz, 2H), 2.89 (t, *J* = 6.8 Hz, 2H), 1.25 (t, *J* = 8.8 Hz, 3H).

¹³C NMR (400 MHz, CDCl₃); δ 169.8, 152.7, 143.7, 133.7, 133.1, 129.8, 128.7, 128.4, 127.9, 126.3, 125.4, 122.6, 122.4, 117.7, 61.1, 32.6, 29.7, 22.1, 14.1.

HRMS calcd. C₂₂H₂₀BrO₃, 411.05958; found 411.05947 [M + H]

2-(1-phenyl-4,5-dihydronaphtho[2,1-b]furan-2-yl)ethan-1-ol (6):

Compound **6** was synthesized according to the general procedure by taking **5a** (200 mg, 0.30 mmol, 1 equiv.), LAH (45 mg 1.20 mmol, 2 equiv.), in THF (4 mL).



Light yellow solid; Yield: 60% (105.0 mg, 0.36 mmol).

IR (neat, cm^{-1}) 3016, 2286, 1727, 1621, 1407, 1271, 1136, 1047.

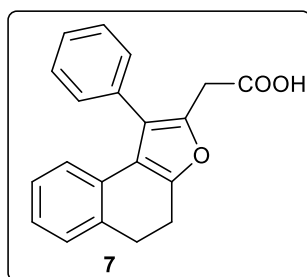
^1H NMR (400 MHz, CDCl_3); δ 7.50 (d, $J = 7.2$ Hz, 2H), 7.46-7.30 (m, 1H), 7.27 (d, $J = 18.8$ Hz, 1H), 7.21 (d, $J = 9.6$ Hz, 1H), 7.10 (d, $J = 8.4$ Hz, 2H), 7.02-6.91 (m, 2H), 4.79 (s, 1H), 3.65 (t, $J = 6.8$ Hz, 2H), 3.02 (t, $J = 8.0$ Hz, 2H), 2.82 (t, $J = 8.0$ Hz, 2H), 2.69 (t, $J = 6.8$ Hz, 2H).

^{13}C NMR (400 MHz, CDCl_3); δ 152.1, 133.8, 133.1, 131.2, 129.8, 128.7, 128.4, 127.9, 127.3, 126.3, 125.4, 123.5, 123.3, 61.1, 33.6, 28.1, 26.3.

HRMS calcd. $\text{C}_{20}\text{H}_{19}\text{O}_2$, 291.13850; found 291.13861 [$\text{M} + \text{H}$]

2-(1-phenyl-4,5-dihydronaphtho[2,1-b]furan-2-yl)acetic acid (7):

Compound **7** was synthesized according to the general procedure by taking **5a** (180mg, 0.54 mmol, 1 equiv.), KOH (30 mg, 0.54 mmol, 1 equiv.) in EtOH/ H_2O (3.6:0.4 ml).



White solid; Yield: 70% (115.0 mg, 0.37 mmol).

IR (neat, cm^{-1}) 3010, 2278, 1715, 1627, 1409, 1271, 1136, 1047.

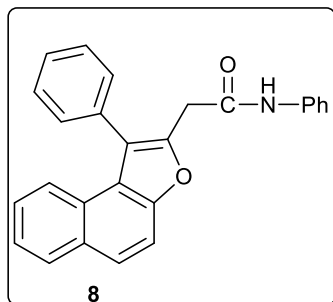
^1H NMR (400 MHz, CDCl_3); δ 12.64 (s, 1H), 7.49-7.39 (m, 3H), 7.36-7.34 (m, 2H), 7.22 (d, $J = 7.2$ Hz, 1H), 7.04-7.00 (m, 1H), 6.93 (t, $J = 7.6$ Hz, 1H), 6.70 (d, $J = 6.8$ Hz, 1H), 3.51 (s, 2H), 3.05 (t, $J = 7.6$ Hz, 2H), 2.86 (t, $J = 7.6$ Hz, 2H).

^{13}C NMR (400 MHz, CDCl_3); δ 170.7, 152.2, 144.7, 133.6, 132.5, 130.6, 129.3, 128.6, 128.2, 127.5, 126.1, 125.5, 121.7, 121.0, 116.9, 32.2, 28.9, 21.4.

HRMS calcd. $\text{C}_{20}\text{H}_{17}\text{O}_3$, 305.11777; found 305.11726 [$\text{M} + \text{H}$]

N-phenyl-2-(1-phenylnaphtho[2,1-b]furan-2-yl)acetamide (8):

Compound **8** was synthesized according to the general procedure by taking **5a** (50 mg, 0.16 mmol, 1 equiv.), aniline (20 μ l, 0.16 mmol, 1 equiv.) and Et₃N (45 μ l, 0.328 mmol, 2 equiv.). SOCl₂ (23 μ l, 0.328 mmol, 2 equiv.) in DCM (3 mL)



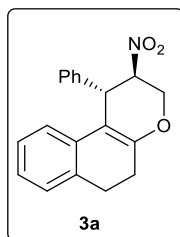
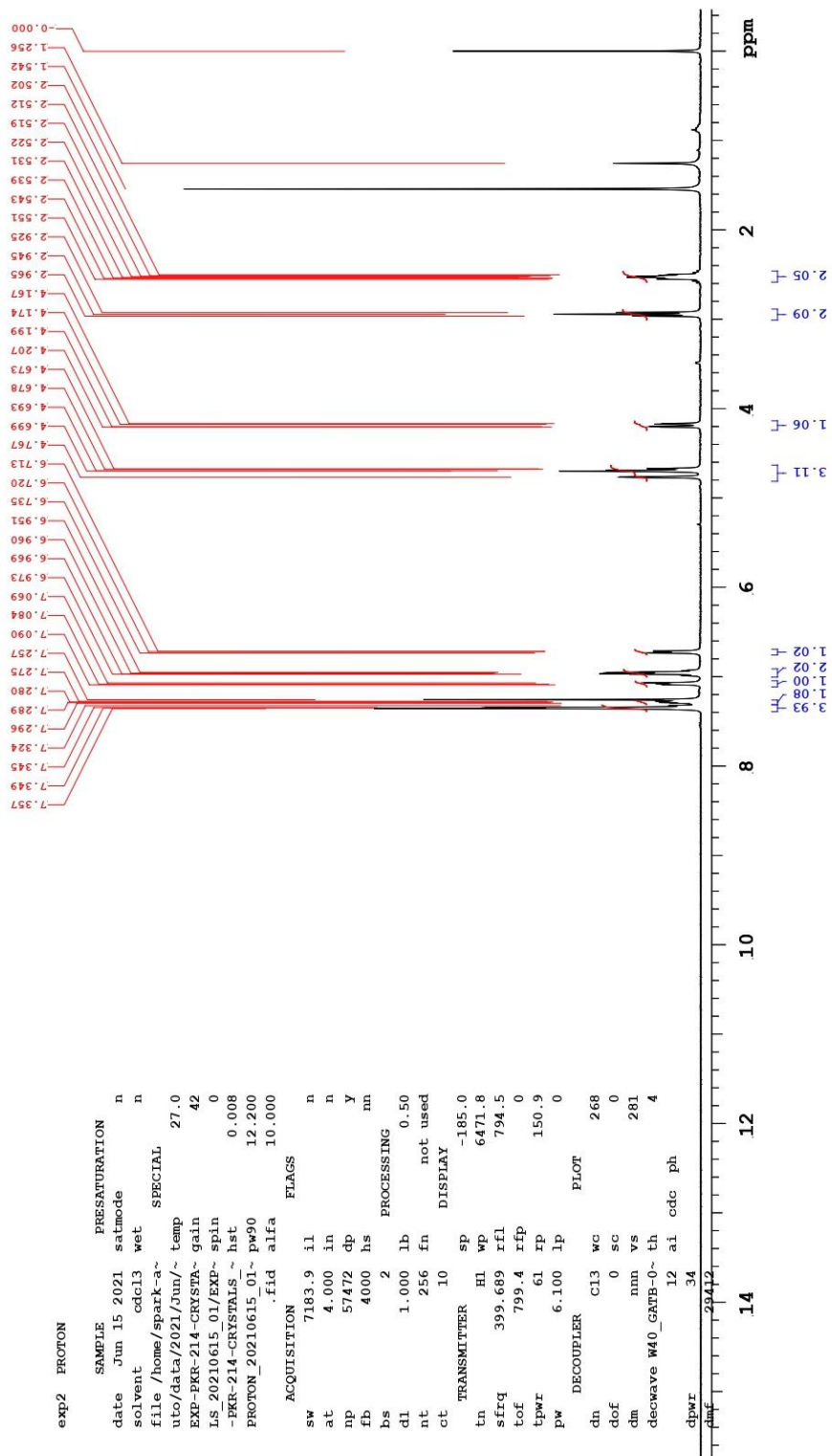
Light yellow solid; Yield: 67% (42.0 mg, 0.11 mmol).

IR (neat, cm⁻¹) 3018, 2284, 1715, 1626, 1410, 1267, 1129, 1047.

¹H NMR (400 MHz, CDCl₃); δ 7.39-7.30 (m, 5H), 7.29-7.16 (m, 4H), 7.15-6.99 (m, 5H), 6.81 (d, *J* = 8.8 Hz, 2H), 5.17 (s, 1H), 2.39 (s, 2H).

¹³C NMR (400 MHz, CDCl₃); δ 170.8, 159.6, 157.5, 136.6, 134.6, 129.8, 128.5, 128.3, 125.8, 125.3, 124.1, 121.1, 114.4, 34.6.

HRMS calcd. C₂₆H₁₉NO₂, 378.14940; found 378.14959 [M + H]

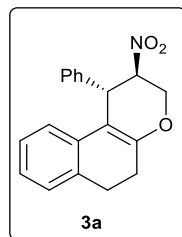


¹H NMR Spectrum of compound **3a**

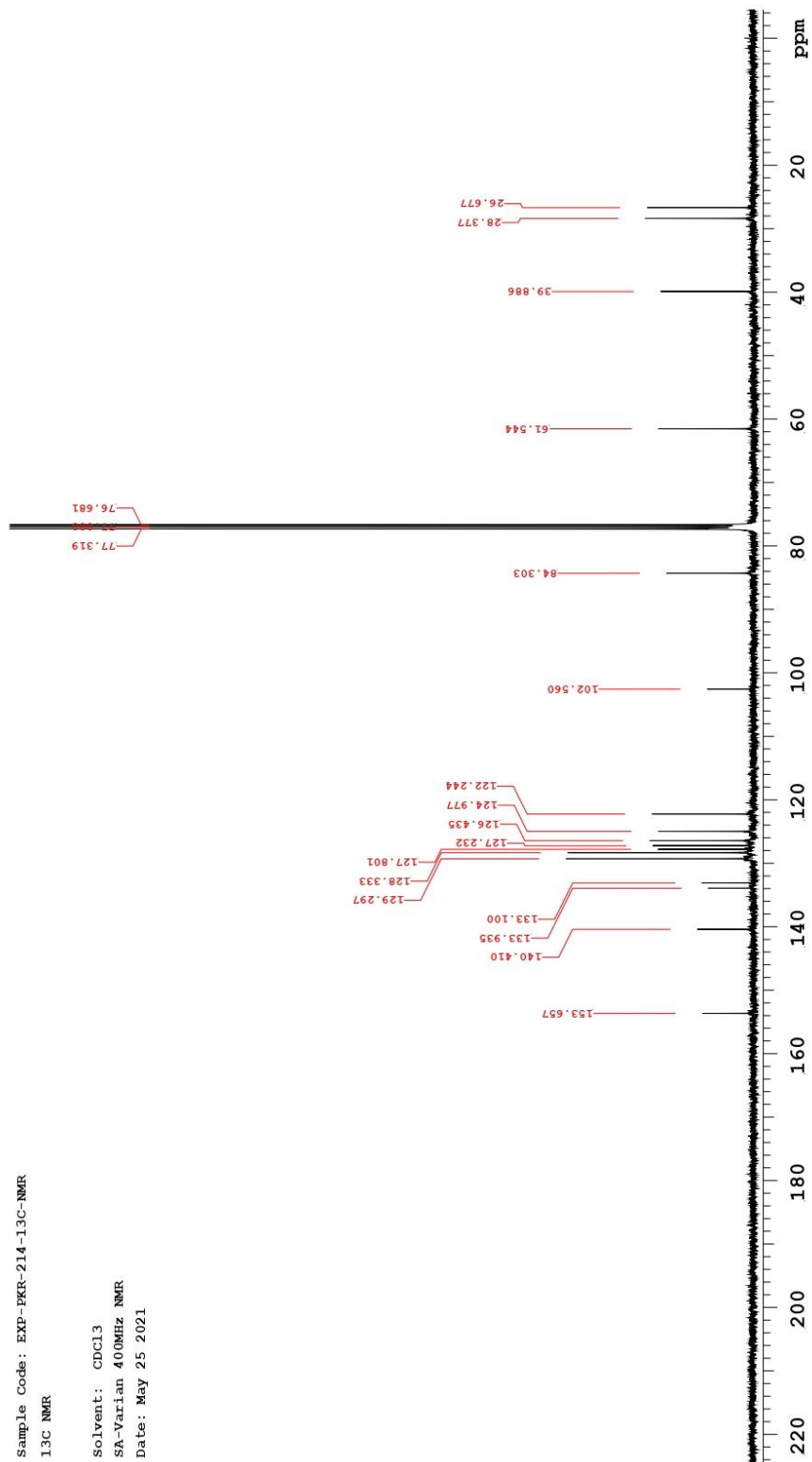
Plotname: EXP-EKR-214-CRYSTALS_PROTON_20210615_01_plot05

Sample Code: EXP-FKR-214-13C-NMR
13C NMR

Solvent: CDCl₃
SA-Varian 400MHz NMR
Date: May 25 2021

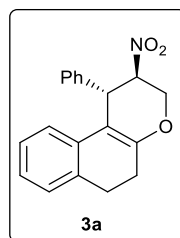
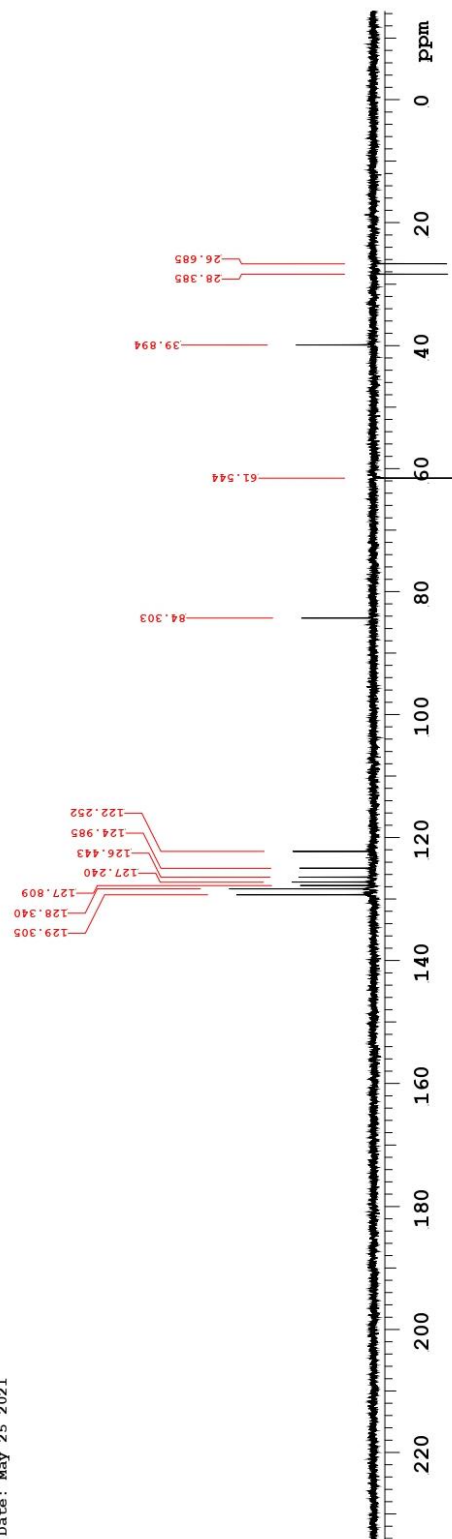


¹³C NMR Spectrum of compound **3a**



Plotname: EXP-FKR-214-13C-NMR_CARBON_20210525_01_plot01

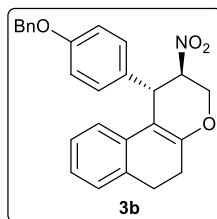
Sample Code: EXP-PKR-214-DEPT-135
DEPT 135
VIGNAN'S UNIVERSITY
Solvent: cdcl3
SA-Varian 400MHz NMR
Date: May 25 2021



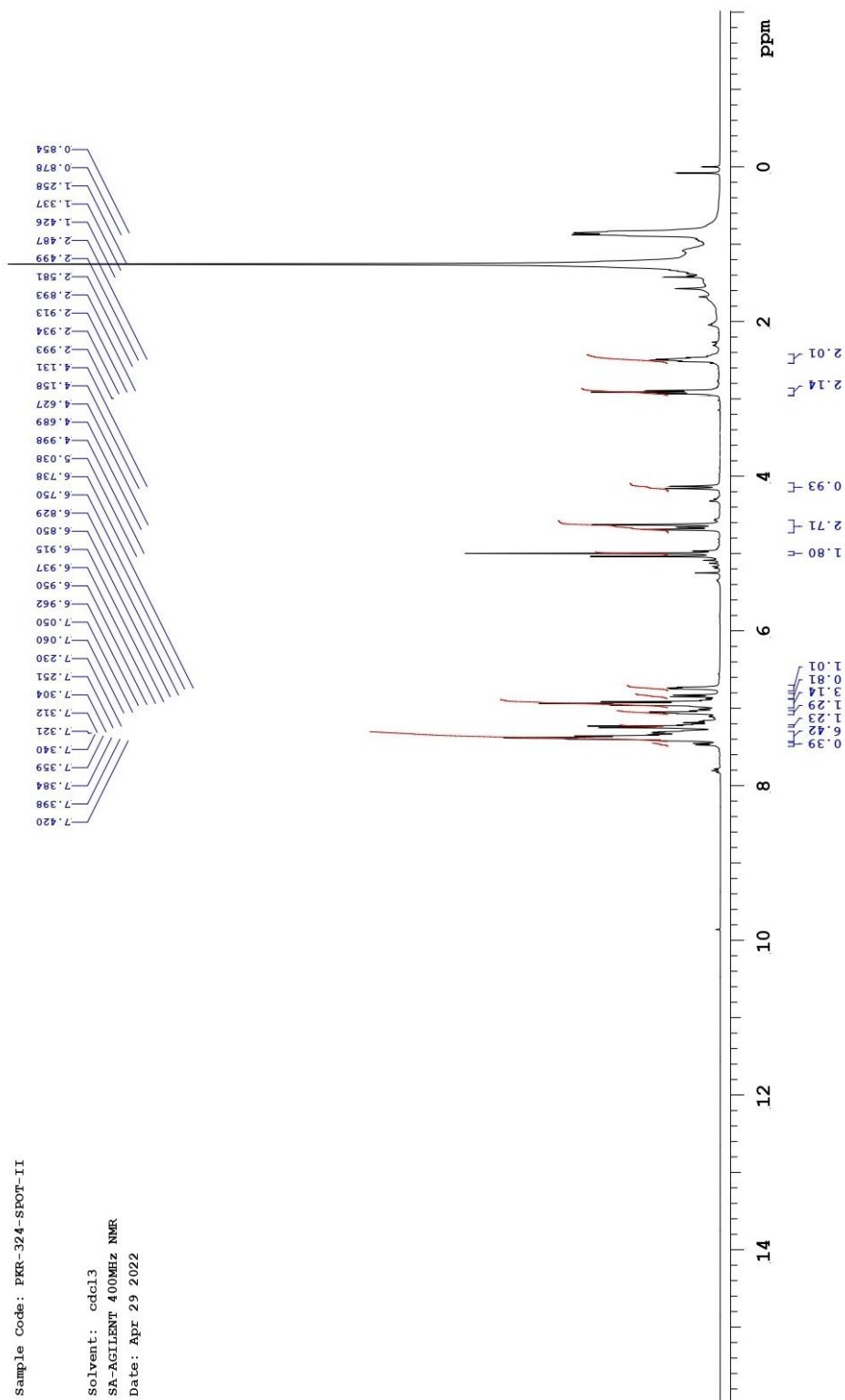
Dept-135 NMR Spectrum of compound **3a**

Sample Code: PKR-324-SPOT-II

Solvent: cdcl3
SA-AGILENT 400MHz NMR
Date: Apr 29 2022

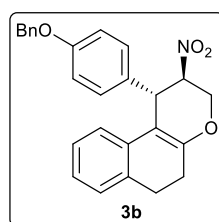


¹H NMR Spectrum of compound **3b**

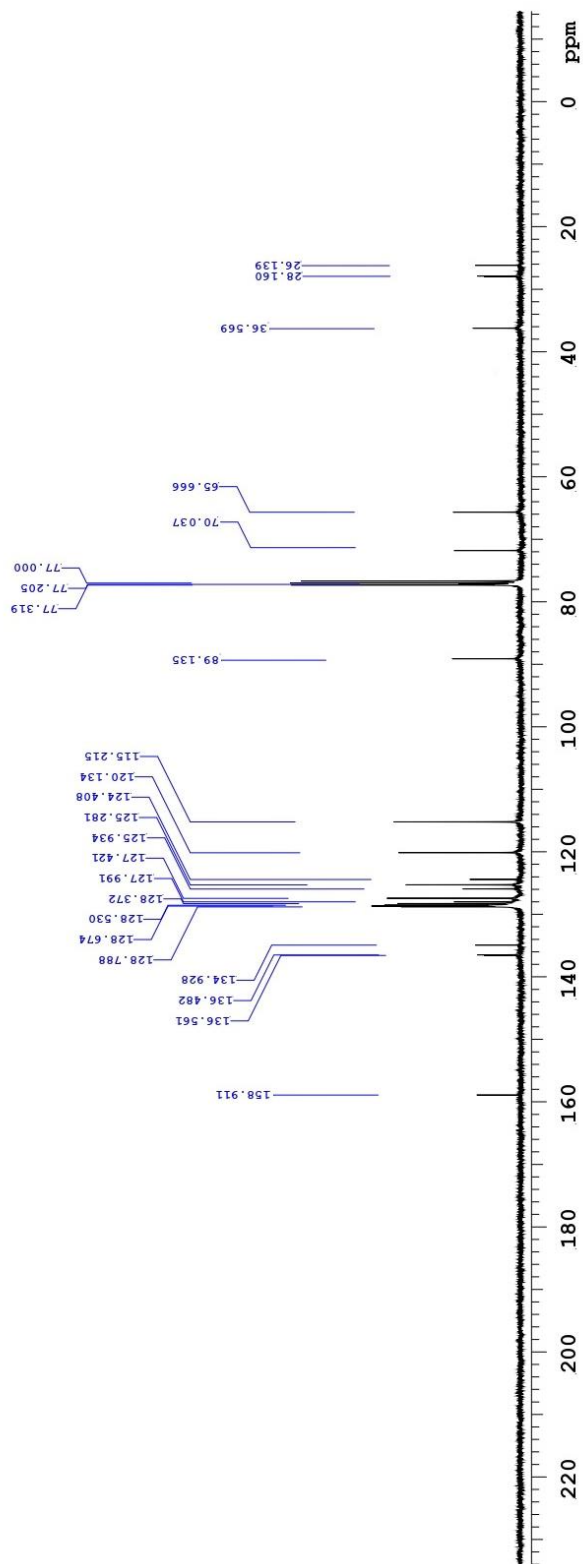


Plotname: PKR-324-SPOT-II_PROTON_20220429_01_plot01

Solvent: cdcl3
SA-Varian 400MHz NMR
Date: Jul 29 2022



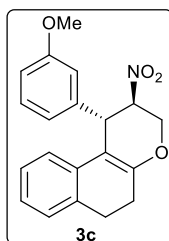
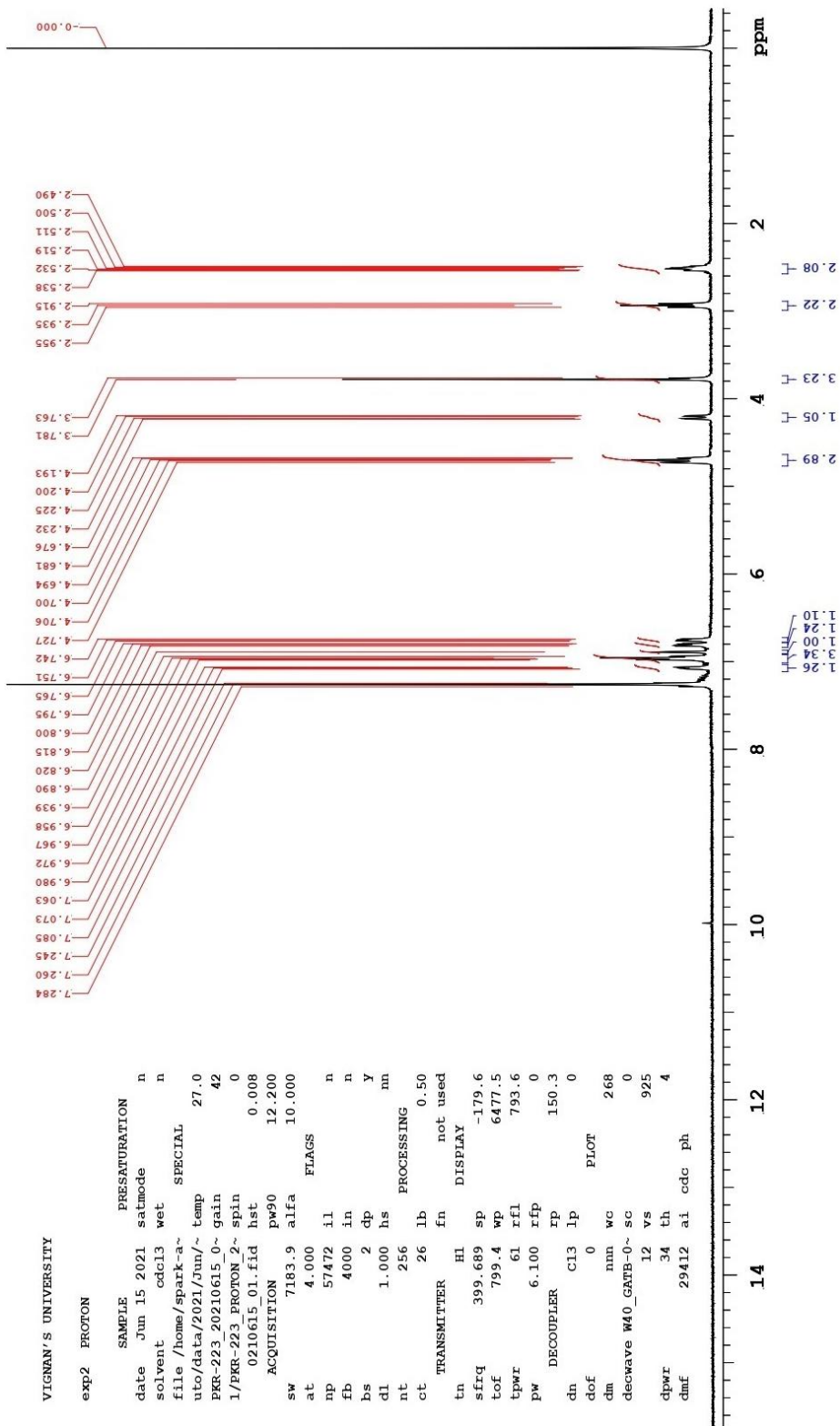
¹³C NMR Spectrum of compound **3b**



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exp2 PROTON

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uto/data/2021/Jun/~ temp 27.0
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1/PKR-223 PROTON 2~ spin 0
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sw 7183.9 alfa 10.000
at 4.000
np 57472 il n
fb 4000 in n
bs 2 dp y
dl 1.000 hs nm
nt 256
ct 26 lb 0.50
tn TRANSMITTER fn not used
HI DISPLAY
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tof 799.4 wp 6477.5
tpwr 61 rfl 793.6
pw 6.100 rfp 0
DECOUPLER rp 150.3
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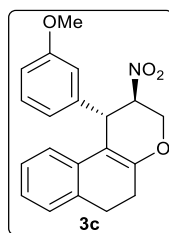


¹H NMR Spectrum of compound 3c

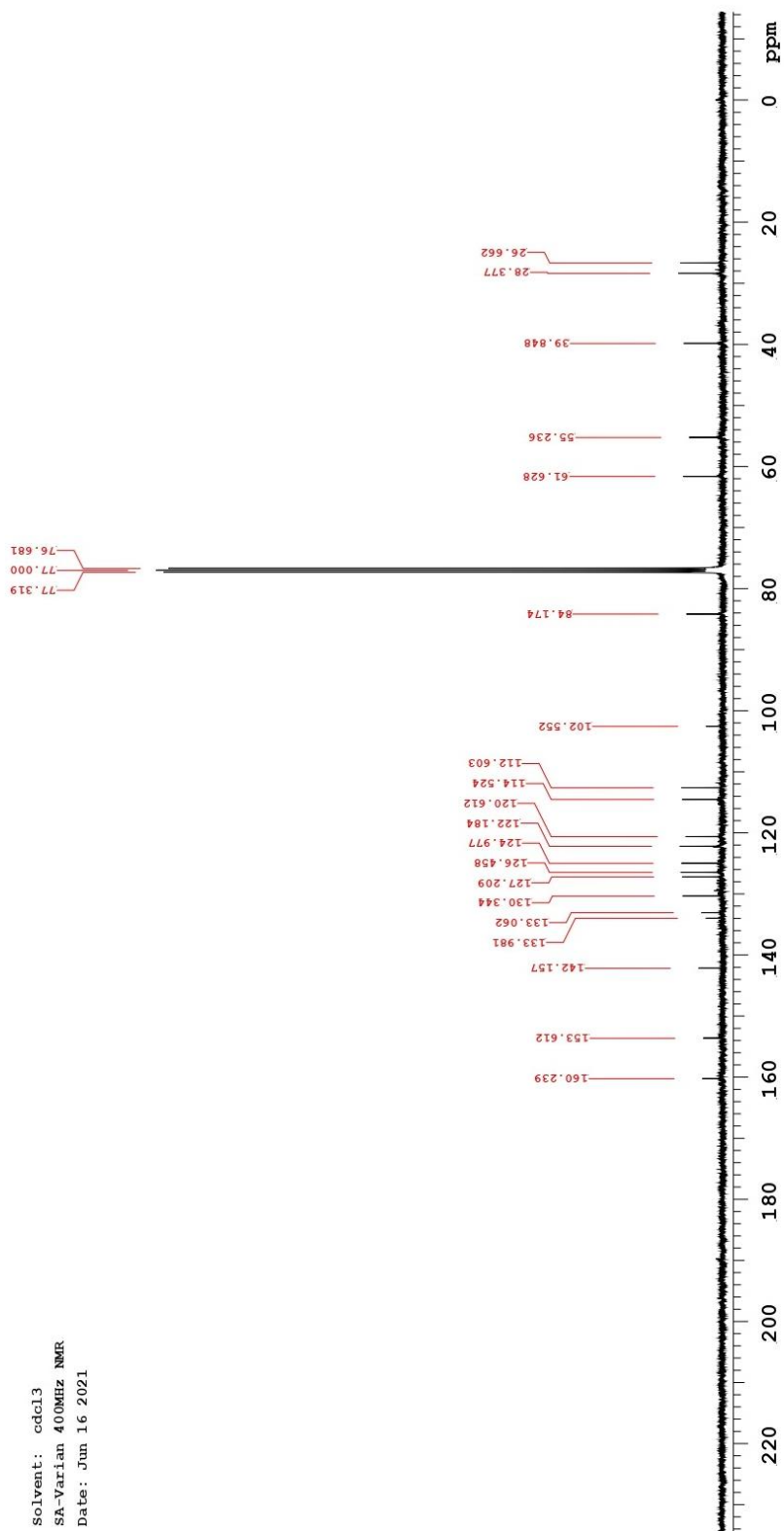
Plotname: PKR-223_PROTON_20210615_01_plot05

Sample Code: PKR-223-13c-NMR
13C NMR

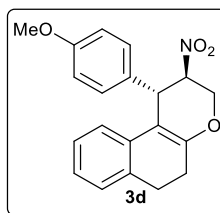
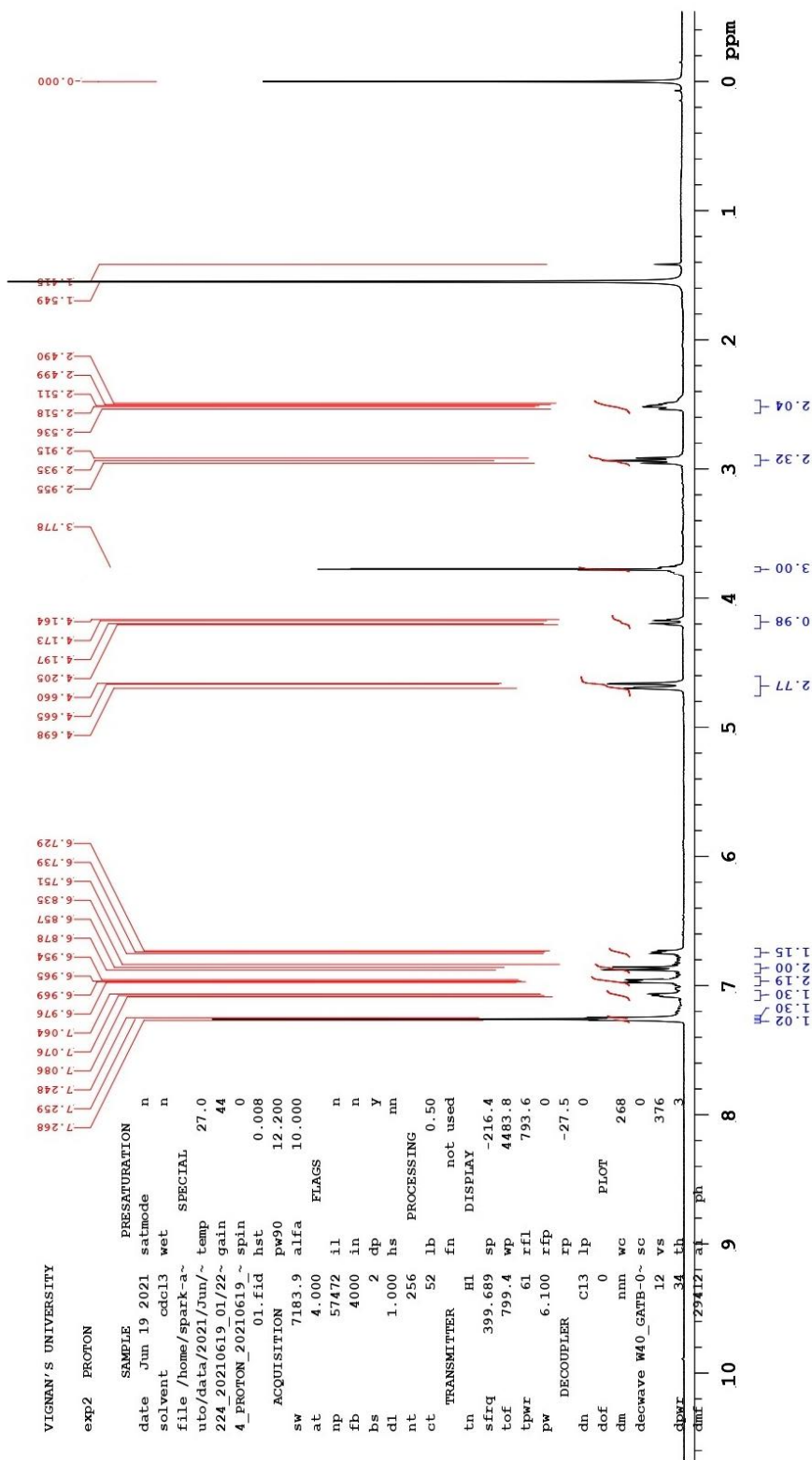
Solvent: cdcl3
SA-Varian 400MHz NMR
Date: Jun 16 2021



¹³C NMR Spectrum of compound **3c**



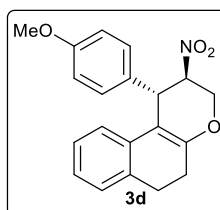
Plotname: PKR-223-13c-NMR_CARBON_20210616_01_plot01



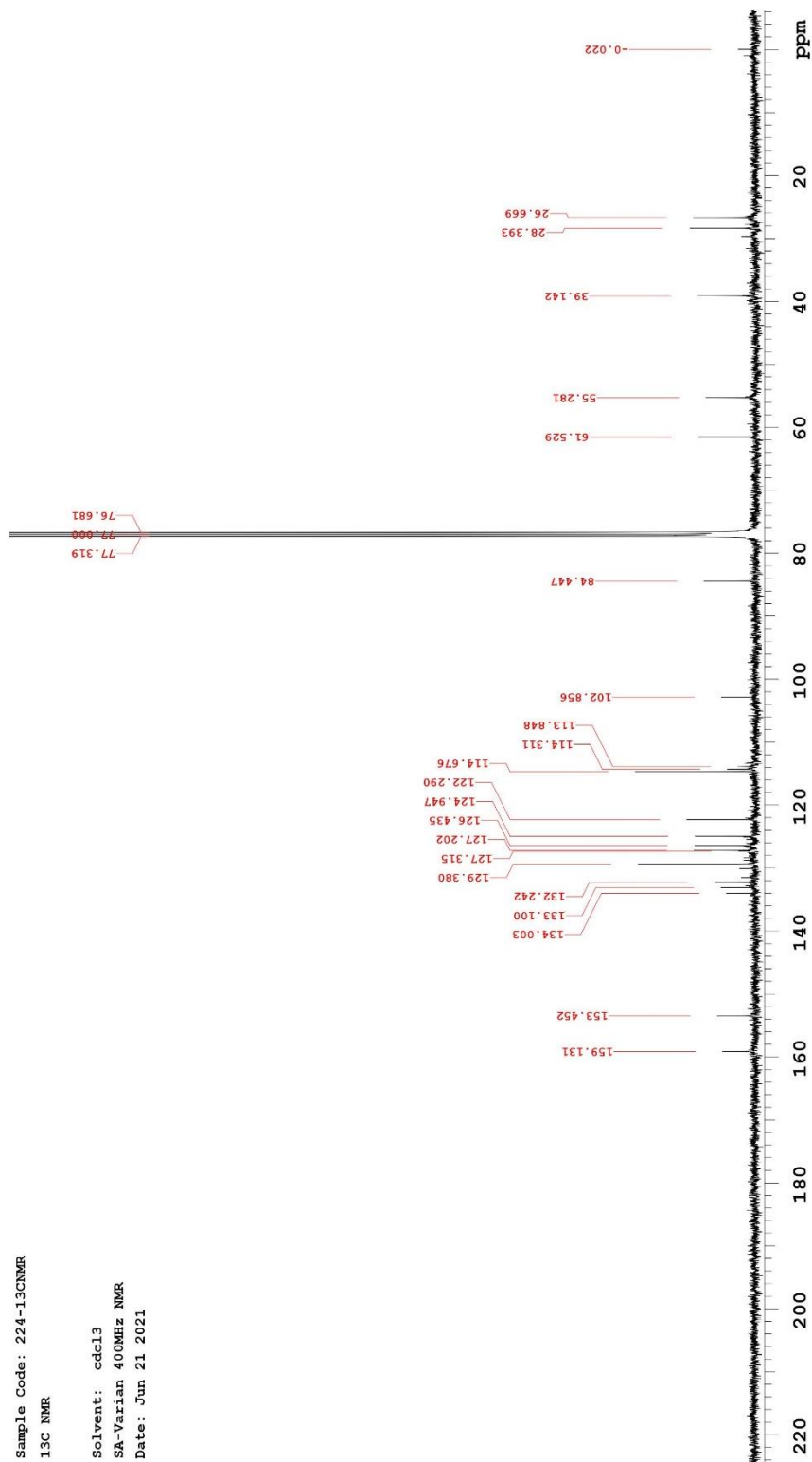
¹H NMR Spectrum of compound **3d**

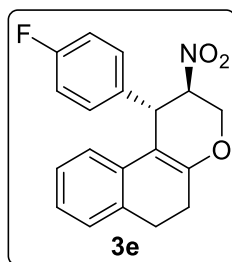
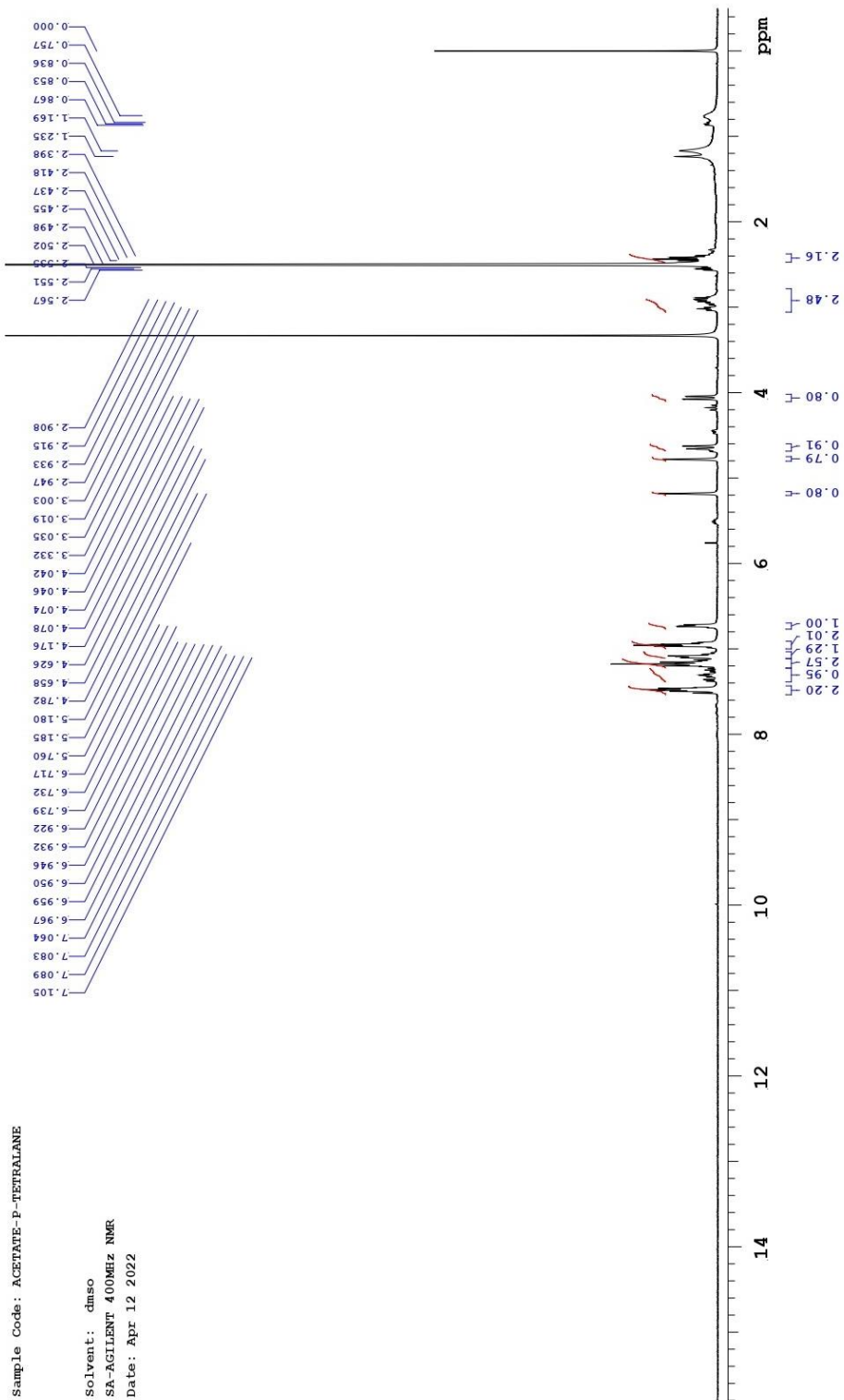
Sample Code: 224-13CNMR
13C NMR

Solvent: cdcl3
SA-Varian 400MHz NMR
Date: Jun 21 2021

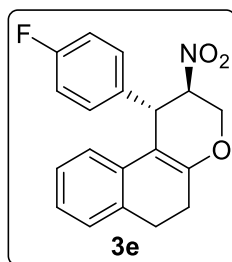
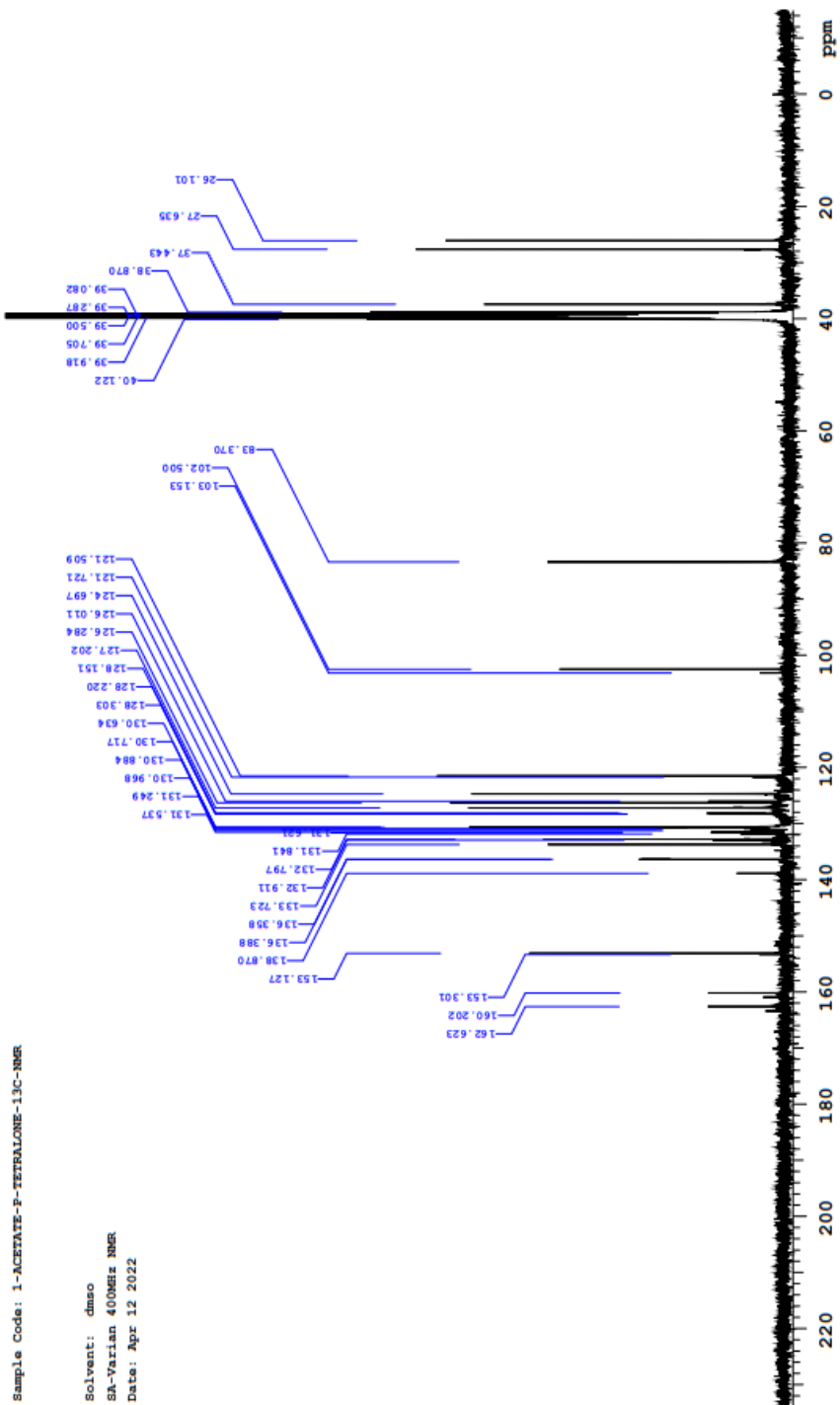


¹³C NMR Spectrum of compound **3d**

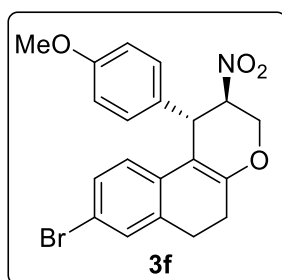
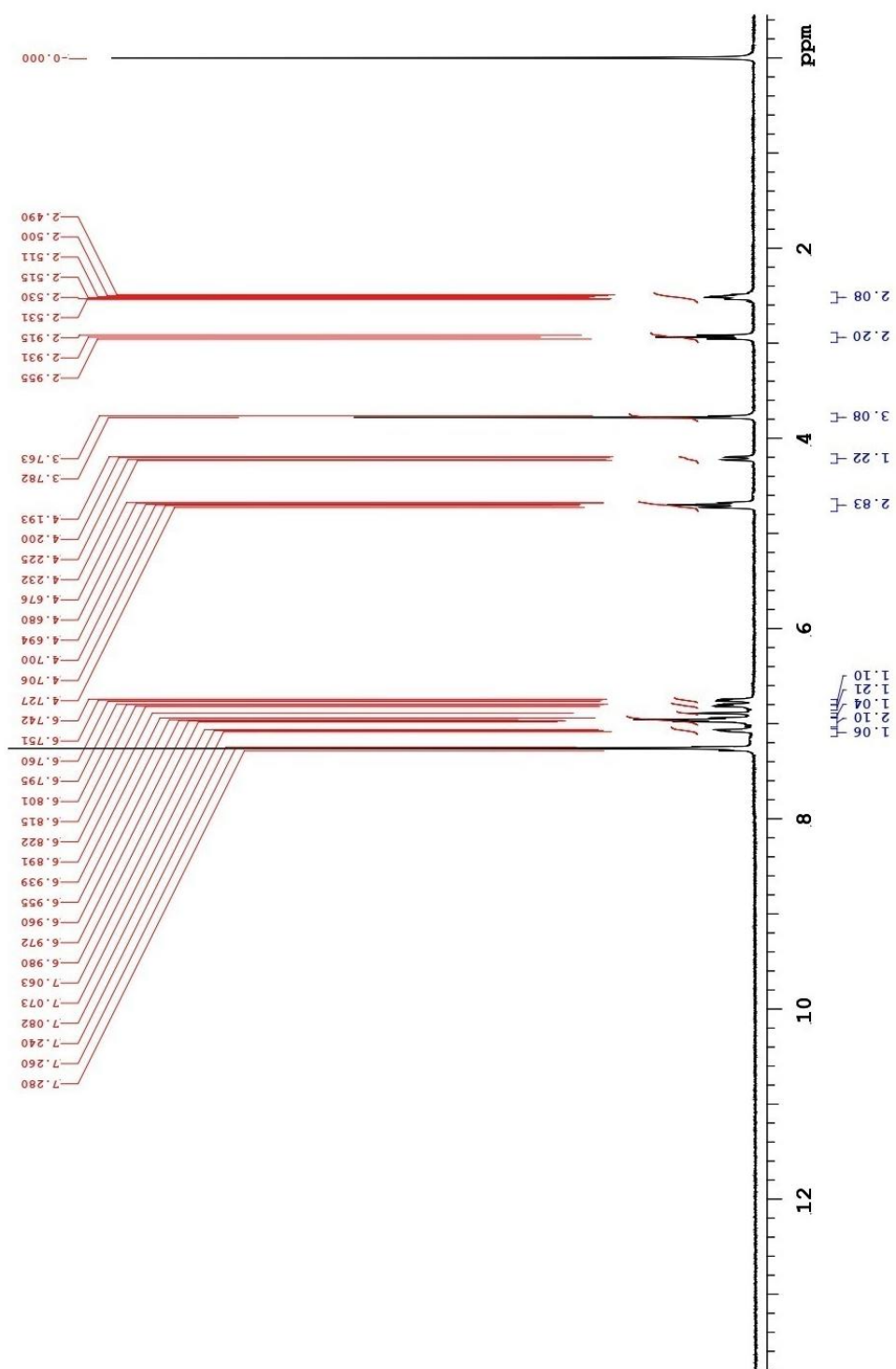




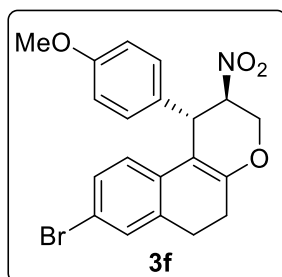
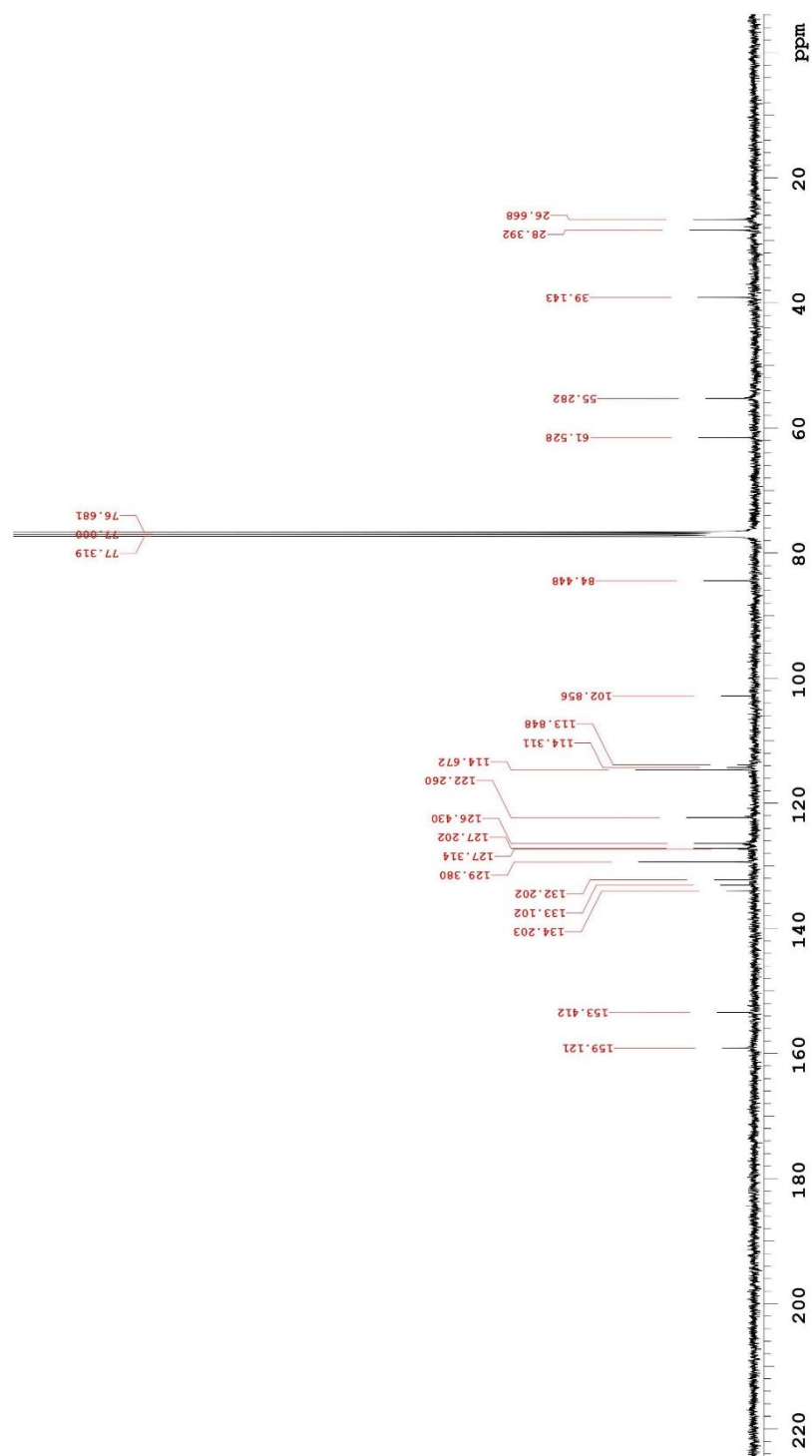
¹H NMR Spectrum of compound **3e**



¹³C NMR Spectrum of compound **3e**



¹H NMR Spectrum of compound 3f



¹³C NMR Spectrum of compound 3e

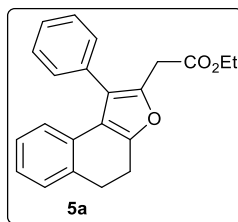
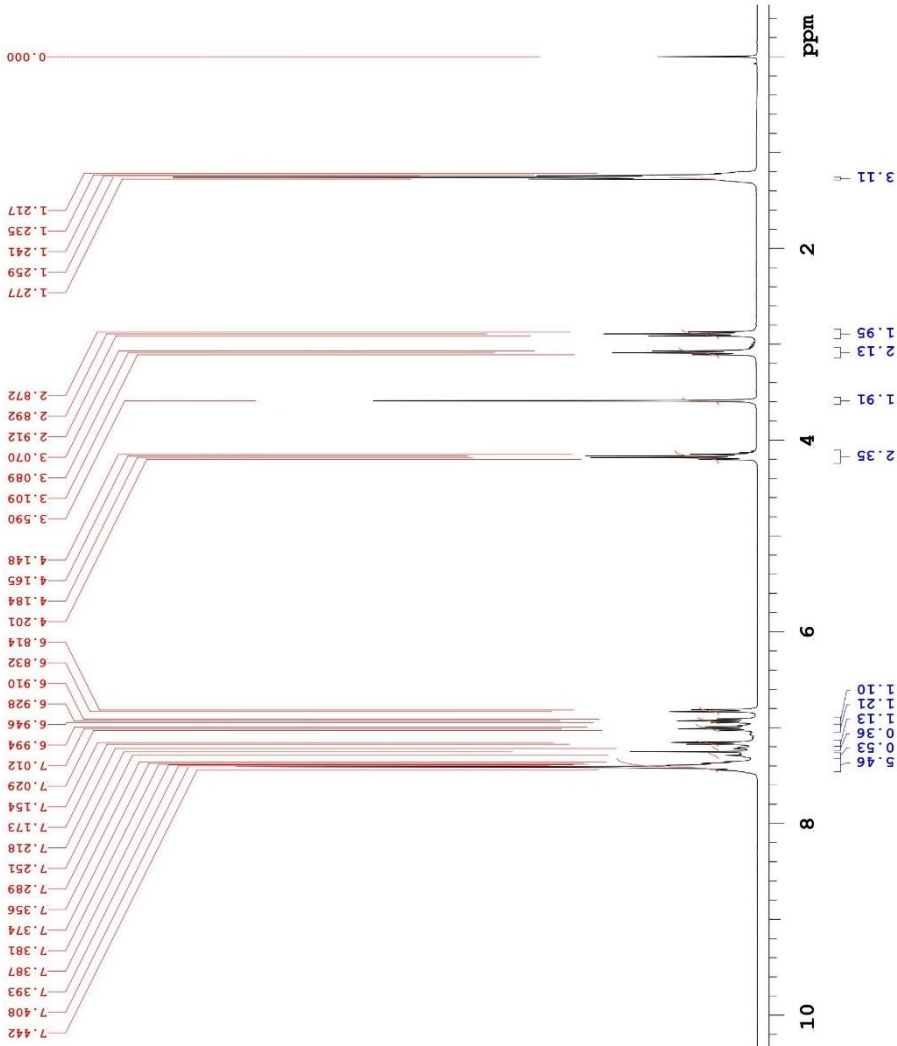
VIGNAN'S UNIVERSITY

exp2 PROTON

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ACQUISITION pw90 12.200
sw 7183.9 alfa 10.000
at 4.000 FLAGS
np 57472 il n
fb 4000 in n
bs 2 dp Y
dl 1.000 hs mn
nt 256 PROCESSING
ct 34 lb 0.50
tn TRANSMITTER fn not used
H1 DISPLAY
sfrq 399.689 sp -215.7
tof 799.3 wp 6553.4
tpwr 61 rfl 797.6
pw 6.100 rfp 0
DECOUPLER rp 66.1
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dmf 29412 ai cdc ph 4

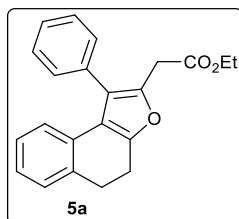
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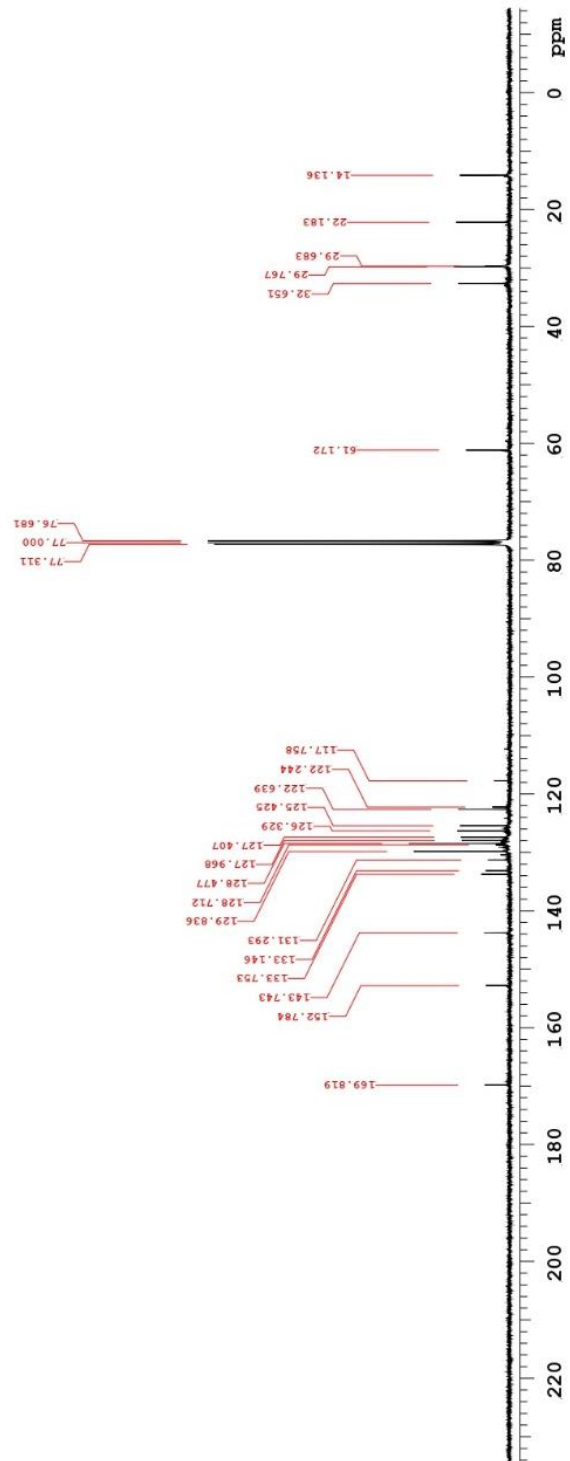
¹H NMR Spectrum of compound **5a**

Plotname: PKR-219_PROTON_20210601_01_plot05

Sample Code: PKR-219-13C-NMR
13C NMR
VIGNAN'S UNIVERSITY
Solvent: cdcl3
SA-Varian 400MHZ NMR
Date: Jun 2 2021

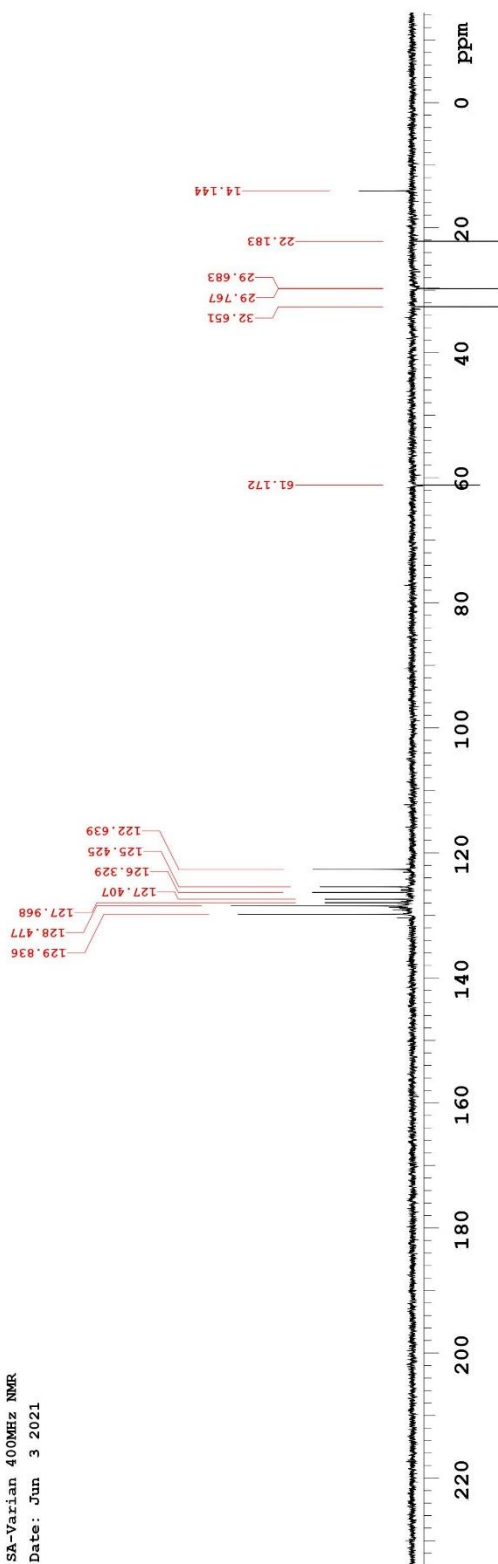
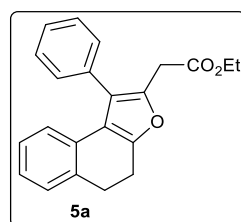


¹³C NMR Spectrum of compound 5a

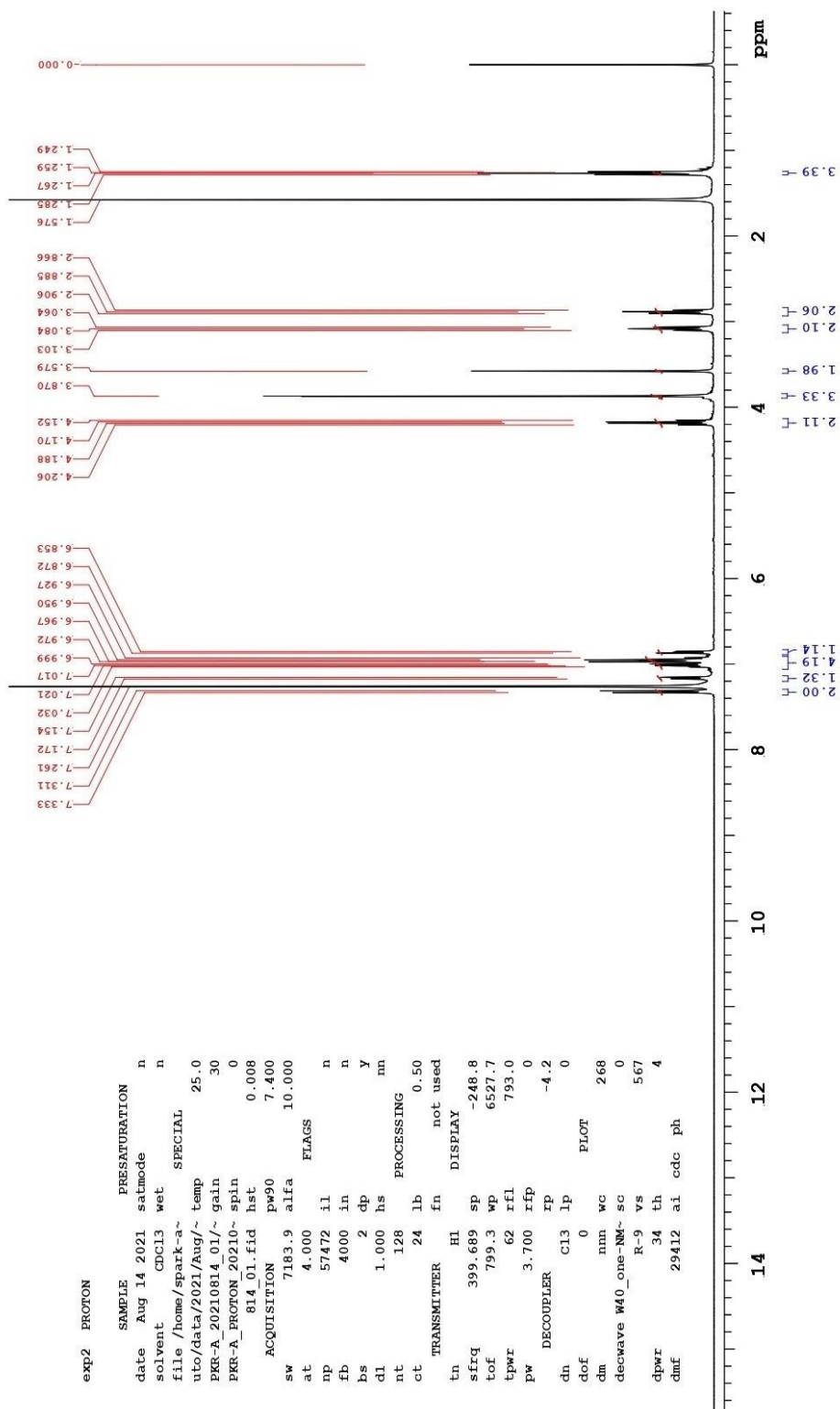


Plotname: PKR-219-13C-NMR CARBON_20210602_01_plot01

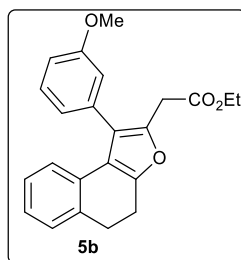
Sample Code: PKR-219-DEPT-135
DEPT 135
VIGNAN'S UNIVERSITY
Solvent: CDCl3
SA-Varian 400MHz NMR
Date: Jun 3 2021



Dept-135 NMR Spectrum of compound 5a



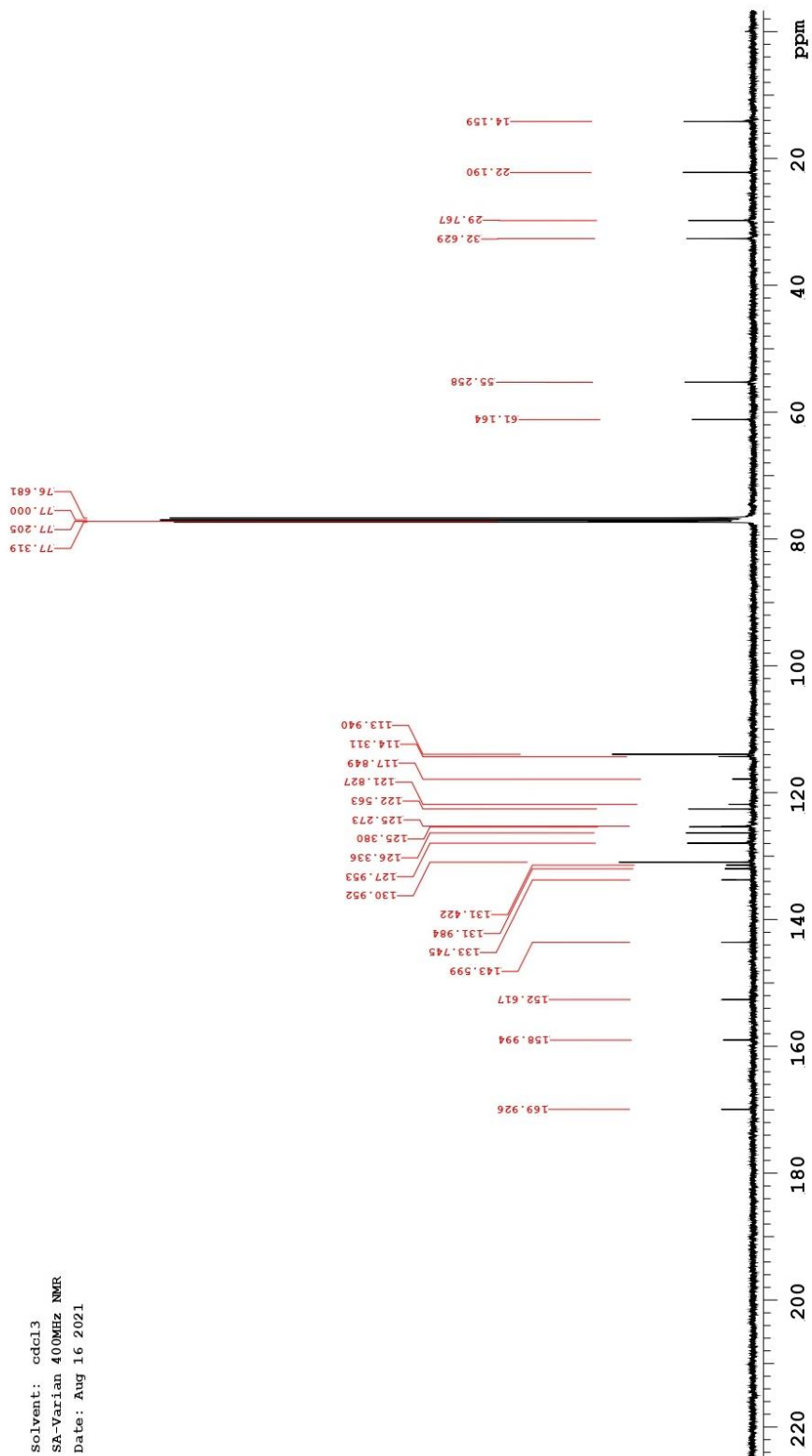
Plotname: PRR-A_PROTON_20210814_01_plot05



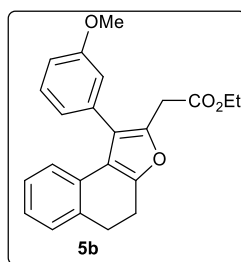
¹H NMR Spectrum of compound **5b**

Sample Code: PKR-A-13CNMR

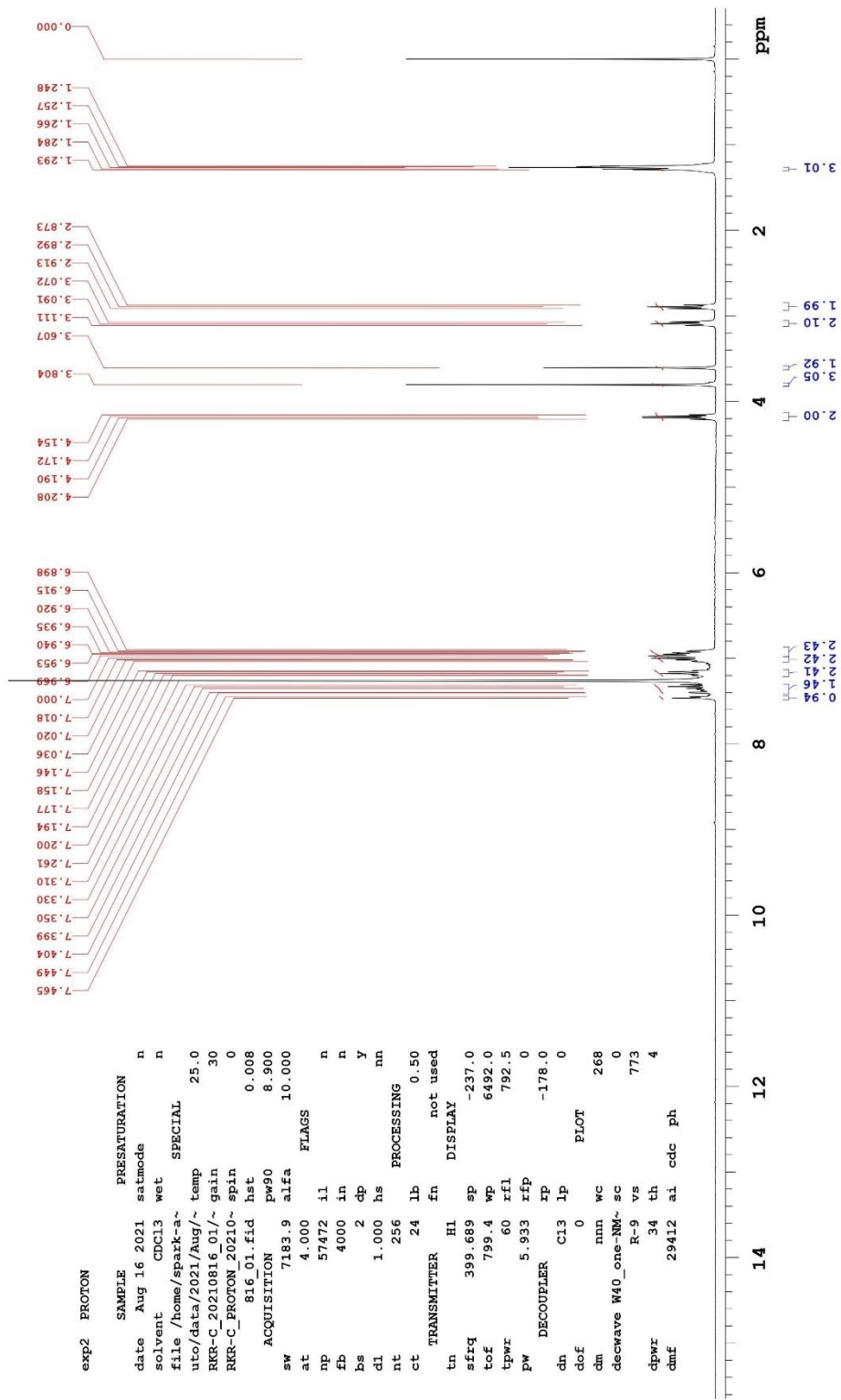
Solvent: cdcl3
SA-Varian 400MHz NMR
Date: Aug 16 2021



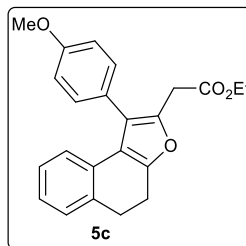
Plotname: PKR-A-13CNMR_CARBON_20210816_01_plot01



^{13}C NMR Spectrum of compound **5b**



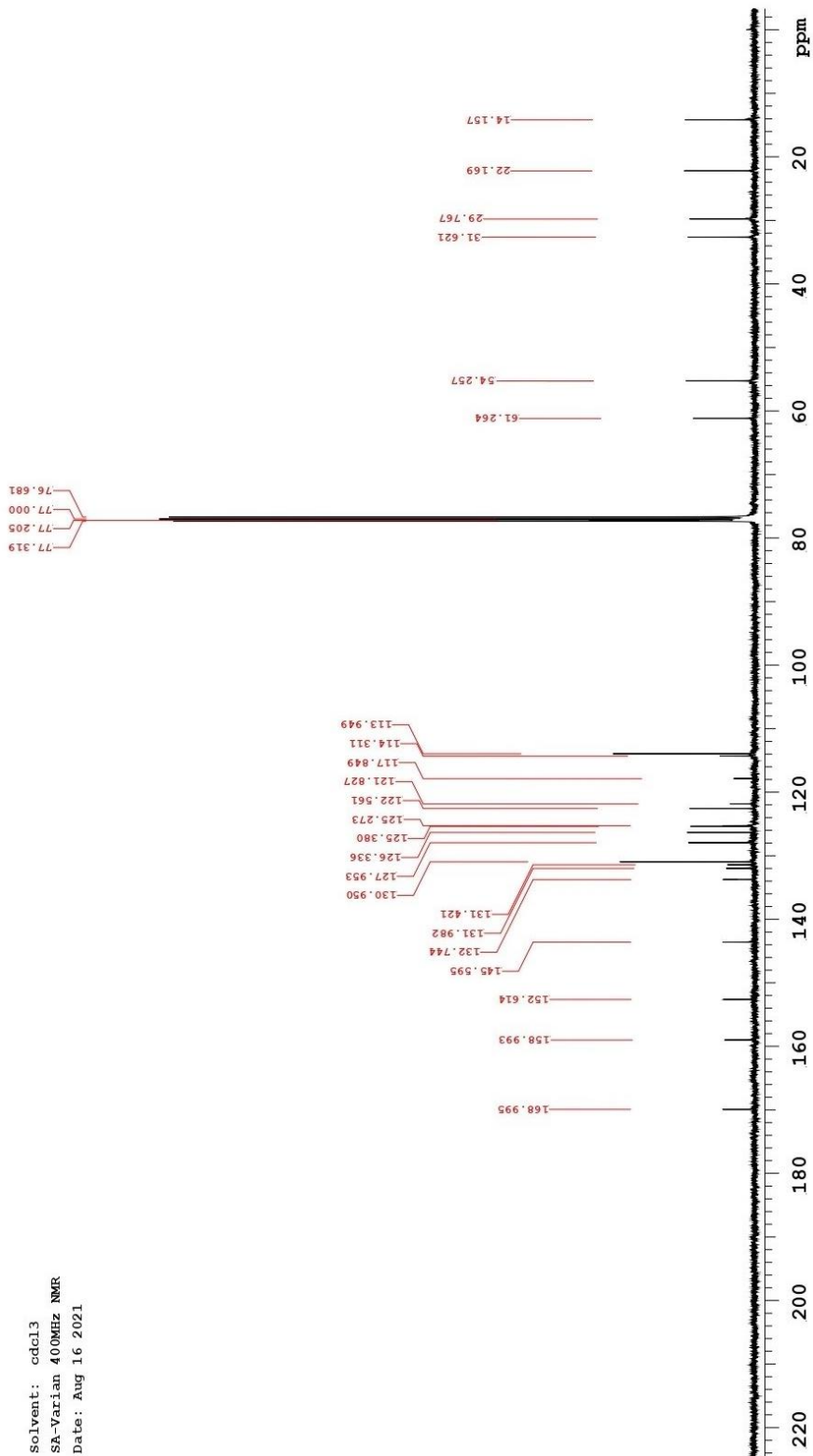
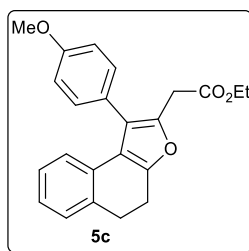
Plotname: RKR-C_PROTON_20210816_01_Plot07



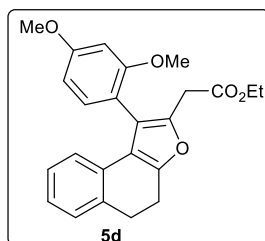
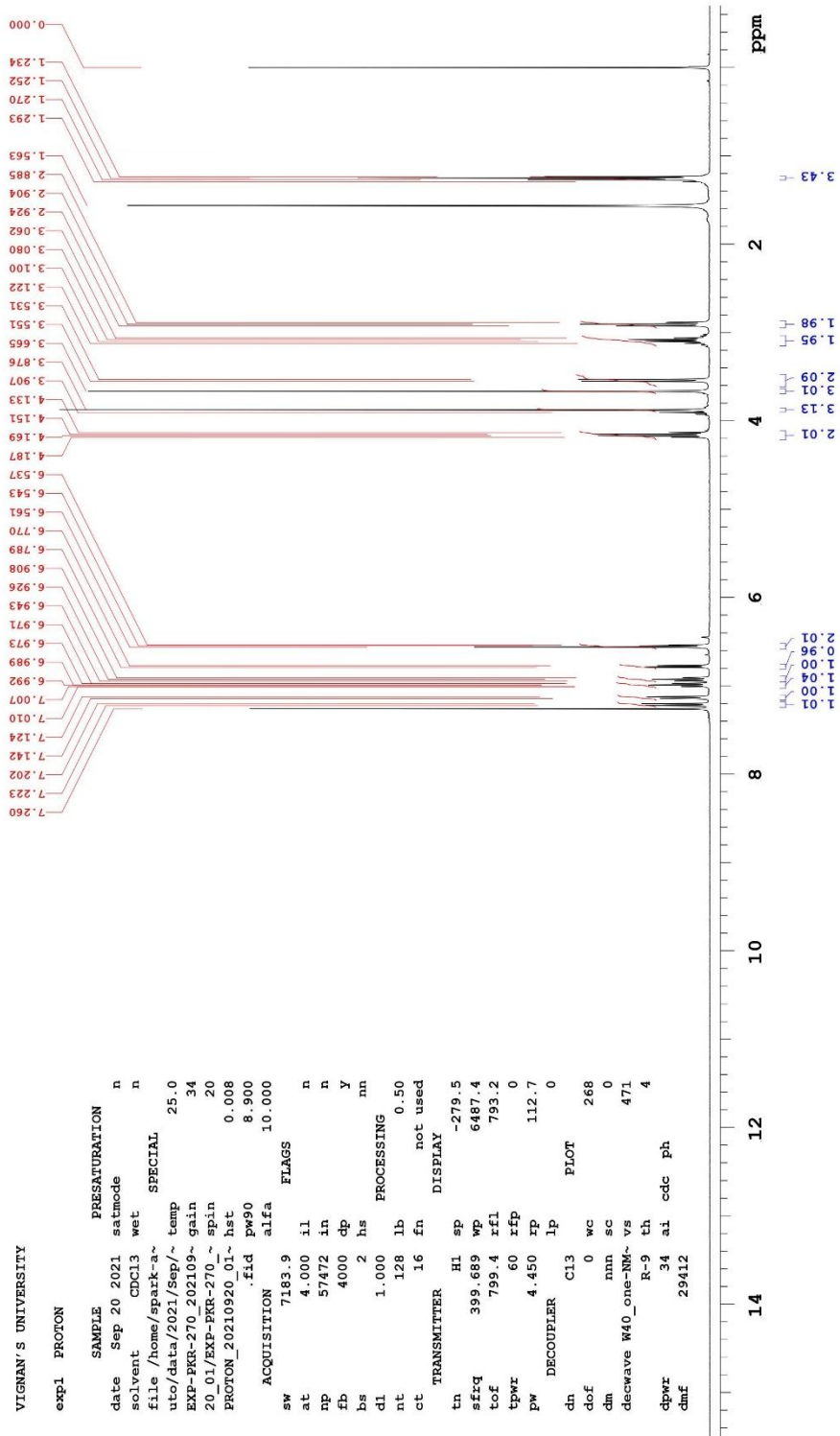
¹H NMR Spectrum of compound 5c

Sample Code : PRR-C-13CNMR

Solvent: cdcl3
SA-Varian 400MHz NMR
Date: Aug 16 2021

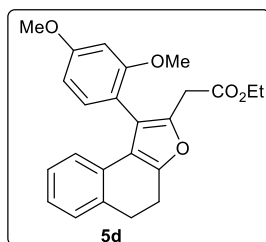


¹³C NMR Spectrum of compound **5c**

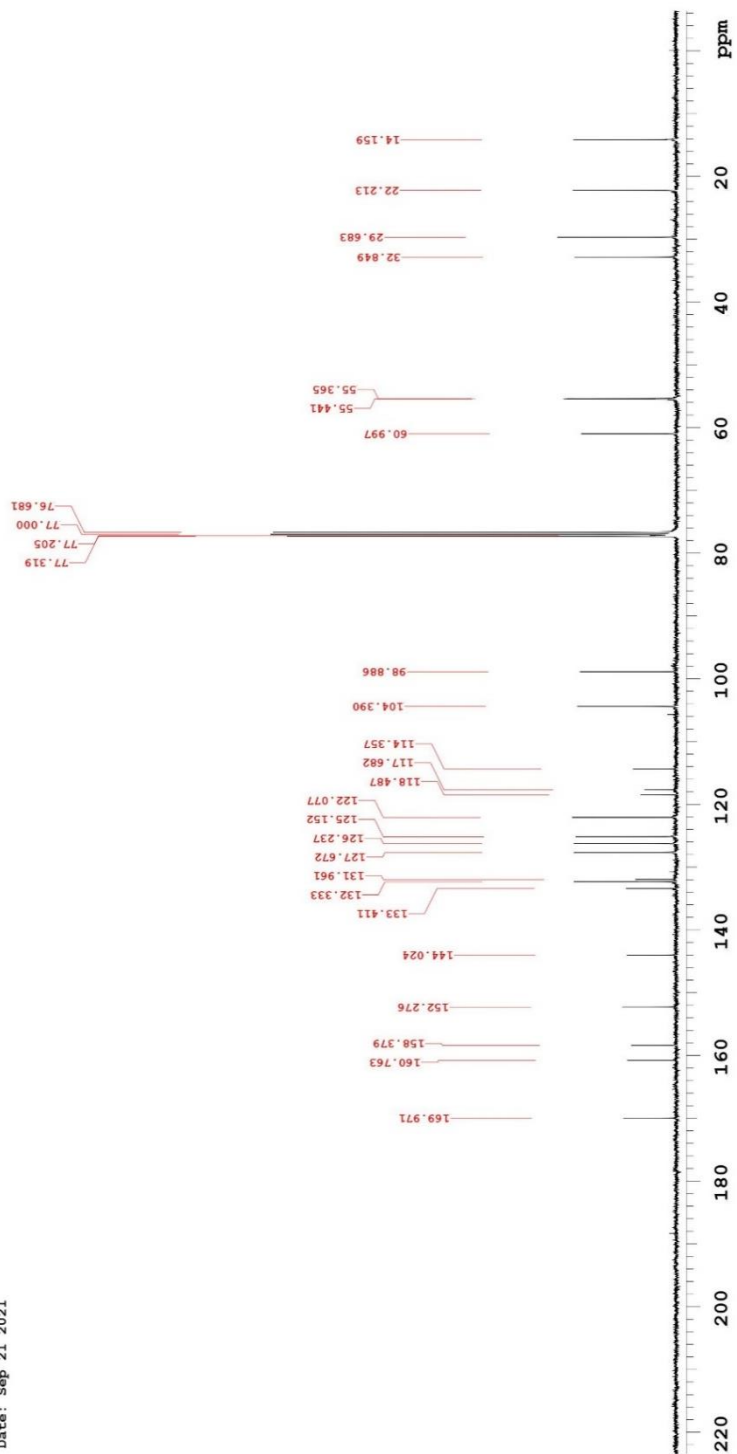


^1H NMR Spectrum of compound **5d**

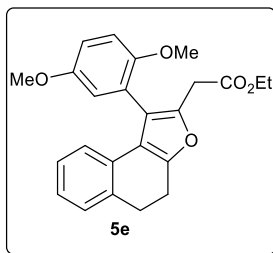
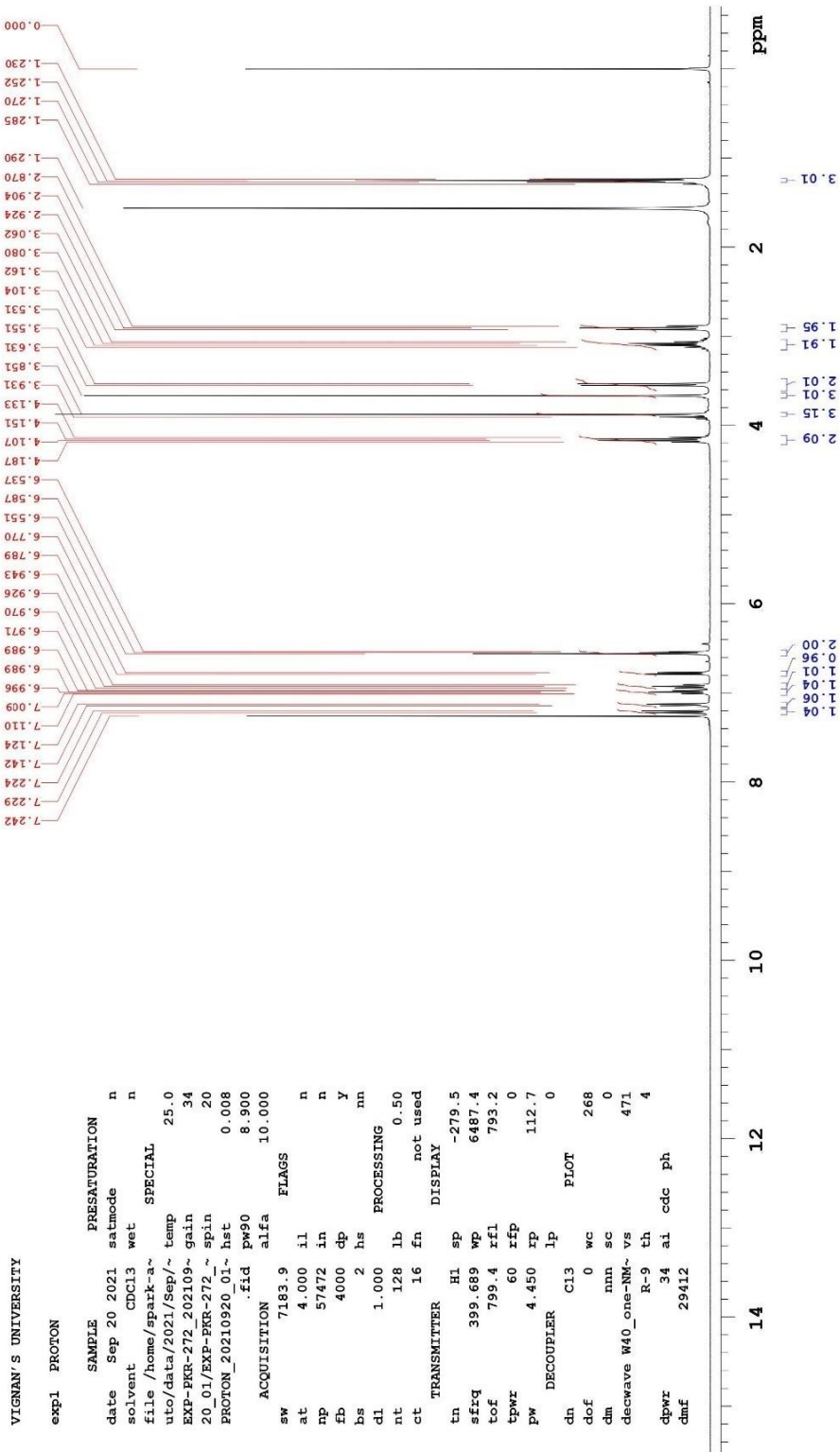
Sample Code: EXP-PKR-270-13C-NMR
13C NMR
VIGNAN'S UNIVERSITY
Solvent: CDCl3
SA-Varian 400MHz NMR
Date: Sep 21 2021



¹³C NMR Spectrum of compound **5d**

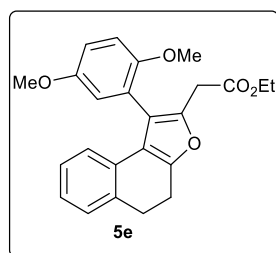


Plotname: EXP-PKR-270-13C-NMR_CARBON_20210921_01_plot01

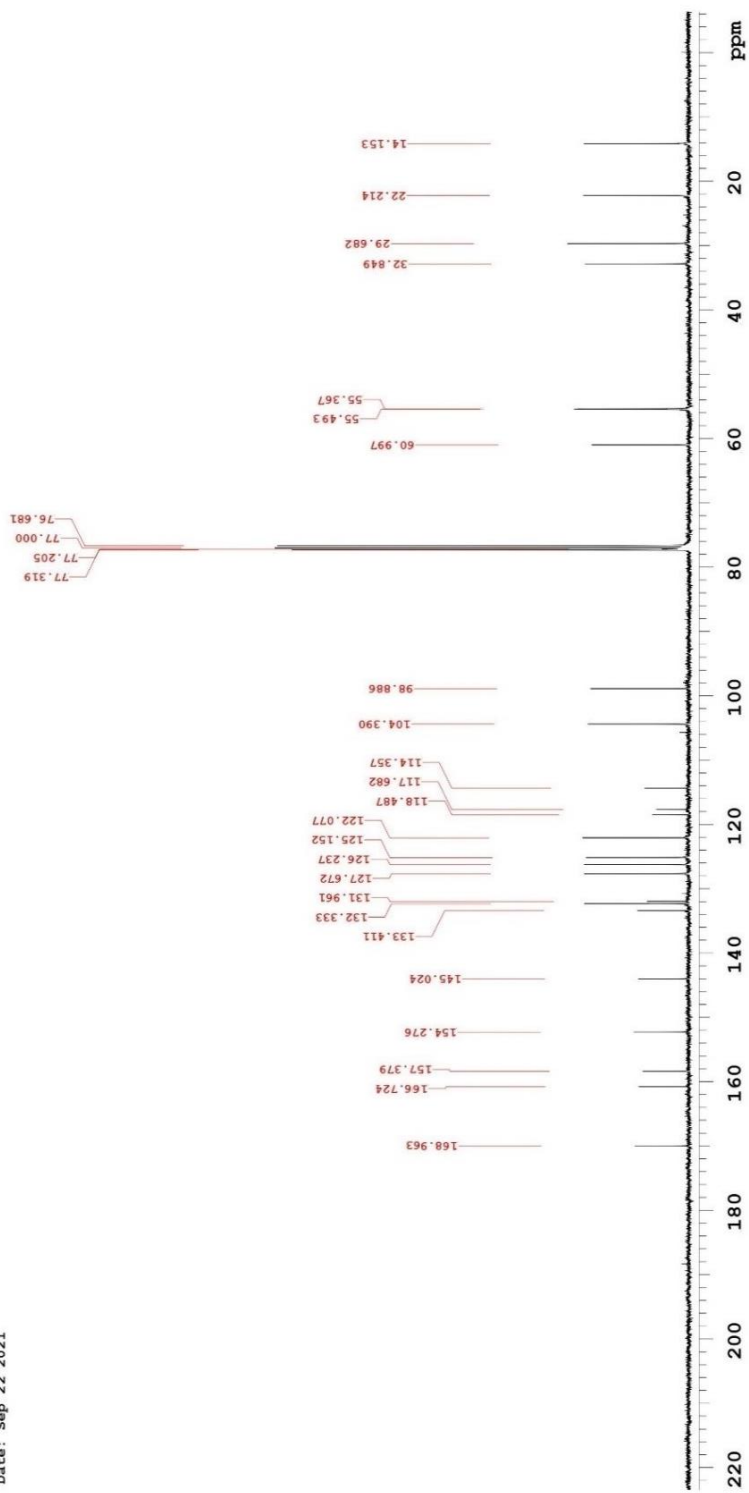


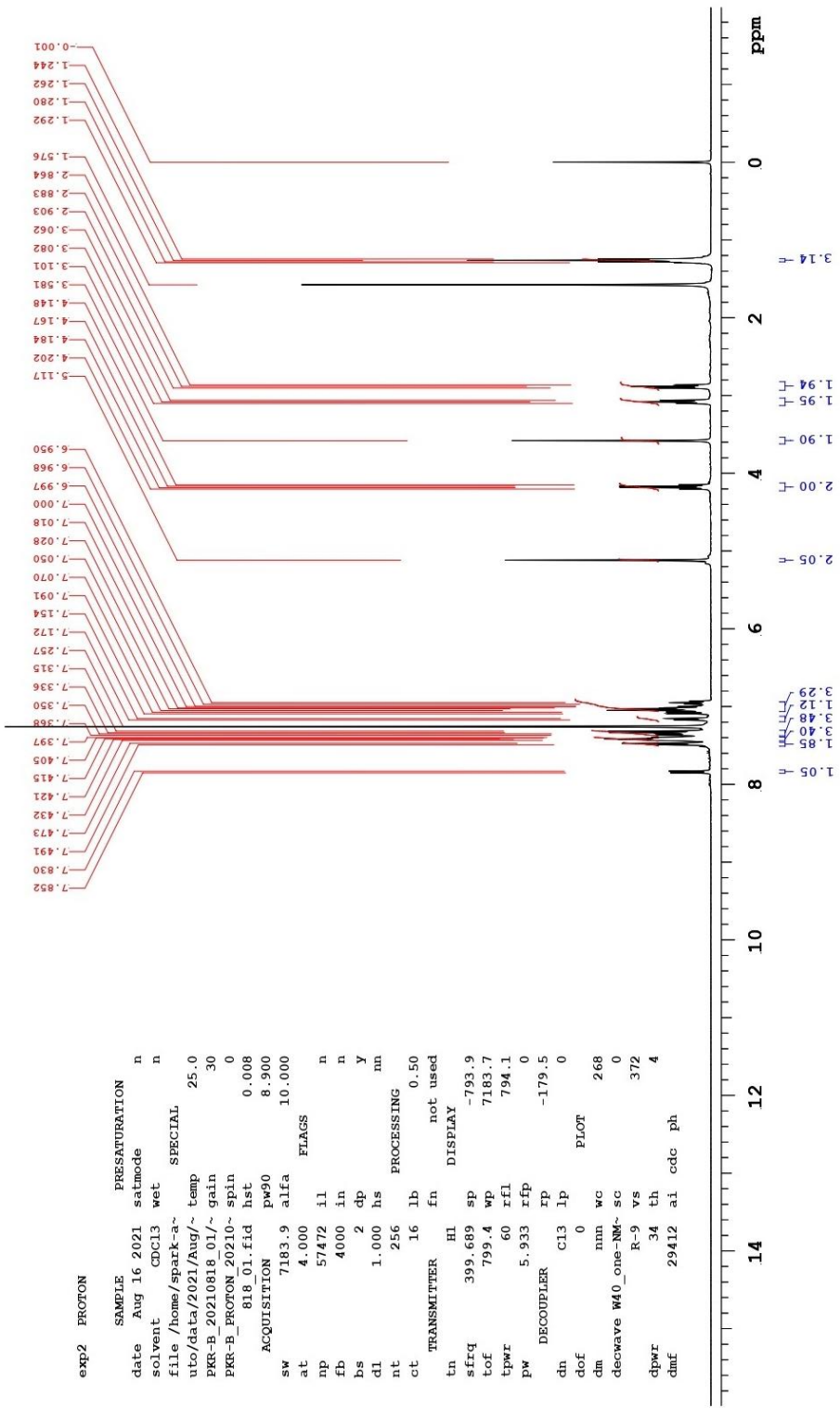
¹H NMR Spectrum of compound 5e

Sample Code: EXP-FMR-272-13C-NMR
13C NMR
VIGNAN'S UNIVERSITY
Solvent: CDCl3
SA-Varian 400MHz NMR
Date: Sep 22 2021



¹³C NMR Spectrum of compound **5e**



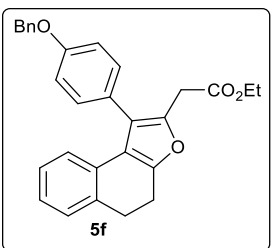


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exp2 PROTON
SAMPLE          PRESATURATION
date   Aug 16 2021   satmode      n
solvent CDC13      wet          n
file   /home/spark-3~
        SPECIAL
uto/data/2021/Aug/~   temp      25.0
PKR-B_20210818_01/~ gain      30
PKR-B PROTON 20210~ spin      0
            818 01.fid hst      0.008
ACQUISITION PW90      8.900
            7183.9 alfa      10.000
at         4.000          FLAGS
np         57472 i1
fb         4000 in n
bs         2 dp y
dl         1.000 hs mn
nt         256          PROCESSING
ct         16 lb 0.50
TRANSMITTER   fn not used
tn            H1 DISPLAY
sfrq         399.689 sp -793.9
tof          799.4 wp 7183.7
tpwr         60 rfl 794.1
pw           5.933 rfp 0
DECOUPLER    rp -179.5
            C13 lp 0
dn           dof 0 PLOT
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decwave W40_one-NM~ sc 0
            R-9 vs 372
dpwr         34 th 4
dmf          29412 ai cdc ph

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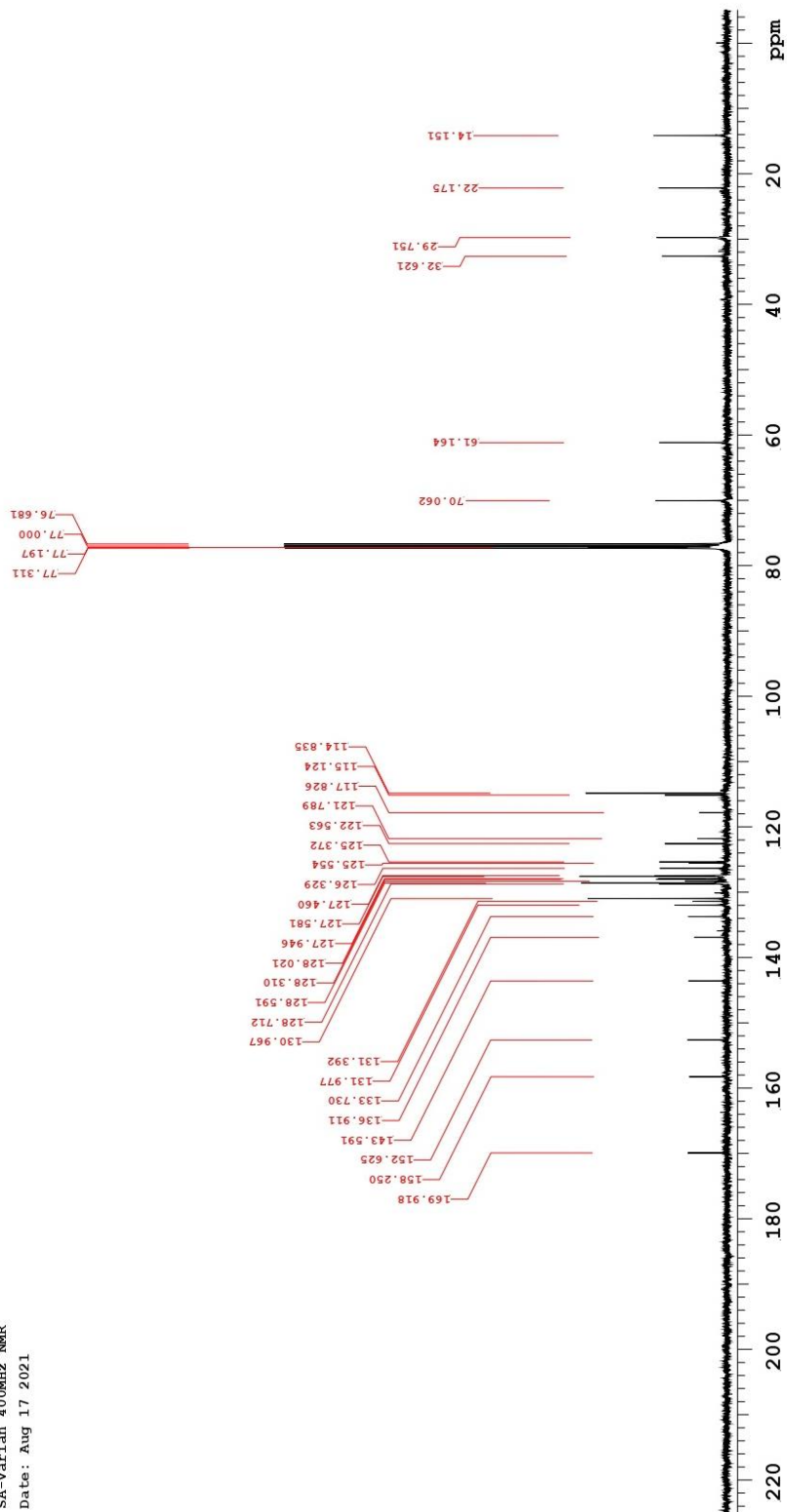
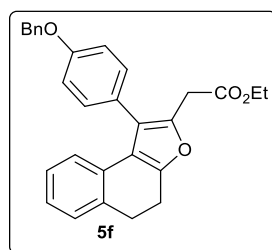
Plotname: PKR-B_PROTON_20210818_01_plot01



¹H NMR Spectrum of compound **5f**

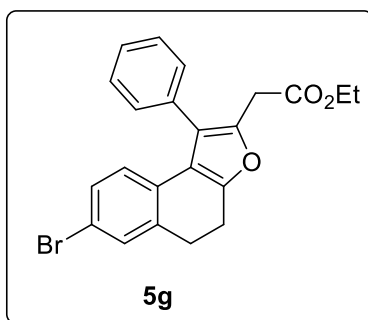
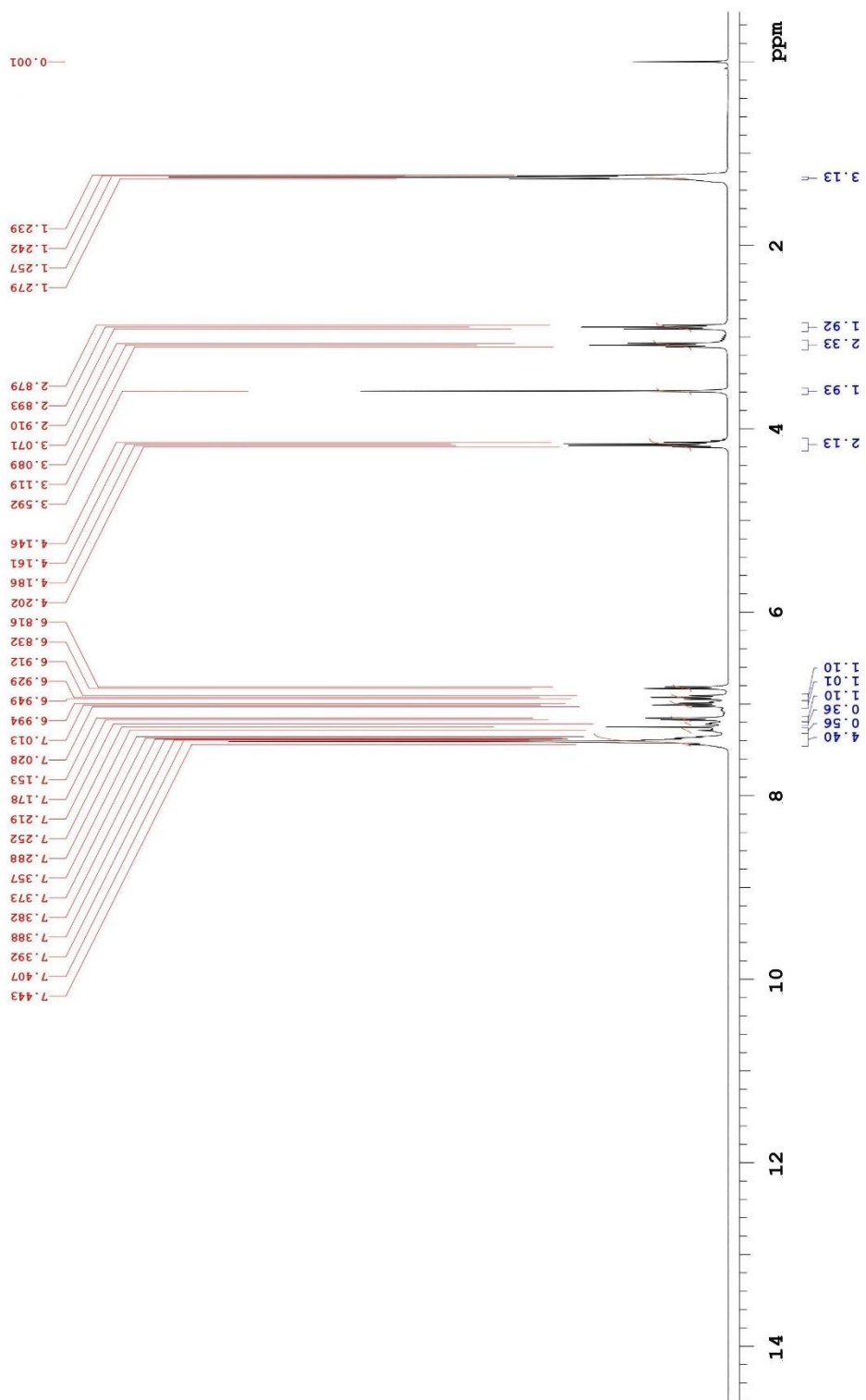
Sample Code: RKR-B-13C-NMR
13C NMR

Solvent: cdcl3
SA-Varian 400MHz NMR
Date: Aug 17 2021

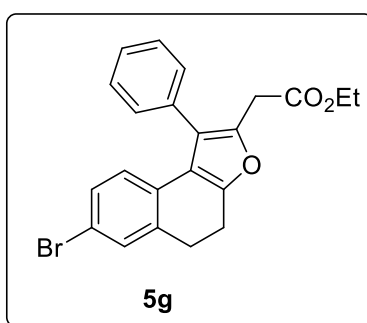
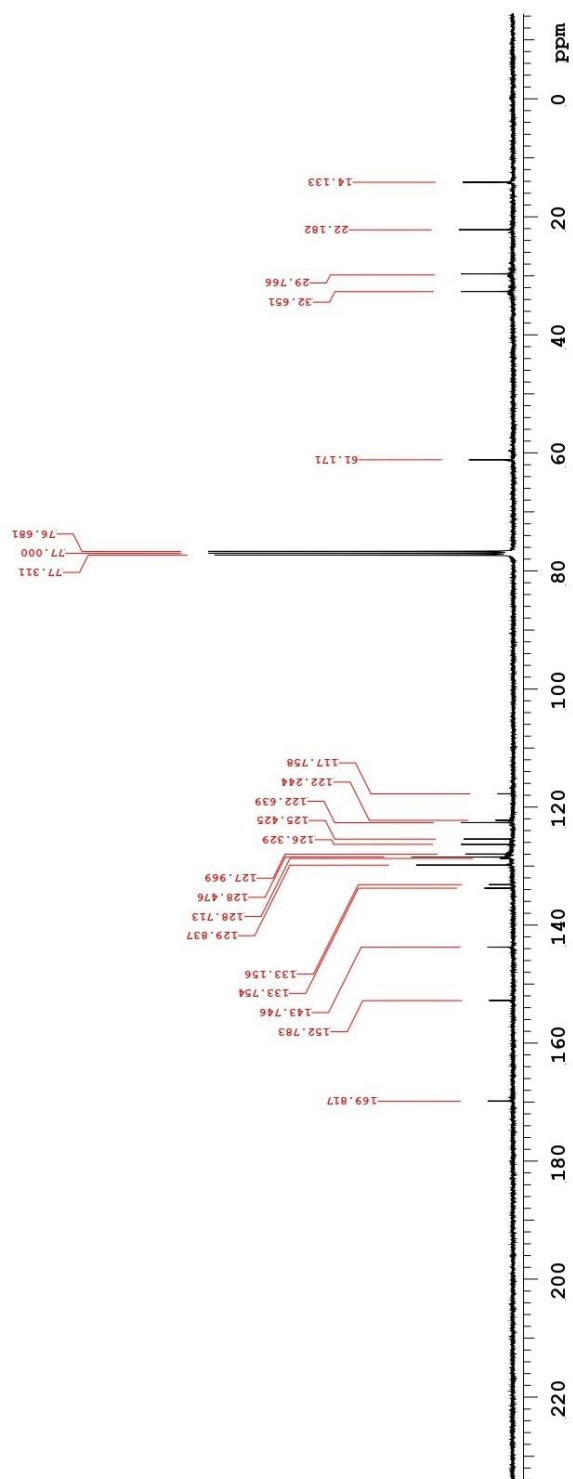


Plotname: RKR-B-13C-NMR_CARBON_20210817_01_plot01

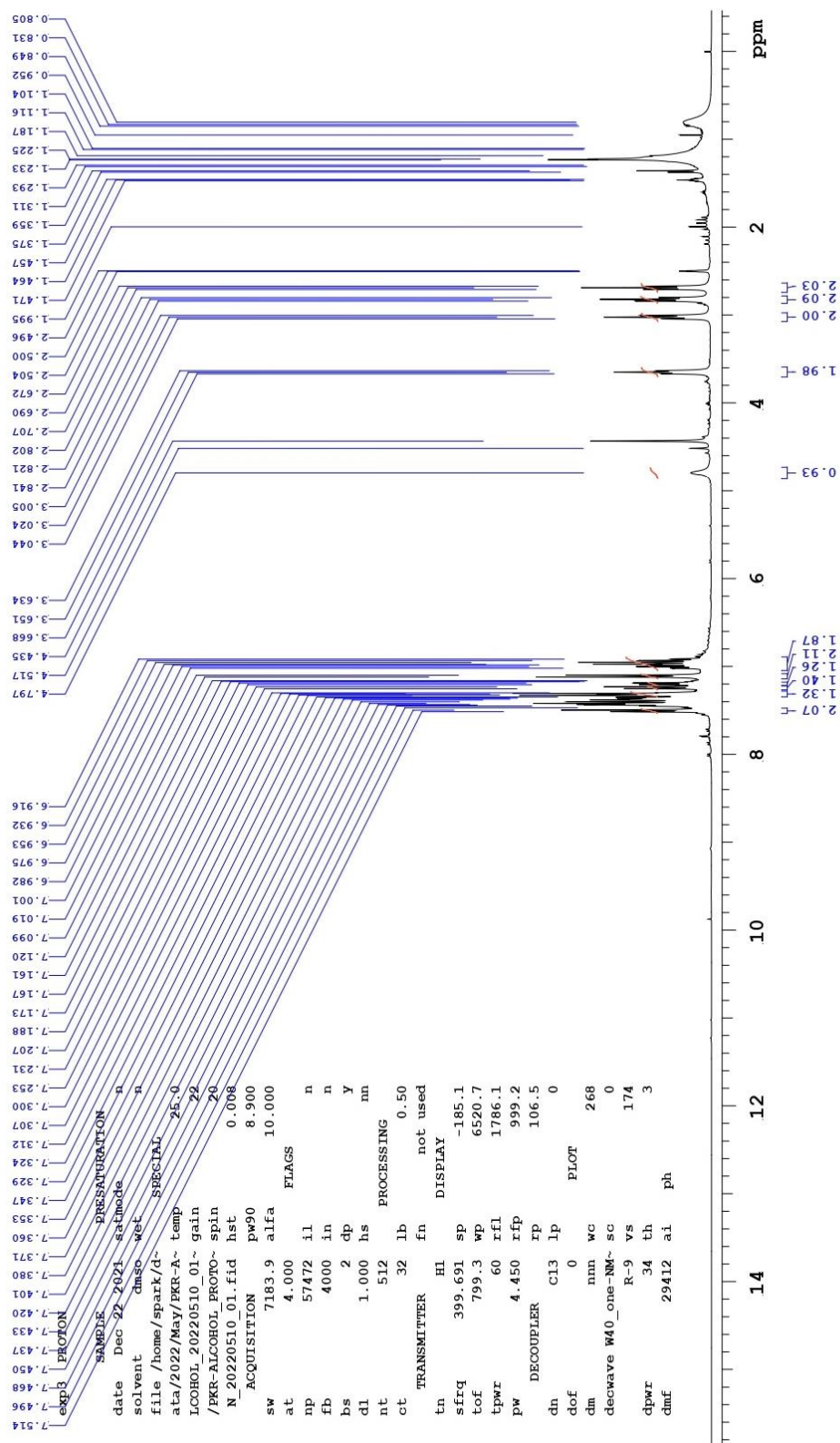
¹³C NMR Spectrum of compound **5f**



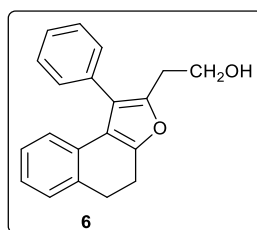
¹H NMR Spectrum of compound 5g



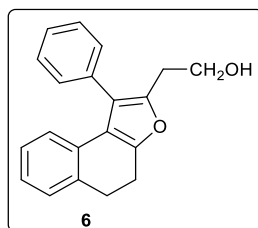
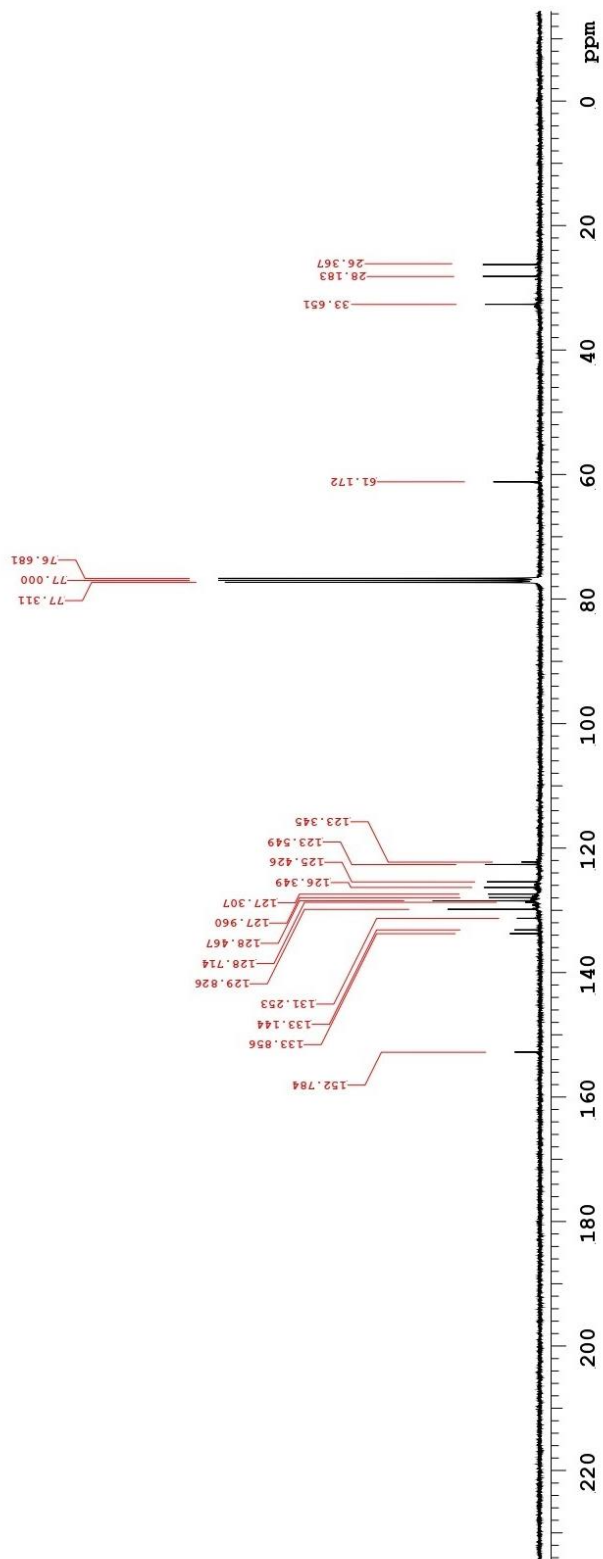
¹³C NMR Spectrum of compound **5g**



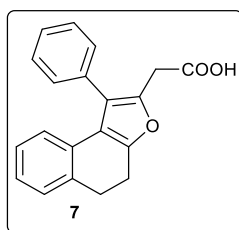
Plotname: EKR-ALCOHOL_PROTON_20220510_01_plot04



¹H NMR Spectrum of compound 6

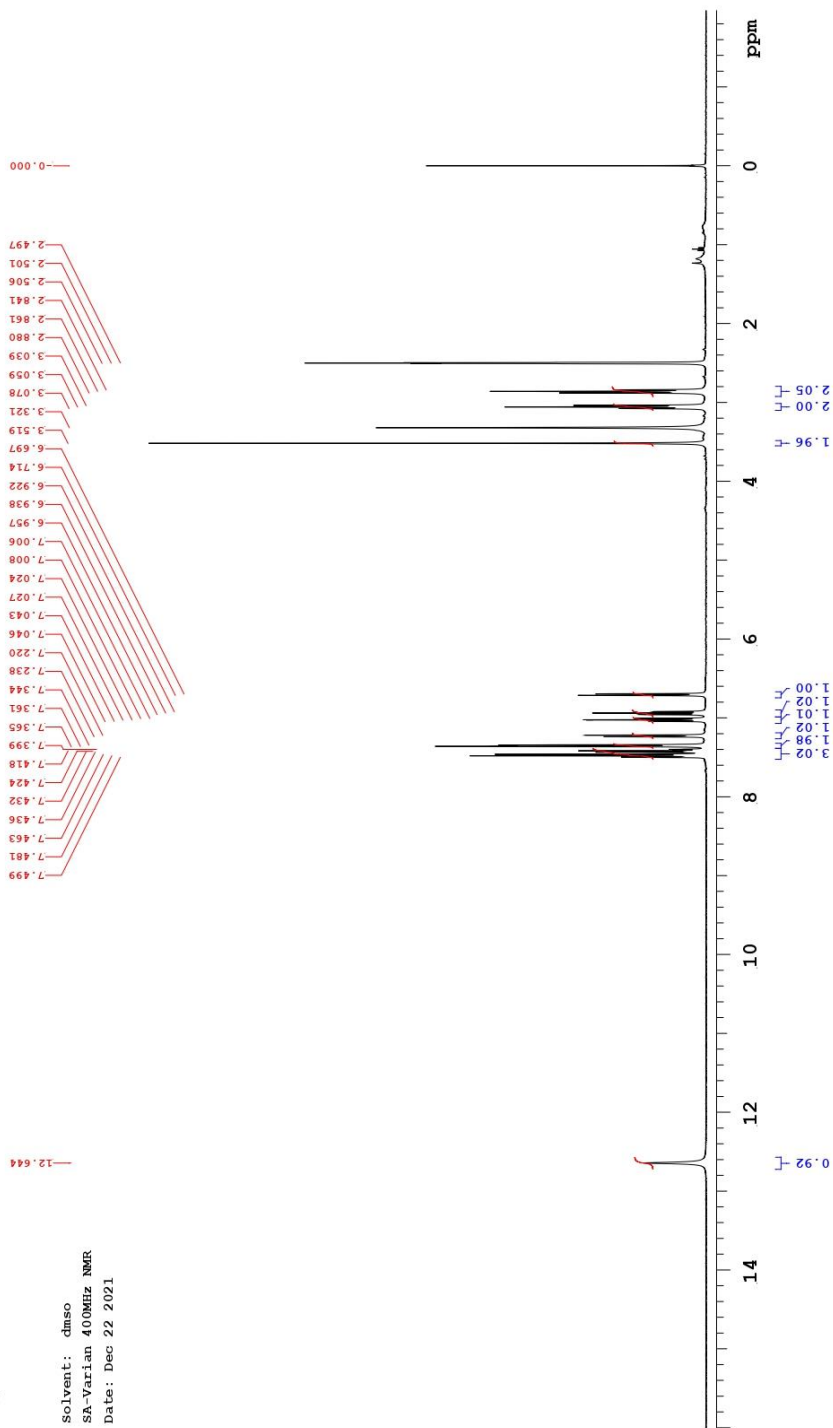


¹³C NMR Spectrum of compound 6



Sample Code: PKR-COOH

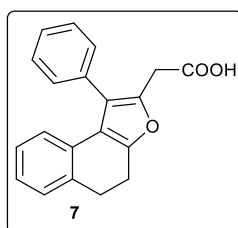
Solvent: dmsc
 SA-Varian 400MHz NMR
 Date: Dec 22 2021



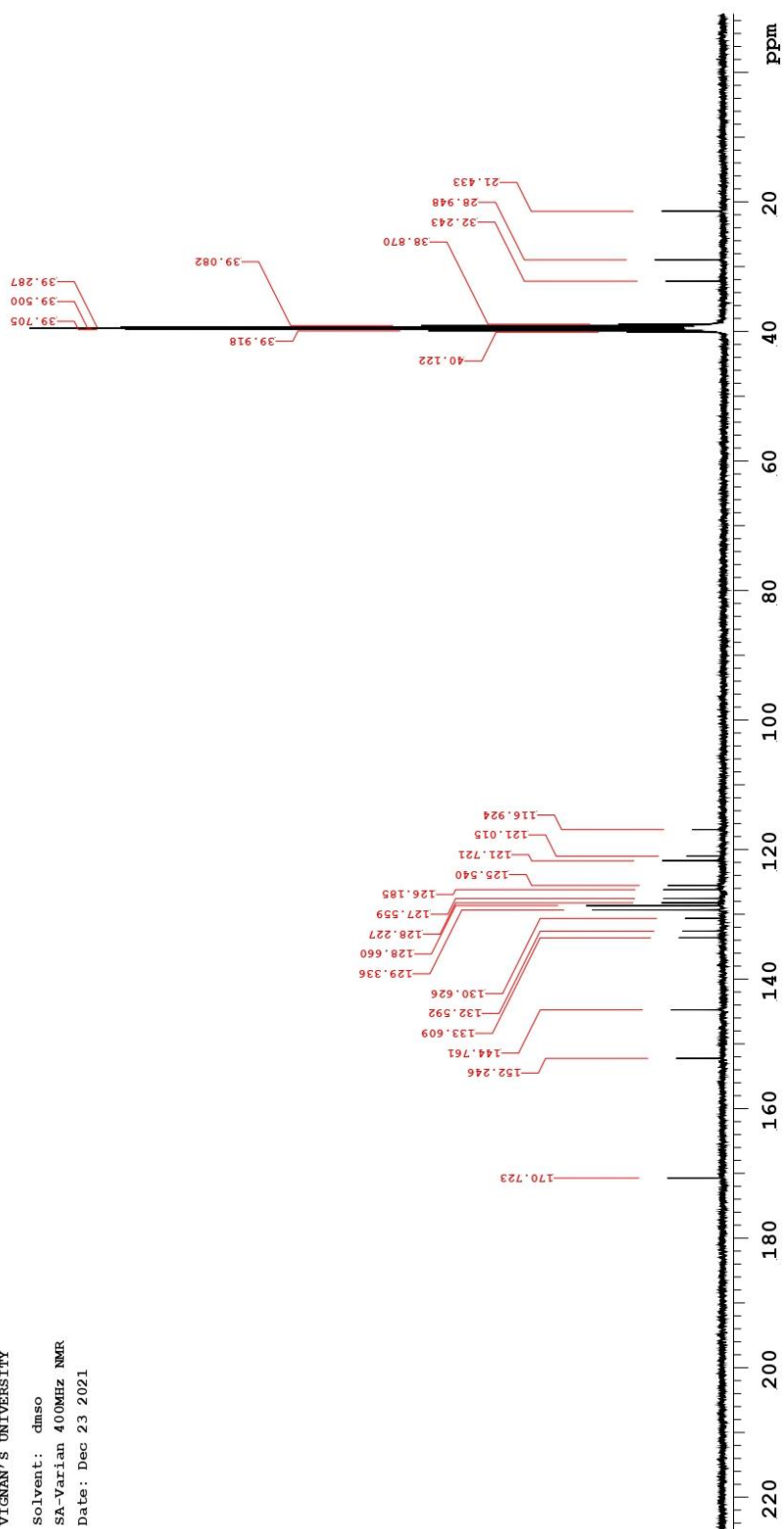
Plotname: PKR-COOH_PROTON_20211222_01_plot05

¹H NMR Spectrum of compound 7

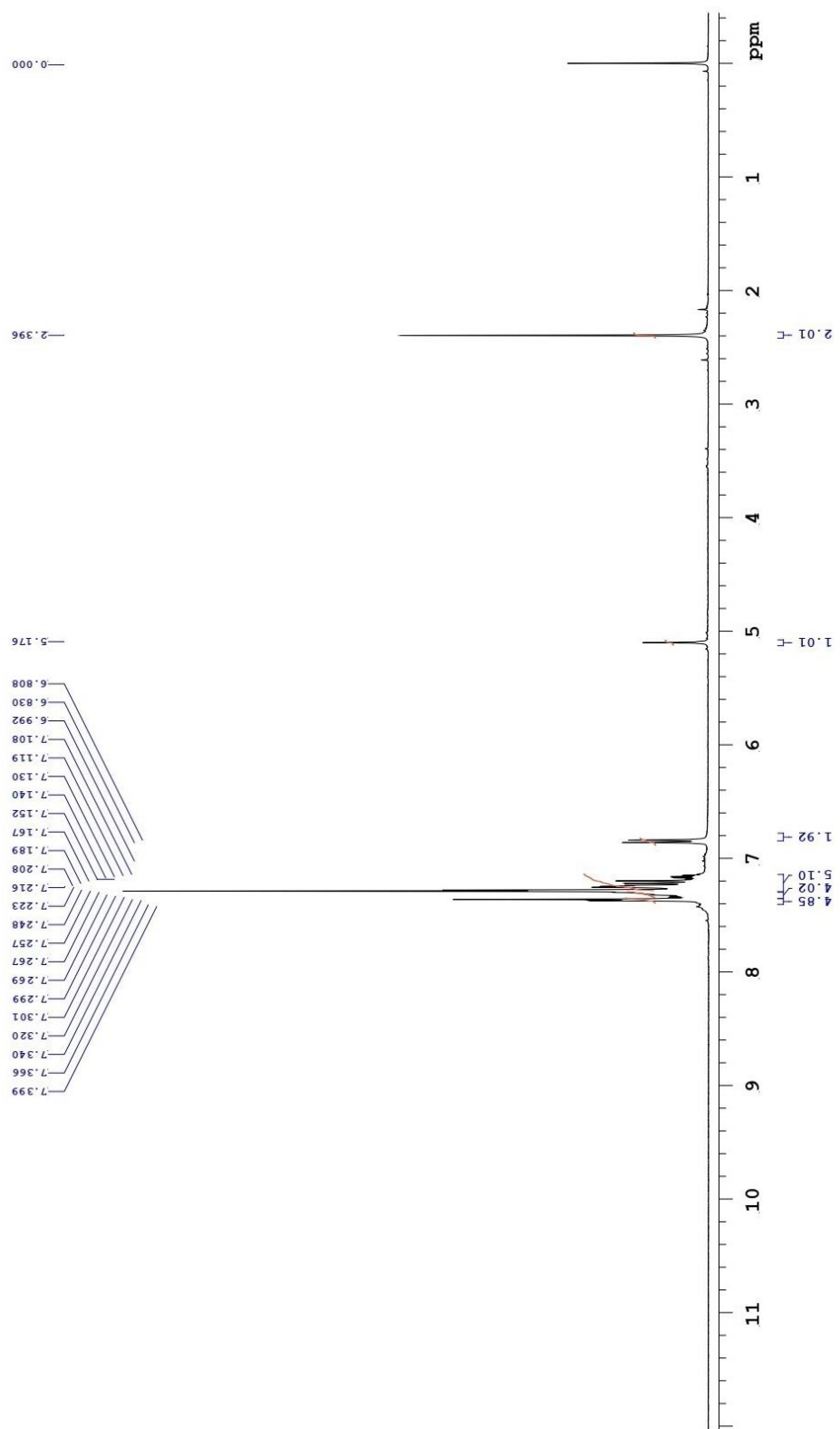
Sample Code: PKR-COOH-13C-NMR
13C NMR
VIGNAN'S UNIVERSITY
Solvent: dms0
SA-Varian 400MHz NMR
Date: Dec 23 2021



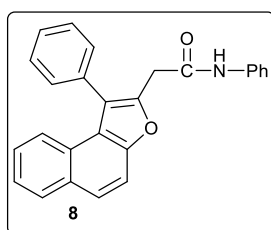
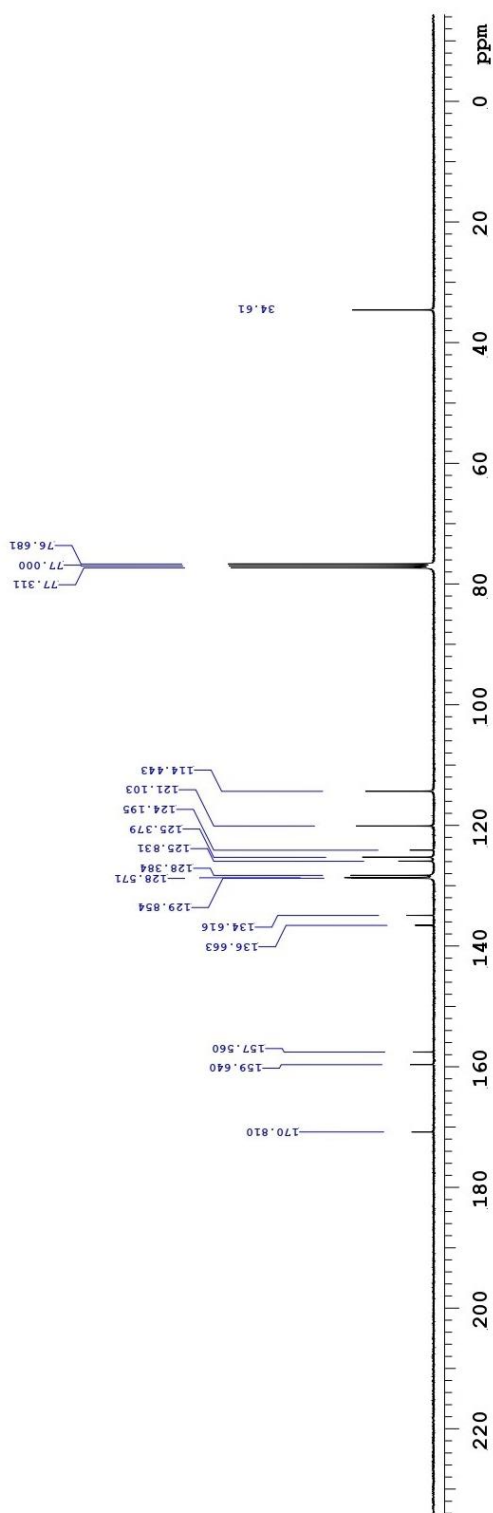
¹³C NMR Spectrum of compound 7



Plotname: PKR-COOH-13C-NMR_CARBON_20211223_01_plot01

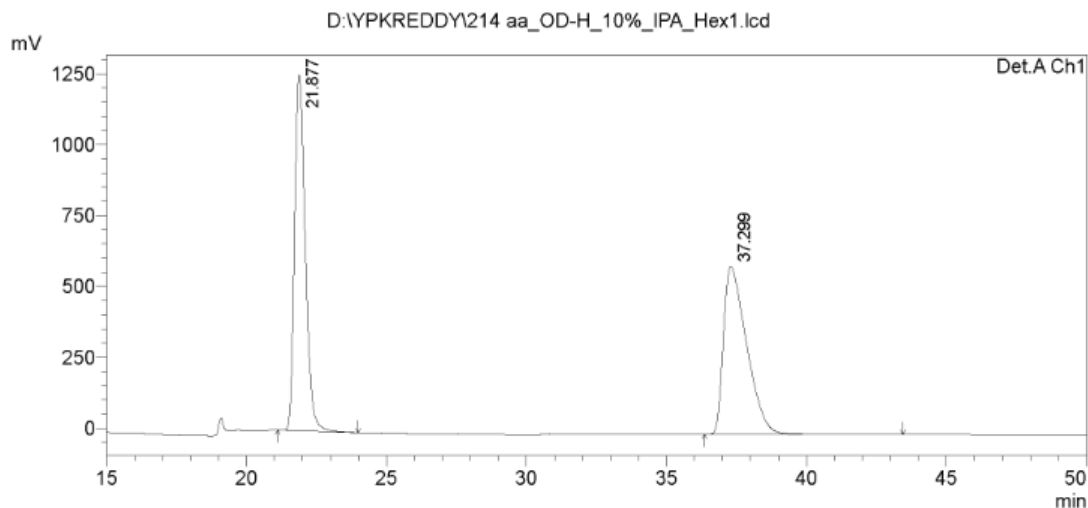


¹H NMR Spectrum of compound **8**
S46



¹³C NMR Spectrum of compound 8

Racemic compound for **3a**



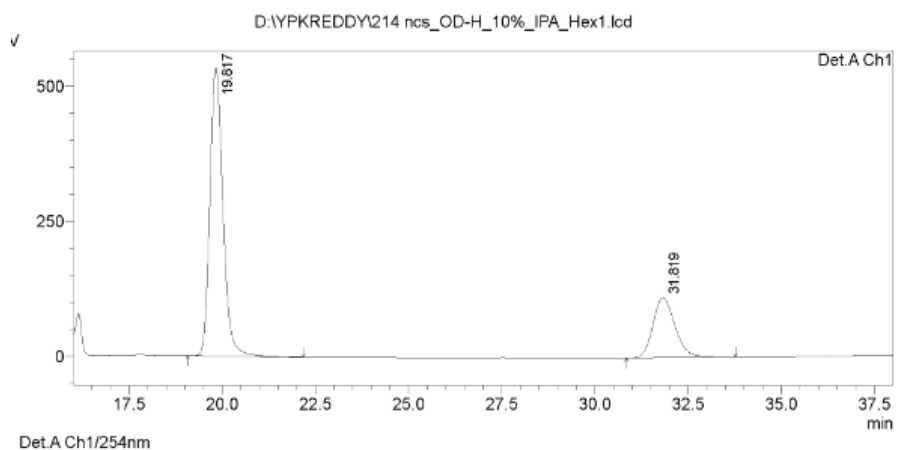
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|-------|-----------|----------|---------|---------|----------|
| 1 | 21.877 | 33484702 | 1253513 | 49.436 | 67.916 |
| 2 | 37.299 | 34248492 | 592168 | 50.564 | 32.084 |
| Total | | 67733194 | 1845681 | 100.000 | 100.000 |

Chiral compound for **3a**



Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

| Peak# | Ret. Time | Area | Height | Area % | Height % |
|-------|-----------|----------|--------|---------|----------|
| 1 | 19.817 | 13028936 | 534334 | 74.101 | 82.790 |
| 2 | 31.819 | 4553836 | 111071 | 25.899 | 17.210 |
| Total | | 17582773 | 645405 | 100.000 | 100.000 |

Crystallographic data of 3a

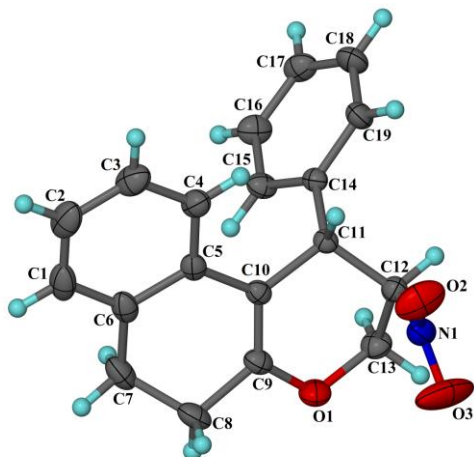


Figure caption: ORTEP diagram of **3a** compound with the atom-numbering. Displacement ellipsoids are drawn at the 35% probability level and H atoms are shown as small spheres of arbitrary radius.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) **3a_0m**

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: KB100_0m

Bond precision: C-C = 0.0035 Å Wavelength=0.71073

Cell: a=10.0111(10) b=11.7592(12) c=13.0970(15) alpha=90 beta=90 gamma=90

Temperature: 293 K

Calculated Reported Volume 1541.8(3) 1541.8(3) Space group P n a 21 P n a 21 Hall group P 2c -2n P 2c -2n Moiety formula C₁₉ H₁₇ N O₃ C₁₉ H₁₇ N O₃ Sum formula C₁₉ H₁₇ N O₃ C₁₉ H₁₇ N O₃ Mr 307.34 307.33 Dx,g cm⁻³ 1.324 1.324 Z 4 4 Mu (mm⁻¹) 0.090 0.090 F000

648.0 648.0 F000' 648.31 h,k,lmax 13,15,17 13,15,17 Nref 3541[1848] 3504 Tmin,Tmax
0.970,0.975 0.673,0.746 Tmin' 0.970

Correction method= # Reported T Limits: Tmin=0.673 Tmax=0.746 AbsCorr = MULTI-
SCAN

Data completeness= 1.90/0.99 Theta(max)= 27.486

R(reflections)= 0.0365(3158)

wR2(reflections)= 0.0985(3504)

S = 1.039 Npar= 208

Crystal data for 3a: C₁₉H₁₇N₁O₃, *M* = 307.33, Orthorhombic, space group *Pna*2₁(No.33), *a* = 10.0111(10)Å, *b* = 11.7592(12)Å, *c* = 13.0970(15)Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, *V* = 1541.8(3)Å³, *Z* = 4, *D*_c = 1.324 g/cm³, *F*₀₀₀ = 648, Bruker D8 QUEST PHOTON-100, Mo-K α radiation, $\lambda = 0.71073$ Å, *T* = 293(2)K, $2\theta_{\max} = 55^\circ$, $\mu = 0.090$ mm⁻¹, 28119 reflections collected, 3504 unique (*R*_{int} = 0.0591), 208 parameters, *R*1 = 0.0365, *wR*2 = 0.0947, *R* indices based on 3158 reflections with *I* > 2 σ (*I*) (refinement on *F*²), Final *Goof* = 1.039, largest difference hole and peak = -0.162 and 0.167 e.Å⁻³. **CCDC 2149875** deposition numbers contain the supplementary crystallographic data for this paper which can be obtained free of charge at <https://www.ccdc.cam.ac.uk/structures/>

Data collection and Structure solution details: Single crystal X-ray data were collected at room temperature on a Bruker D8 QUEST equipped with a four-circle kappa diffractometer and Photon 100 detector. An I μ s microfocus Mo source ($\lambda=0.71073$ Å) supplied the multi-mirror monochromated incident beam. A combination of Phi and Omega scans were used to collect the necessary data. Integration and scaling of intensity data were accomplished using SAINT program.¹ The structures were solved by Direct Methods using SHELXS97² and refinement was carried out by full-matrix least-squares technique using SHELXL-2014/7.²⁻³ Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms, with C-H distances of 0.93--0.97 Å, and with *U*_{iso}(H) = 1.2*U*_{eq}(C) or 1.5*U*_{eq} for methyl atoms. **CCDC 2149875** deposition numbers contain the supplementary crystallographic data for this paper which can be obtained free of charge at <https://www.ccdc.cam.ac.uk/structures/>

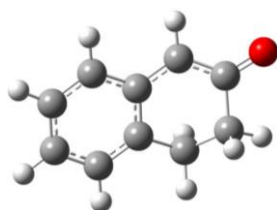
SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.

Sheldrick, G. M. SHELXS97 and SHELXL Version 2014/7, <http://shelx.uni-ac.gwdg.de/SHELX/index.php>

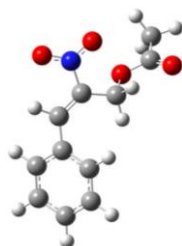
Muller, P, Herbst-Imer, R, Spek, A. L, Schneider, T. R, and Sawaya, M. R. Crystal Structure Refinement: A Crystallographer's Guide to SHELXL. Muller, P. Ed. 2006 Oxford University Press: Oxford, New York, pp. 57–91.

A. L. Spek, Acta Cryst. 2009, D65, 148-155.

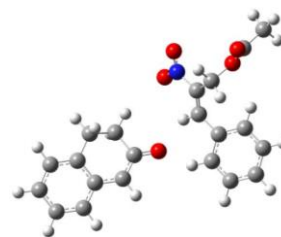
Figure-1: Optimized structures of primary acetate path



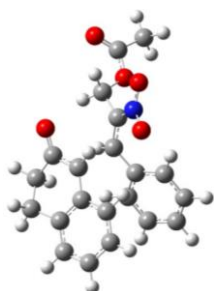
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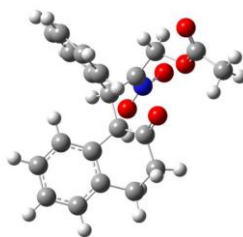
2a



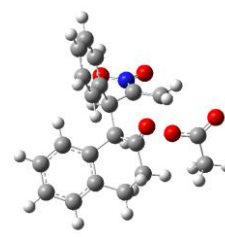
P-Cmplx



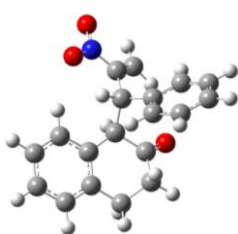
P-Ts1 (Imaginary Frequency-159.73)



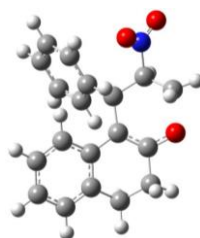
P-Int1



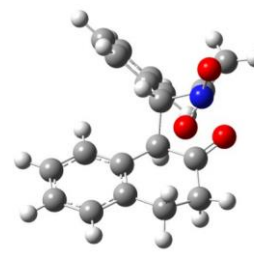
P-Ts2 (I.F-137.61)



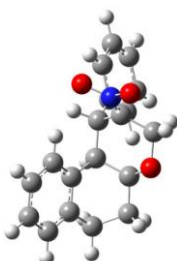
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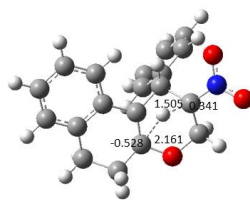
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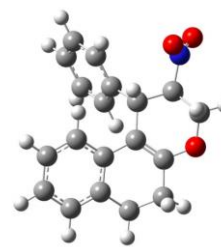
P-Ts3a (I.F-475.30)



P-Int3

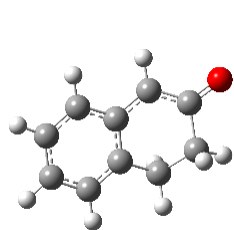


P-Ts4 (I.F -1765.18)

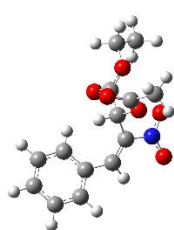


3a

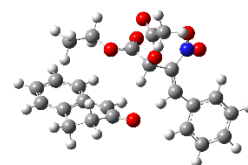
Figure-2: Optimized structures of secondary acetate path



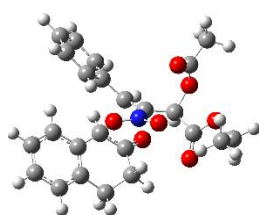
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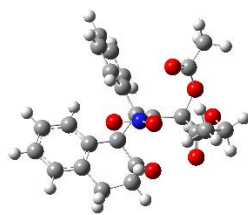
4a



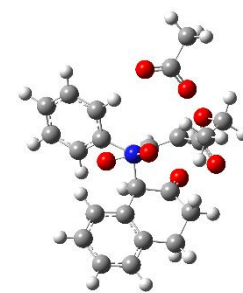
S-Cmplx



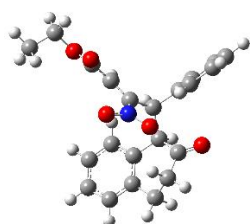
S-Ts1 (I.F-162.38)



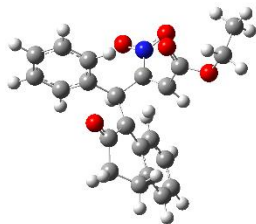
S-Int1



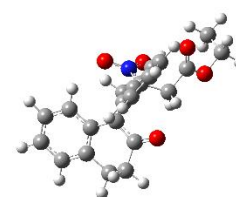
S-Ts2 (I.F- 37.44)



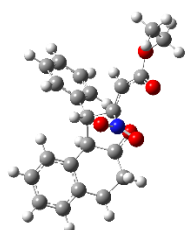
S-Int2



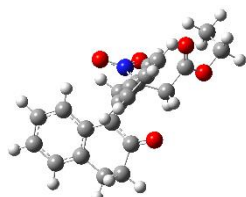
S-Ts3 (I.F-1438.90)



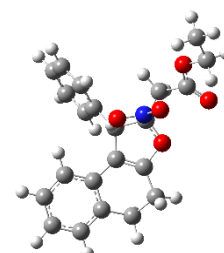
S-Int3



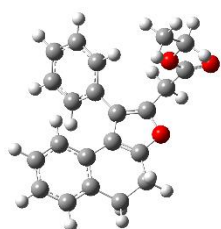
S-Ts4 (I.F-267.42)



S-Int4



S-Ts5 (I.F -490.31)



5a

Cartesian coordinates of primary acetate path optimized structures

| | | | |
|---|-------------|-------------|-------------|
| 1 | | | |
| C | 2.72589500 | -0.97164700 | 0.09079000 |
| C | 2.93823300 | 0.41151700 | 0.12096400 |
| C | 1.81770600 | 1.25225700 | 0.01789600 |
| C | 0.52897100 | 0.74888100 | -0.09725300 |
| C | 0.28860500 | -0.66617400 | -0.09197600 |
| C | 1.44241700 | -1.49732500 | -0.01362200 |
| C | -0.67281700 | 1.63487400 | -0.33054500 |
| C | -1.92959000 | 1.09336900 | 0.35929200 |
| C | -2.19383900 | -0.39729600 | 0.03375800 |
| C | -1.03861100 | -1.18212800 | -0.17311400 |
| O | -3.38182400 | -0.80229800 | 0.04289200 |
| H | 3.57564500 | -1.65145300 | 0.15808100 |
| H | 3.93963800 | 0.82524100 | 0.21227600 |
| H | 1.95605900 | 2.33473900 | 0.01217900 |
| H | 1.30161900 | -2.57732700 | -0.02207300 |
| H | -0.87736500 | 1.66362000 | -1.41556800 |
| H | -0.45725200 | 2.66987600 | -0.02803000 |
| H | -2.82104800 | 1.66296500 | 0.07319000 |
| H | -1.82692300 | 1.18943400 | 1.45225600 |
| H | -1.17759400 | -2.25667600 | -0.28258600 |

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|---|-------------|-------------|-------------|
| C | 3.44022600 | -1.50418100 | -0.84048000 |
| C | 4.42489500 | -1.22123700 | 0.10760000 |
| C | 4.25864900 | -0.14279300 | 0.97953100 |
| C | 3.11134200 | 0.64145500 | 0.90725100 |
| C | 2.09098900 | 0.34405900 | -0.01638100 |
| C | 2.28361100 | -0.73001300 | -0.90484000 |
| C | 0.90527800 | 1.20660500 | -0.03056300 |
| C | -0.37580100 | 0.87974800 | -0.27447200 |
| C | -0.98660400 | -0.46359800 | -0.51883600 |
| O | -1.92654200 | -0.71547400 | 0.54708000 |
| O | -3.18110500 | -1.96172800 | -0.87091500 |
| C | -3.02155900 | -1.45082000 | 0.21374200 |
| C | -3.98187900 | -1.51892200 | 1.37396300 |
| N | -1.34971600 | 1.99697600 | -0.28546800 |
| O | -1.00100400 | 3.10118000 | 0.13175500 |
| O | -2.46768400 | 1.74463800 | -0.73639700 |
| H | 3.57710000 | -2.32300100 | -1.54011700 |
| H | 5.32447600 | -1.82723500 | 0.15581500 |
| H | 5.02745700 | 0.09255600 | 1.70906900 |
| H | 2.98770700 | 1.48514000 | 1.58035400 |
| H | 1.55036300 | -0.93179500 | -1.67822900 |
| H | 1.07229400 | 2.25393900 | 0.20841800 |
| H | -0.21652000 | -1.23547600 | -0.48838500 |
| H | -1.50914200 | -0.51872200 | -1.47546700 |
| H | -3.45656500 | -1.78994500 | 2.29314500 |
| H | -4.42820000 | -0.53144000 | 1.52767700 |

H -4.76515900 -2.24359600 1.15472200

P-cmplx

C 7.14445400 0.53190600 0.95527900

C 7.29577500 -0.85350900 0.84858600

C 6.18372700 -1.62060500 0.47094500

C 4.95346800 -1.03658000 0.19395200

C 4.79194100 0.38117000 0.26993500

C 5.92230900 1.13578400 0.67279900

C 3.71491900 -1.84989300 -0.10528100

C 2.78308100 -1.15165100 -1.10297200

C 2.51074100 0.31169100 -0.72641800

C 3.52987300 0.98663400 -0.04849400

O 1.41868500 0.83265200 -1.12034600

C -1.09896500 3.99783700 -0.02764700

C -2.42213900 4.41158000 0.14719900

C -3.45692800 3.47853200 0.04761700

C -3.17024400 2.13787500 -0.19935500

C -1.83561200 1.70560900 -0.35101700

C -0.79970600 2.66254200 -0.28805100

C -1.47247400 0.31273100 -0.62983700

C -2.14114700 -0.78483800 -0.20028500

C -3.24491400 -0.85172800 0.79876000

O -4.51975900 -0.99916600 0.09857100

C -5.56723500 -1.39306100 0.84896900

C -6.79167600 -1.60028000 -0.01592600

O -5.52520900 -1.56584000 2.04868400

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|---|-------------|-------------|-------------|
| N | -1.69809700 | -2.09210300 | -0.68901100 |
| O | -2.24196900 | -3.09624400 | -0.19856400 |
| O | -0.83663500 | -2.14814300 | -1.56992000 |
| H | 7.99034200 | 1.14950800 | 1.25402100 |
| H | 8.25041700 | -1.32901600 | 1.05898700 |
| H | 6.27565100 | -2.70465900 | 0.40217500 |
| H | 5.82410800 | 2.21734500 | 0.74788400 |
| H | 3.15654100 | -1.98478700 | 0.83650000 |
| H | 3.98498600 | -2.85652000 | -0.45052800 |
| H | 1.82309700 | -1.67163300 | -1.17952700 |
| H | 3.22983100 | -1.16300800 | -2.10952800 |
| H | 3.40144800 | 2.05223200 | 0.13199800 |
| H | -0.29162300 | 4.72302600 | 0.03087300 |
| H | -2.64839100 | 5.45673000 | 0.34330100 |
| H | -4.49091500 | 3.79694200 | 0.15289400 |
| H | -3.98331500 | 1.42942400 | -0.31946100 |
| H | 0.22363200 | 2.31799900 | -0.45197600 |
| H | -3.27943000 | 0.06361400 | 1.39105500 |
| H | -3.12155200 | -1.70776200 | 1.46000500 |
| H | -7.65581500 | -1.79636400 | 0.61857600 |
| H | -6.97153100 | -0.72230600 | -0.64210700 |
| H | -6.62484400 | -2.45016000 | -0.68489400 |
| H | -0.54234600 | 0.16756700 | -1.18710300 |

P-TS1

| | | | |
|---|------------|------------|-------------|
| C | 1.29937800 | 2.87276300 | 1.16230200 |
| C | 0.46099600 | 2.41119300 | -0.04168300 |
| C | 2.80090200 | 2.87527900 | 0.85178000 |

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|---|-------------|-------------|-------------|
| C | 3.26556900 | 1.58181400 | 0.21577200 |
| C | 2.36352400 | 0.86344000 | -0.61310600 |
| C | 0.97102200 | 1.26575300 | -0.75306300 |
| C | 1.13999500 | -3.64630100 | 0.19370300 |
| C | 1.95728200 | -3.56339300 | 1.32211200 |
| C | 1.98118700 | -2.37552500 | 2.05465100 |
| C | 1.19204500 | -1.29908300 | 1.66172600 |
| C | 0.35941600 | -1.36182500 | 0.52513000 |
| C | 0.35672600 | -2.56503300 | -0.20723700 |
| C | -0.50452100 | -0.19158300 | 0.25697800 |
| C | -1.68257900 | -0.08205700 | -0.51270400 |
| C | -2.82897300 | 0.74497600 | -0.05046900 |
| O | -3.83339800 | -0.14549400 | 0.58244100 |
| C | -5.06965100 | 0.33709300 | 0.72679200 |
| C | -6.00018400 | -0.73702900 | 1.26234900 |
| O | -5.42312700 | 1.47026600 | 0.46089200 |
| C | 4.58612100 | 1.14980200 | 0.34416000 |
| C | 5.05553900 | 0.02784800 | -0.34361300 |
| C | 4.18196300 | -0.66760000 | -1.18430000 |
| C | 2.85951800 | -0.25721400 | -1.31535400 |
| O | -0.62389600 | 2.96245600 | -0.28156600 |
| N | -1.81330600 | -0.60600800 | -1.79972500 |
| O | -0.79575600 | -1.05933400 | -2.39851400 |
| O | -2.93785100 | -0.58062700 | -2.35653000 |
| H | 1.10032700 | 2.19030800 | 2.00245900 |
| H | 0.94435700 | 3.86360600 | 1.46048600 |
| H | 3.38816500 | 3.09144000 | 1.75368200 |
| H | 3.00690000 | 3.70112600 | 0.15177500 |

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|---|-------------|-------------|-------------|
| H | 0.47777900 | 0.99343200 | -1.67863100 |
| H | 1.11181600 | -4.56418000 | -0.38880200 |
| H | 2.56904600 | -4.40962300 | 1.62456000 |
| H | 2.61311600 | -2.28664800 | 2.93468600 |
| H | 1.21305100 | -0.38306600 | 2.24600900 |
| H | -0.24927900 | -2.63457200 | -1.10024600 |
| H | -3.32454800 | 1.26404300 | -0.86788900 |
| H | -2.51333500 | 1.47191200 | 0.69753000 |
| H | -6.16620200 | -1.49095200 | 0.48616100 |
| H | -5.54967400 | -1.24464700 | 2.11951100 |
| H | -6.95341800 | -0.28833800 | 1.54405200 |
| H | 5.26405400 | 1.71409700 | 0.98355000 |
| H | 6.08735700 | -0.29429200 | -0.22796700 |
| H | 4.53084800 | -1.53980400 | -1.73215300 |
| H | 2.17405600 | -0.80547400 | -1.95445400 |
| H | -0.59070700 | 0.41565500 | 1.15440800 |

P-Int1

| | | | |
|---|-------------|-------------|-------------|
| C | -4.25075100 | 1.30706300 | -0.07852000 |
| C | -5.11698600 | 0.30106400 | 0.34560400 |
| C | -4.61686300 | -0.98258300 | 0.57398100 |
| C | -3.26459200 | -1.26464000 | 0.37598300 |
| C | -2.38274700 | -0.24669600 | -0.04824800 |
| C | -2.89306200 | 1.03634700 | -0.26973700 |
| C | -2.67573200 | -2.63901500 | 0.59318900 |
| C | -1.37787500 | -2.54512700 | 1.41261100 |
| C | -0.47312000 | -1.37212800 | 1.00537000 |
| C | -0.91869200 | -0.63970000 | -0.25483700 |

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|---|-------------|-------------|-------------|
| O | 0.49386600 | -1.09775000 | 1.69281900 |
| C | 0.67693500 | 4.12811300 | -0.60486100 |
| C | 0.80232900 | 4.31757700 | 0.77351200 |
| C | 0.68866100 | 3.21754600 | 1.62166100 |
| C | 0.44574300 | 1.94041100 | 1.10759200 |
| C | 0.30333700 | 1.73448500 | -0.27167200 |
| C | 0.43214200 | 2.85410200 | -1.11360000 |
| C | 0.03701500 | 0.38751800 | -0.93827100 |
| C | 1.30542400 | -0.27708400 | -1.44497400 |
| C | 2.65003300 | -0.11706700 | -0.88537900 |
| O | 2.97908500 | -1.22968700 | 0.07901600 |
| C | 3.68820000 | -0.92911200 | 1.16143800 |
| C | 3.71749300 | -2.10797700 | 2.11929200 |
| O | 4.22687600 | 0.14110500 | 1.39526000 |
| N | 1.15609100 | -1.11281500 | -2.51289300 |
| O | -0.02311000 | -1.31183900 | -2.98876300 |
| O | 2.15535800 | -1.68844000 | -3.04081200 |
| H | -4.62636900 | 2.31122300 | -0.25773500 |
| H | -6.17223800 | 0.51144300 | 0.49991600 |
| H | -5.28335000 | -1.77638800 | 0.90578300 |
| H | -2.23017200 | 1.83145500 | -0.58893800 |
| H | -2.45059700 | -3.09091400 | -0.38318800 |
| H | -3.39665400 | -3.30091400 | 1.08583100 |
| H | -0.78111300 | -3.46094900 | 1.32287700 |
| H | -1.59626900 | -2.41693400 | 2.47902500 |
| H | -0.94222600 | -1.42401600 | -1.03760400 |
| H | 0.76837900 | 4.97259600 | -1.28398300 |
| H | 0.99234800 | 5.30868800 | 1.17805400 |

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|---|-------------|-------------|-------------|
| H | 0.79826300 | 3.34634400 | 2.69576300 |
| H | 0.39008300 | 1.09216200 | 1.77720900 |
| H | 0.34163000 | 2.71128400 | -2.18777800 |
| H | 2.77364900 | 0.80863200 | -0.32482700 |
| H | 3.40727500 | -0.20161500 | -1.66520000 |
| H | 4.45966100 | -1.93400600 | 2.90019000 |
| H | 2.72283600 | -2.20707600 | 2.56500600 |
| H | 3.93636500 | -3.03580800 | 1.58375700 |
| H | -0.52208300 | 0.61878900 | -1.85486100 |

P-Ts2

| | | | |
|---|-------------|-------------|-------------|
| C | 3.23877000 | -2.44948700 | 1.51650200 |
| C | 2.90190600 | -3.78093500 | 1.27924100 |
| C | 1.69348000 | -4.08198900 | 0.64742500 |
| C | 0.81998900 | -3.06518800 | 0.25855200 |
| C | 1.15979700 | -1.71559000 | 0.49701200 |
| C | 2.37446000 | -1.42376800 | 1.12486600 |
| C | -0.50315700 | -3.33687000 | -0.41868300 |
| C | -0.69013500 | -2.41831900 | -1.63767800 |
| C | -0.24969200 | -0.97311600 | -1.38931100 |
| C | 0.13618900 | -0.66400800 | 0.06424100 |
| O | -0.21438800 | -0.17612300 | -2.30612000 |
| C | 3.37496800 | 1.78800800 | -1.83835800 |
| C | 3.55968800 | 3.12270800 | -1.48404000 |
| C | 2.72177800 | 3.68879300 | -0.52011400 |
| C | 1.71223300 | 2.93097700 | 0.06903200 |
| C | 1.50435900 | 1.58658800 | -0.28725400 |

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|---|-------------|-------------|-------------|
| C | 2.36258000 | 1.02958800 | -1.24374300 |
| C | 0.40988000 | 0.81217200 | 0.46204300 |
| C | -0.90687400 | 1.56713600 | 0.60012500 |
| C | -1.94304600 | 1.53794300 | -0.31916400 |
| O | -2.87800500 | -0.18686300 | -0.18487200 |
| C | -4.14354900 | -0.12735900 | -0.46909500 |
| C | -4.88777500 | -1.43729700 | -0.14931100 |
| O | -4.75898500 | 0.83543800 | -0.93103800 |
| N | -1.15328300 | 2.17331500 | 1.85415800 |
| O | -0.20590000 | 2.25714000 | 2.68547100 |
| O | -2.27687900 | 2.65227600 | 2.11266000 |
| H | 4.17770300 | -2.20166800 | 2.00434000 |
| H | 3.57399000 | -4.58032500 | 1.58031300 |
| H | 1.42239700 | -5.11814600 | 0.45547300 |
| H | 2.65516200 | -0.39219200 | 1.30445800 |
| H | -1.32048000 | -3.14474200 | 0.29043300 |
| H | -0.58268900 | -4.38962100 | -0.71109400 |
| H | -1.74102600 | -2.37040200 | -1.94114200 |
| H | -0.11966100 | -2.78413800 | -2.49910200 |
| H | -0.79446400 | -0.91365200 | 0.59771900 |
| H | 4.01581400 | 1.32762400 | -2.58670400 |
| H | 4.34516400 | 3.71358300 | -1.94885800 |
| H | 2.85573400 | 4.72609000 | -0.22233600 |
| H | 1.08130700 | 3.36927300 | 0.83510600 |
| H | 2.24213400 | -0.00278600 | -1.54581000 |
| H | -1.70050400 | 1.34196400 | -1.35315800 |
| H | -2.82417000 | 2.13459400 | -0.13267300 |
| H | -4.85857400 | -1.62213200 | 0.92998600 |

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|---|-------------|-------------|-------------|
| H | -5.92711900 | -1.37176300 | -0.47863400 |
| H | -4.39874000 | -2.28813700 | -0.63611800 |
| H | 0.76916500 | 0.75852400 | 1.49616100 |

P-int2

| | | | |
|---|-------------|-------------|-------------|
| C | -1.10281100 | 2.38323200 | 1.11943000 |
| C | -0.28381100 | 1.19670800 | 1.59632800 |
| C | -2.59339400 | 2.01971800 | 1.09500100 |
| C | -2.85027900 | 0.77140300 | 0.27688700 |
| C | -1.86805500 | -0.23338400 | 0.17534100 |
| C | -0.52756800 | -0.13901600 | 0.90296700 |
| C | 1.80130400 | 2.42459800 | -2.08919100 |
| C | 3.04123900 | 2.75245000 | -1.53846800 |
| C | 3.54305400 | 1.98246900 | -0.48789000 |
| C | 2.81381000 | 0.90446800 | 0.01714200 |
| C | 1.56176700 | 0.56922800 | -0.51524100 |
| C | 1.07701100 | 1.34373900 | -1.58427400 |
| C | 0.71062500 | -0.59902600 | -0.01962900 |
| C | 1.46226500 | -1.75440200 | 0.60164400 |
| C | 2.05517200 | -1.71568000 | 1.84208300 |
| C | -4.08040000 | 0.60832400 | -0.37503100 |
| C | -4.36094500 | -0.54051600 | -1.10909200 |
| C | -3.39266100 | -1.54281700 | -1.20282600 |
| C | -2.16069000 | -1.39101500 | -0.57124000 |
| O | 0.52868200 | 1.31381400 | 2.50054800 |
| N | 1.43277100 | -2.94248500 | -0.14016000 |
| O | 0.71115500 | -3.02009300 | -1.21935500 |
| O | 2.09635800 | -3.94794400 | 0.27824500 |
| H | -0.77013300 | 2.63370700 | 0.10348800 |

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|---|-------------|-------------|-------------|
| H | -0.89227800 | 3.23399900 | 1.77317700 |
| H | -3.18399900 | 2.85531700 | 0.70024800 |
| H | -2.93900400 | 1.86551300 | 2.12856100 |
| H | 1.40236900 | 3.00063100 | -2.92109400 |
| H | 3.61297900 | 3.59039400 | -1.93004100 |
| H | 4.51315700 | 2.21934900 | -0.05709000 |
| H | 3.21530300 | 0.29771500 | 0.82125000 |
| H | 0.12190000 | 1.08061400 | -2.03297200 |
| H | 1.98748800 | -0.81918300 | 2.44640200 |
| H | 2.53585900 | -2.60142300 | 2.23263800 |
| H | -4.82382200 | 1.40021200 | -0.30035600 |
| H | -5.32027800 | -0.64910000 | -1.60919700 |
| H | -3.59070100 | -2.44449500 | -1.77627000 |
| H | -1.40265400 | -2.16750700 | -0.67742400 |
| H | 0.27078000 | -1.03453200 | -0.91682200 |
| H | -0.52972000 | -0.87291600 | 1.71747100 |

P-TS3

| | | | |
|---|-------------|-------------|-------------|
| C | 2.41443500 | -2.38381800 | 0.91108500 |
| C | 0.95975700 | -2.01027700 | 0.64030800 |
| C | 3.26900700 | -1.15487900 | 1.20772700 |
| C | 3.09495900 | -0.12328500 | 0.12240900 |
| C | 1.78329900 | 0.06001700 | -0.40070900 |
| C | 0.67101400 | -0.79051500 | 0.04692000 |
| C | -1.05691700 | 2.68271200 | 2.02619600 |
| C | -1.98128900 | 3.47732400 | 1.34513100 |
| C | -2.49287400 | 3.03455300 | 0.12426400 |

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|---|-------------|-------------|-------------|
| C | -2.08209500 | 1.81298800 | -0.41173600 |
| C | -1.14835400 | 1.00970100 | 0.26077100 |
| C | -0.64695000 | 1.46267100 | 1.48791900 |
| C | -0.74820100 | -0.35413000 | -0.31804500 |
| C | -1.83809400 | -1.38877300 | 0.05544800 |
| C | -1.45546700 | -2.78065100 | -0.19650100 |
| C | 4.15849500 | 0.65417900 | -0.32642900 |
| C | 3.97895800 | 1.64915100 | -1.29298900 |
| C | 2.69735800 | 1.85666500 | -1.80113600 |
| C | 1.62344800 | 1.08245500 | -1.36373400 |
| O | 0.12083100 | -2.95999500 | 0.93781100 |
| N | -3.09970300 | -1.16920500 | -0.77954400 |
| O | -4.19528900 | -1.46164600 | -0.23212800 |
| O | -2.98263100 | -0.87277600 | -2.00526300 |
| H | 2.80723200 | -2.91580000 | 0.03032200 |
| H | 2.42889300 | -3.09600500 | 1.74233400 |
| H | 4.32693600 | -1.41918400 | 1.33003700 |
| H | 2.93419500 | -0.72841200 | 2.16776100 |
| H | -2.18065800 | -1.25957000 | 1.08407700 |
| H | -0.64953400 | 3.01574300 | 2.97825200 |
| H | -2.29903300 | 4.43029200 | 1.76178200 |
| H | -3.21811400 | 3.64055300 | -0.41403400 |
| H | -2.49557700 | 1.45685200 | -1.35128700 |
| H | 0.07953300 | 0.84781700 | 2.01113500 |
| H | -2.06178600 | -3.55666700 | 0.25483000 |
| H | -1.02510100 | -3.01077200 | -1.16621300 |
| H | 5.14733500 | 0.48093000 | 0.09675300 |
| H | 4.81953200 | 2.24850900 | -1.63320900 |

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|---|-------------|-------------|-------------|
| H | 2.52519400 | 2.62746800 | -2.54945800 |
| H | 0.64221900 | 1.27579100 | -1.78085700 |
| H | -0.82956300 | -0.27429200 | -1.41017200 |

P-TS3a

| | | | |
|---|-------------|-------------|-------------|
| C | -2.38499000 | -1.16483800 | -1.71077900 |
| C | -1.02366400 | -1.21228300 | -1.10635900 |
| C | -3.33123100 | -0.30091600 | -0.85544100 |
| C | -2.70201100 | 0.97136900 | -0.31581300 |
| C | -1.31014500 | 1.12697500 | -0.17245100 |
| C | -0.35375200 | 0.05845100 | -0.66949100 |
| C | 3.97302500 | 0.97953800 | -1.37724600 |
| C | 4.55794700 | 1.67283900 | -0.31445100 |
| C | 3.93358900 | 1.67649000 | 0.93189900 |
| C | 2.72737300 | 0.99547500 | 1.11284500 |
| C | 2.12685000 | 0.30764900 | 0.05213500 |
| C | 2.77009500 | 0.30055800 | -1.19413900 |
| C | 0.80675400 | -0.41728200 | 0.26920900 |
| C | 0.92877300 | -1.91672200 | 0.06185800 |
| C | 1.96155000 | -2.74538200 | 0.13157700 |
| C | -3.54110700 | 2.01443700 | 0.09940300 |
| C | -3.02848100 | 3.18536700 | 0.65033100 |
| C | -1.64806700 | 3.33569300 | 0.78822200 |
| C | -0.79962600 | 2.31333600 | 0.37165800 |
| O | -0.26657200 | -2.21525500 | -1.17891000 |
| N | -0.64265900 | -2.49788200 | 1.18208700 |
| O | -1.70215900 | -1.85899200 | 0.97857300 |

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|---|-------------|-------------|-------------|
| O | -0.48043500 | -3.23189000 | 2.13527400 |
| H | -2.76580100 | -2.17884900 | -1.84882100 |
| H | -2.26569500 | -0.71399700 | -2.70764000 |
| H | -3.67235000 | -0.90634200 | -0.00986400 |
| H | -4.21842800 | -0.05124400 | -1.44660600 |
| H | 4.45800500 | 0.96277600 | -2.34887600 |
| H | 5.49567900 | 2.20130000 | -0.45777200 |
| H | 4.38291900 | 2.20624800 | 1.76671200 |
| H | 2.24704700 | 0.99814700 | 2.08782000 |
| H | 2.33720600 | -0.25734700 | -2.02006700 |
| H | 1.85286700 | -3.81196900 | -0.01714800 |
| H | 2.93708900 | -2.35202500 | 0.39143000 |
| H | -4.61667400 | 1.89739500 | -0.00909500 |
| H | -3.70157500 | 3.97739900 | 0.96485300 |
| H | -1.23334500 | 4.24588200 | 1.21081000 |
| H | 0.27514200 | 2.43675200 | 0.46474900 |
| H | 0.48602800 | -0.24158200 | 1.30022500 |
| H | 0.11655100 | 0.43720900 | -1.59260600 |

P-int3

| | | | |
|---|-------------|-------------|-------------|
| C | -1.69344700 | -2.27338100 | 1.44424000 |
| C | -0.57381000 | -1.28182200 | 1.21377700 |
| C | -2.54479400 | -2.47765500 | 0.16422500 |
| C | -2.87529900 | -1.14013800 | -0.45684800 |
| C | -1.81092700 | -0.22564100 | -0.61968200 |
| C | -0.42970300 | -0.74767700 | -0.21113200 |
| C | 3.74589800 | -2.13925500 | -0.37019500 |
| C | 4.72948100 | -1.32443100 | -0.92699000 |

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|---|-------------|-------------|-------------|
| C | 4.40337500 | -0.01233800 | -1.29035100 |
| C | 3.11068200 | 0.46788200 | -1.10324700 |
| C | 2.10338300 | -0.34942900 | -0.55792600 |
| C | 2.44464500 | -1.65706500 | -0.18871200 |
| C | 0.71873700 | 0.27215000 | -0.36577300 |
| C | 0.70806400 | 1.20014700 | 0.81409100 |
| C | 0.63969500 | 0.58573100 | 2.15182600 |
| C | -4.17406700 | -0.76764400 | -0.80629800 |
| C | -4.43435900 | 0.51219300 | -1.30212300 |
| C | -3.38910900 | 1.42773200 | -1.42277100 |
| C | -2.08187500 | 1.06931400 | -1.07865800 |
| O | -0.43681200 | -0.41867900 | 2.26426700 |
| N | 0.64788300 | 2.53884800 | 0.64728100 |
| O | 0.60800200 | 3.32083100 | 1.65253800 |
| O | 0.64748000 | 3.03017300 | -0.54636300 |
| H | -2.33302500 | -1.87805600 | 2.24493300 |
| H | -1.31867100 | -3.24692400 | 1.79637800 |
| H | -3.45762700 | -3.03959000 | 0.39394400 |
| H | -1.97243200 | -3.09256600 | -0.54639100 |
| H | 3.98708200 | -3.15756000 | -0.07220100 |
| H | 5.73934100 | -1.70083500 | -1.07218700 |
| H | 5.16282600 | 0.63747600 | -1.71956600 |
| H | 2.85290900 | 1.49302100 | -1.35792400 |
| H | 1.69154900 | -2.29559300 | 0.26431400 |
| H | 1.55862100 | 0.04187000 | 2.43123800 |
| H | 0.42451600 | 1.34575300 | 2.90124700 |
| H | -4.98758400 | -1.47982400 | -0.67751700 |
| H | -5.44891200 | 0.79652500 | -1.57158100 |

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|---|-------------|-------------|-------------|
| H | -3.58713000 | 2.43585900 | -1.77834400 |
| H | -1.28816200 | 1.81101800 | -1.14693900 |
| H | 0.53491600 | 0.88250100 | -1.25093000 |
| H | -0.22216500 | -1.61563100 | -0.85768200 |

P-TS4

| | | | |
|---|-------------|-------------|-------------|
| C | 2.00156700 | -1.28672900 | 2.12741000 |
| C | 0.69607700 | -0.94650100 | 1.47937200 |
| C | 3.04313400 | -0.21425800 | 1.79631100 |
| C | 3.10792700 | 0.07501500 | 0.31086400 |
| C | 1.93489400 | -0.03953400 | -0.48437900 |
| C | 0.67510200 | -0.58203600 | 0.07809200 |
| C | -1.62413900 | 3.05752000 | 1.34692800 |
| C | -2.81591300 | 3.40335200 | 0.71089200 |
| C | -3.30958500 | 2.58225500 | -0.30720400 |
| C | -2.61626300 | 1.43403100 | -0.68536600 |
| C | -1.41244900 | 1.07497100 | -0.05135900 |
| C | -0.92991800 | 1.90433600 | 0.96974600 |
| C | -0.69544200 | -0.18768700 | -0.51299300 |
| C | -1.36395400 | -1.53247500 | -0.23108100 |
| C | -1.55832800 | -1.81517400 | 1.23787100 |
| C | 4.30296800 | 0.51110300 | -0.26585000 |
| C | 4.38198400 | 0.86592600 | -1.61309900 |
| C | 3.22967400 | 0.77968300 | -2.39737900 |
| C | 2.03462300 | 0.33362900 | -1.84106200 |
| O | -0.32274000 | -1.74180100 | 1.97844300 |
| N | -2.37397000 | -1.99258200 | -1.07710000 |

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|---|-------------|-------------|-------------|
| O | -2.52246200 | -1.45376700 | -2.21966200 |
| O | -3.06487900 | -2.99693400 | -0.72889300 |
| H | 2.36312500 | -2.27377800 | 1.77691200 |
| H | 1.86506600 | -1.37822000 | 3.21240500 |
| H | 4.03506100 | -0.50474300 | 2.16575100 |
| H | 2.77181900 | 0.71056300 | 2.32832000 |
| H | -1.22873400 | 3.68602100 | 2.14195300 |
| H | -3.35529600 | 4.30126700 | 1.00372400 |
| H | -4.23950000 | 2.83910900 | -0.80988400 |
| H | -2.99603700 | 0.78651400 | -1.47168100 |
| H | -0.00979900 | 1.62958200 | 1.47481100 |
| H | -1.95532700 | -2.82024300 | 1.37655900 |
| H | -2.26541200 | -1.09692700 | 1.69069600 |
| H | 5.18901500 | 0.58465600 | 0.36359700 |
| H | 5.32308200 | 1.20232200 | -2.04067500 |
| H | 3.26177200 | 1.05220100 | -3.44984400 |
| H | 1.15764700 | 0.25732400 | -2.47526300 |
| H | -0.60924200 | -0.14467400 | -1.60039000 |
| H | 0.09943800 | -1.84743600 | -0.39268400 |

P-Pdt

| | | | |
|---|------------|-------------|-------------|
| C | 2.22659300 | -2.51353700 | 0.80455600 |
| C | 0.86269400 | -2.01992600 | 0.41626300 |
| C | 3.11900300 | -1.34120000 | 1.22130000 |
| C | 3.05285400 | -0.21814100 | 0.21078700 |
| C | 1.80562300 | 0.07106200 | -0.39212500 |
| C | 0.63418900 | -0.78559000 | -0.08918900 |

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|---|-------------|-------------|-------------|
| C | -1.12981000 | 2.67503500 | 1.96925600 |
| C | -1.89697800 | 3.55728200 | 1.20579600 |
| C | -2.28141200 | 3.19634700 | -0.08533700 |
| C | -1.89965700 | 1.96049100 | -0.61014100 |
| C | -1.12760400 | 1.07074800 | 0.14693800 |
| C | -0.74900400 | 1.44138500 | 1.44348400 |
| C | -0.77598500 | -0.30537300 | -0.41910200 |
| C | -1.79541500 | -1.34475200 | 0.09065800 |
| C | -1.29258400 | -2.76954300 | -0.15516300 |
| C | 4.17129700 | 0.55064000 | -0.10588800 |
| C | 4.08482500 | 1.61033300 | -1.01151200 |
| C | 2.85948400 | 1.90139100 | -1.60706200 |
| C | 1.73248800 | 1.13908200 | -1.29987300 |
| O | -0.10176600 | -2.97784300 | 0.59153600 |
| N | -3.12732200 | -1.19537200 | -0.60855400 |
| O | -4.13341400 | -1.21209800 | 0.09147100 |
| O | -3.11482200 | -1.11701800 | -1.83711100 |
| H | 2.66676800 | -3.05537500 | -0.04583200 |
| H | 2.11989300 | -3.24000500 | 1.61651500 |
| H | 4.15191700 | -1.67388300 | 1.36256600 |
| H | 2.77088300 | -0.96822800 | 2.19639000 |
| H | -2.01713200 | -1.20727900 | 1.14887000 |
| H | -0.82376200 | 2.94951000 | 2.97464500 |
| H | -2.19087500 | 4.51943900 | 1.61467800 |
| H | -2.87874900 | 3.87513800 | -0.68696700 |
| H | -2.20809500 | 1.68141200 | -1.61436700 |
| H | -0.14345100 | 0.76246000 | 2.03741000 |
| H | -2.01338400 | -3.51195700 | 0.19416500 |

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|---|-------------|-------------|-------------|
| H | -1.10220100 | -2.91614400 | -1.22578000 |
| H | 5.12337100 | 0.31660500 | 0.36458000 |
| H | 4.96612100 | 2.19911800 | -1.24774500 |
| H | 2.77543500 | 2.72096800 | -2.31468000 |
| H | 0.78903900 | 1.38192200 | -1.77520000 |
| H | -0.89811400 | -0.26482400 | -1.50839600 |

Cartesian coordinates of secondary acetate path optimized structures

1

| | | | |
|---|-------------|-------------|-------------|
| C | -2.72584200 | -0.97160800 | -0.09077900 |
| C | -2.93821500 | 0.41149500 | -0.12083600 |
| C | -1.81767800 | 1.25226600 | -0.01775400 |
| C | -0.52898000 | 0.74888400 | 0.09713900 |
| C | -0.28852300 | -0.66628100 | 0.09174100 |
| C | -1.44238500 | -1.49735400 | 0.01352700 |
| C | 0.67282100 | 1.63475300 | 0.33062900 |
| C | 1.92948400 | 1.09333900 | -0.35952700 |
| C | 2.19382300 | -0.39720500 | -0.03386900 |
| C | 1.03860500 | -1.18199600 | 0.17330700 |
| O | 3.38176000 | -0.80228100 | -0.04274600 |
| H | -3.57561000 | -1.65143300 | -0.15841200 |
| H | -3.93964800 | 0.82517100 | -0.21243200 |
| H | -1.95609600 | 2.33476400 | -0.01156500 |
| H | -1.30167000 | -2.57738400 | 0.02198500 |

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|---|------------|-------------|-------------|
| H | 0.87759000 | 1.66315900 | 1.41567400 |
| H | 0.45729600 | 2.66993400 | 0.02845100 |
| H | 2.82086100 | 1.66323300 | -0.07373800 |
| H | 1.82635800 | 1.18950600 | -1.45254500 |
| H | 1.17818600 | -2.25645800 | 0.28308300 |

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|---|-------------|-------------|-------------|
| C | -3.53077100 | 0.79668300 | -1.81724000 |
| C | -4.76409500 | 0.88016200 | -1.16890900 |
| C | -4.94844100 | 0.24503600 | 0.06204600 |
| C | -3.90090100 | -0.46201200 | 0.64392200 |
| C | -2.64054700 | -0.51795100 | 0.01944300 |
| C | -2.47281600 | 0.10274000 | -1.23307600 |
| C | -1.56815300 | -1.26880800 | 0.67738000 |
| C | -0.25395800 | -0.99056300 | 0.70000300 |
| C | 0.44727800 | 0.23767700 | 0.19248200 |
| O | 1.16987300 | 0.81448600 | 1.28850000 |
| O | 0.76448500 | 2.88251600 | 0.44851800 |
| C | 1.27917100 | 2.17444000 | 1.28275700 |
| C | 2.12601300 | 2.63437600 | 2.44002800 |
| N | 0.63299000 | -1.99186100 | 1.32299100 |
| O | 0.14901800 | -2.84301500 | 2.06687200 |
| O | 1.82780300 | -1.91629400 | 1.02922900 |
| H | -3.39329100 | 1.26323600 | -2.78785100 |
| H | -5.58460200 | 1.42328800 | -1.62814200 |
| H | -5.91063100 | 0.29401800 | 0.56261700 |
| H | -4.04616700 | -0.96282900 | 1.59709500 |
| H | -1.53376400 | -0.00918900 | -1.76623600 |

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|---|-------------|-------------|-------------|
| H | -1.86023500 | -2.16373700 | 1.22173500 |
| H | -0.30541800 | 0.95522300 | -0.14431700 |
| H | 2.09416600 | 3.72135600 | 2.50358600 |
| H | 1.77530400 | 2.18565500 | 3.37283100 |
| H | 3.15716000 | 2.30263400 | 2.28457400 |
| C | 1.33103800 | -0.04429500 | -1.02962600 |
| O | 0.88452200 | -0.62119400 | -2.00072900 |
| O | 2.55775200 | 0.46150900 | -0.91753000 |
| C | 3.45506400 | 0.24464700 | -2.04145000 |
| H | 2.87841500 | 0.31508000 | -2.96629600 |
| H | 4.15731100 | 1.07879400 | -1.98469600 |
| C | 4.15803900 | -1.09683900 | -1.92043000 |
| H | 4.87932000 | -1.20831400 | -2.73674500 |
| H | 4.69375200 | -1.17157300 | -0.97050800 |
| H | 3.43859000 | -1.91643000 | -1.98144600 |

S-Cmplx

| | | | |
|---|-------------|-------------|-------------|
| C | -4.59820500 | -1.54903800 | -2.21396000 |
| C | -5.66182600 | -1.48336900 | -1.30924100 |
| C | -5.37695000 | -1.55207400 | 0.06182000 |
| C | -4.07314200 | -1.67299300 | 0.53174400 |
| C | -2.97404000 | -1.71328600 | -0.38002700 |
| C | -3.28541800 | -1.66150700 | -1.76208700 |
| C | -3.74924600 | -1.86078000 | 1.99604000 |
| C | -2.43443800 | -1.17582500 | 2.38224900 |
| C | -1.28090300 | -1.52875300 | 1.43053500 |

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|---|-------------|-------------|-------------|
| C | -1.62318000 | -1.79977300 | 0.10758800 |
| O | -0.09791400 | -1.46190000 | 1.91326500 |
| H | -4.79212800 | -1.50474300 | -3.28447000 |
| H | -6.68681200 | -1.38667100 | -1.65773300 |
| H | -6.19281800 | -1.52366900 | 0.78434300 |
| H | -2.46847400 | -1.69975500 | -2.47983700 |
| H | -3.63524800 | -2.94107900 | 2.18971500 |
| H | -4.58079800 | -1.51740300 | 2.62589700 |
| H | -2.12897100 | -1.44175000 | 3.39983000 |
| H | -2.55806400 | -0.08146100 | 2.36345600 |
| H | -0.82272800 | -1.96095200 | -0.61189800 |
| C | 5.38197700 | -2.68220200 | -0.65599100 |
| C | 4.98940400 | -3.92522300 | -0.15227200 |
| C | 3.73468100 | -4.06232700 | 0.44309500 |
| C | 2.88539300 | -2.96331100 | 0.53490500 |
| C | 3.25972300 | -1.70388600 | 0.01343200 |
| C | 4.52988300 | -1.58332600 | -0.58486600 |
| C | 2.25934900 | -0.65342800 | 0.23100800 |
| C | 2.05306700 | 0.63575300 | -0.12121000 |
| C | 0.82056900 | 1.32947300 | 0.42312400 |
| O | 1.15746700 | 2.41479200 | 1.32700400 |
| O | 0.48188700 | 4.11959800 | -0.03092600 |
| C | 1.02969400 | 3.70998600 | 0.96619800 |
| C | 1.68033800 | 4.58915100 | 2.01150300 |
| N | 2.91352200 | 1.41096300 | -1.00810800 |
| O | 3.56344700 | 0.82750900 | -1.87998100 |
| O | 2.95681200 | 2.63278700 | -0.83691700 |
| H | 6.35920600 | -2.56884800 | -1.11807400 |

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|---|-------------|-------------|-------------|
| H | 5.65848400 | -4.77906000 | -0.22366200 |
| H | 3.41929400 | -5.02203500 | 0.84301500 |
| H | 1.91406600 | -3.05020000 | 1.01573400 |
| H | 4.84130500 | -0.63504400 | -0.99877700 |
| H | 1.44509400 | -1.01557300 | 0.87562200 |
| H | 0.33168100 | 0.59642800 | 1.07390700 |
| H | 1.38799500 | 5.62635300 | 1.84724500 |
| H | 1.40469800 | 4.26608000 | 3.01828300 |
| H | 2.76694500 | 4.49695500 | 1.91607600 |
| C | -0.19254500 | 1.67313400 | -0.68099300 |
| O | 0.03140400 | 1.56535100 | -1.86619200 |
| O | -1.38809100 | 1.95543500 | -0.14264600 |
| C | -2.45058700 | 2.21775800 | -1.08685000 |
| H | -2.18159100 | 3.10700700 | -1.66704300 |
| H | -2.52924400 | 1.36809000 | -1.76985800 |
| C | -3.72780400 | 2.41261500 | -0.29359000 |
| H | -4.55160600 | 2.64810300 | -0.97555400 |
| H | -3.98626500 | 1.49854300 | 0.24709900 |
| H | -3.62353700 | 3.23475700 | 0.42164900 |

S-TS1

| | | | |
|---|-------------|-------------|-------------|
| C | -4.70663800 | -0.75992900 | 1.19380300 |
| C | -4.61096500 | -2.10132400 | 1.57016000 |
| C | -3.68623400 | -2.92323100 | 0.92114900 |
| C | -2.84940900 | -2.43170000 | -0.08006900 |
| C | -2.91144800 | -1.05962900 | -0.43975900 |
| C | -3.87255500 | -0.25000700 | 0.20370900 |
| C | -1.95662200 | -3.36447400 | -0.87139200 |

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|---|-------------|-------------|-------------|
| C | -0.73519600 | -2.66554700 | -1.48158700 |
| C | -1.08594500 | -1.34919800 | -2.16540100 |
| C | -2.03431500 | -0.51431800 | -1.46848700 |
| O | -0.47791700 | -0.98811200 | -3.18942600 |
| H | -5.42857500 | -0.10622400 | 1.67800100 |
| H | -5.24995400 | -2.50489100 | 2.35146500 |
| H | -3.62053600 | -3.97678300 | 1.18899700 |
| H | -3.94877200 | 0.79536000 | -0.07963400 |
| H | -2.55549000 | -3.80131000 | -1.68752300 |
| H | -1.64117200 | -4.20786000 | -0.24518700 |
| H | -0.22454300 | -3.30469500 | -2.20788400 |
| H | -0.00057200 | -2.43562600 | -0.69681600 |
| H | -2.39871500 | 0.34411000 | -2.02266700 |
| C | -2.38158900 | 3.33598600 | 1.52967500 |
| C | -2.85888200 | 4.19203300 | 0.53776200 |
| C | -2.52935500 | 3.93304300 | -0.79569300 |
| C | -1.73802900 | 2.83519400 | -1.11530700 |
| C | -1.24889000 | 1.95245800 | -0.12534300 |
| C | -1.59295100 | 2.22905300 | 1.21160300 |
| C | -0.37458200 | 0.85590000 | -0.60408700 |
| C | 0.71167800 | 0.20981000 | 0.03317300 |
| C | 1.93203500 | -0.04978600 | -0.80547700 |
| O | 2.70291500 | 1.14623600 | -1.18580300 |
| O | 2.85289600 | 2.05198600 | 0.90817100 |
| C | 3.09119900 | 2.06420600 | -0.27573000 |
| C | 3.89054300 | 3.14983900 | -0.97569900 |
| N | 0.74277000 | -0.19797200 | 1.36802300 |
| O | -0.31837100 | -0.22789300 | 2.03688100 |

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|---|-------------|-------------|-------------|
| O | 1.83316700 | -0.58120500 | 1.86246000 |
| H | -2.62768900 | 3.52427200 | 2.57186800 |
| H | -3.47643900 | 5.04859700 | 0.79635000 |
| H | -2.88328700 | 4.59048800 | -1.58613300 |
| H | -1.48105100 | 2.64908400 | -2.15534900 |
| H | -1.23817100 | 1.56603800 | 1.98786600 |
| H | -0.13899000 | 1.00009100 | -1.65482500 |
| H | 1.58654700 | -0.38931500 | -1.78560800 |
| H | 4.12873100 | 3.93923600 | -0.26243400 |
| H | 4.81462500 | 2.72418200 | -1.37937300 |
| H | 3.32299200 | 3.55892300 | -1.81626000 |
| C | 2.85423000 | -1.16511300 | -0.30949000 |
| O | 2.51947900 | -2.33159800 | -0.31953900 |
| O | 4.10245700 | -0.73628700 | -0.02755300 |
| C | 5.00053700 | -1.72623400 | 0.51016500 |
| H | 4.80671700 | -2.68470000 | 0.02123900 |
| H | 5.99894100 | -1.37440500 | 0.23260600 |
| C | 4.84618900 | -1.83749300 | 2.02006200 |
| H | 5.56988000 | -2.55991900 | 2.41646100 |
| H | 5.01636600 | -0.86826100 | 2.49642900 |
| H | 3.83590800 | -2.16284600 | 2.27429200 |

S-int1

| | | | |
|---|-------------|-------------|------------|
| C | -4.69109600 | -0.09362200 | 1.18827600 |
| C | -4.87146300 | -1.40023900 | 1.64254400 |
| C | -4.04639600 | -2.40680200 | 1.14965900 |
| C | -3.03179900 | -2.13747200 | 0.22255800 |

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|---|-------------|-------------|-------------|
| C | -2.82006700 | -0.81302000 | -0.20626500 |
| C | -3.68368500 | 0.18673100 | 0.26941300 |
| C | -2.24077600 | -3.30121200 | -0.34287600 |
| C | -0.92909600 | -2.89371200 | -1.03054800 |
| C | -1.13969500 | -1.68924800 | -1.91823200 |
| C | -1.78684200 | -0.46477000 | -1.27073700 |
| O | -0.79665900 | -1.66081800 | -3.09020000 |
| H | -5.33286700 | 0.70755800 | 1.54612800 |
| H | -5.64920600 | -1.63385400 | 2.36541200 |
| H | -4.18856500 | -3.43292400 | 1.48420100 |
| H | -3.55807100 | 1.20348400 | -0.08519300 |
| H | -2.87414000 | -3.83178100 | -1.07043300 |
| H | -2.02864600 | -4.02350000 | 0.45390100 |
| H | -0.51862500 | -3.70526900 | -1.63677900 |
| H | -0.18251400 | -2.62657500 | -0.27649100 |
| H | -2.32231400 | 0.04142700 | -2.08390000 |
| C | -1.44765600 | 3.53296200 | 1.31287400 |
| C | -1.89872300 | 4.46337700 | 0.37397300 |
| C | -1.92286800 | 4.11273300 | -0.97661800 |
| C | -1.49797300 | 2.84322000 | -1.37225000 |
| C | -1.04864600 | 1.89715300 | -0.43761100 |
| C | -1.02756800 | 2.26218800 | 0.91701100 |
| C | -0.57212000 | 0.53133800 | -0.93903600 |
| C | 0.63377200 | -0.05916000 | -0.24414100 |
| C | 1.93916000 | -0.02439500 | -0.93213500 |
| O | 2.64614500 | 1.29547300 | -0.98838900 |
| O | 2.54187200 | 1.76469400 | 1.24891100 |
| C | 2.84522200 | 2.04353300 | 0.11266400 |

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|---|-------------|-------------|-------------|
| C | 3.52088300 | 3.34780300 | -0.28637900 |
| N | 0.56189300 | -0.60835100 | 0.99359500 |
| O | -0.56374800 | -0.66592700 | 1.58965400 |
| O | 1.59452900 | -1.11034300 | 1.53752700 |
| H | -1.42185500 | 3.79621700 | 2.36740400 |
| H | -2.22359900 | 5.45180600 | 0.69023200 |
| H | -2.26064500 | 4.82817900 | -1.72307000 |
| H | -1.50745100 | 2.58162600 | -2.42905700 |
| H | -0.70168800 | 1.53107000 | 1.64710100 |
| H | -0.20642900 | 0.72939200 | -1.95358000 |
| H | 1.77310200 | -0.17572300 | -2.00363400 |
| H | 3.71016700 | 3.94381400 | 0.60698800 |
| H | 4.46133600 | 3.14286000 | -0.80686100 |
| H | 2.87829300 | 3.90572500 | -0.97442300 |
| C | 2.89743700 | -1.15145100 | -0.53821800 |
| O | 2.68806400 | -2.30541000 | -0.85632900 |
| O | 4.05606300 | -0.71059000 | 0.00064800 |
| C | 4.95358500 | -1.72964400 | 0.47418800 |
| H | 4.90656800 | -2.58787500 | -0.20212200 |
| H | 5.94872900 | -1.27695300 | 0.41337100 |
| C | 4.61053900 | -2.13473900 | 1.90097100 |
| H | 5.32894100 | -2.88208400 | 2.26039100 |
| H | 4.63981500 | -1.26578800 | 2.56371200 |
| H | 3.60150200 | -2.54831200 | 1.94244200 |

S-TS2

| | | | |
|---|------------|-------------|-------------|
| C | 4.06194000 | -0.40023100 | -1.94556400 |
| C | 4.50226500 | -1.71512100 | -1.79305400 |

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|---|-------------|-------------|-------------|
| C | 4.08174100 | -2.44389300 | -0.68666700 |
| C | 3.23498100 | -1.88240100 | 0.28004500 |
| C | 2.77945700 | -0.55692300 | 0.12629100 |
| C | 3.21243000 | 0.16434400 | -0.99926600 |
| C | 2.85938200 | -2.71689400 | 1.48625500 |
| C | 1.51673700 | -2.29310500 | 2.09195800 |
| C | 1.51415700 | -0.80642600 | 2.35233300 |
| C | 1.92458000 | 0.12661900 | 1.19931800 |
| O | 1.18618400 | -0.33680300 | 3.42957800 |
| H | 4.36489600 | 0.18496000 | -2.80925400 |
| H | 5.15609000 | -2.17006900 | -2.53271200 |
| H | 4.40991000 | -3.47346400 | -0.55850600 |
| H | 2.85545900 | 1.17365200 | -1.15034800 |
| H | 3.64406900 | -2.62800000 | 2.25316700 |
| H | 2.82719700 | -3.77636200 | 1.20849800 |
| H | 1.30589000 | -2.80950600 | 3.03224900 |
| H | 0.70241300 | -2.51734800 | 1.38887100 |
| H | 2.54854100 | 0.87615200 | 1.70248500 |
| C | -0.25012800 | 4.28603700 | -0.77219800 |
| C | 0.93605400 | 5.01184100 | -0.63508300 |
| C | 2.04693800 | 4.38939400 | -0.07185500 |
| C | 1.97087000 | 3.05624400 | 0.34440200 |
| C | 0.79120700 | 2.31655500 | 0.19633100 |
| C | -0.32808600 | 2.95666800 | -0.36313800 |
| C | 0.60908300 | 0.90022100 | 0.76216300 |
| C | -0.38413400 | 0.00821600 | 0.03452700 |
| C | -1.38622600 | -0.62232200 | 0.72202700 |
| O | -3.11712200 | 0.52515800 | 1.36050200 |

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|---|-------------|-------------|-------------|
| O | -3.29780400 | 1.90390500 | -0.43866300 |
| C | -3.72008000 | 1.35675600 | 0.59306500 |
| C | -5.16212600 | 1.66972100 | 1.05381000 |
| N | -0.28523500 | -0.17119900 | -1.37907900 |
| O | 0.54133100 | 0.50418300 | -2.01369800 |
| O | -1.01649900 | -1.01504000 | -1.93265300 |
| H | -1.13303700 | 4.75370300 | -1.19988600 |
| H | 0.99141700 | 6.04817200 | -0.95974500 |
| H | 2.98014000 | 4.93461200 | 0.04949400 |
| H | 2.85599800 | 2.60438800 | 0.78093100 |
| H | -1.27598500 | 2.42614600 | -0.46485400 |
| H | 0.12508400 | 1.08758800 | 1.72819800 |
| H | -1.31854700 | -0.60062600 | 1.80012500 |
| H | -5.56652200 | 2.52263300 | 0.50278300 |
| H | -5.79573400 | 0.79336400 | 0.87333300 |
| H | -5.18675800 | 1.87032800 | 2.12976600 |
| C | -2.11531400 | -1.84196700 | 0.23300100 |
| O | -1.64808400 | -2.94512100 | 0.47426300 |
| O | -3.29484800 | -1.63969300 | -0.35711900 |
| C | -3.96426900 | -2.81042700 | -0.86187300 |
| H | -3.81667900 | -3.63889200 | -0.16356000 |
| H | -5.02168300 | -2.53241800 | -0.87377300 |
| C | -3.47079000 | -3.17213100 | -2.25569400 |
| H | -4.04985800 | -4.01705000 | -2.64750500 |
| H | -3.57968500 | -2.32226800 | -2.93391400 |
| H | -2.41524500 | -3.44866900 | -2.22676800 |

S-Int2

| | | | |
|---|-------------|-------------|-------------|
| C | -3.17608900 | -0.95582800 | -1.57279900 |
| C | -2.77044900 | 0.15467600 | -0.62114500 |
| C | -3.56841600 | -2.19954400 | -0.76555300 |
| C | -2.43129500 | -2.65043600 | 0.12435300 |
| C | -1.55789600 | -1.70440200 | 0.70251900 |
| C | -1.80441000 | -0.20063500 | 0.52933200 |
| C | -1.21803000 | 4.22785800 | 1.86080200 |
| C | -1.18141100 | 4.97624000 | 0.68499100 |
| C | -0.93894500 | 4.32915300 | -0.52907200 |
| C | -0.73813700 | 2.95060600 | -0.57525900 |
| C | -0.77166500 | 2.18794200 | 0.60055500 |
| C | -1.00816900 | 2.84857700 | 1.81319400 |
| C | -0.49521800 | 0.68042200 | 0.62085100 |
| C | 0.69410700 | 0.25247000 | -0.23202400 |
| C | 1.94415200 | 0.18286500 | 0.38224400 |
| C | -2.24120100 | -4.01584900 | 0.36968900 |
| C | -1.20873600 | -4.47091000 | 1.18470100 |
| C | -0.34161100 | -3.54274800 | 1.75868300 |
| C | -0.51826700 | -2.18201500 | 1.51610000 |
| O | -3.32059100 | 1.24188000 | -0.63906400 |
| N | 0.46532000 | -0.08865500 | -1.55665000 |
| O | -0.64890000 | 0.29608500 | -2.08934200 |
| O | 1.29576200 | -0.76669800 | -2.20835400 |
| H | -2.32263100 | -1.17439800 | -2.21999500 |
| H | -4.00612500 | -0.58632100 | -2.18138800 |
| H | -3.85921300 | -3.01634300 | -1.43645500 |
| H | -4.45686400 | -1.97565200 | -0.15424700 |

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|---|-------------|-------------|-------------|
| H | -1.39758100 | 4.71543100 | 2.81633500 |
| H | -1.33641500 | 6.05218500 | 0.71383200 |
| H | -0.90853600 | 4.90302900 | -1.45208600 |
| H | -0.57297900 | 2.43986500 | -1.51724400 |
| H | -1.02206300 | 2.27471600 | 2.73847500 |
| H | 1.94475500 | 0.23702100 | 1.46691300 |
| H | -2.91742300 | -4.72918000 | -0.09741100 |
| H | -1.07485000 | -5.53558400 | 1.35807900 |
| H | 0.48274600 | -3.87297000 | 2.38485400 |
| H | 0.18481300 | -1.48681200 | 1.95790700 |
| H | -0.14674000 | 0.50235100 | 1.64417800 |
| H | -2.38086400 | 0.11943200 | 1.41165800 |
| C | 3.26746300 | 0.18588200 | -0.18979200 |
| O | 4.19319300 | -0.14170600 | 0.81832900 |
| C | 5.56130500 | -0.09945900 | 0.42097400 |
| C | 6.00192700 | -1.40282000 | -0.23874800 |
| O | 3.65023900 | 0.47078600 | -1.31463000 |
| H | 5.71955100 | 0.73777000 | -0.26647200 |
| H | 6.12799300 | 0.08132000 | 1.34236600 |
| H | 5.44400100 | -1.55182200 | -1.16591400 |
| H | 7.07327300 | -1.37401900 | -0.47402900 |
| H | 5.81623600 | -2.25448000 | 0.42411800 |

S-TS3

| | | | |
|---|-------------|-------------|-------------|
| C | -3.02706800 | -2.18692800 | -2.23404800 |
| C | -3.96906400 | -2.84112900 | -1.44198000 |
| C | -4.01287900 | -2.54640800 | -0.07871300 |

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|---|-------------|-------------|-------------|
| C | -3.14684700 | -1.61481800 | 0.49459300 |
| C | -2.20671600 | -0.91211400 | -0.30462900 |
| C | -2.16203000 | -1.24786000 | -1.67455500 |
| C | -3.18207200 | -1.33997400 | 1.97745300 |
| C | -2.95861300 | 0.14716300 | 2.24629900 |
| C | -1.65794500 | 0.65629700 | 1.61657600 |
| C | -1.25847500 | 0.06239900 | 0.32151600 |
| O | -0.99583100 | 1.49289400 | 2.22666400 |
| H | -2.95683300 | -2.40656900 | -3.29657800 |
| H | -4.64928100 | -3.57156400 | -1.87180400 |
| H | -4.73160800 | -3.05327500 | 0.56312200 |
| H | -1.43001700 | -0.77875700 | -2.32184100 |
| H | -2.38612000 | -1.91332500 | 2.47776100 |
| H | -4.13027000 | -1.68352900 | 2.40858000 |
| H | -2.91794300 | 0.37803400 | 3.31430400 |
| H | -3.78858300 | 0.72453100 | 1.81239800 |
| H | -0.15497000 | -0.70400500 | 0.67721300 |
| C | 1.48781800 | 3.95275500 | 0.71238700 |
| C | 0.60812000 | 4.98660400 | 0.38136800 |
| C | -0.58473200 | 4.68360700 | -0.27402600 |
| C | -0.88684000 | 3.35925900 | -0.59466700 |
| C | -0.01638000 | 2.31772400 | -0.25881100 |
| C | 1.17985200 | 2.63106400 | 0.39864500 |
| C | -0.38077600 | 0.88285900 | -0.66247900 |
| C | 0.83825900 | 0.01017100 | -0.90724700 |
| C | 1.01498400 | -1.14314800 | -0.04783400 |
| N | 1.71161600 | 0.32057600 | -1.95082100 |
| O | 2.72609100 | -0.39312600 | -2.14174700 |

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|---|-------------|-------------|-------------|
| O | 1.41945700 | 1.29412900 | -2.69417100 |
| H | 2.42148500 | 4.17663100 | 1.22261300 |
| H | 0.85323600 | 6.01713900 | 0.62755500 |
| H | -1.27693000 | 5.47729200 | -0.54650900 |
| H | -1.81280500 | 3.13029500 | -1.11835800 |
| H | 1.86781100 | 1.83386700 | 0.66601000 |
| H | -0.93478800 | 1.00163100 | -1.59999500 |
| H | 0.49323400 | -2.06546400 | -0.32406900 |
| C | 2.31896000 | -1.37441000 | 0.57169000 |
| O | 3.12096800 | -0.52535800 | 0.93321100 |
| O | 2.52867700 | -2.71798600 | 0.81273200 |
| C | 3.76187100 | -3.04210900 | 1.46503500 |
| H | 3.98271100 | -2.28374600 | 2.22199800 |
| H | 3.58093500 | -4.00289600 | 1.95916300 |
| C | 4.90881000 | -3.14443100 | 0.46637900 |
| H | 5.83493800 | -3.43805700 | 0.97540900 |
| H | 4.68571500 | -3.88832000 | -0.30489400 |
| H | 5.06444800 | -2.17781300 | -0.01757200 |

S-Ts3a

| | | | |
|---|------------|-------------|-------------|
| C | 3.72951000 | -1.85357800 | 2.01843000 |
| C | 4.59406200 | -2.16576700 | 0.96723900 |
| C | 4.12189000 | -2.11119200 | -0.34098500 |
| C | 2.79984100 | -1.74299800 | -0.63162900 |
| C | 1.93538200 | -1.39503300 | 0.42507700 |
| C | 2.41911200 | -1.47467200 | 1.74058500 |
| C | 2.31474100 | -1.80085300 | -2.06934200 |
| C | 1.09444500 | -0.90297500 | -2.33884000 |

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|---|-------------|-------------|-------------|
| C | 0.07542200 | -1.11485000 | -1.25363300 |
| C | 0.48756500 | -1.00722600 | 0.18380000 |
| O | -1.18827900 | -1.20071600 | -1.52866500 |
| H | 4.07406200 | -1.90480300 | 3.04817700 |
| H | 5.62323100 | -2.45440100 | 1.16581800 |
| H | 4.78642800 | -2.36686200 | -1.16440700 |
| H | 1.74527500 | -1.23544900 | 2.55902700 |
| H | 2.04404900 | -2.84150300 | -2.30064200 |
| H | 3.13939800 | -1.54107400 | -2.74579100 |
| H | 0.64440400 | -1.14031000 | -3.30864000 |
| H | 1.43106200 | 0.14422700 | -2.37880100 |
| H | -0.15232500 | -1.69455000 | 0.75050100 |
| C | 1.81340600 | 3.14310300 | -1.39769900 |
| C | 2.93630500 | 3.44851000 | -0.62560200 |
| C | 3.11058900 | 2.80321800 | 0.59850600 |
| C | 2.18089500 | 1.85802700 | 1.03423200 |
| C | 1.05912800 | 1.52634400 | 0.26375400 |
| C | 0.88815000 | 2.19934300 | -0.95484700 |
| C | 0.08389100 | 0.44222200 | 0.74007300 |
| C | -1.34947800 | 0.71910500 | 0.34034400 |
| C | -2.21918300 | -0.19995600 | -0.36264800 |
| N | -1.87627400 | 1.95981500 | 0.59358700 |
| O | -1.19156200 | 2.80721500 | 1.23532300 |
| O | -3.06463400 | 2.24495500 | 0.20821400 |
| H | 1.64826700 | 3.65275100 | -2.34423500 |
| H | 3.65635400 | 4.18825700 | -0.96713900 |
| H | 3.97117500 | 3.03697500 | 1.22125000 |
| H | 2.32584600 | 1.37325900 | 1.99509700 |

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|---|-------------|-------------|-------------|
| H | 0.00151100 | 1.99147500 | -1.54602000 |
| H | 0.18399200 | 0.40186600 | 1.83589200 |
| H | -2.89478100 | 0.31778100 | -1.03181800 |
| C | -2.84946500 | -1.33655900 | 0.38094200 |
| O | -2.26662600 | -2.12906800 | 1.09723000 |
| O | -4.20560500 | -1.49976700 | 0.25528300 |
| C | -5.03929500 | -0.46677000 | -0.30708300 |
| H | -4.68929100 | 0.51930800 | 0.01704600 |
| H | -4.98793100 | -0.50842700 | -1.40385700 |
| C | -6.45870000 | -0.73845600 | 0.16455900 |
| H | -7.14327200 | 0.00647600 | -0.25556700 |
| H | -6.79278700 | -1.73336300 | -0.14718100 |
| H | -6.51638600 | -0.68521100 | 1.25569800 |

S-Int3

| | | | |
|---|------------|-------------|-------------|
| C | 3.94079800 | -1.51992900 | 2.00540000 |
| C | 4.83739600 | -2.09120400 | 1.10170200 |
| C | 4.58743300 | -1.95192500 | -0.26633300 |
| C | 3.48149900 | -1.25057800 | -0.73723700 |
| C | 2.57533200 | -0.62195500 | 0.17302700 |
| C | 2.83551000 | -0.80544800 | 1.55517800 |
| C | 3.18859100 | -1.17639000 | -2.21527100 |
| C | 2.62391800 | 0.19304100 | -2.58537000 |
| C | 1.40716100 | 0.54101300 | -1.72229200 |
| C | 1.46110200 | 0.17356200 | -0.32859300 |
| O | 0.47227200 | 1.17351900 | -2.25002500 |
| H | 4.09774900 | -1.63250600 | 3.07539600 |

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|---|-------------|-------------|-------------|
| H | 5.70524200 | -2.64472500 | 1.45057200 |
| H | 5.26139300 | -2.40894600 | -0.98933600 |
| H | 2.14441900 | -0.41144200 | 2.28763200 |
| H | 2.44027000 | -1.94311500 | -2.47204500 |
| H | 4.08842400 | -1.41096200 | -2.79726200 |
| H | 2.31202800 | 0.24537600 | -3.63241700 |
| H | 3.39316500 | 0.96478700 | -2.43176700 |
| H | -1.45964900 | 0.39518800 | -1.45245200 |
| C | -1.69094100 | 3.89689200 | 0.76695100 |
| C | -0.70761700 | 4.86320300 | 0.55551700 |
| C | 0.60636800 | 4.45353300 | 0.31660200 |
| C | 0.92394200 | 3.09717400 | 0.28678100 |
| C | -0.05718200 | 2.11785700 | 0.49474500 |
| C | -1.37020200 | 2.53731600 | 0.74275100 |
| C | 0.33670500 | 0.64517900 | 0.58869200 |
| C | -0.74283800 | -0.37741300 | 0.38133600 |
| C | -1.62678300 | -0.48379300 | -0.82283100 |
| N | -0.86728000 | -1.39798900 | 1.29994700 |
| O | -1.73717300 | -2.29746300 | 1.07704700 |
| O | -0.15005400 | -1.42467900 | 2.34418600 |
| H | -2.71926400 | 4.19798000 | 0.95375300 |
| H | -0.95965600 | 5.92094600 | 0.57406500 |
| H | 1.38629100 | 5.19306300 | 0.14841600 |
| H | 1.94663700 | 2.78423200 | 0.09467800 |
| H | -2.14768800 | 1.79681000 | 0.90876700 |
| H | 0.65091200 | 0.49722300 | 1.62305600 |
| H | -1.38833200 | -1.37055500 | -1.42016700 |
| C | -3.09980400 | -0.57093300 | -0.46661700 |

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|---|-------------|-------------|-------------|
| O | -3.68160900 | 0.10279100 | 0.36065400 |
| O | -3.74006400 | -1.47063600 | -1.26237600 |
| C | -5.11965300 | -1.72180500 | -0.94348100 |
| H | -5.59168200 | -0.78896100 | -0.62363000 |
| H | -5.57299600 | -2.05240500 | -1.88336600 |
| C | -5.23226200 | -2.78888900 | 0.13728000 |
| H | -6.28592700 | -2.98501500 | 0.36940800 |
| H | -4.76583600 | -3.72204900 | -0.19114500 |
| H | -4.72235100 | -2.45829900 | 1.04470200 |

S-TS4

| | | | |
|---|-------------|-------------|-------------|
| C | 2.13445700 | -1.83603600 | 1.94696200 |
| C | 1.25222000 | -0.64893200 | 1.67014200 |
| C | 3.60713100 | -1.47510600 | 1.71203500 |
| C | 3.82108500 | -0.87710600 | 0.33804600 |
| C | 2.86376300 | 0.00953300 | -0.19927900 |
| C | 1.63063600 | 0.37626300 | 0.61959300 |
| C | -0.89785900 | 3.86872900 | 1.48440500 |
| C | -1.01060700 | 4.73759300 | 0.39496000 |
| C | -0.72513600 | 4.26827400 | -0.88646700 |
| C | -0.32482200 | 2.94259000 | -1.07408400 |
| C | -0.19642700 | 2.06604300 | 0.00912200 |
| C | -0.49438600 | 2.54858500 | 1.29477600 |
| C | 0.29187700 | 0.64472700 | -0.19516100 |
| C | -0.76454100 | -0.40874400 | 0.18924100 |
| C | -2.12969000 | -0.11942800 | 0.14927400 |
| C | 4.96860000 | -1.18194800 | -0.40340700 |

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|---|-------------|-------------|-------------|
| C | 5.19717800 | -0.61450500 | -1.65633600 |
| C | 4.26476400 | 0.28001400 | -2.17969800 |
| C | 3.11532800 | 0.58705300 | -1.45147400 |
| O | -0.04261000 | -0.70046900 | 1.88337000 |
| N | -0.39201900 | -1.75255000 | -0.47022400 |
| O | -0.20579100 | -1.70055700 | -1.69164000 |
| O | -0.32168000 | -2.77602700 | 0.18894200 |
| H | 1.85354800 | -2.68660000 | 1.30183800 |
| H | 1.98366000 | -2.18040000 | 2.97939900 |
| H | 4.25449200 | -2.35105500 | 1.84017800 |
| H | 3.91811100 | -0.74269600 | 2.47311200 |
| H | -1.13043500 | 4.22101200 | 2.48637900 |
| H | -1.32376700 | 5.76780300 | 0.54482000 |
| H | -0.81604100 | 4.93102800 | -1.74366600 |
| H | -0.11277700 | 2.58054400 | -2.07728400 |
| H | -0.42541000 | 1.86025400 | 2.13218900 |
| H | -2.42008800 | 0.91508700 | 0.26588600 |
| H | 5.69239900 | -1.87934600 | 0.01395600 |
| H | 6.09273100 | -0.86983200 | -2.21741700 |
| H | 4.42669200 | 0.73642300 | -3.15299800 |
| H | 2.40178000 | 1.29348600 | -1.86474400 |
| H | 0.48006600 | 0.49715200 | -1.26041400 |
| H | 1.86788100 | 1.33835800 | 1.10718400 |
| C | -3.19725900 | -1.05868800 | 0.04819400 |
| O | -4.42919400 | -0.38161900 | 0.12614000 |
| C | -5.58238100 | -1.20361100 | -0.01527300 |
| C | -5.94303300 | -1.43329000 | -1.48085200 |
| O | -3.17430100 | -2.27657000 | -0.11541500 |

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|---|-------------|-------------|-------------|
| H | -5.41460600 | -2.16509500 | 0.48019800 |
| H | -6.38853600 | -0.66941600 | 0.50238300 |
| H | -5.14235100 | -1.99252000 | -1.97033700 |
| H | -6.87440900 | -2.00745800 | -1.56681000 |
| H | -6.07559200 | -0.47902200 | -2.00178200 |

S-Int4

| | | | |
|---|-------------|-------------|-------------|
| C | 1.44602800 | -2.59152500 | 1.33632400 |
| C | 0.79801900 | -1.45449400 | 0.62928100 |
| C | 2.85982600 | -2.15541500 | 1.77361200 |
| C | 3.61378200 | -1.34610600 | 0.73000900 |
| C | 2.89876700 | -0.45128900 | -0.10584800 |
| C | 1.44035300 | -0.47789500 | -0.02784600 |
| C | 0.59530300 | 3.48687800 | 1.62365000 |
| C | 0.26152900 | 4.51788800 | 0.74357500 |
| C | -0.00929400 | 4.22360700 | -0.59349200 |
| C | 0.05151300 | 2.90484200 | -1.04466100 |
| C | 0.38259100 | 1.86235300 | -0.16860900 |
| C | 0.65604600 | 2.16886100 | 1.17054300 |
| C | 0.42157600 | 0.42986200 | -0.68610300 |
| C | -0.89056000 | -0.42073700 | -0.42467800 |
| C | -2.14647900 | 0.34004500 | -0.03650300 |
| C | 5.00252700 | -1.39707000 | 0.63715700 |
| C | 5.69808600 | -0.57358000 | -0.25414000 |
| C | 4.99520800 | 0.31911200 | -1.06096100 |
| C | 3.60307500 | 0.37832000 | -0.98814200 |
| O | -0.57675900 | -1.38806200 | 0.54641400 |

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|---|-------------|-------------|-------------|
| N | -1.15409500 | -1.18213900 | -1.76958900 |
| O | -1.62855900 | -0.49311400 | -2.67046800 |
| O | -0.81268500 | -2.34635300 | -1.85442300 |
| H | 1.48212800 | -3.45183800 | 0.65244300 |
| H | 0.85191700 | -2.90358500 | 2.20121900 |
| H | 3.44695900 | -3.02904300 | 2.07236100 |
| H | 2.75523700 | -1.53015200 | 2.67308600 |
| H | 0.81404200 | 3.70898100 | 2.66409200 |
| H | 0.21812100 | 5.54405500 | 1.09624900 |
| H | -0.26373300 | 5.01985700 | -1.28691000 |
| H | -0.15928600 | 2.67908900 | -2.08722300 |
| H | 0.92995500 | 1.37063300 | 1.85399200 |
| H | -2.39556700 | 1.04749400 | -0.83214200 |
| H | 5.55195800 | -2.08563800 | 1.27486400 |
| H | 6.78095000 | -0.62951700 | -0.31181500 |
| H | 5.52647100 | 0.96686000 | -1.75206600 |
| H | 3.05915400 | 1.07163000 | -1.62291800 |
| H | 0.56483200 | 0.48301400 | -1.76993400 |
| H | -1.94412300 | 0.92309700 | 0.86311000 |
| C | -3.34890300 | -0.56047000 | 0.19196200 |
| O | -4.22524600 | 0.04090100 | 1.02133600 |
| C | -5.46351300 | -0.67239400 | 1.27847500 |
| C | -6.49418200 | -0.39860700 | 0.19508600 |
| O | -3.51415400 | -1.64597600 | -0.31783600 |
| H | -5.24203500 | -1.73920300 | 1.35507700 |
| H | -5.79121300 | -0.29743200 | 2.25055100 |
| H | -6.15687700 | -0.79313500 | -0.76630700 |
| H | -7.43956000 | -0.88725700 | 0.45268800 |

H -6.67921300 0.67475200 0.09436800

S-TS5

C -4.59000600 0.31608500 1.59679700

C -5.40262400 -0.74641600 1.20470700

C -4.90600300 -1.71663400 0.32914300

C -3.60420600 -1.64269200 -0.16234800

C -2.77911300 -0.56362600 0.24384900

C -3.28268300 0.40647400 1.11944800

C -3.09006200 -2.64783300 -1.18323000

C -1.57840600 -2.94832000 -1.07116100

C -0.88832600 -1.65321000 -0.84164500

C -1.40326500 -0.55616200 -0.25306100

O 0.45591300 -1.47321600 -1.15977700

H -4.96801200 1.07166500 2.27875600

H -6.41921200 -0.82475400 1.57823900

H -5.54304800 -2.54317900 0.02396100

H -2.64532700 1.22661600 1.43342700

H -3.27963000 -2.23962400 -2.18684900

H -3.66088200 -3.57842000 -1.11396600

H -1.21489500 -3.43673500 -1.98065600

H -1.37247600 -3.63368900 -0.23630200

H 1.97842000 0.46294600 -2.31471100

C 0.06696800 4.18570000 0.40268300

C -0.69564700 4.67657800 -0.65732900

C -1.33518700 3.78446500 -1.52066900

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|---|-------------|-------------|-------------|
| C | -1.20698100 | 2.40932200 | -1.32905200 |
| C | -0.44199400 | 1.90794400 | -0.26619600 |
| C | 0.18976300 | 2.80940300 | 0.60165100 |
| C | -0.28406200 | 0.41588200 | -0.06718000 |
| C | 0.82643700 | -0.27369600 | -0.71407500 |
| C | 2.10305300 | 0.29472300 | -1.23576300 |
| N | 1.68970700 | -0.77227400 | 1.51107300 |
| O | 0.85685900 | -0.13898100 | 2.24287600 |
| O | 2.59675900 | -1.39442700 | 2.04114800 |
| H | 0.56209600 | 4.87264100 | 1.08264900 |
| H | -0.79500700 | 5.74733400 | -0.80854400 |
| H | -1.93343000 | 4.15906900 | -2.34619600 |
| H | -1.70729800 | 1.71792800 | -2.00109200 |
| H | 0.77016800 | 2.42762300 | 1.43654300 |
| H | 0.06097000 | 0.26366100 | 1.10040300 |
| H | 2.28510000 | 1.25602300 | -0.75652300 |
| C | 3.29912100 | -0.64008000 | -1.04819000 |
| O | 3.40623200 | -1.72059700 | -1.57982400 |
| O | 4.19790800 | -0.08537800 | -0.22556300 |
| C | 5.30463900 | -0.94042100 | 0.16863300 |
| H | 4.88533900 | -1.87719000 | 0.54142300 |
| H | 5.91016900 | -1.15667300 | -0.71720500 |
| C | 6.08278000 | -0.20126000 | 1.23783400 |
| H | 6.93220300 | -0.81019800 | 1.56256400 |
| H | 6.46673700 | 0.75186100 | 0.86220200 |
| H | 5.44552400 | -0.00755900 | 2.10442100 |

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|---|-------------|-------------|-------------|
| C | -4.04163000 | 1.01939100 | 1.47468500 |
| C | -5.00025000 | 0.01894300 | 1.32801600 |
| C | -4.68041800 | -1.14222700 | 0.61981100 |
| C | -3.42024700 | -1.31598800 | 0.04906200 |
| C | -2.44698100 | -0.29321600 | 0.19111900 |
| C | -2.77316700 | 0.86174000 | 0.91523600 |
| C | -3.09653800 | -2.55906100 | -0.76446300 |
| C | -1.64002400 | -3.03814200 | -0.59385100 |
| C | -0.76926000 | -1.83672700 | -0.70211400 |
| C | -1.11563000 | -0.55609600 | -0.37725700 |
| O | 0.52523000 | -1.90857100 | -1.10812700 |
| H | -4.27375100 | 1.92217300 | 2.03232500 |
| H | -5.98760800 | 0.13439400 | 1.76532200 |
| H | -5.42404700 | -1.92803900 | 0.50935000 |
| H | -2.02692900 | 1.63574000 | 1.05163500 |
| H | -3.25346800 | -2.32911200 | -1.82861700 |
| H | -3.79260300 | -3.36468400 | -0.51143100 |
| H | -1.38503700 | -3.78015800 | -1.35728900 |
| H | -1.50509500 | -3.52533400 | 0.38371900 |
| H | 2.56276800 | -0.92818200 | -2.51790700 |
| C | 1.52450200 | 3.62694800 | 0.30424900 |
| C | 0.62776500 | 4.49623900 | -0.31704300 |
| C | -0.45991100 | 3.97565200 | -1.02235700 |
| C | -0.64618800 | 2.59754200 | -1.10927900 |
| C | 0.25053500 | 1.71039400 | -0.48815900 |
| C | 1.33675700 | 2.24612800 | 0.22431100 |
| C | 0.07280300 | 0.24740900 | -0.61223100 |

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|---|-------------|-------------|-------------|
| C | 1.02995300 | -0.63073900 | -1.05199700 |
| C | 2.42935000 | -0.46787600 | -1.53472100 |
| H | 2.36946900 | 4.02273300 | 0.86070300 |
| H | 0.77253900 | 5.57059700 | -0.25146400 |
| H | -1.16203600 | 4.64476200 | -1.51153900 |
| H | -1.48819600 | 2.19769200 | -1.66593800 |
| H | 2.02376700 | 1.57080200 | 0.72491000 |
| H | 2.63767000 | 0.60276600 | -1.63449000 |
| C | 3.50955500 | -1.06485500 | -0.63475000 |
| O | 4.45862700 | -1.69907200 | -1.03741400 |
| O | 3.29992500 | -0.76861400 | 0.66591200 |
| C | 4.28629500 | -1.28062500 | 1.59547700 |
| H | 4.36381100 | -2.36336000 | 1.46029200 |
| H | 5.26056400 | -0.84754800 | 1.34776200 |
| C | 3.83376600 | -0.90972800 | 2.99391900 |
| H | 4.55108800 | -1.29055000 | 3.72750100 |
| H | 3.76720700 | 0.17565800 | 3.11197000 |
| H | 2.85339000 | -1.34093200 | 3.21423100 |