# Cp*Co(III)-Catalyzed coupling of benzamides with α,β-unsaturated carbonyl compounds: Preparation of aliphatic ketones and azepinones

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**Citation:**

# Cp*Co(III)-Catalyzed Coupling of Benzamides with α,β-unsaturated Carbonyl Compounds: Preparation of Aliphatic Ketones and Azepinones

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## *Contents:*

## [1] General Experimental Considerations:

All solvents and reagents were purchased from Sigma-Aldrich, Fisher Scientific or Fluorochem and used without further purification. $^1$H, $^{13}$C{$^1$H} and $^{19}$F NMR spectra were recorded on a Bruker AV-400 spectrometer in CDCl$_3$ (99.8% D, containing 0.03% v/v TMS). High Resolution Mass Spectra (HRMS) were recorded on a Xevo G2-Xs QTof Mass Spectrometer at Sheffield Hallam University.

## [2] General Procedure for the Optimization of Cp*Co(III)-Catalyzed Coupling of *N*-isopropylbenzamide and Methyl Vinyl Ketone:

A 10 mL screw top vial was charged with benzamide substrate (0.2 mmol), [Cp*Co(CO)I$_2$], silver salt, base, MVK and 2 mL solvent under air. The vial was sealed and the reaction mixture heated with stirring for 18 hours. After this period, the solvent was removed under reduced pressure. The residue was suspended in 2 mL of ethyl acetate and passed through a plug of silica, which was washed with a further 3 mL of ethyl acetate. The ethyl acetate was removed and the yield calculated from the $^1$H NMR spectrum using mesitylene as internal standard.

## [3] Optimization of Cp*Co(III)-Catalyzed coupling of *N*-isopropylbenzamide and Methyl Vinyl Ketone:
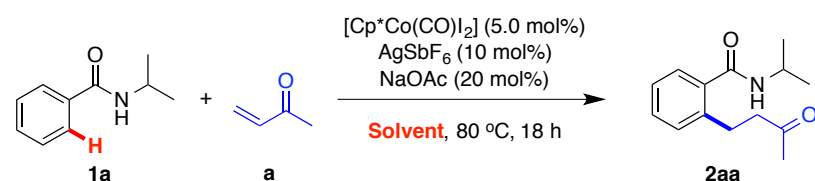


| Entry | Solvent | 2aa [%][a] |
|:-----:|:-------:|:----------:|
| 1 | 1,2-dichloroethane | 53 |
| 2 | 1,4-dioxane | 10 |
| 3 | acetonitrile | trace |
| 4 | toluene | 11 |
| **6** | **chloroform** | **63** |
| 5 | 2,2,2-trifluoroethanol | trace |

[a] Yield determined by $^1$H NMR spectroscopy of the crude reaction mixture using mesitylene as internal standard.
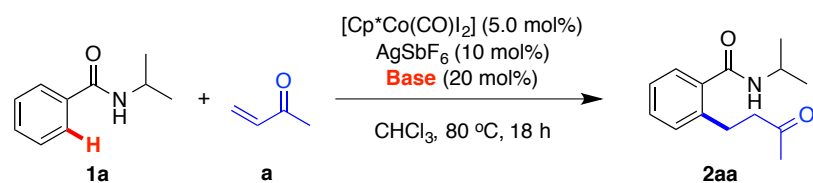
| Entry | Base | 2aa [%][a] |
|-------|------|-----------|
| 1 | - | 49 |
| 2 | NaOAc | 63 |
| **3** | **CsOAc** | **72** |
| 4 | AgOAc | 64 |
| 5 | KOPiv | trace |
| 6 | NaOPiv | trace |
| 7 | Cs$_2$CO$_3$ | trace |
| 8[b] | CsOAc | trace |

[a] Yield determined by ^{1}H NMR spectroscopy of the crude reaction mixture using mesitylene as internal standard. [b] 50 mol% CsOAc used.
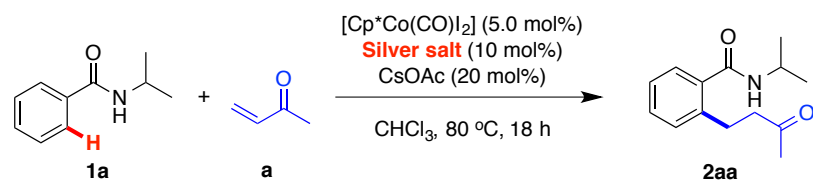


| Entry | Silver salt | 2aa [%][a] |
|-------|-------------|-----------|
| 1 | - | trace |
| 2 | AgSbF$_6$ | 72 |
| 3 | AgNTf$_2$ | 8 |
| 4 | AgBF$_4$ | 13 |
| 5 | AgOTf | 5 |
| 6 | AgOAc | trace |
| 7 | AgPF$_6$ | trace |
| **8[b]** | **AgSbF$_6$** | **82** |

[a] Yield determined by ^{1}H NMR spectroscopy of the crude reaction mixture using mesitylene as internal standard. [b] 10 mol% [Cp*Co(CO)I$_2$], 20 mol% AgSbF$_6$.
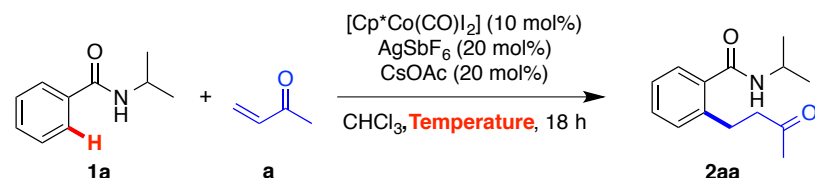
| Entry | Temperature [$^\circ$C] | 2aa [%][a] |
|:-----:|:-----------------------:|:----------:|
| 1 | 60 | 13 |
| **2** | **80** | **82** |
| 3 | 100 | 43 |

[a] Yield determined by $^1$H NMR spectroscopy of the crude reaction mixture using mesitylene as internal standard.

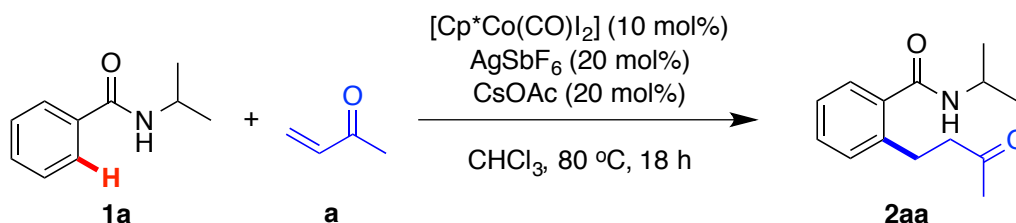## [4] Optimized Procedure for Cp*Co(III)-Catalyzed Coupling of Benzamides and Vinyl Ketones/Aldehydes:



A 20 mL screw top vial was charged with benzamide substrate (0.8 mmol), [Cp*Co(CO)I$_2$] (38.0 mg, 0.08 mmol, 10 mol%), AgSbF$_6$ (55.2 mg, 0.16 mmol, 20 mol%), CsOAc (30.8 mg, 0.16 mmol, 20 mol%), vinyl ketone/aldehyde (0.12 mmol, 1.5 equiv.) and 8 mL CHCl$_3$. The vial was sealed and the reaction mixture heated to 80 $^\circ$C with stirring for 18 hours. After this period the solvent was removed under reduced pressure and the crude product purified by column chromatography (Hexane:EtOAc; alkylation 60:40 and cyclization 80:20).

## [5] Characterization Data for Aliphatic Ketone Products:

### *N*-isopropyl-2-(3-oxobutyl)benzamide (2aa)
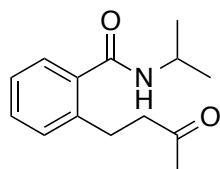


This compound was prepared by the general alkylation protocol described above starting from substrate **1a** (130 mg, 0.8 mmol) to yield an off-white powder (153 mg, 82 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.36-7.28 (m, 2H), 7.23-7.18 (m, 2H), 6.20-6.00 (br d, 1H, $^3J_{HH}$ = 6.1 Hz), 4.31-4.18 (m, 1H), 3.00-2.93 (m, 2H), 2.92-2.86 (m, 2H), 2.12 (s, 3H), 1.26 (d, 6H, $^3J_{HH}$ = 6.7 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.5, 169.2, 138.8, 137.0, 130.0, 129.8, 127.1, 126.3, 45.1, 41.9, 30.0, 27.2, 22.8. HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{19}$NO$_2$+H = 234.1494; obtained = 234.1488 [M+H]$^+$. $R_f$ = 0.36 (EtOAc:Hexane 40:60).

**N-isopropyl-5-methyl-2-(3-oxobutyl)benzamide (2ca)**
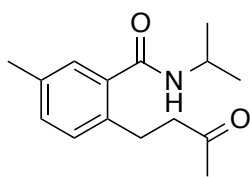


This compound was prepared by the general alkylation protocol described above starting from substrate **1c** (142 mg, 0.8 mmol) to yield an off-white powder (156 mg, 79 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.16-7.05 (m, 3H), 6.20-6.07 (br d, 1H, $^3J_{HH}$ = 6.5 Hz), 4.30-4.18 (m, 1H), 2.96-2.89 (m, 2H), 2.89-2.82 (m, 2H), 2.31 (s, 3H), 2.11 (s, 3H), 1.26 (d, 6H, $^3J_{HH}$ = 6.2 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.7, 169.3, 136.9, 136.0, 135.6, 130.6, 129.7, 127.2, 45.3, 41.8, 30.1, 26.8, 22.8, 20.9. HR-MS (ASAP+, $m/z$); calcd. for C$_{15}$H$_{21}$NO$_2$+H = 248.1651; obtained = 248.1647 [M+H]$^+$. $R_f$ = 0.34 (EtOAc:Hexane 40:60).

**N-isopropyl-4-methyl-2-(3-oxobutyl)benzamide (2da)**



This compound was prepared by the general alkylation protocol described above starting from substrate **1d** (142 mg, 0.8 mmol) to yield an off-white powder (178 mg, 90 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.25-7.21 (m, 1H), 7.02-6.98 (m, 2H), 6.12-5.97 (br d, 1H, $^3J_{HH}$ = 6.8 Hz), 4.30-4.16 (m, 1H), 2.97-2.90 (m, 2H), 2.90-2.84 (m, 2H), 2.32 (s, 3H), 2.13 (s, 3H), 1.26 (d, 6H, $^3J_{HH}$ = 6.5 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.6, 169.3, 140.0, 139.0, 134.1, 130.6, 127.2, 127.0, 45.4, 41.8, 30.0, 27.3, 22.8, 21.3. HR-MS (ASAP+, $m/z$); calcd. for C$_{15}$H$_{21}$NO$_2$+H = 248.1651; obtained = 248.1645 [M+H]$^+$. $R_f$ = 0.31 (EtOAc:Hexane 40:60).

**4-(tert-butyl)-N-isopropyl-2-(3-oxobutyl)benzamide (2ea)**
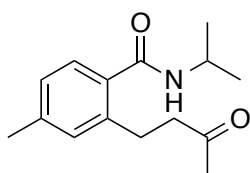


This compound was prepared by the general alkylation protocol described above starting from substrate **1e** (175 mg, 0.8 mmol) to yield an off-white powder (192 mg, 83 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.30-7.26 (m, 1H), 7.24-7.20 (m, 2H), 6.01-5.90 (br d, 1H, $^3J_{HH}$ = 7.4 Hz), 4.31-4.17 (m, 1H), 3.01-2.94 (m, 2H), 2.91-2.85 (m, 2H), 2.13 (s, 3H), 1.29 (s, 9H), 1.25 (d, 6H, $^3J_{HH}$ = 6.5 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.6, 169.3, 153.2, 138.8, 134.1, 127.1, 126.9, 123.3, 45.7, 41.8, 34.7, 31.2, 30.0, 27.9, 22.8. HR-MS (ASAP+, $m/z$); calcd. for C$_{18}$H$_{27}$NO$_2$+H = 290.2120; obtained = 290.2116 [M+H]$^+$. $R_f$ = 0.45 (EtOAc:Hexane 40:60).

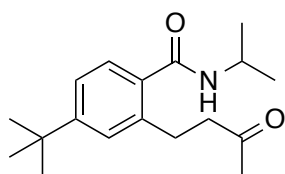### *N*-isopropyl-3-(3-oxobutyl)-[1,1'-biphenyl]-4-carboxamide (2fa)



This compound was prepared by the general alkylation protocol described above starting from substrate **1f** (191 mg, 0.8 mmol) to yield an off-white powder (193 mg, 78 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.58-7.52 (m, 2H), 7.48-7.40 (m, 5H), 7.39-7.33 (m, 1H), 6.23-6.08 (br d, 1H, $^3J_{HH}$ = 8.0 Hz), 4.34-4.21 (m, 1H), 3.08-3.00 (m, 2H), 3.00-2.91 (m, 2H), 2.14 (s, 3H), 1.28 (d, 6H, $^3J_{HH}$ = 6.6 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.5, 169.0, 142.8, 140.3, 139.5, 135.8, 128.9, 128.7, 127.8, 127.7, 127.2, 125.0, 45.4, 41.9, 30.0, 27.4, 22.8. HR-MS (ASAP+, *m/z*); calcd. for C$_{20}$H$_{23}$NO$_2$+H = 310.1807; obtained = 310.1800 [M+H]$^+$. *R$_f$* = 0.34 (EtOAc:Hexane 40:60).

### *N*-isopropyl-4-(methylthio)-2-(3-oxobutyl)benzamide (2ha)
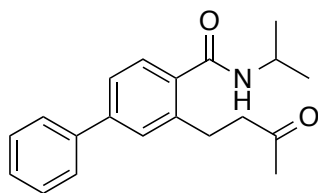


This compound was prepared by the general alkylation protocol described above starting from substrate **1h** (167 mg, 0.8 mmol) to yield an off-white powder (147 mg, 66 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.29-7.24 (m, 1H), 7.08-7.03 (m, 2H), 6.18-6.04 (br d, 1H, $^3J_{HH}$ = 7.4 Hz), 4.29-4.16 (m, 1H), 2.98-2.91 (m, 2H), 2.91-2.85 (m, 2H), 2.47 (s, 3H), 2.13 (s, 3H), 1.25 (d, 6H, $^3J_{HH}$ = 6.2 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.4, 168.7, 141.0, 139.8, 133.4, 127.7, 127.3, 123.6, 45.2, 41.9, 30.0, 27.3, 22.8, 15.4. HR-MS (ASAP+, *m/z*); calcd. for C$_{15}$H$_{21}$NO$_2$S+H = 280.1371; obtained = 280.1379 [M+H]$^+$. *R$_f$* = 0.26 (EtOAc:Hexane 40:60).

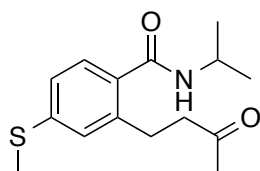### *N*-isopropyl-4-methoxy-2-(3-oxobutyl)benzamide (2ia)



This compound was prepared by the general alkylation protocol described above starting from substrate **1i** (155 mg, 0.8 mmol) to yield an off-white powder (181 mg, 86 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.31 (d, 1H, $^3J_{HH}$ = 8.2 Hz), 6.75-6.69 (m, 2H), 6.14-5.98 (br d, 1H, $^3J_{HH}$ = 7.1 Hz), 4.29-4.16 (m, 1H), 3.80 (s, 3H), 3.01-2.93 (m, 2H), 2.93-2.85 (m, 2H), 2.13 (s, 3H), 1.25 (d, 6H, $^3J_{HH}$ = 6.6 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.5, 168.9, 160.6, 141.4, 129.4, 128.8, 115.5, 111.3, 55.3, 45.3, 41.8, 30.0, 27.6, 22.8. HR-MS (ASAP+, *m/z*); calcd. for C$_{16}$H$_{11}$N$_3$O$_3$+H = 264.1600; obtained = 264.1597 [M+H]$^+$. *R$_f$* = 0.20 (EtOAc:Hexane 40:60).

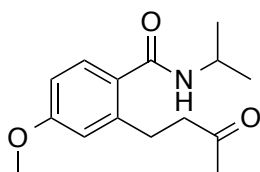### 4-bromo-*N*-isopropyl-2-(3-oxobutyl)benzamide (2ja)



This compound was prepared by the general alkylation protocol described above starting from substrate **1j** (193 mg, 0.8 mmol) to yield an off-white powder (172 mg, 69 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.37-7.31 (m, 2H), 7.22 (d, 1H, $^3J_{HH}$ = 7.7 Hz), 6.34-6.21 (br d, 1H, $^3J_{HH}$ = 7.0 Hz), 4.29-4.17 (m, 1H), 2.96-2.86 (m, 4H), 2.14 (s, 3H), 1.25 (d, 6H, $^3J_{HH}$ = 7.0 Hz). $^{13}$C $\{^1$H$\}$ NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.1, 168.2, 141.1, 136.0, 132.6, 129.4, 128.9, 124.0, 44.8, 42.0, 30.0, 26.8, 22.7. HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{18}$NO$_2$Br+H = 312.0599; obtained = 312.0600 [M+H]$^+$. $R_f$ = 0.39 (EtOAc:Hexane 40:60).

### *N*-isopropyl-2-(3-oxobutyl)-4-(trifluoromethyl)benzamide (2ka)



This compound was prepared by the general alkylation protocol described above starting from substrate **1k** (185 mg, 0.8 mmol) to yield an off-white powder (173 mg, 72 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.48-7.44 (m, 3H), 6.43-6.30 (br d, 1H, $^3J_{HH}$ = 6.9 Hz), 4.33-4.20 (m, 1H), 3.04-2.96 (m, 2H), 2.96-2.90 (m, 2H), 2.14 (s, 3H), 1.27 (d, 6H, $^3J_{HH}$ = 6.9 Hz). $^{13}$C $\{^1$H$\}$ NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.0, 168.0, 140.5, 139.6, 131.8 (q, $^2J_{CF}$ = 33.6 Hz), 127.82, 126.3 (q, $^3J_{CF}$ = 3.7 Hz), 123.7 (q, $^1J_{CF}$ = 273.0 Hz), 123.3 (q, $^3J_{CF}$ = 3.8 Hz), 44.7, 42.1, 30.0, 26.8, 22.7. $^{19}$F $\{^1$H$\}$ NMR (CDCl$_3$, 376 MHz, 298 K); δ 62.83 (s, 1F). HR-MS (ASAP+, *m/z*); calcd. for C$_{15}$H$_{18}$NO$_2$F$_3$+H = 302.1368; obtained = 302.1372 [M+H]$^+$. $R_f$ = 0.47 (EtOAc:Hexane 40:60).

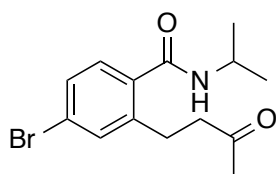### 3-fluoro-*N*-isopropyl-2-(3-oxobutyl)benzamide (2la)



This compound was prepared by the general alkylation protocol described above starting from substrate **1l** (145 mg, 0.8 mmol) to yield an off-white powder (170 mg, 85 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.22-7.15 (m, 1H), 7.13 (dd, 1H, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 1.5 Hz) 7.07-7.01 (m, 1H), 6.41-6.23 (br d, 1H, $^3J_{HH}$ = 6.4 Hz), 4.29-4.16 (m, 1H), 2.99-2.92 (m, 2H), 2.92-2.86 (m, 2H), 2.14 (s, 3H), 1.25 (d, 6H, $^3J_{HH}$ = 6.5 Hz). $^{13}$C $\{^1$H$\}$ NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.5, 167.9 (d, $^4J_{CF}$ = 2.9 Hz), 161.4 (d, $^1J_{CF}$ = 246.0 Hz), 139.5 (d, $^4J_{CF}$ = 4.0 Hz), 127.8 (d, $^3J_{CF}$ = 9.8 Hz), 126.1 (d, $^2J_{CF}$ = 17.5 Hz), 122.8 (d, $^3J_{CF}$ = 6.2 Hz), 116.7 (d, $^2J_{CF}$ = 22.4 Hz), 43.6 (d, $^3J_{CF}$ = 2.6 Hz), 42.0, 29.9, 22.7, 21.0 (d, $^4J_{CF}$ = 2.2 Hz). $^{19}$F $\{^1$H$\}$ NMR (CDCl$_3$, 376 MHz, 298 K); δ 116.19 (s, 1F). HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{18}$NO$_2$F+H = 252.1400; obtained = 252.1403 [M+H]$^+$. $R_f$ = 0.35 (EtOAc:Hexane 40:60).

### *N*-isopropyl-3-(3-oxobutyl)thiophene-2-carboxamide (2ma)
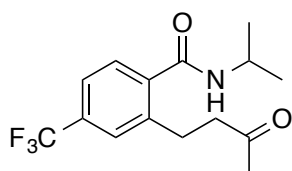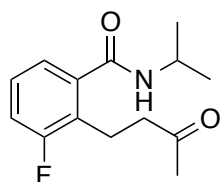


This compound was prepared by the general alkylation protocol described above starting from substrate **1m** (108 mg, 0.8 mmol) to yield an off-white powder containing a minor alkenylation impurity which could not be removed by either column chromatography or recrystallization (141 mg, 74 %) *Spectral data for the target alkylation product*: $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.18 (d, 1H, $^3J_{HH}$ = 5.2 Hz), 7.08-7.03 (br s, 1H), 6.79 (d, 1H, $^3J_{HH}$ = 5.2 Hz), 4.23-4.09 (m, 1H), 3.01 (t, 2H, $^3J_{HH}$ = 6.7 Hz), 2.84 (t, 2H, $^3J_{HH}$ = 6.7 Hz), 2.07 (s, 3H), 1.21 (d, 6H, $^3J_{HH}$ = 6.6 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 209.1, 162.2, 142.3, 133.6, 129.8, 126.8, 44.1, 42.0, 30.0, 23.1, 22.8. HR-MS (ASAP+, *m/z*); calcd. for C$_{12}$H$_{17}$NO$_2$S+H = 240.1058; obtained = 240.1051 [M+H]$^+$. $R_f$ = 0.24 (EtOAc:Hexane 40:60).

### *N*-methyl-2-(3-oxobutyl)benzamide (2oa)

*This product was obtained from **1o** (64 %) as a mixture with 11 % of product **3oa** for which characterization can be found in the next section of this document.*



This compound was prepared by the general alkylation protocol described above starting from substrate **1o** (108 mg, 0.8 mmol) to yield an off-white powder (104 mg, 64 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.36-7.27 (m, 2H), 7.22-7.16 (m, 2H), 6.51-6.31 (br s, 1H), 2.98 (d, 3H, $^3J_{HH}$ = 4.8 Hz), 2.98-2.92 (m, 2H), 2.91-2.85 (m, 2H), 2.12 (s, 3H). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.8, 170.7, 138.9, 136.7, 130.0, 129.8, 127.2, 126.3, 45.3, 30.0, 27.2, 26.7. HR-MS (ASAP+, *m/z*); calcd. for C$_{12}$H$_{15}$NO$_2$+H = 206.1181; obtained = 206.1177 [M+H]$^+$. $R_f$ = 0.11 (EtOAc:Hexane 40:60).

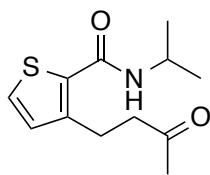### *N*-(*tert*-butyl)-2-(3-oxobutyl)benzamide (2pa)
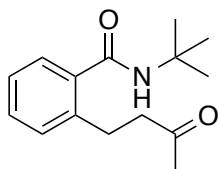


This compound was prepared by the general alkylation protocol described above starting from substrate **1p** (142 mg, 0.8 mmol) to yield an off-white powder (158 mg, 80 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.33-7.26 (m, 2H), 7.22-7.16 (m, 2H), 6.01-5.89 (br s, 1H), 3.00-2.93 (m, 2H), 2.90-2.84 (m, 2H), 2.12 (s, 3H), 1.46 (s, 9H). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.4, 169.6, 138.6, 138.0, 129.8, 129.7, 126.9, 126.2, 51.8, 45.3, 30.0, 28.8, 27.3. HR-MS (ASAP+, *m/z*); calcd. for C$_{15}$H$_{21}$NO$_2$+H = 248.1651; obtained = 248.1659 [M+H]$^+$. $R_f$ = 0.47 (EtOAc:Hexane 40:60).

### *N*-cyclohexyl-2-(3-oxobutyl)benzamide (2qa)



This compound was prepared by the general alkylation protocol described above starting from substrate **1q** (163 mg, 0.8 mmol) to yield an off-white powder (164 mg, 75 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.36-7.28 (m, 2H), 7.23-7.17 (m, 2H), 6.21-6.07 (br d, 1H, $^3J_{HH}$ = 7.8 Hz), 4.00-3.88 (m, 1H), 3.00-2.93 (m, 2H), 2.92-2.85 (m, 2H), 2.12 (s, 3H), 2.07-1.98 (m, 2H), 1.79-1.70 (m, 2H), 1.66-1.59 (m, 1H), 1.48-1.35 (m, 2H), 1.29-1.13 (m, 3H). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.5, 169.1, 138.8, 137.1, 129.9, 129.8, 127.1, 126.3, 48.7, 45.3, 33.1, 30.0, 27.2, 25.6, 24.9. HR-MS (ASAP+, *m/z*); calcd. for C$_{17}$H$_{23}$NO$_2$+H = 274.1807; obtained = 274.1803 [M+H]$^+$. $R_f$ = 0.40 (EtOAc:Hexane 40:60).

### 2-(3-oxobutyl)-*N*-(tetrahydro-2*H*-pyran-4-yl)benzamide (2ra)



This compound was prepared by the general alkylation protocol described above starting from substrate **1r** (164 mg, 0.8 mmol) to yield an off-white powder (88 mg, 40 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.39-7.30 (m, 2H), 7.24-7.19 (m, 2H), 6.50-6.40 (br d, 1H, $^3J_{HH}$ = 7.2 Hz), 4.24-4.12 (m, 1H), 4.02-3.95 (m, 2H), 3.57-3.48 (m, 2H), 3.00-2.88 (m, 4H), 2.13 (s, 3H), 2.05-1.97 (m, 2H), 1.63-1.52 (m, 2H). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 208.6, 169.3, 138.7, 136.7, 130.1, 129.6, 127.3, 126.4, 66.8, 46.2, 45.1, 33.1, 30.1, 27.0. HR-MS (ASAP+, *m/z*); calcd. for C$_{16}$H$_{21}$NO$_3$+H = 276.1600; obtained = 276.1593 [M+H]$^+$. $R_f$ = 0.08 (EtOAc:Hexane 40:60).

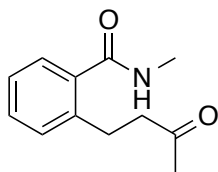### *N*-isopropyl-2-(3-oxopentyl)benzamide (2ac)



This compound was prepared by the general alkylation protocol described above starting from substrate **1a** (130 mg, 0.8 mmol) to yield an off-white powder (170 mg, 86 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.35-7.27 (m, 2H), 7.22-7.16 (m, 2H), 6.22-6.06 (br d, 1H, $^3J_{HH}$ = 6.9 Hz), 4.31-4.18 (m, 1H), 3.00-2.94 (m, 2H), 2.88-2.81 (m, 2H), 2.39 (q, 2H, $^3J_{HH}$ = 6.9 Hz), 1.26 (d, 6H, $^3J_{HH}$ = 6.5 Hz), 1.01, (t, 3H, $^3J_{HH}$ = 6.9 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 211.2, 169.2, 139.0, 137.1, 130.0, 129.8, 127.1, 126.2, 43.9, 41.8, 36.0, 27.3, 22.8, 7.8. HR-MS (ASAP+, *m/z*); calcd. for C$_{15}$H$_{21}$NO$_2$+H = 248.1651; obtained = 248.1646 [M+H]$^+$. $R_f$ = 0.44 (EtOAc:Hexane 40:60).

## [6] Characterization Data for Azepinone Products:

### 2,3-dimethyl-2,5-dihydro-1H-benzo[c]azepin-1-one (3oa)

*This product was obtained from 1o (11 %) as a mixture with 64 % of product 2oa for which characterization can be found in the previous section of this document.*
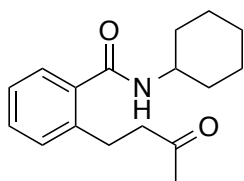


This compound was prepared by the general alkylation protocol described above starting from substrate **1o** (130 mg, 0.8 mmol) to yield an off-white powder (19 mg, 11 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.85 (dd, 1H, $^3J_{HH}$ = 7.4, $^4J_{HH}$ = 1.7 Hz), 7.34 (ddd, 1H, $^3J_{HH}$ = 7.4, $^3J_{HH}$ = 7.4, $^4J_{HH}$ = 1.4 Hz), 7.27 (ddd, 1H, $^3J_{HH}$ = 7.4, $^3J_{HH}$ = 7.4, $^4J_{HH}$ = 1.5 Hz), 7.04 (dd, 1H, $^3J_{HH}$ = 7.4, $^4J_{HH}$ = 1.4 Hz), 5.59-5.53 (m, 1H), 3.51-2.99 (br s, 1H), 3.28 (s, 3H), 3.27-2.77 (br s, 1H), 1.88 (d, 3H, $^4J_{HH}$ = 0.9 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 169.2, 144.5, 136.4, 133.6, 131.2, 131.2, 126.4, 125.5, 119.1, 32.9, 31.3, 19.8. HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{17}$NO+H = 216.1388; obtained = 216.1382 [M+H]$^+$. $R_f$ = 0.31 (EtOAc:Hexane 40:60).

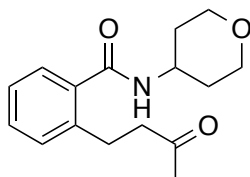### 2-isopropyl-2,5-dihydro-1H-benzo[c]azepin-1-one (3ab)
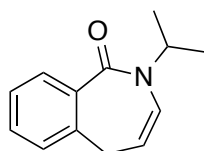


This compound was prepared by the general alkylation protocol described above starting from substrate **1a** (130 mg, 0.8 mmol) to yield an off-white powder (114 mg, 71 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.86 (dd, 1H, $^3J_{HH}$ = 7.8, $^4J_{HH}$ = 1.4 Hz), 7.36 (ddd, 1H, $^3J_{HH}$ = 7.8, $^3J_{HH}$ = 7.8, $^4J_{HH}$ = 1.4 Hz), 7.28 (ddd, 1H, $^3J_{HH}$ = 7.8, $^3J_{HH}$ = 7.8, $^4J_{HH}$ = 1.2 Hz), 7.05 (dd, 1H, $^3J_{HH}$ = 7.8, $^4J_{HH}$ = 1.2 Hz), 6.01 (d, 1H, $^3J_{HH}$ = 7.5 Hz), 5.81 (dt, 1H, $^3J_{HH}$ = 7.5, $^3J_{HH}$ = 7.5 Hz), 5.19 (h, 1H, $^3J_{HH}$ = 7.4 Hz), 3.20 (d, 2H, $^3J_{HH}$ = 7.5), 1.25 (d, 6H, $^3J_{HH}$ = 7.4 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 168.5, 143.5, 134.2, 131.5, 131.3, 126.5, 125.8, 124.6, 120.5, 45.7, 31.3, 20.7. HR-MS (ASAP+, *m/z*); calcd. for C$_{13}$H$_{15}$NO+H = 202.1232; obtained = 202.1239 [M+H]$^+$. $R_f$ = 0.58 (EtOAc:Hexane 20:80).

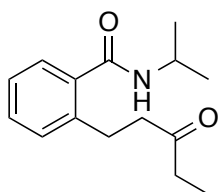### 2-isopropyl-8-methyl-2,5-dihydro-1H-benzo[c]azepin-1-one (3cb)



This compound was prepared by the general alkylation protocol described above starting from substrate **1c** (142 mg, 0.8 mmol) to yield an off-white powder (127 mg, 74 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.68 (d, 1H, $^4J_{HH}$ = 1.3 Hz), 7.16 (dd, 1H, $^3J_{HH}$ = 7.3, $^4J_{HH}$ = 1.3 Hz), 6.94 (d, 1H, $^3J_{HH}$ = 7.3 Hz), 5.98 (d, 1H, $^3J_{HH}$ = 7.7 Hz), 5.80 (dt, 1H, $^3J_{HH}$ = 7.7, $^3J_{HH}$ = 7.7 Hz), 5.18 (h, 1H, $^3J_{HH}$ = 7.2 Hz), 3.17 (d, 2H, $^3J_{HH}$ = 7.7), 2.34 (s, 3H), 1.25 (d, 6H, $^3J_{HH}$ = 7.2 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 168.6, 140.8, 136.1, 134.0, 132.0, 131.9, 125.8, 124.5, 120.8, 45.6, 30.8, 20.9, 20.7. HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{17}$NO+H = 216.1388; obtained = 216.1387 [M+H]$^+$. $R_f$ = 0.64 (EtOAc:Hexane 20:80).

**2-isopropyl-7-methyl-2,5-dihydro-1*H*-benzo[*c*]azepin-1-one (3db)**



This compound was prepared by the general alkylation protocol described above starting from substrate **1d** (142 mg, 0.8 mmol) to yield an off-white powder (126 mg, 73 %). ^{1}H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.76 (d, 1H, $^3J_{HH}$ = 8.1 Hz), 7.09 (d, 1H, $^3J_{HH}$ = 8.1Hz), 6.87 (s, 1H), 6.00 (d, 1H, $^3J_{HH}$ = 7.5 Hz), 5.78 (dt, 1H, $^3J_{HH}$ = 7.5, $^3J_{HH}$ = 7.5 Hz), 5.18 (h, 1H, $^3J_{HH}$ = 7.0 Hz), 3.16 (d, 2H, $^3J_{HH}$ = 7.5), 2.34 (s, 3H), 1.25 (d, 6H, $^3J_{HH}$ = 7.0 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 168.4, 143.4, 141.7, 131.6, 131.5, 127.3, 126.5, 124.8, 120.2, 45.6, 31.3, 21.3, 20.7. HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{17}$NO+H = 216.1388; obtained = 216.1390 [M+H]$^+$. *R$_f$* = 0.56 (EtOAc:Hexane 20:80).

**7-(*tert*-butyl)-2-isopropyl-2,5-dihydro-*1H*-benzo[*c*]azepin-1-one (3eb)**
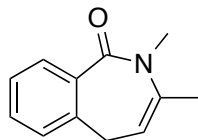


This compound was prepared by the general alkylation protocol described above starting from substrate **1e** (175 mg, 0.8 mmol) to yield an off-white powder (134 mg, 65 %). ^{1}H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.81 (d, 1H, $^3J_{HH}$ = 8.2 Hz), 7.32 (dd, 1H, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 1.8Hz), 7.05 (d, 1H, $^4J_{HH}$ = 1.8 Hz), 6.01 (d, 1H, $^3J_{HH}$ = 8.2 Hz), 5.81 (dt, 1H, $^3J_{HH}$ = 8.1, $^3J_{HH}$ = 8.1 Hz), 5.19 (h, 1H, $^3J_{HH}$ = 7.0 Hz), 3.21 (d, 2H, $^3J_{HH}$ = 8.2), 1.31 (s, 9H), 1.25 (d, 6H, $^3J_{HH}$ = 7.0 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 168.4, 154.8, 143.2, 131.4, 131.3, 124.7, 123.7, 122.8, 120.2, 45.6, 34.8, 31.7, 31.2, 20.7. HR-MS (ASAP+, *m/z*); calcd. for C$_{17}$H$_{23}$NO+H = 258.1858; obtained = 258.1861 [M+H]$^+$. *R$_f$* = 0.65 (EtOAc:Hexane 20:80).

**2-isopropyl-7-phenyl-2,5-dihydro-1H-benzo[*c*]azepin-1-one (3fb)**



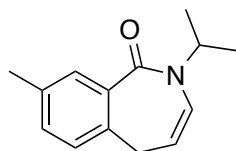This compound was prepared by the general alkylation protocol described above starting from substrate **1f** (191 mg, 0.8 mmol) to yield an off-white powder (160 mg, 72 %). ^{1}H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.95 (d, 1H, $^3J_{HH}$ = 8.3 Hz), 7.61-7.56 (m, 2H), 7.52 (dd, 1H, $^3J_{HH}$ = 8.3, $^4J_{HH}$ = 1.9 Hz), 7.47-7.41 (m, 2H), 7.39-7.34 (m, 1H), 7.29 (d, 1H, $^4J_{HH}$ = 1.9 Hz), 6.05 (d, 1H, $^3J_{HH}$ = 7.4 Hz), 5.87 (dt, 1H, $^3J_{HH}$ = 7.4, $^3J_{HH}$ = 7.4 Hz), 5.21 (h, 1H, $^3J_{HH}$ = 6.9 Hz), 3.28 (d, 2H, $^3J_{HH}$ = 7.4), 1.28 (d, 6H, $^3J_{HH}$ = 6.9 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 168.2, 144.1, 143.9, 140.2, 133.0, 132.1, 128.9, 127.9, 127.2, 125.2, 124.8, 124.5, 120.3, 45.7, 31.5, 20.7. HR-MS (ASAP+, *m/z*); calcd. for C$_{19}$H$_{19}$NO+H = 278.1545; obtained = 278.1544 [M+H]$^+$. *R$_f$* = 0.57 (EtOAc:Hexane 20:80).

**2-isopropyl-7-(methylthio)-2,5-dihydro-1*H*-benzo[*c*]azepin-1-one (3hb)**

This compound was prepared by the general alkylation protocol described above starting from substrate **1h** (167 mg, 0.8 mmol) to yield an off-white powder (136 mg, 69 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.79 (d, 1H, $^3J_{HH}$ = 8.5 Hz), 7.12 (dd, 1H, $^3J_{HH}$ = 8.5, $^4J_{HH}$ = 1.8Hz), 6.89 (d, 1H, $^4J_{HH}$ = 1.8 Hz), 6.01 (d, 1H, $^3J_{HH}$ = 7.4 Hz), 5.77 (dt, 1H, $^3J_{HH}$ = 7.4, $^3J_{HH}$ = 7.4 Hz), 5.16 (h, 1H, $^3J_{HH}$ = 6.7 Hz), 3.17 (d, 2H, $^3J_{HH}$ = 7.4), 2.48 (s, 3H), 1.25 (d, 6H, $^3J_{HH}$ = 6.7 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 168.0, 143.7, 142.9, 132.0, 130.6, 125.0, 123.5, 122.7, 119.8, 45.7, 31.4, 20.7, 15.1. HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{17}$NOS+H = 248.1109; obtained = 248.1107 [M+H]$^+$. $R_f$ = 0.47 (EtOAc:Hexane 20:80).

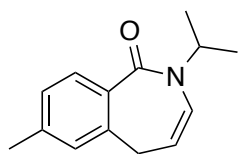**2-isopropyl-7-methoxy-2,5-dihydro-1*H*-benzo[*c*]azepin-1-one (3ib)**

This compound was prepared by the general alkylation protocol described above starting from substrate **1i** (155 mg, 0.8 mmol) to yield an off-white powder (112 mg, 61 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.84 (d, 1H, $^3J_{HH}$ = 8.6 Hz), 6.80 (dd, 1H, $^3J_{HH}$ = 8.6, $^4J_{HH}$ = 2.3Hz), 6.57 (d, 1H, $^4J_{HH}$ = 2.3 Hz), 6.02 (d, 1H, $^3J_{HH}$ = 7.8 Hz), 5.77 (dt, 1H, $^3J_{HH}$ = 7.8, $^3J_{HH}$ = 7.8 Hz), 5.16 (h, 1H, $^3J_{HH}$ = 6.7 Hz), 3.82 (s, 3H), 3.18 (d, 2H, $^3J_{HH}$ = 7.8), 1.25 (d, 6H, $^3J_{HH}$ = 6.7 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 168.0, 161.9, 145.2, 133.5, 126.9, 125.1, 119.6, 111.7, 111.1 55.4, 45.6, 31.6, 20.7 HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{17}$NO$_2$+H = 232.1338; obtained = 232.1334 [M+H]$^+$. $R_f$ = 0.40 (EtOAc:Hexane 20:80).

**7-bromo-2-isopropyl-2,5-dihydro-1*H*-benzo[*c*]azepin-1-one (3jb)**
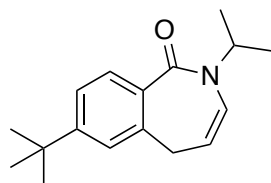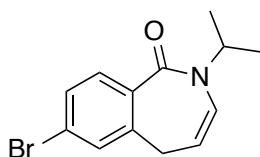
This compound was prepared by the general alkylation protocol described above starting from substrate **1j** (194 mg, 0.8 mmol) to yield an off-white powder (118 mg, 53 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.72 (d, 1H, $^3J_{HH}$ = 8.3 Hz), 7.41 (dd, 1H, $^3J_{HH}$ = 8.3, $^4J_{HH}$ = 2.3Hz), 7.23 (d, 1H, $^4J_{HH}$ = 2.3 Hz), 6.01 (d, 1H, $^3J_{HH}$ = 7.7 Hz), 5.79 (dt, 1H, $^3J_{HH}$ = 7.7, $^3J_{HH}$ = 7.7 Hz), 5.15 (h, 1H, $^3J_{HH}$ = 7.2 Hz), 3.17 (d, 2H, $^3J_{HH}$ = 7.7), 1.25 (d, 6H, $^3J_{HH}$ = 7.2 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 167.5, 145.0, 133.1, 133.1, 129.7, 128.8, 125.6, 125.1, 119.9, 45.9, 31.0, 20.6. HR-MS (ASAP+, *m/z*); calcd. for C$_{13}$H$_{14}$NOBr+H = 280.0337; obtained = 280.0343 [M+H]$^+$. $R_f$ = 0.62 (EtOAc:Hexane 20:80).

### 2-isopropyl-7-(trifluoromethyl)-2,5-dihydro-1*H*-benzo[*c*]azepin-1-one (3kb)
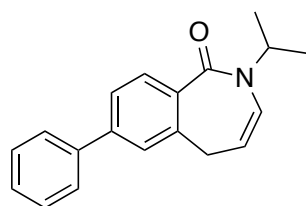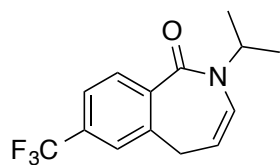


This compound was prepared by the general alkylation protocol described above starting from substrate **1k** (185 mg, 0.8 mmol) to yield an off-white powder (124 mg, 58 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.96 (d, 1H, $^3J_{HH}$ = 8.6 Hz), 7.53 (d, 1H, $^3J_{HH}$ = 8.6 Hz), 7.33 (s, 1H), 6.04 (d, 1H, $^3J_{HH}$ = 7.6 Hz), 5.83 (dt, 1H, $^3J_{HH}$ = 7.6, $^3J_{HH}$ = 7.6 Hz), 5.18 (h, 1H, $^3J_{HH}$ = 6.6 Hz), 3.26 (d, 2H, $^3J_{HH}$ = 7.6), 1.27 (d, 6H, $^3J_{HH}$ = 6.6 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 167.3, 144.0, 137.5, 132.8 (q, $^2J_{CF}$ = 32.0 Hz), 132.1, 124.9, 123.7 (q, $^1J_{CF}$ = 273.9 Hz), 123.3 (q, $^3J_{CF}$ = 3.5 Hz), 122.7 (q, $^3J_{CF}$ = 3.8 Hz), 12.2, 46.0, 31.1, 20.6. $^{19}$F {$^1$H} NMR (CDCl$_3$, 376 MHz, 298 K); δ 62.84 (s, 1F). HR-MS (ASAP+, *m/z*); calcd. for C$_{14}$H$_{14}$NOF$_3$+H = 270.1106; obtained = 270.1103 [M+H]$^+$. $R_f$ = 0.58 (EtOAc:Hexane 20:80).

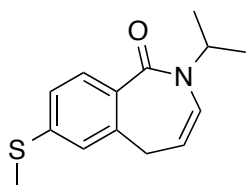### 6-fluoro-2-isopropyl-2,5-dihydro-1*H*-benzo[*c*]azepin-1-one (3lb)
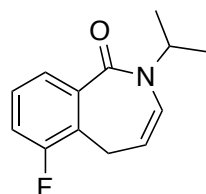


This compound was prepared by the general alkylation protocol described above starting from substrate **1l** (145 mg, 0.8 mmol) to yield an off-white powder (98 mg, 56 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.65 (d, 1H, $^3J_{HH}$ = 7.5 Hz), 7.24-7.17 (m, 1H), 7.16-7.09 (m, 1H), 6.04 (d, 1H, $^3J_{HH}$ = 7.5 Hz), 5.81 (dt, 1H, $^3J_{HH}$ = 7.5, $^3J_{HH}$ = 7.5 Hz), 5.17 (h, 1H, $^3J_{HH}$ = 7.1 Hz), 3.28 (d, 2H, $^3J_{HH}$ = 7.5), 1.26 (d, 6H, $^3J_{HH}$ = 7.1 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 167.4 (d, $^4J_{CF}$ = 3.3 Hz), 157.2 (d, $^1J_{CF}$ = 243.0 Hz), 136.6 (d, $^4J_{CF}$ = 3.2 Hz), 130.5 (d, $^2J_{CF}$ = 18.0 Hz), 127.1 (d, $^3J_{CF}$ = 8.2 Hz), 126.9 (d, $^3J_{CF}$ = 5.0 Hz), 125.5, 120.2, 117.6 (d, $^2J_{CF}$ = 23.8 Hz), 46.0, 21.6 (d, $^3J_{CF}$ = 5.3 Hz), 20.6. $^{19}$F {$^1$H} NMR (CDCl$_3$, 376 MHz, 298 K); δ 122.75 (s, 1F). HR-MS (ASAP+, *m/z*); calcd. for C$_{13}$H$_{14}$NOF+H = 220.1138; obtained = 220.1147 [M+H]$^+$. $R_f$ = 0.61 (EtOAc:Hexane 20:80).

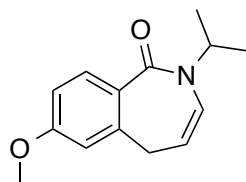### 7-isopropyl-4,7-dihydro-8H-thieno[2,3-*c*]azepin-8-one (4.11)
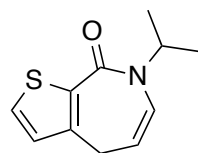


This compound was prepared by the general alkylation protocol described above starting from substrate **1m** (135 mg, 0.8 mmol) to yield an off-white powder (81 mg, 49 %). $^1$H NMR (CDCl$_3$, 400 MHz, 298 K); δ 7.43 (d, 1H, $^3J_{HH}$ = 4.8 Hz), 6.79 (d, 1H, $^3J_{HH}$ = 4.8 Hz), 6.01 (d, 1H, $^3J_{HH}$ = 8.2 Hz), 5.51 (dt, 1H, $^3J_{HH}$ = 6.7, $^3J_{HH}$ = 8.2 Hz), 5.01 (h, 1H, $^3J_{HH}$ = 7.2 Hz), 3.26 (d, 2H, $^3J_{HH}$ = 6.7 Hz), 1.26 (d, 6H, $^3J_{HH}$ = 7.2 Hz). $^{13}$C {$^1$H} NMR (CDCl$_3$, 100 MHz, 298 K); δ = 162.4, 144.9, 135.0, 130.9, 127.4, 125.5, 115.7, 46.3, 26.0, 20.6. HR-MS (ASAP+, *m/z*); calcd. for C$_{11}$H$_{13}$NOS+H = 208.0796; obtained = 208.0794 [M+H]$^+$. $R_f$ = 0.54 (EtOAc:Hexane 20:80).

## [7] Original NMR Spectra for all Compounds:

This section contains the original $^1$H, $^{13}$C {$^1$H} and COSY NMR spectra obtained for all alkylation and cyclization products reported in this manuscript.
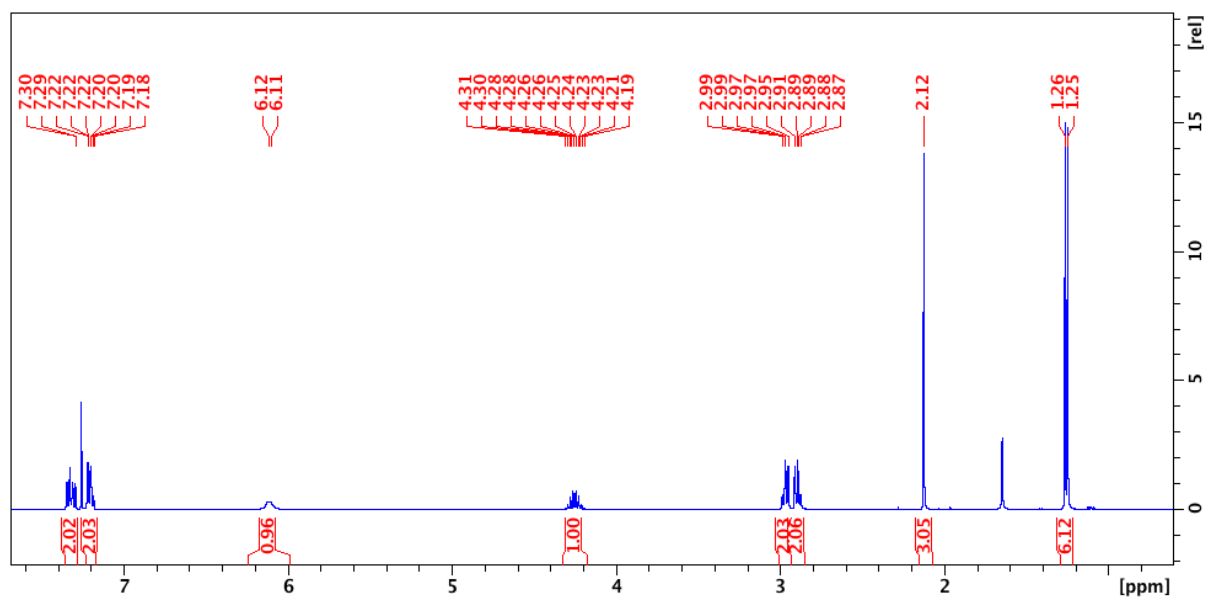


*Figure S1: $^1$H NMR spectrum of compound **2aa** in CDCl$_3$ at 298 K.*



*Figure S2: $^{13}$C {$^1$H} NMR spectrum of compound **2aa** in CDCl$_3$ at 298 K.*

*Figure S3: COSY NMR spectrum of compound **2aa** in CDCl₃ at 298 K.*



*Figure S4: ¹H NMR spectrum of compound **2ca** in CDCl₃ at 298 K.*

*Figure S5: $^{13}C$ {$^1H$} NMR spectrum of compound **2ca** in CDCl$_3$ at 298 K.*
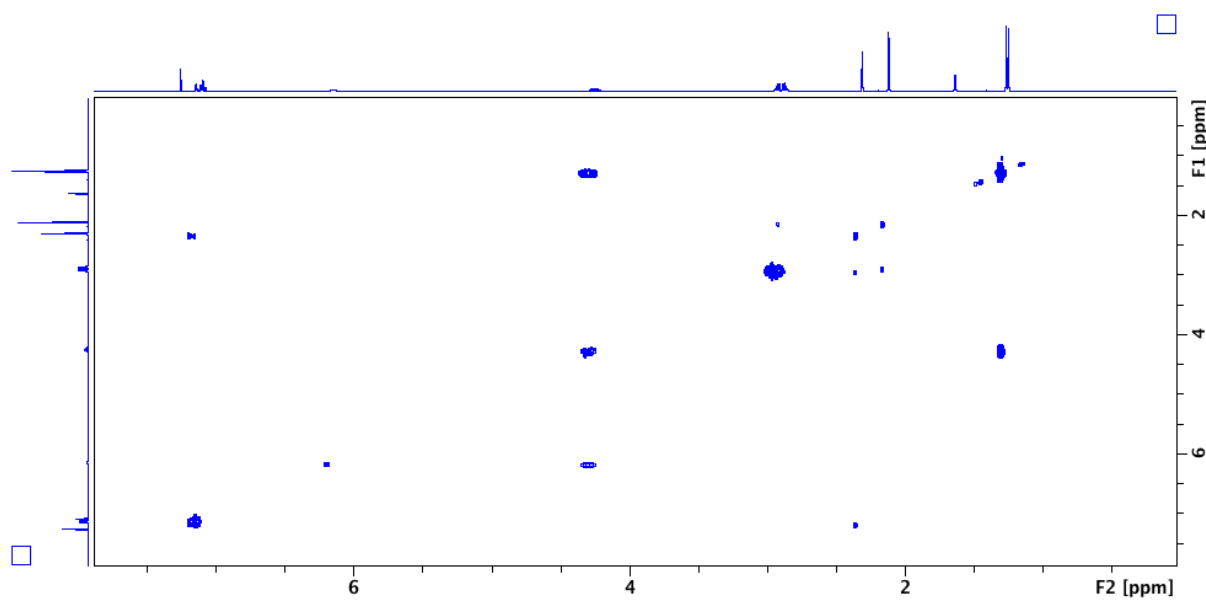


*Figure S6: COSY NMR spectrum of compound **2ca** in CDCl$_3$ at 298 K.*
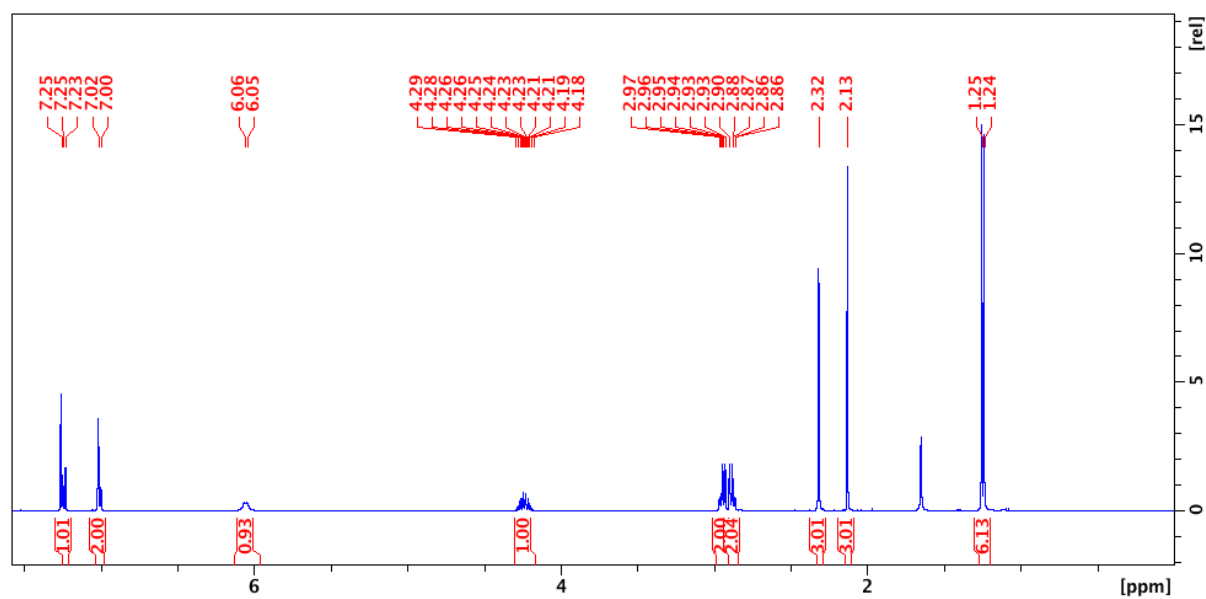
*Figure S7: $^1H$ NMR spectrum of compound **2da** in CDCl$_3$ at 298 K.*
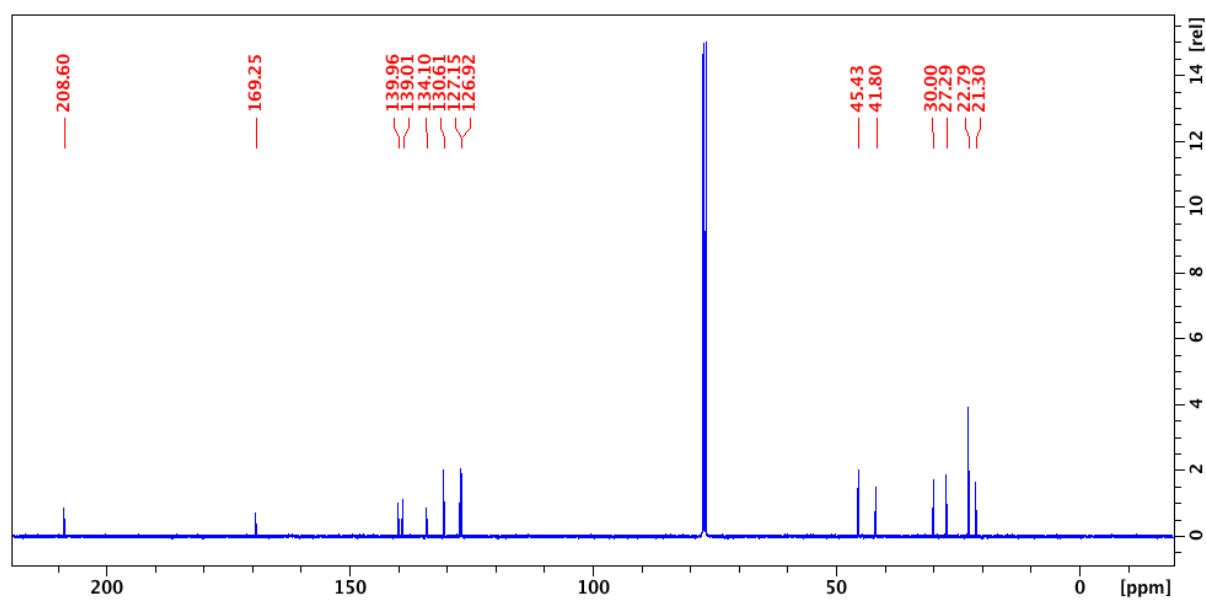


*Figure S8: $^{13}C$ {$^1H$} NMR spectrum of compound **2da** in CDCl$_3$ at 298 K.*
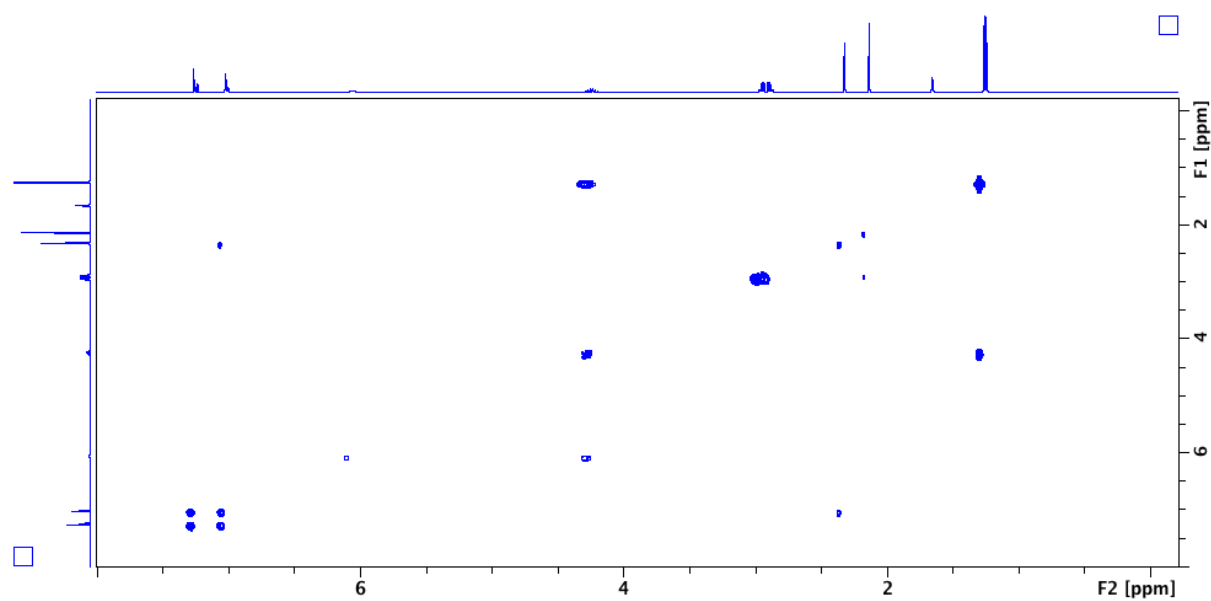
*Figure S9: COSY NMR spectrum of compound **2da** in CDCl₃ at 298 K.*
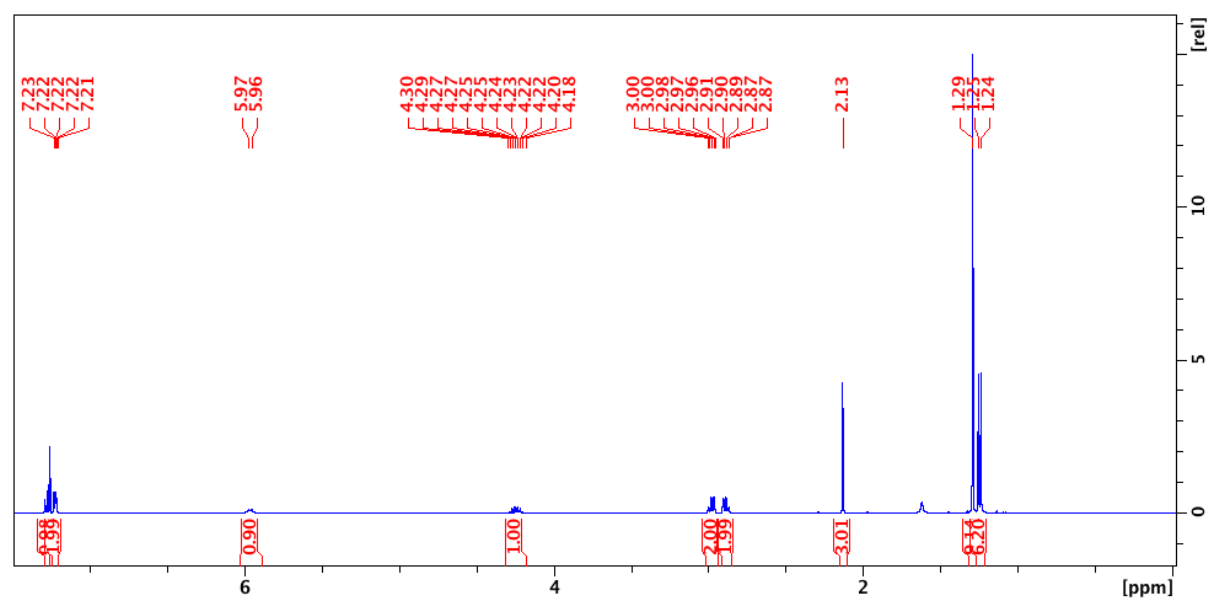


*Figure S10: ¹H NMR spectrum of compound **2ea** in CDCl₃ at 298 K.*
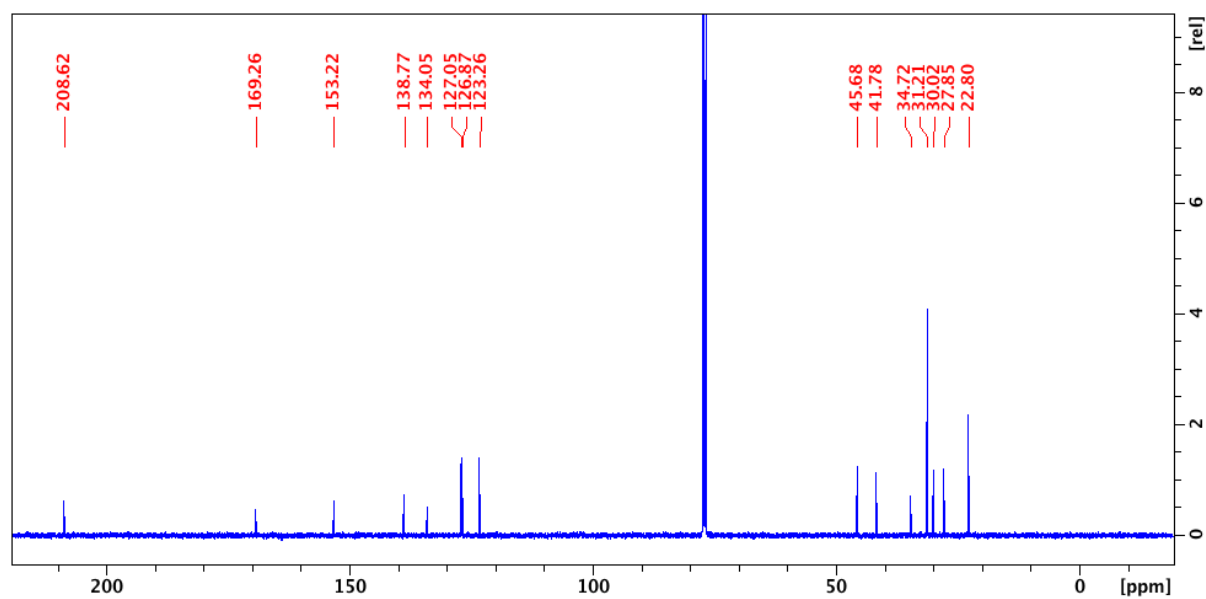
Figure S11: $^{13}C$ {$^1H$} NMR spectrum of compound **2ea** in CDCl$_3$ at 298 K.
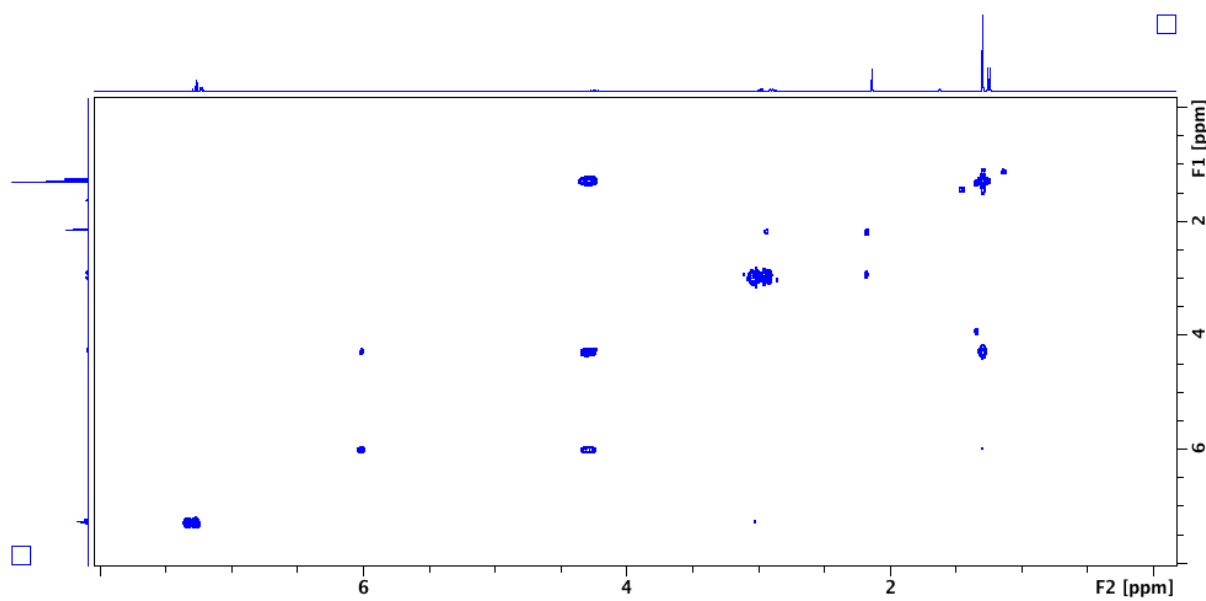


Figure S12: COSY NMR spectrum of compound **2ea** in CDCl$_3$ at 298 K.
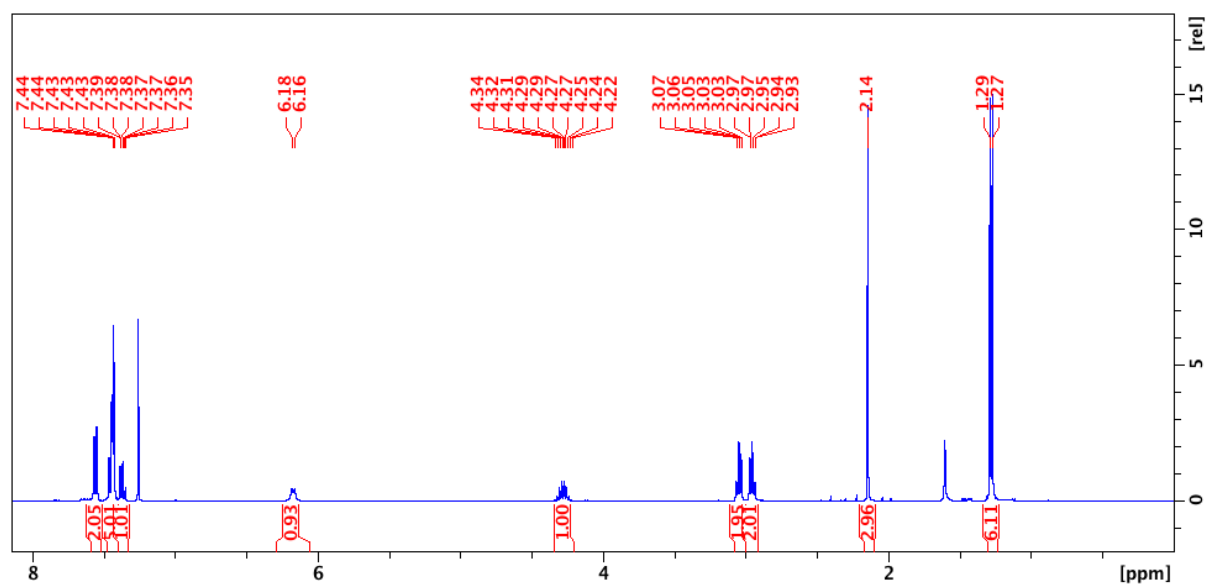
*Figure S13: $^1H$ NMR spectrum of compound **2fa** in CDCl$_3$ at 298 K.*
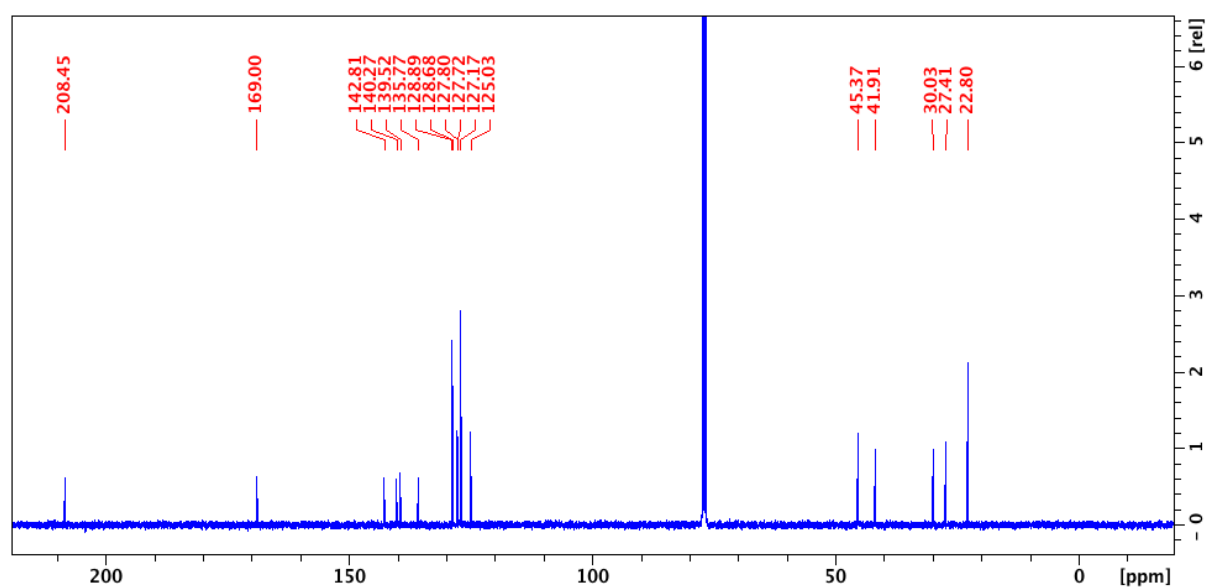


*Figure S14: $^{13}C$ {$^1H$} NMR spectrum of compound **2fa** in CDCl$_3$ at 298 K.*
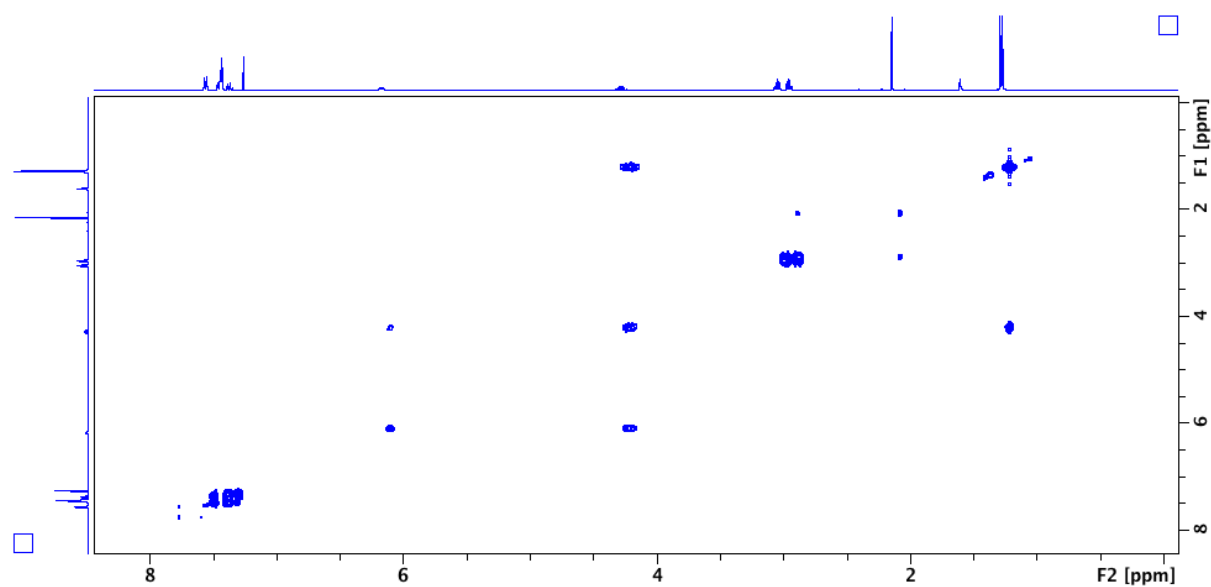
*Figure S15: COSY NMR spectrum of compound **2fa** in CDCl$_3$ at 298 K.*
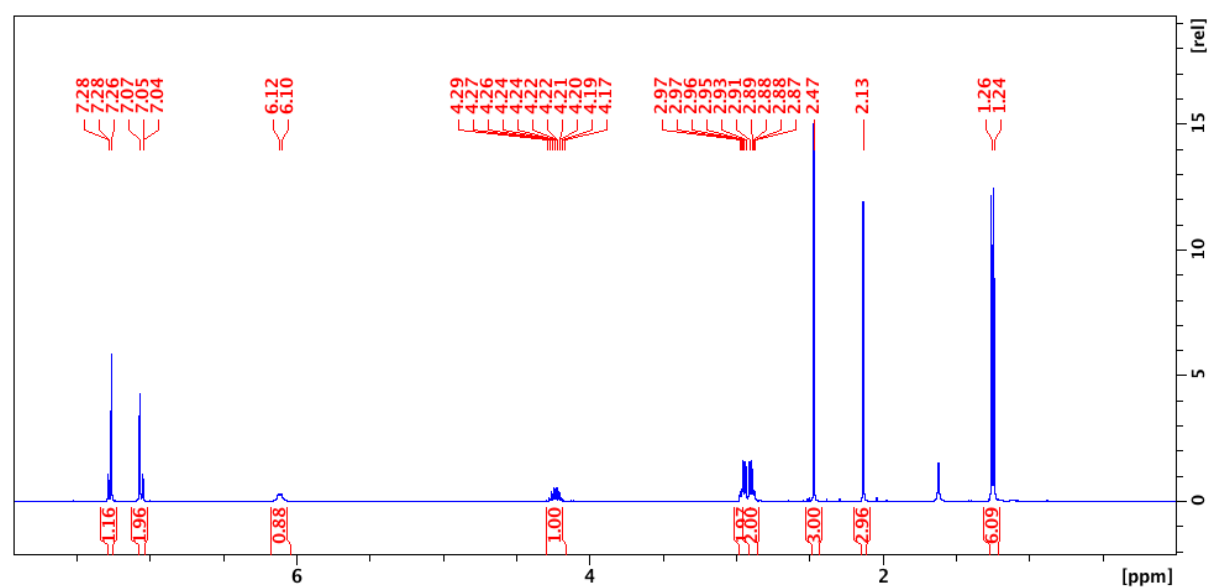


*Figure S16: $^1$H NMR spectrum of compound **2ha** in CDCl$_3$ at 298 K.*
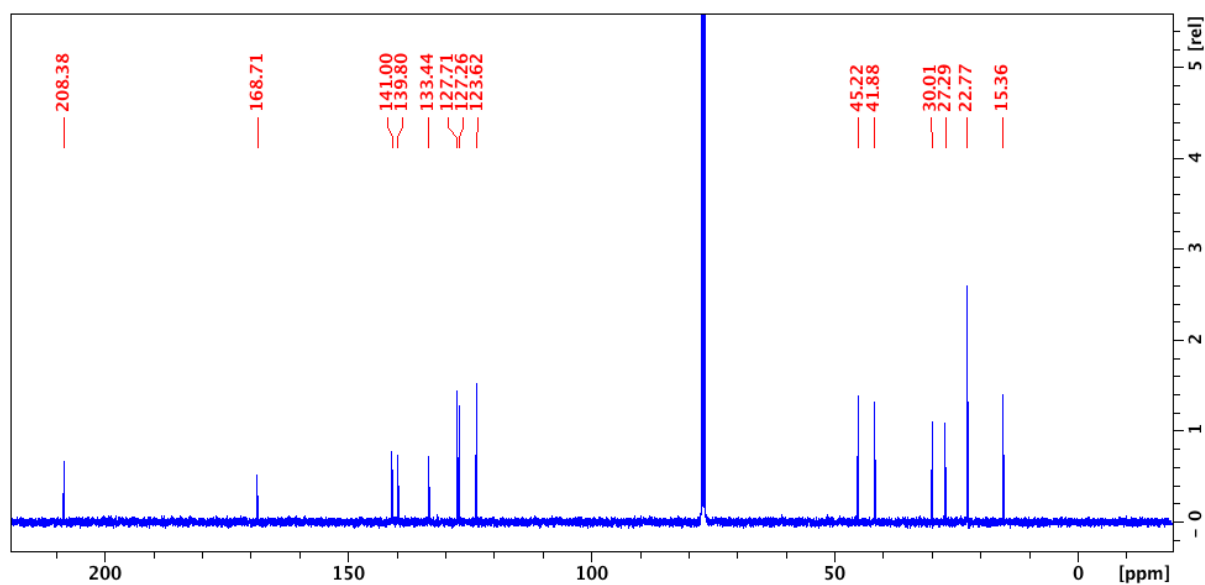
*Figure S17: $^{13}C$ {$^1H$} NMR spectrum of compound **2ha** in CDCl$_3$ at 298 K.*
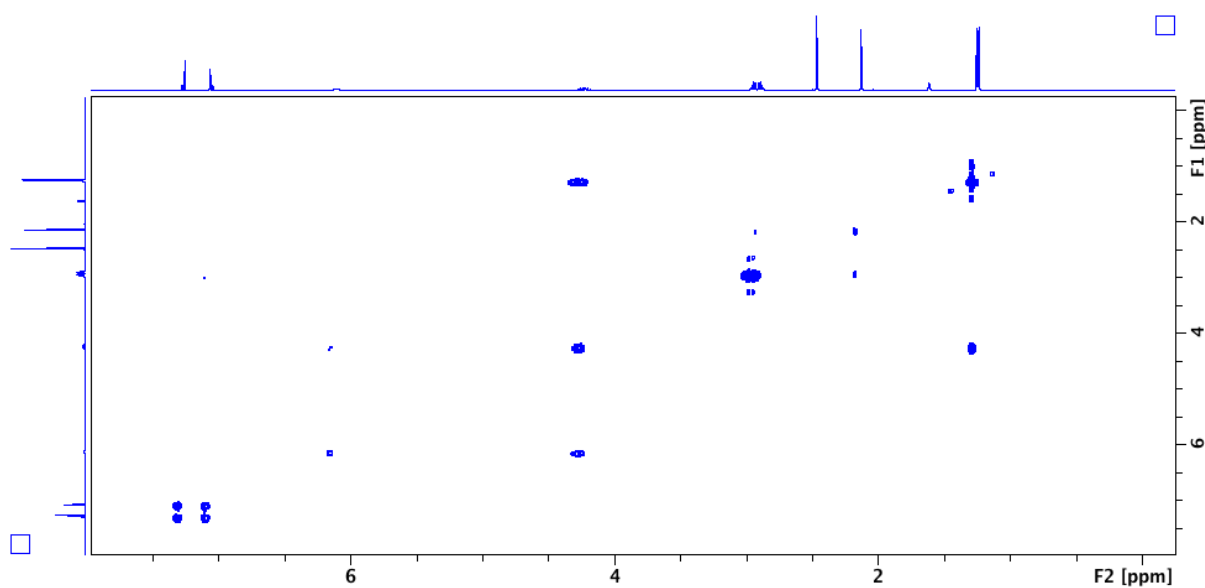


*Figure S18: COSY NMR spectrum of compound **2ha** in CDCl$_3$ at 298 K.*
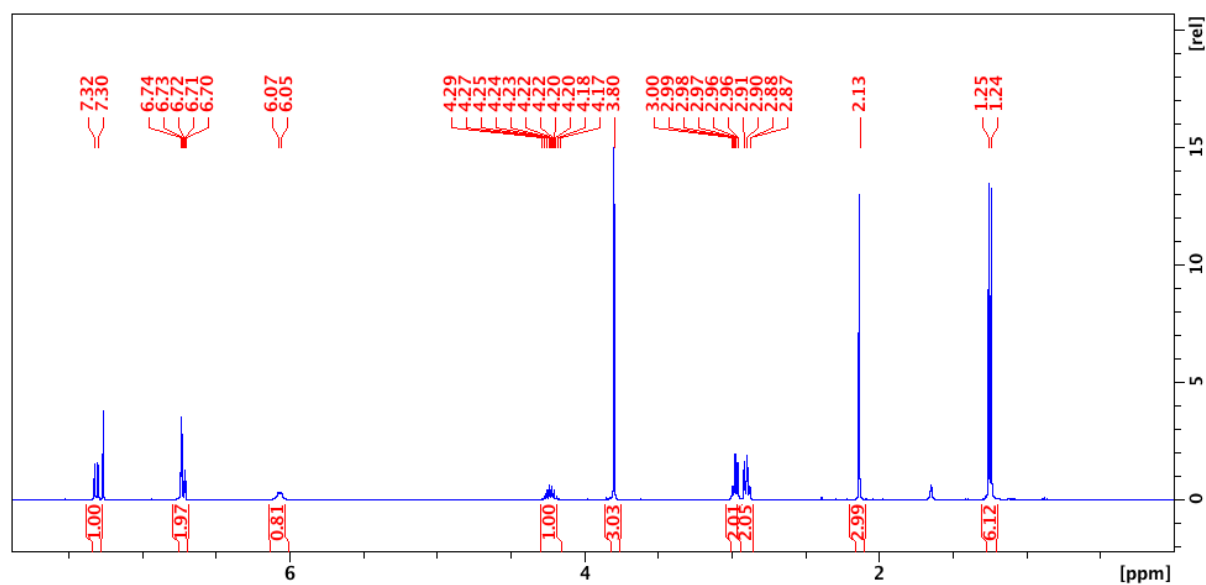
Figure S19: $^1H$ NMR spectrum of compound **2ia** in CDCl₃ at 298 K.
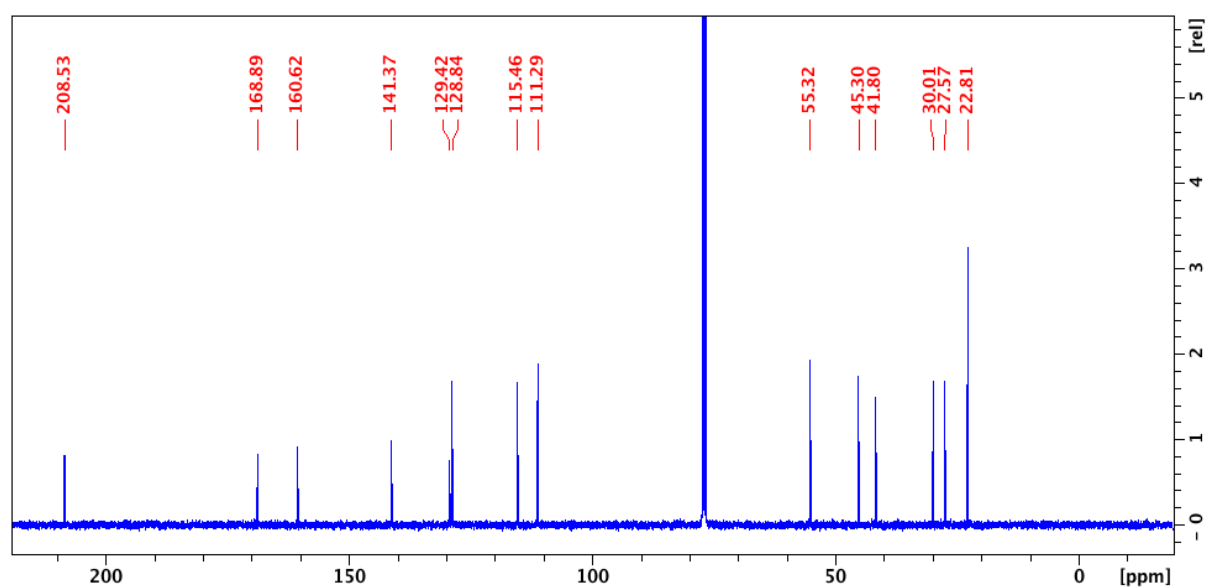


Figure S20: $^{13}C$ {$^1H$} NMR spectrum of compound **2ia** in CDCl₃ at 298 K.
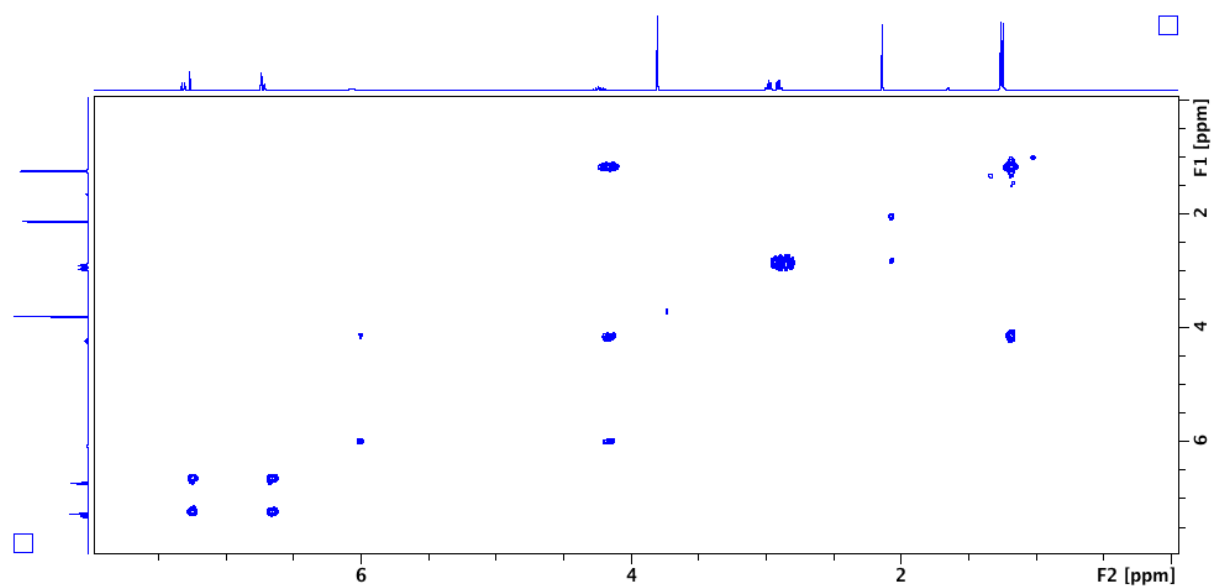
*Figure S21: COSY NMR spectrum of compound **2ia** in CDCl₃ at 298 K.*
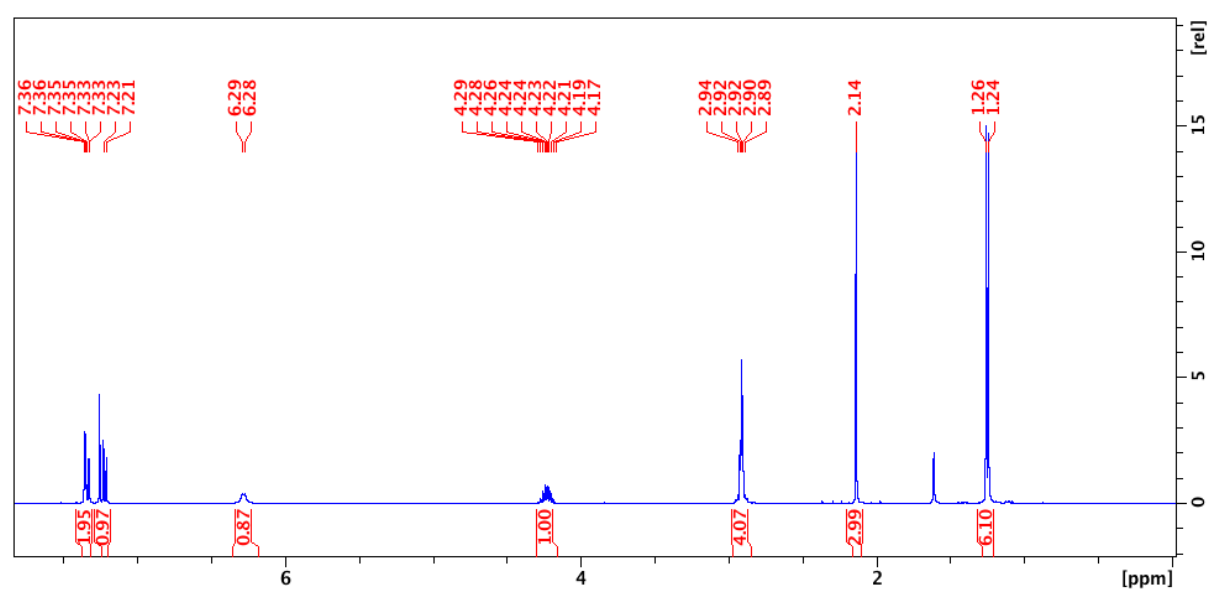


*Figure S22: ¹H NMR spectrum of compound **2ja** in CDCl₃ at 298 K.*
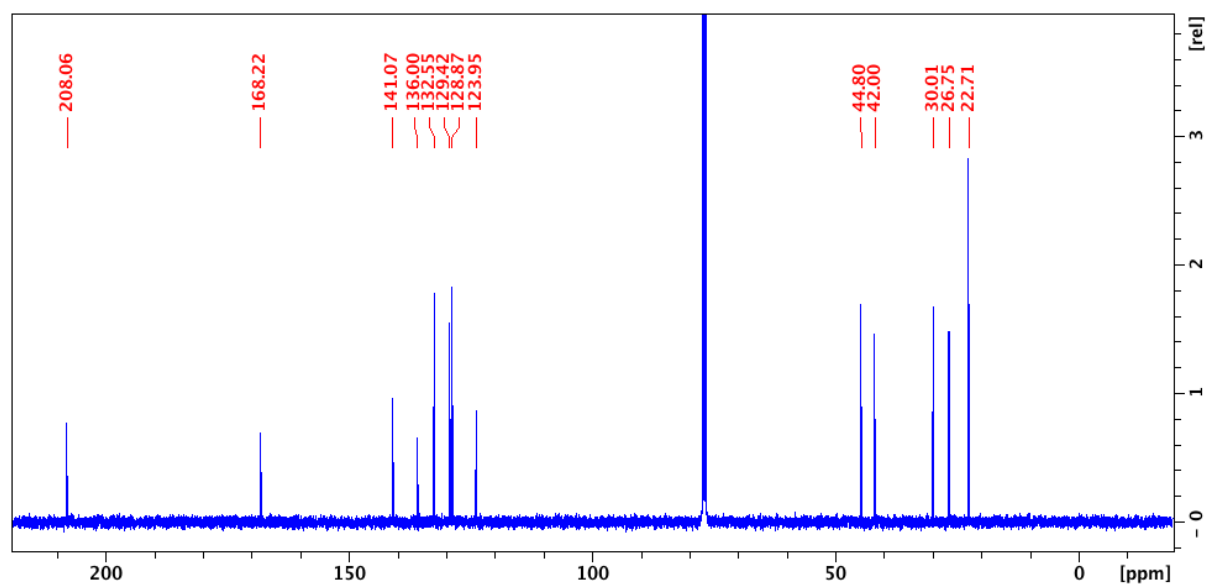
*Figure S23: $^{13}C$ {$^1H$} NMR spectrum of compound **2ja** in CDCl$_3$ at 298 K.*
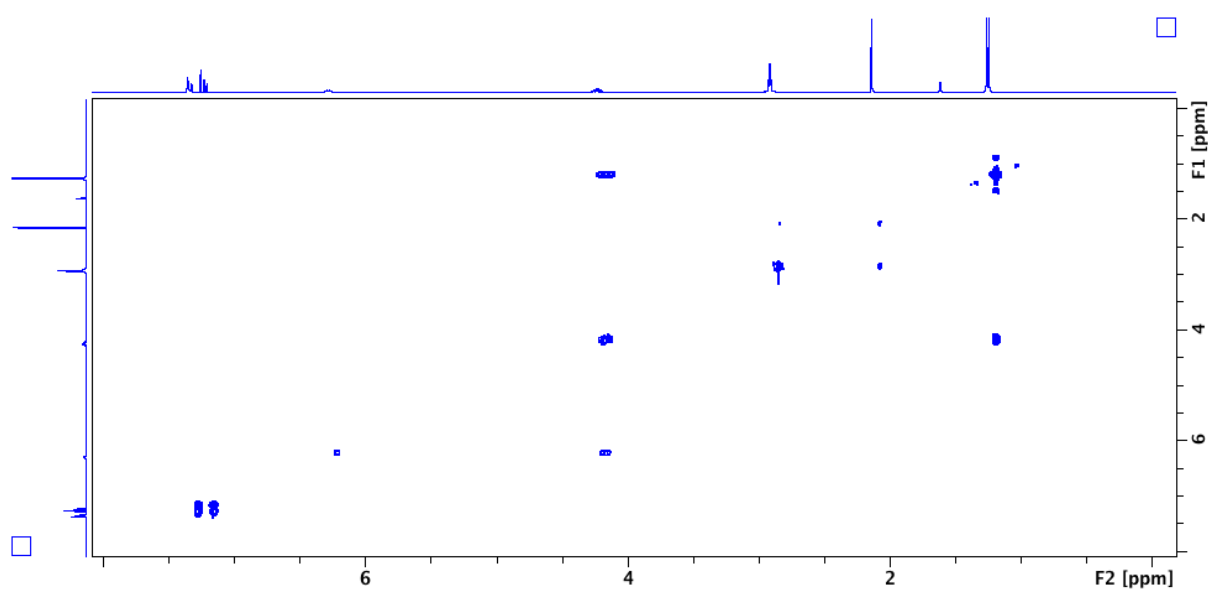


*Figure S24: COSY NMR spectrum of compound **2ja** in CDCl$_3$ at 298 K.*
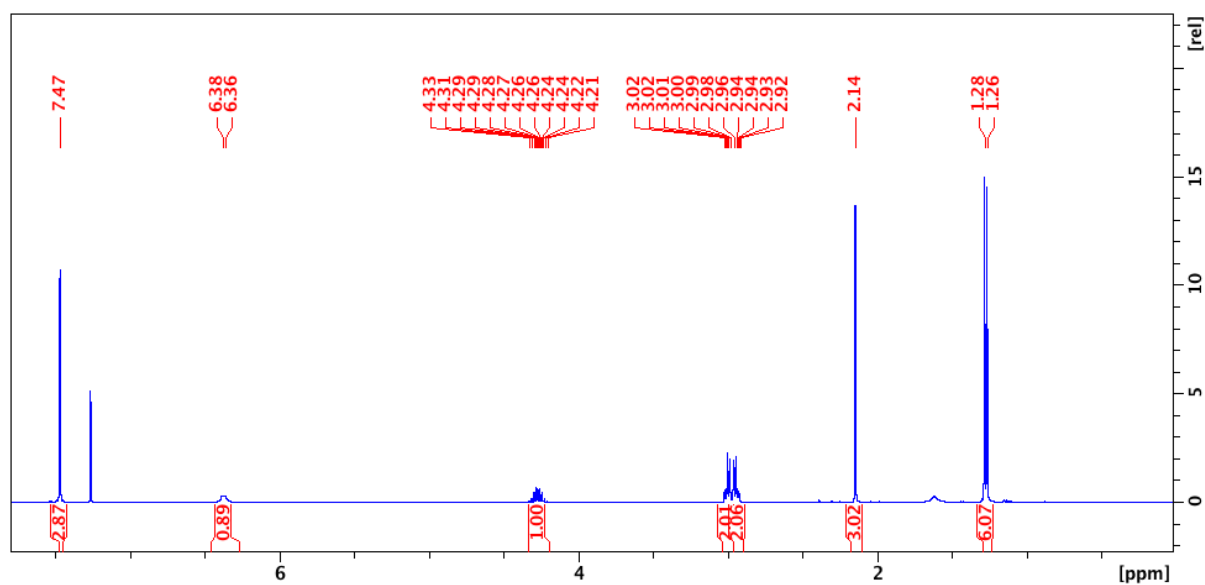
*Figure S25: $^1H$ NMR spectrum of compound **2ka** in CDCl$_3$ at 298 K.*
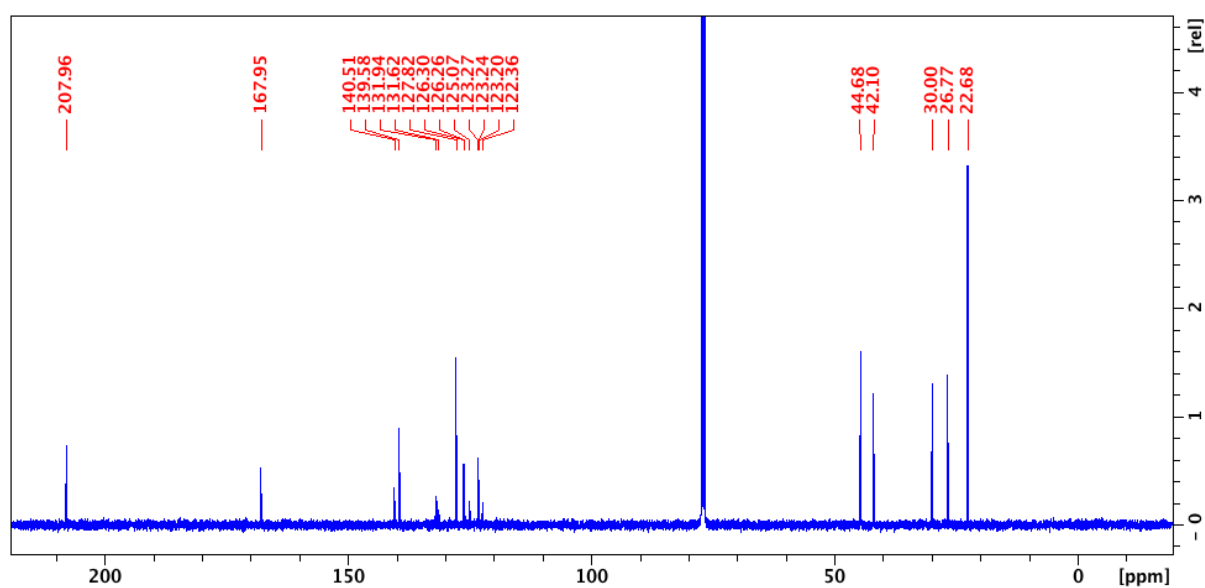


*Figure S26: $^{13}C$ {$^1H$} NMR spectrum of compound **2ka** in CDCl$_3$ at 298 K.*
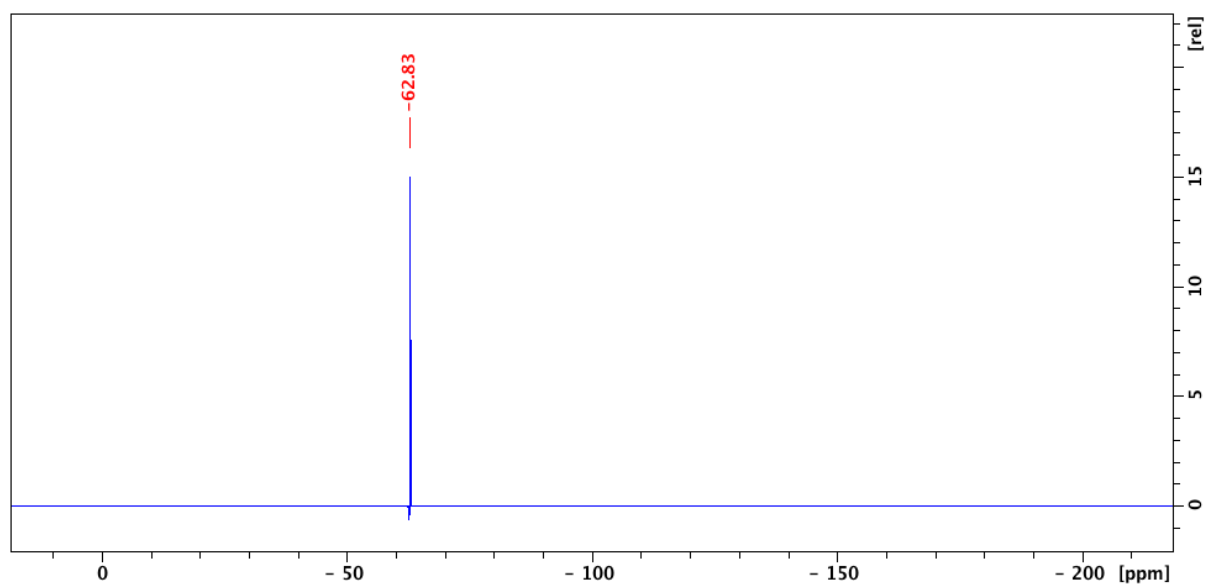
*Figure S27: $^{19}F$ {$^{1}H$} NMR spectrum of compound **2ka** in CDCl$_3$ at 298 K.*
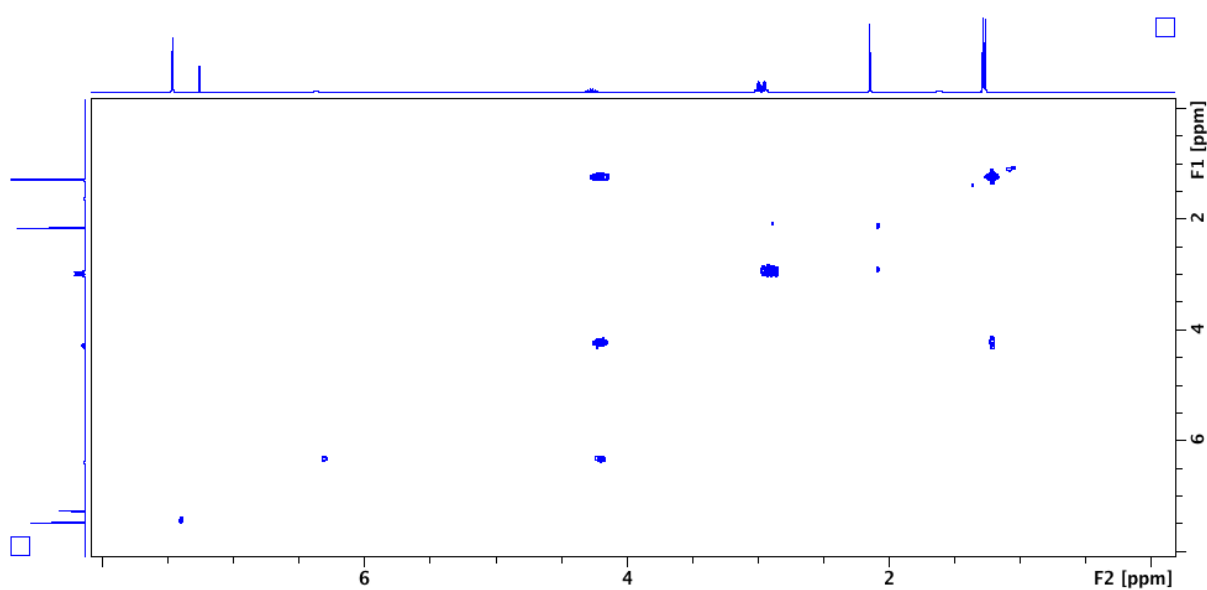


*Figure S28: COSY NMR spectrum of compound **2ka** in CDCl$_3$ at 298 K.*
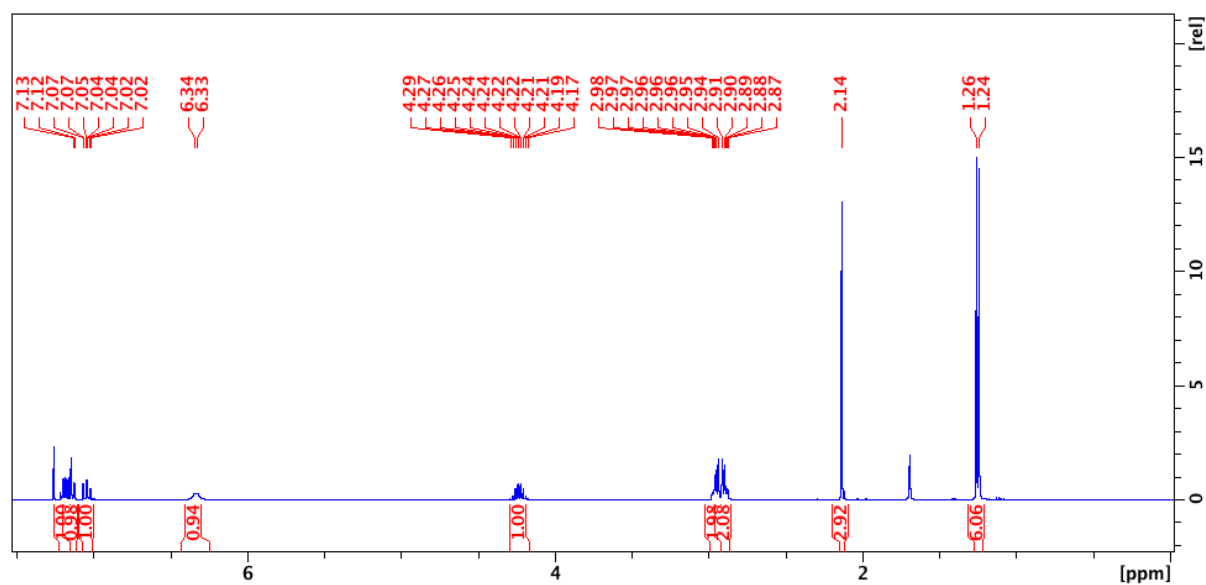
Figure S29: $^1$H NMR spectrum of compound **2la** in CDCl$_3$ at 298 K.
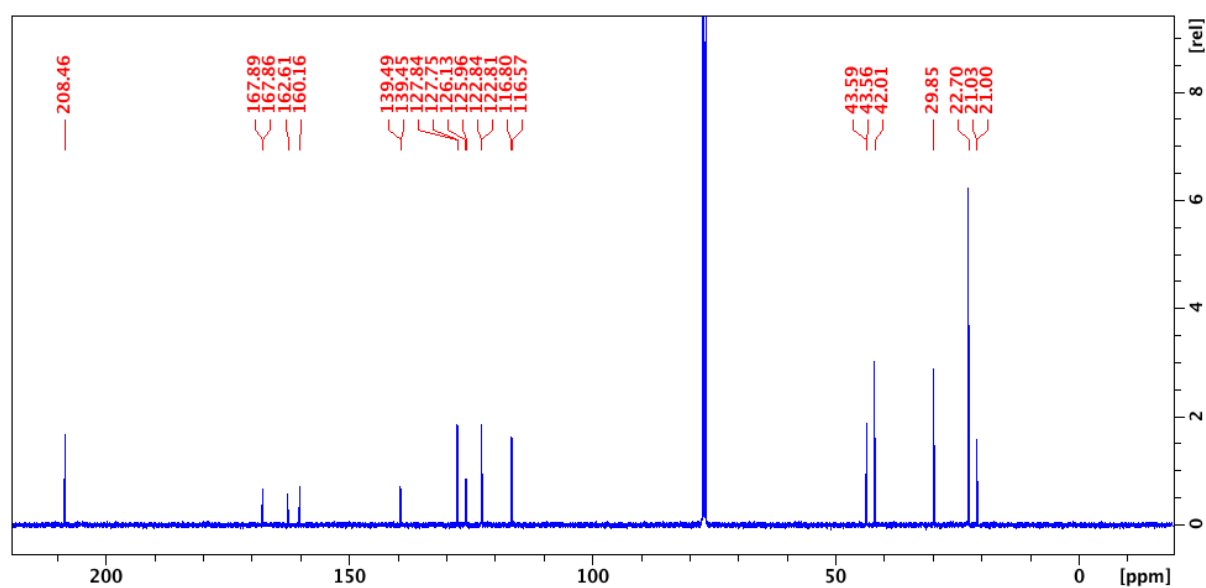


Figure S30: $^{13}$C {$^1$H} NMR spectrum of compound **2la** in CDCl$_3$ at 298 K.
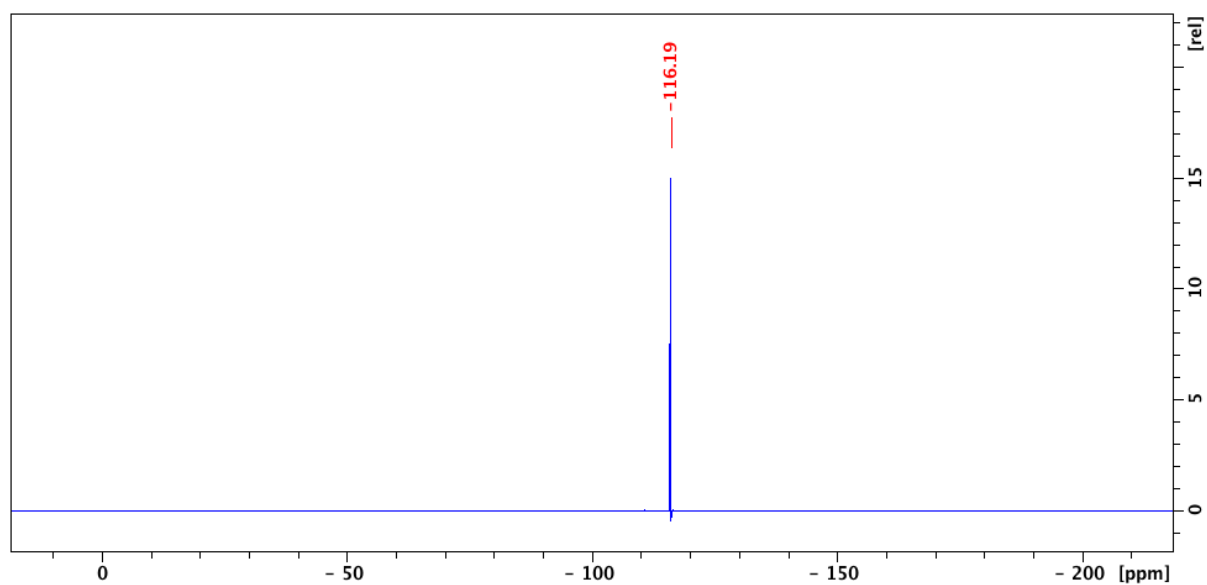
*Figure S31: $^{19}F$ {$^1H$} NMR spectrum of compound **2la** in CDCl$_3$ at 298 K.*
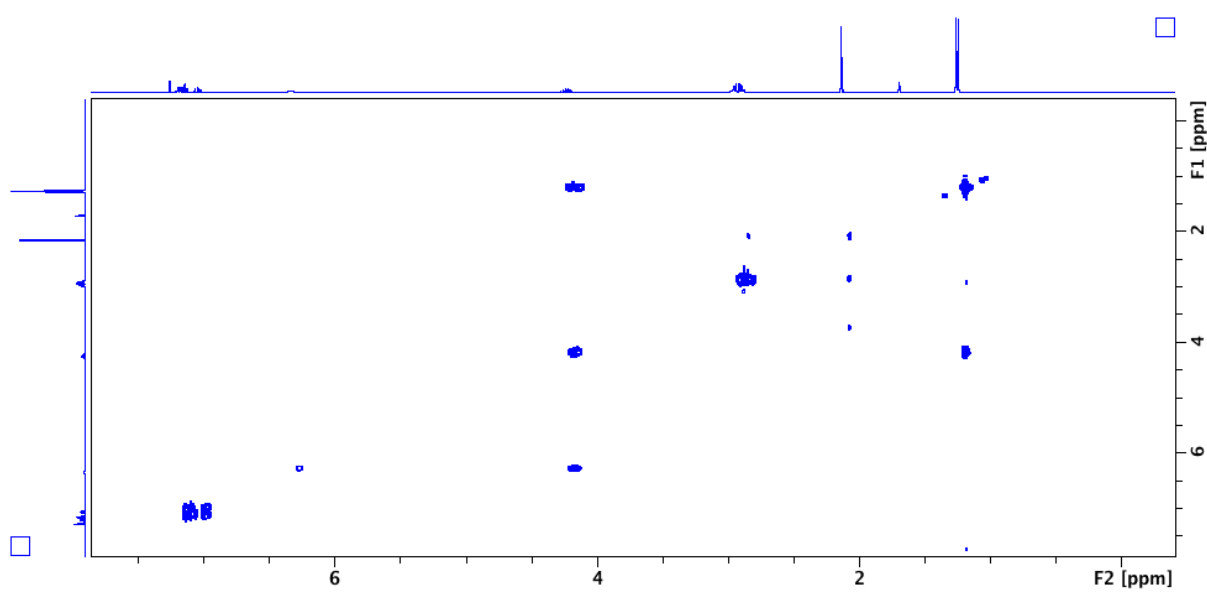


*Figure S32: COSY NMR spectrum of compound **2la** in CDCl$_3$ at 298 K.*
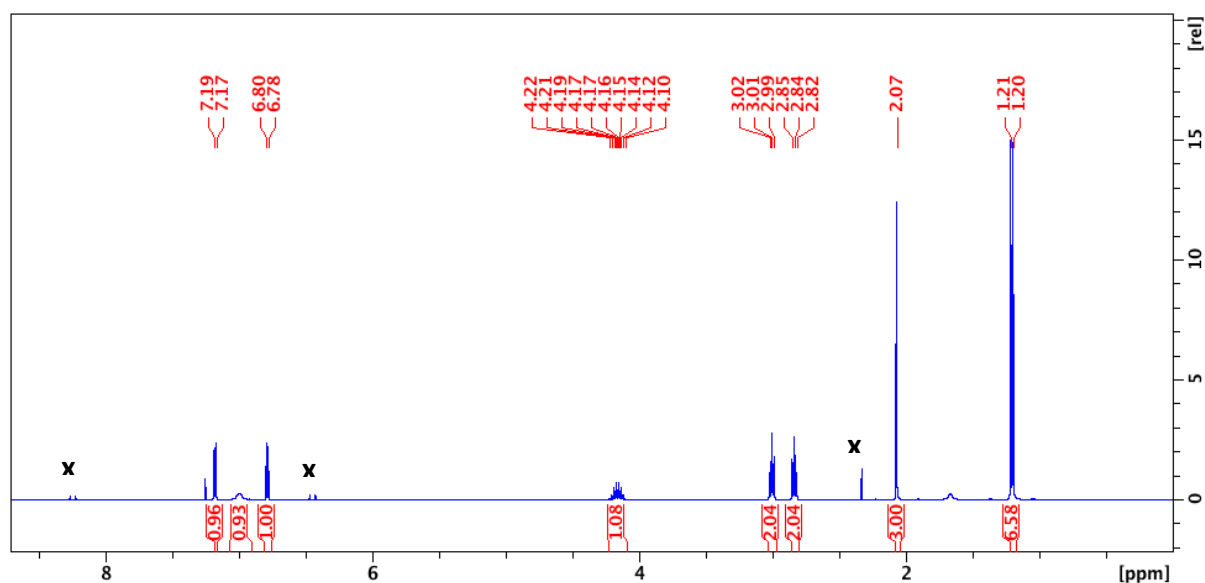
*Figure S33: ¹H NMR spectrum of impure compound **2ma** in CDCl₃ at 298 K. **X** indicates peaks from minor alkenylation purities which could not be removed by either column chromatography or recrystallization; peaks which have been picked and integrated are consistent with those expected for the desired alkylation product.*
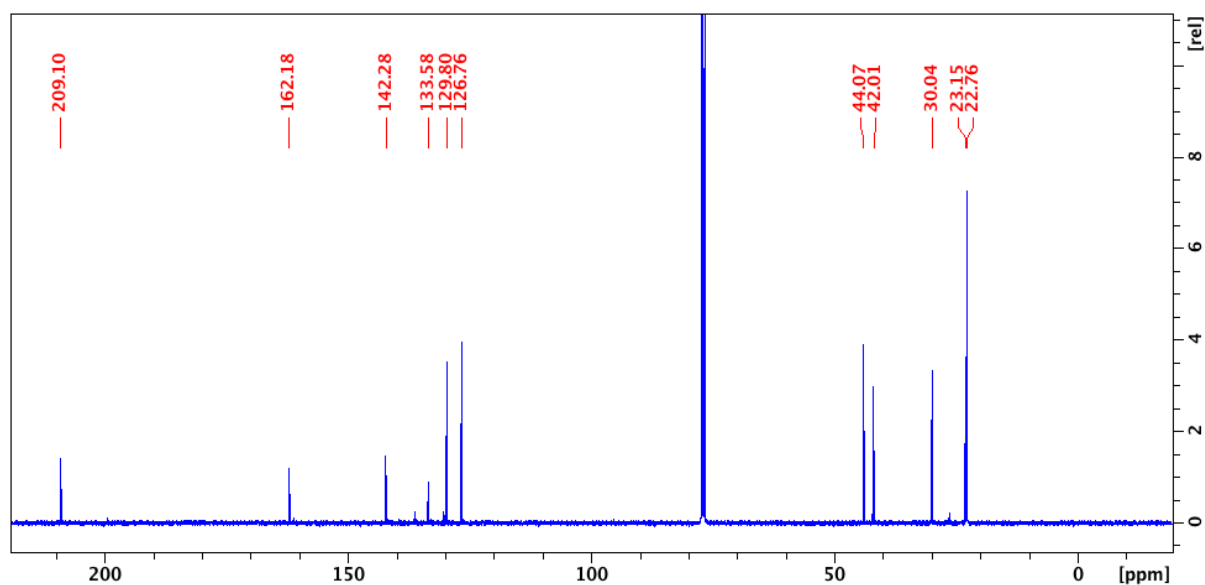


*Figure S34: ¹³C {¹H} NMR spectrum of compound **2ma** in CDCl₃ at 298 K. Presence of minor alkenylation purities which could not be removed by either column chromatography or recrystallization; peaks which have been picked are consistent with those expected for the desired alkylation product.*
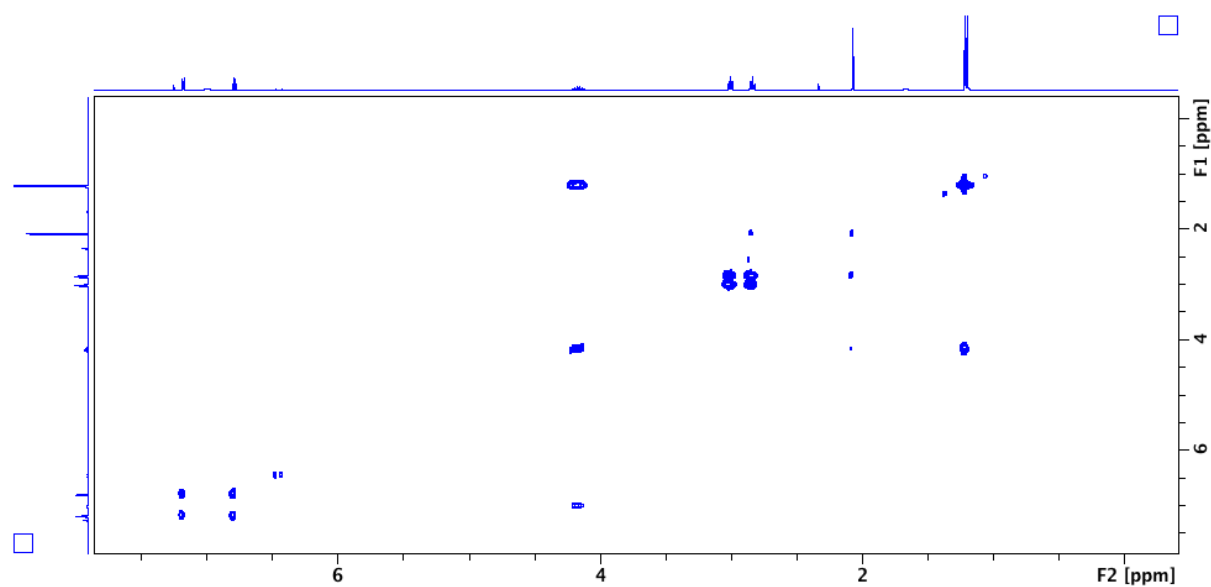
*Figure S32: COSY NMR spectrum of compound **2ma** in CDCl₃ at 298 K.*
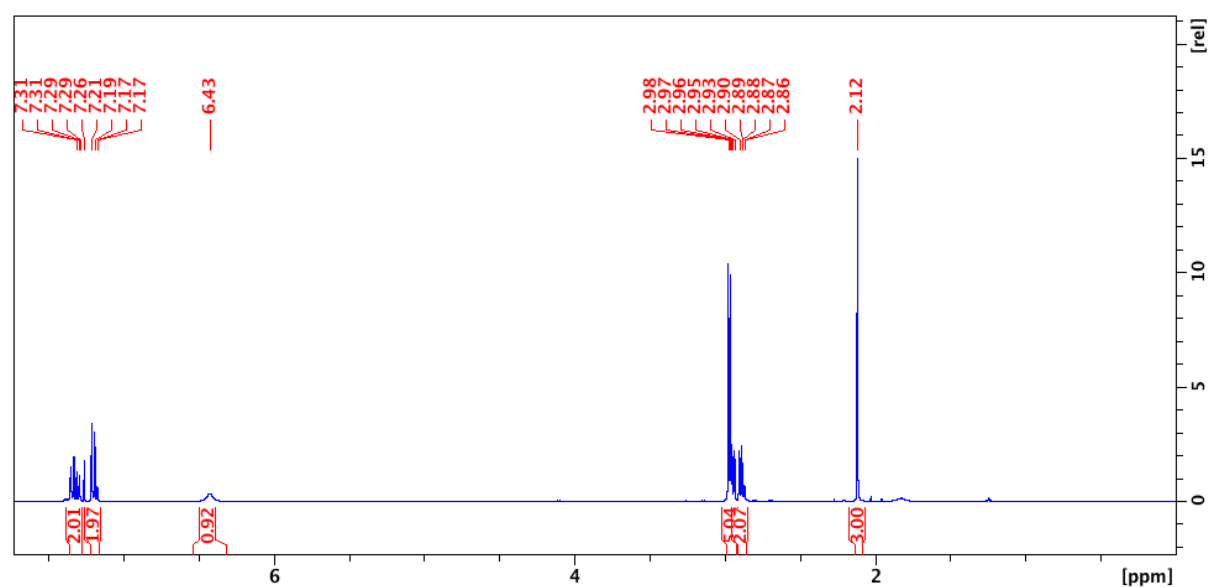


*Figure S33: ¹H NMR spectrum of compound **2oa** in CDCl₃ at 298 K.*
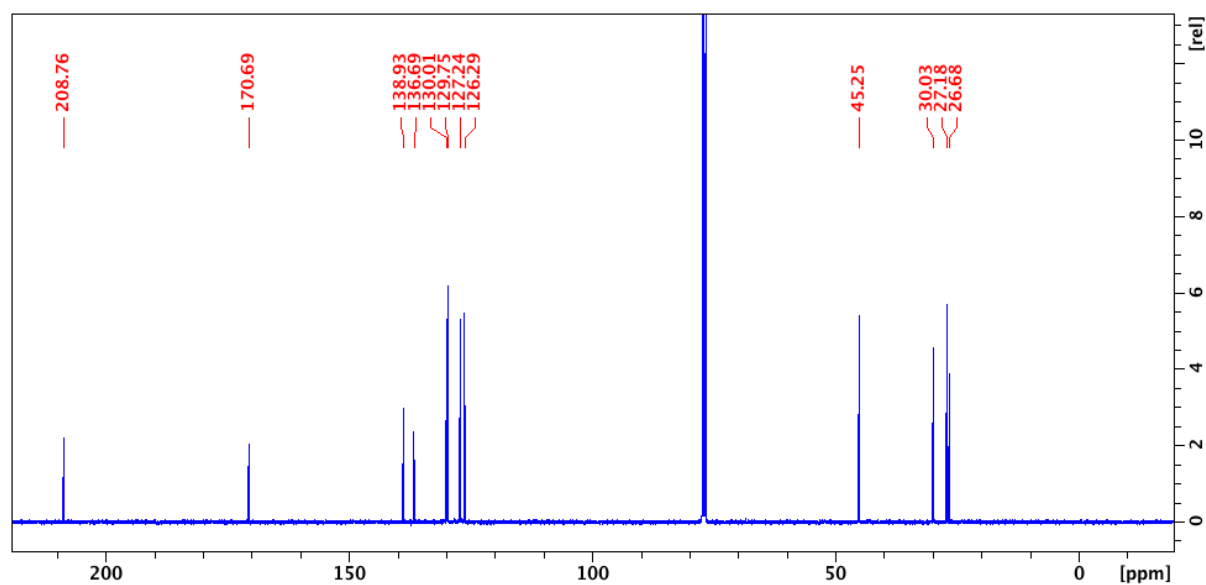
*Figure S34: $^{13}C\{^1H\}$ NMR spectrum of compound **2oa** in CDCl$_3$ at 298 K.*
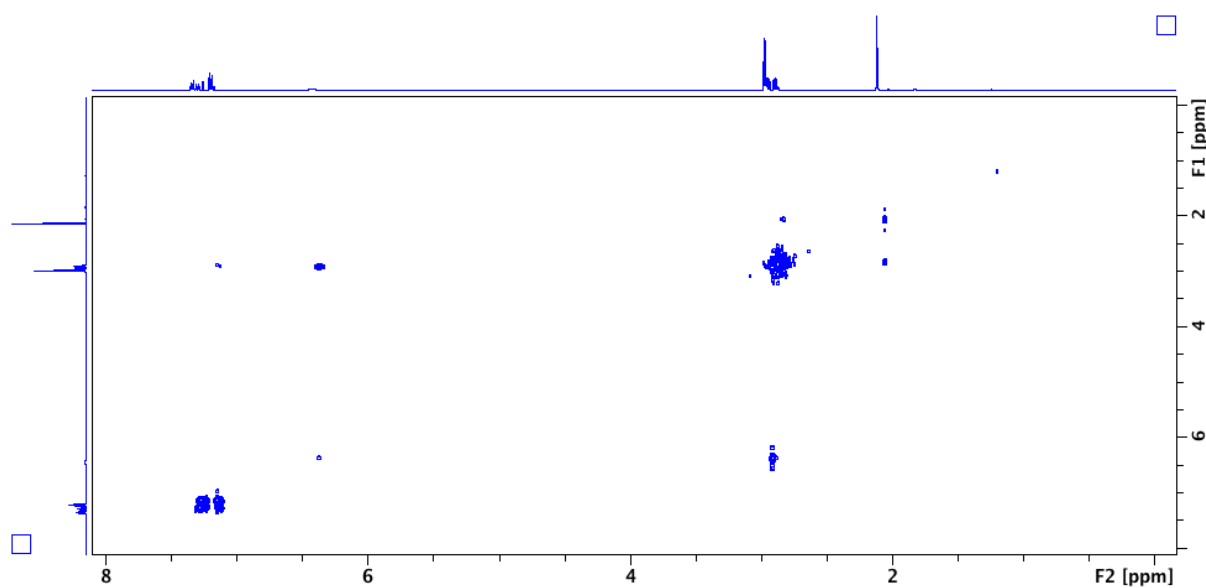


*Figure S35: COSY NMR spectrum of compound **2oa** in CDCl$_3$ at 298 K.*
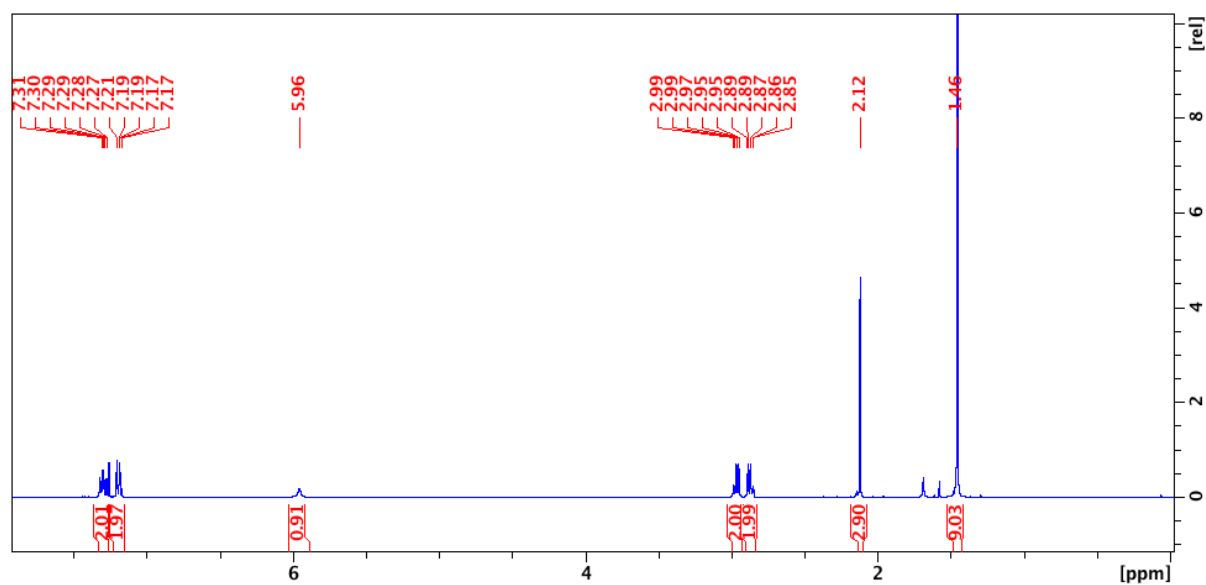
Figure S36: $^1H$ NMR spectrum of compound **2pa** in CDCl$_3$ at 298 K.
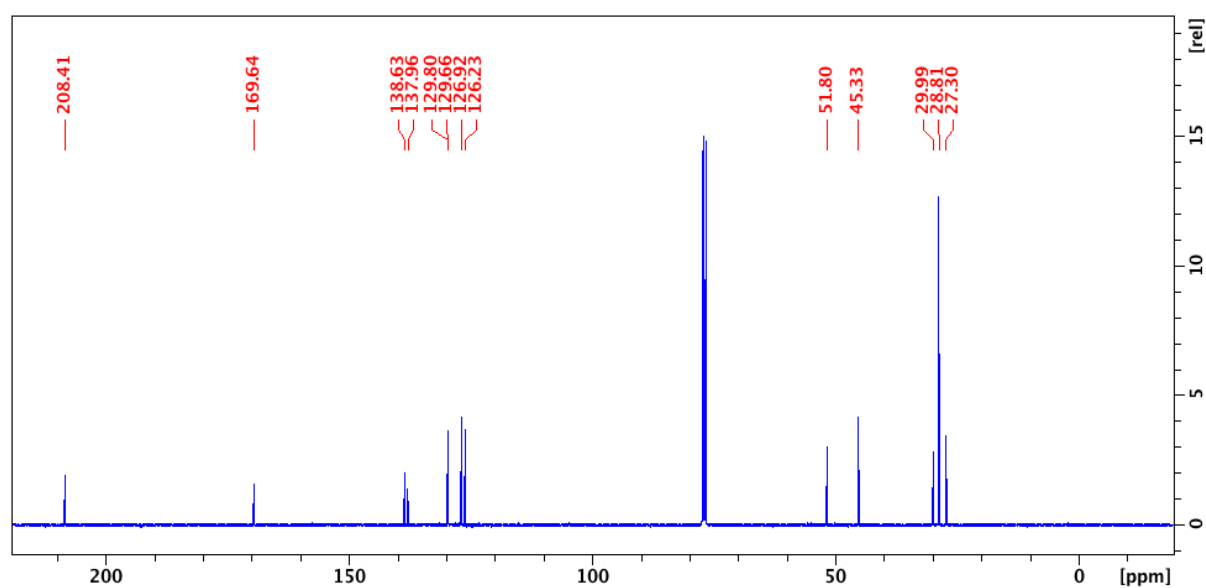


Figure S37: $^{13}C$ {$^1H$} NMR spectrum of compound **2pa** in CDCl$_3$ at 298 K.
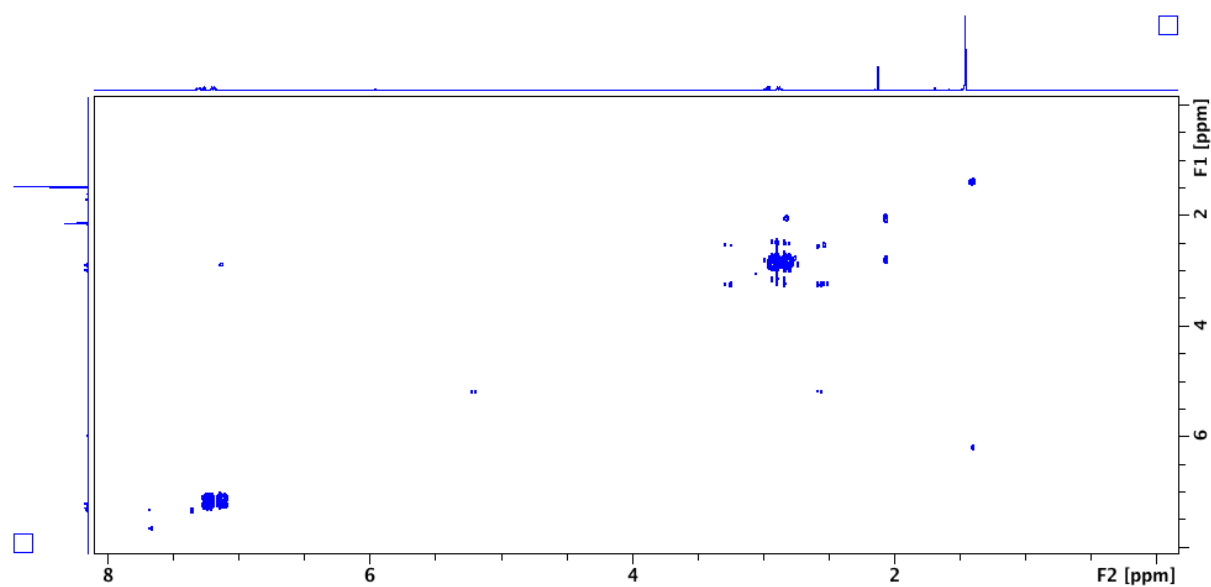
*Figure S38: COSY NMR spectrum of compound **2pa** in CDCl$_3$ at 298 K.*
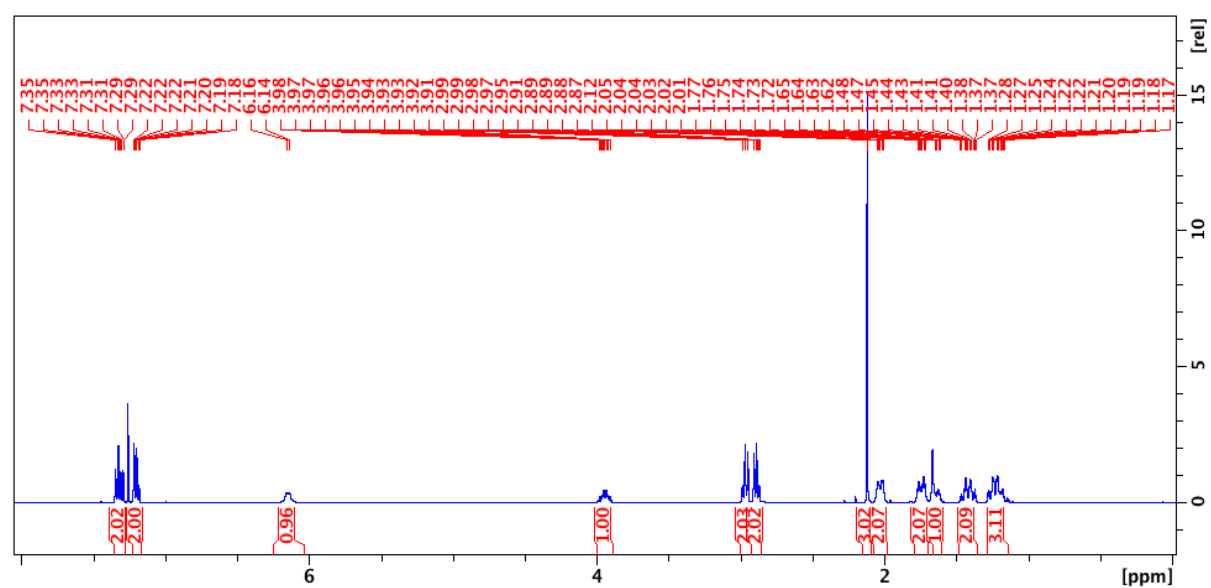


*Figure S39: $^1$H NMR spectrum of compound **2qa** in CDCl$_3$ at 298 K.*
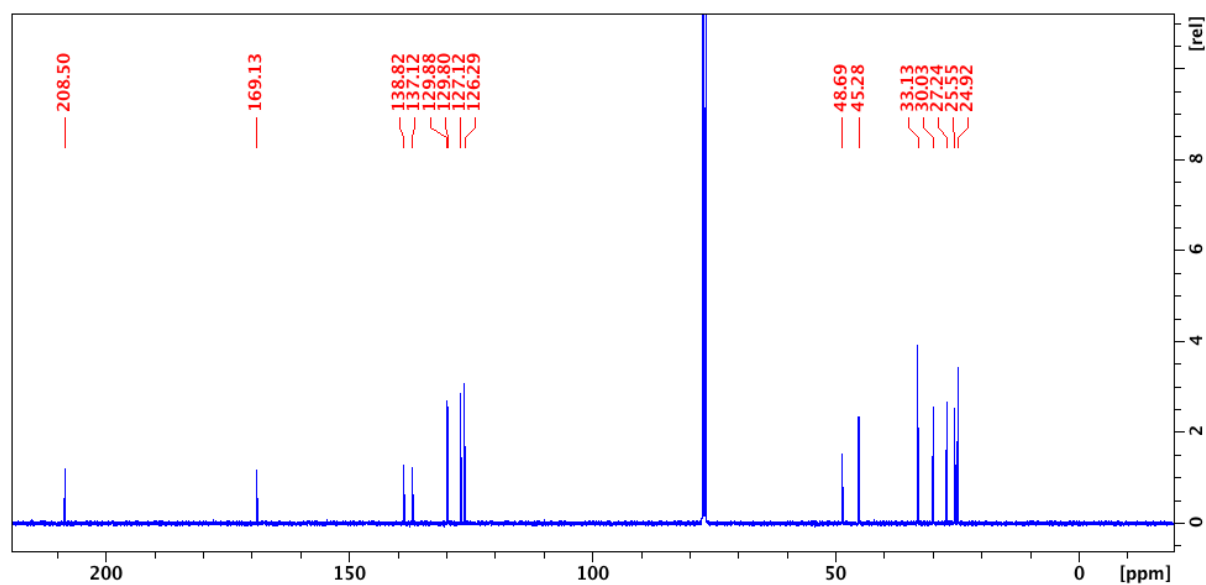
Figure S40: $^{13}C$ {$^1H$} NMR spectrum of compound **2qa** in CDCl$_3$ at 298 K.
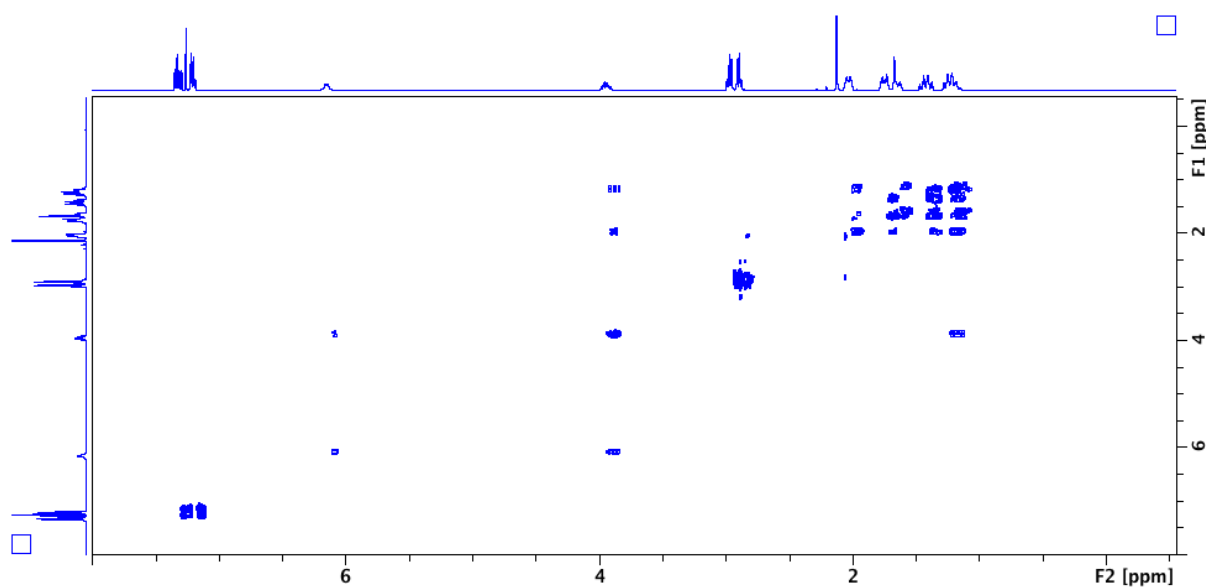


Figure S41: COSY NMR spectrum of compound **2qa** in CDCl$_3$ at 298 K.
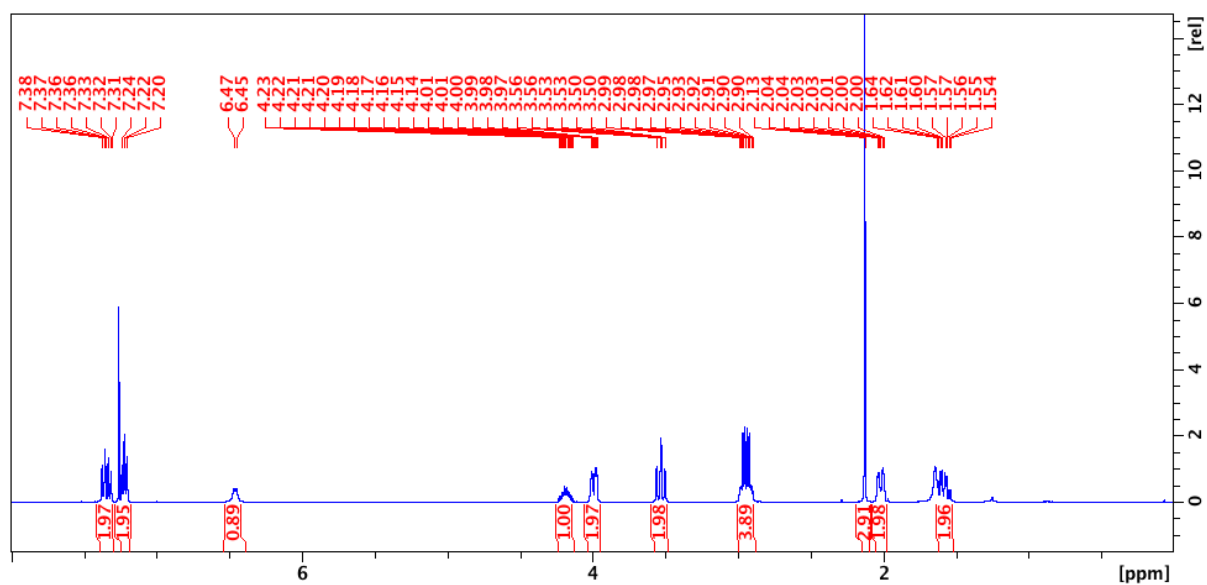
Figure S42: $^1H$ NMR spectrum of compound *2ra* in CDCl$_3$ at 298 K.
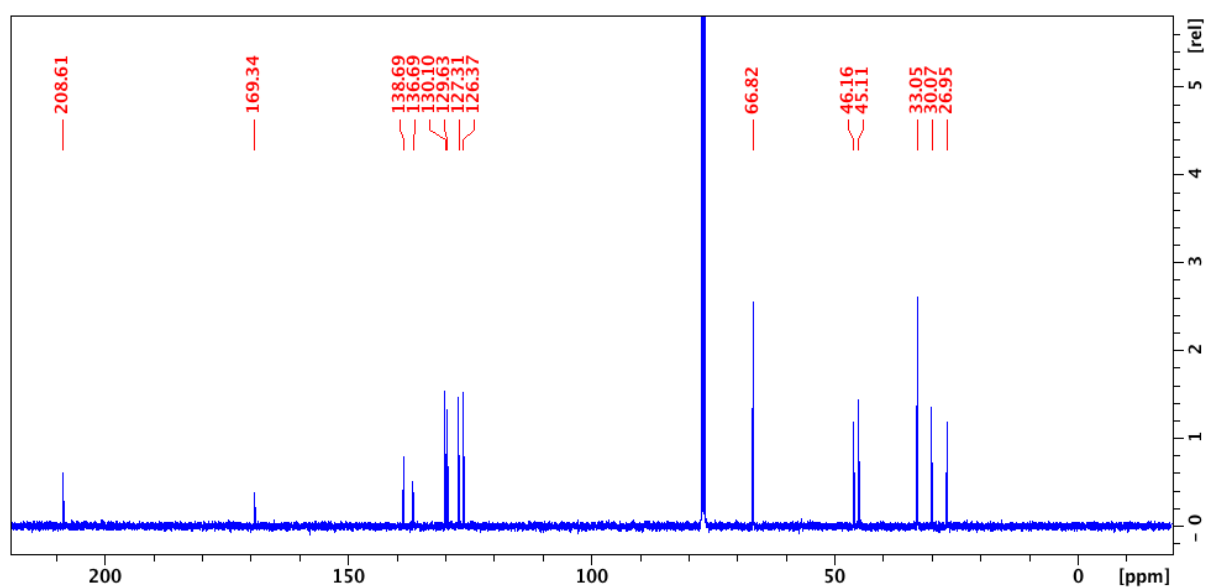


Figure S43: $^{13}C$ {$^1H$} NMR spectrum of compound *2ra* in CDCl$_3$ at 298 K.
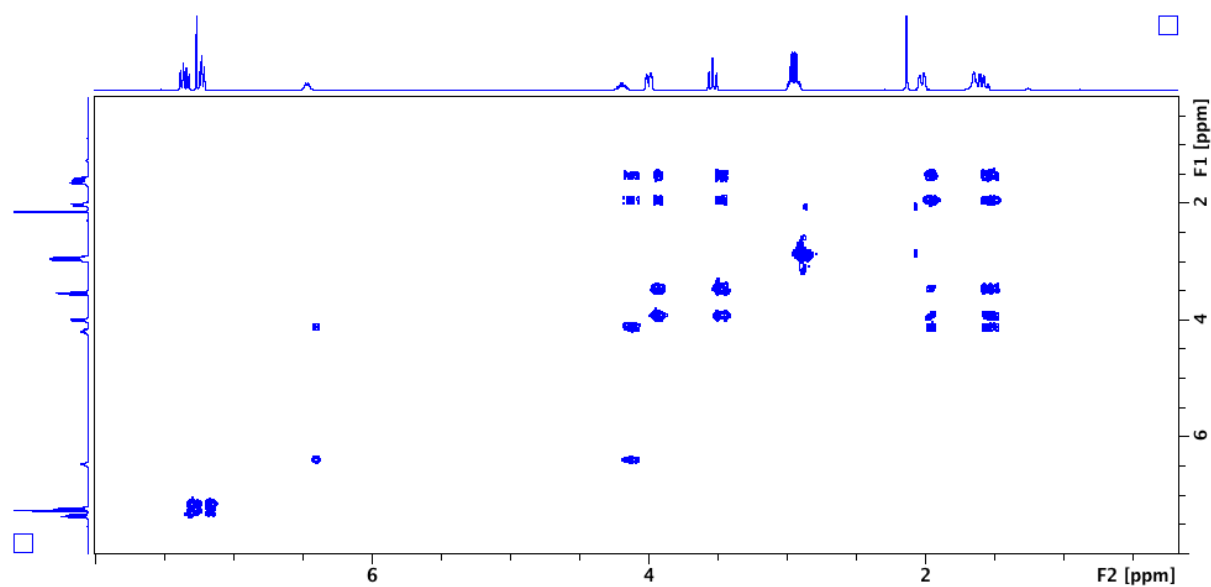
*Figure S44: COSY NMR spectrum of compound **2ra** in CDCl₃ at 298 K.*
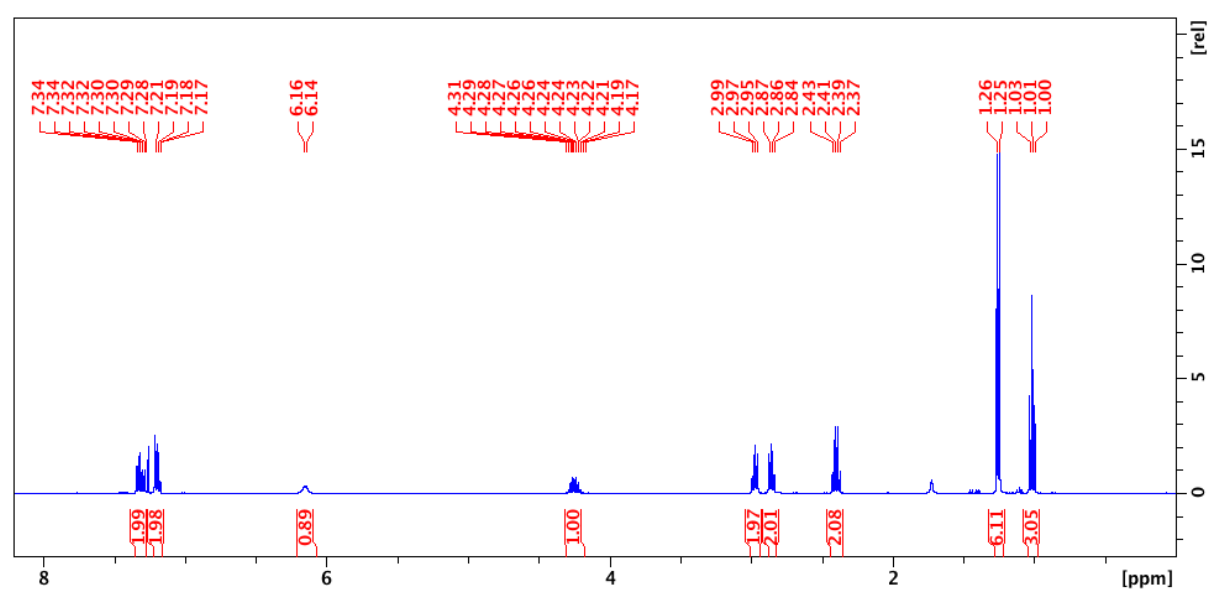


*Figure S45: ¹H NMR spectrum of compound **2ac** in CDCl₃ at 298 K.*
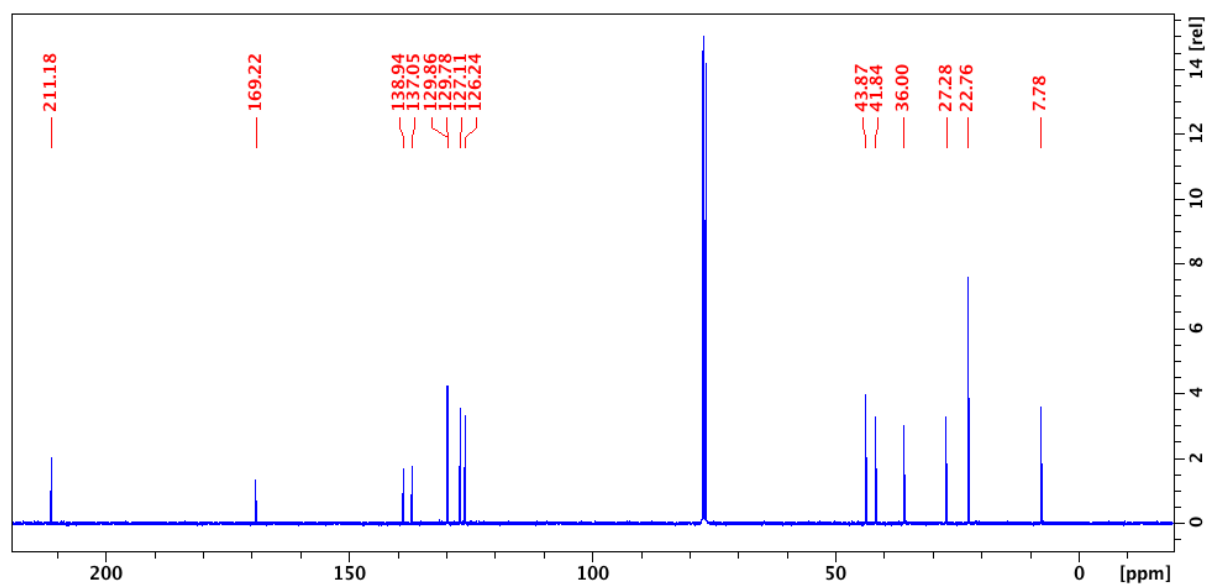
*Figure S46: $^{13}C$ {$^1H$} NMR spectrum of compound **2ac** in CDCl$_3$ at 298 K.*
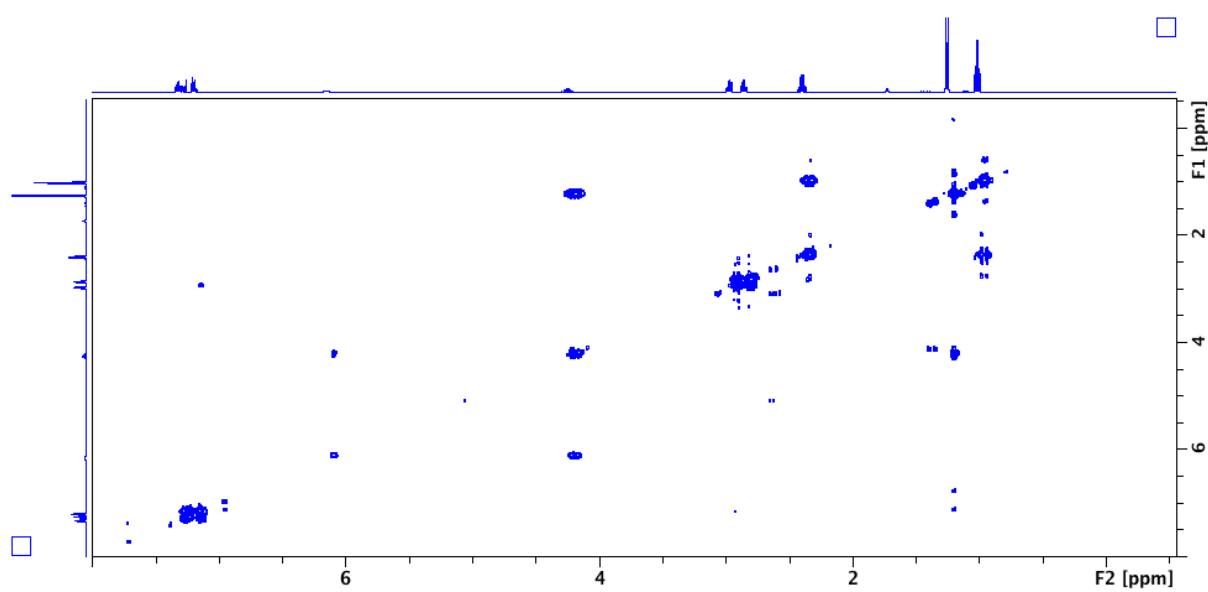


*Figure S47: COSY NMR spectrum of compound **2ac** in CDCl$_3$ at 298 K.*

*Figure S48: $^1$H NMR spectrum of compound **3oa** in CDCl$_3$ at 298 K.*



*Figure S49: Zoomed $^1$H NMR spectrum of compound **3oa** in CDCl$_3$ at 298 K to see broad signals exhibited by the CH$_2$ protons of the ring system.*
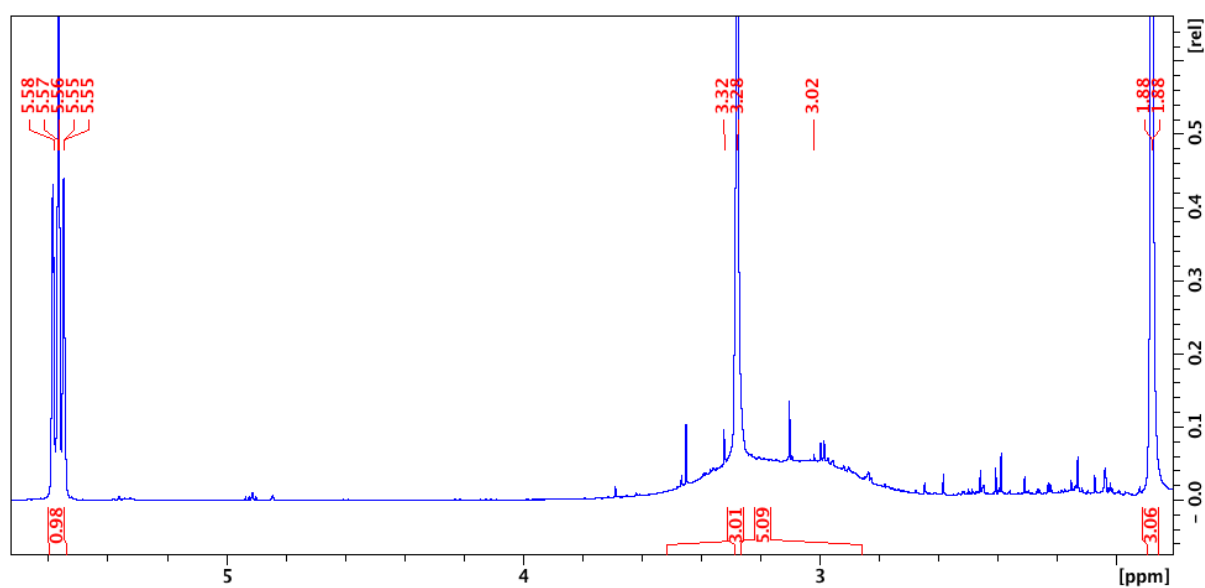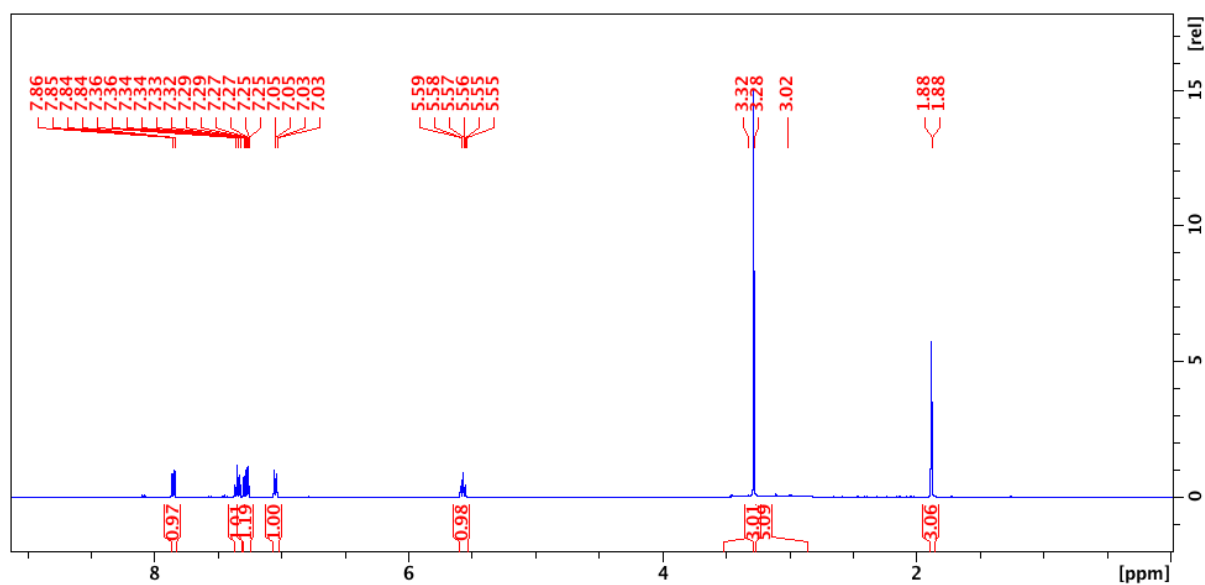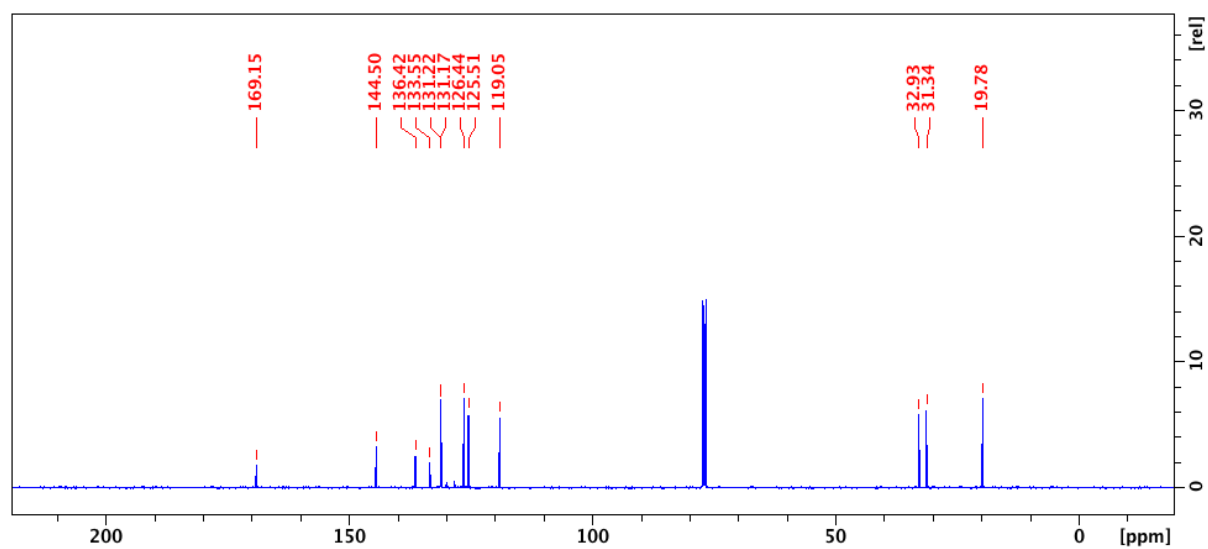
Figure S50: $^{13}C$ {$^1H$} NMR spectrum of compound **3oa** in CDCl$_3$ at 298 K.
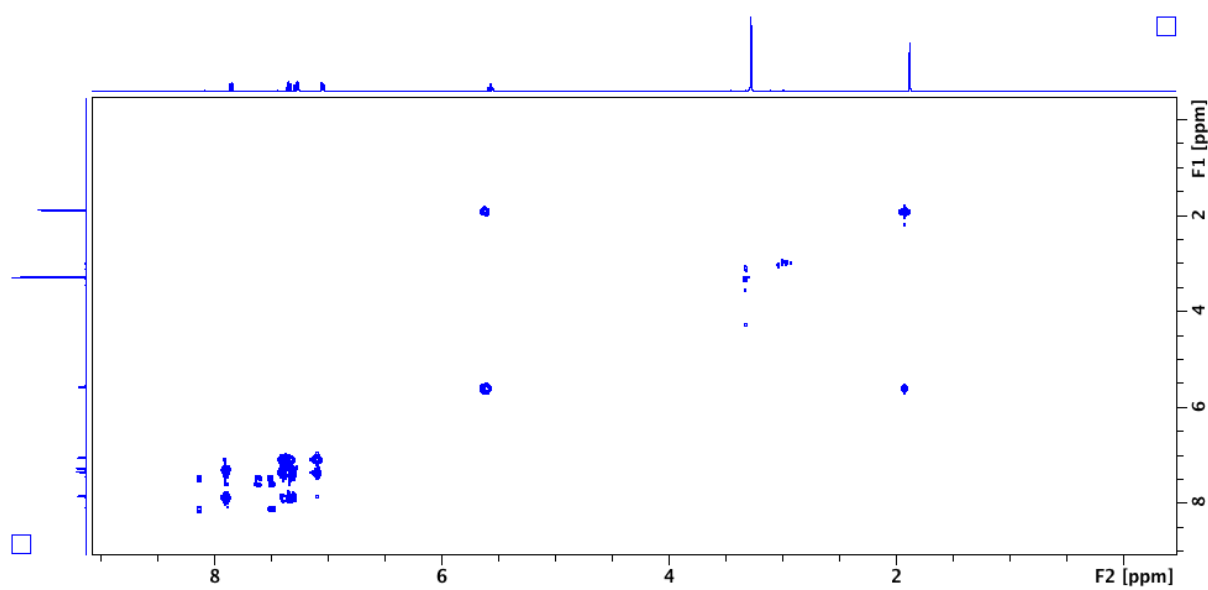


Figure S51: COSY NMR spectrum of compound **3oa** in CDCl$_3$ at 298 K.
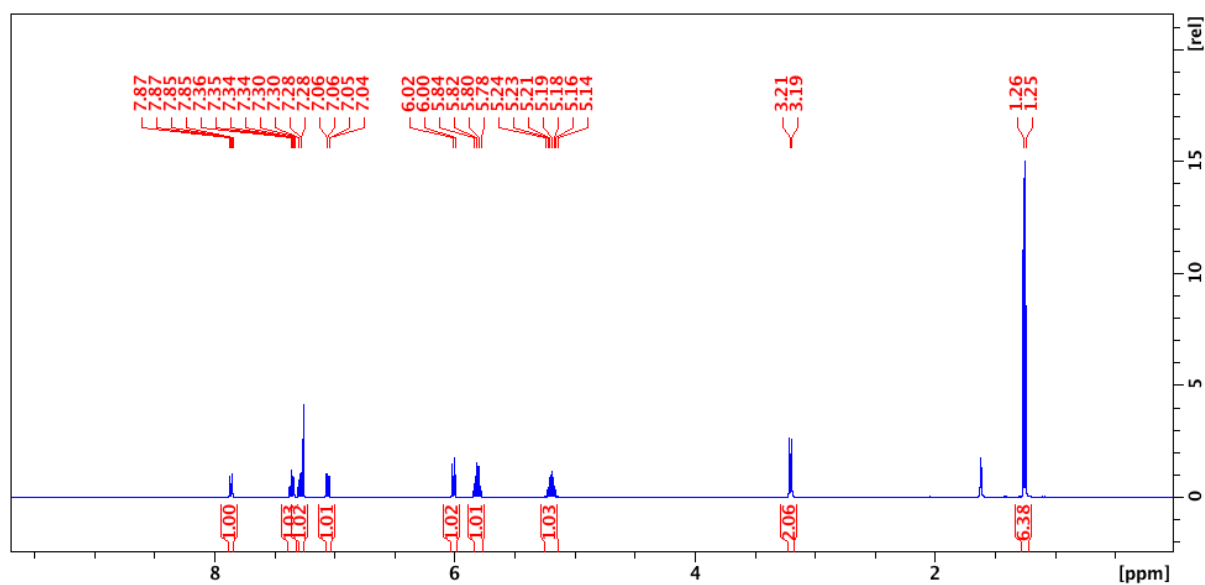
Figure S52: $^1H$ NMR spectrum of compound **3ab** in CDCl$_3$ at 298 K.
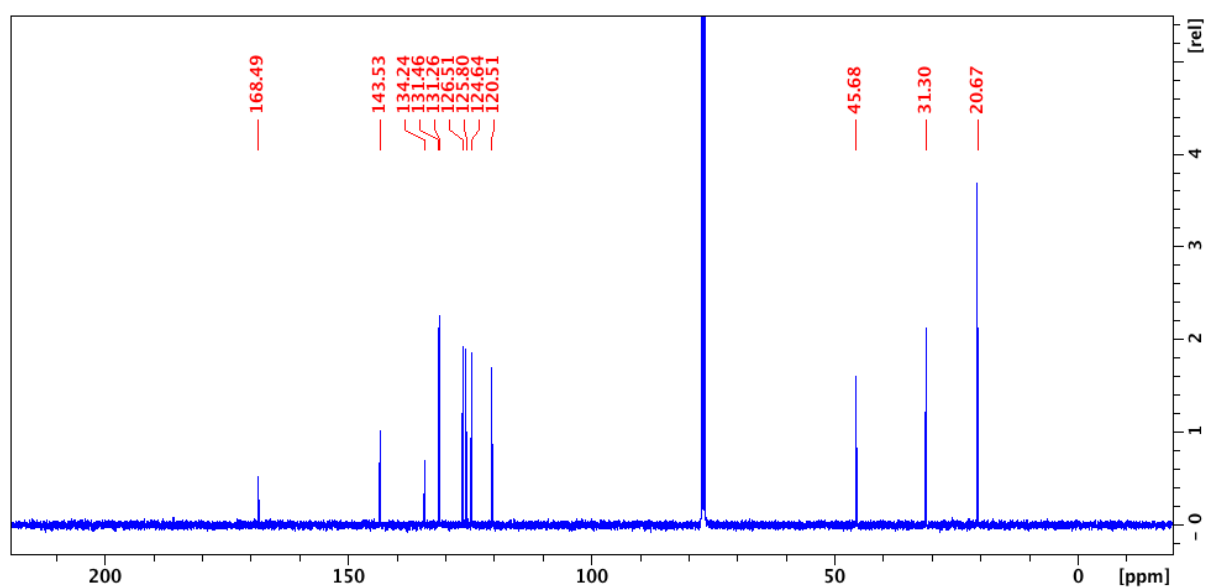


Figure S53: $^{13}C$ {$^1H$} NMR spectrum of compound **3ab** in CDCl$_3$ at 298 K.
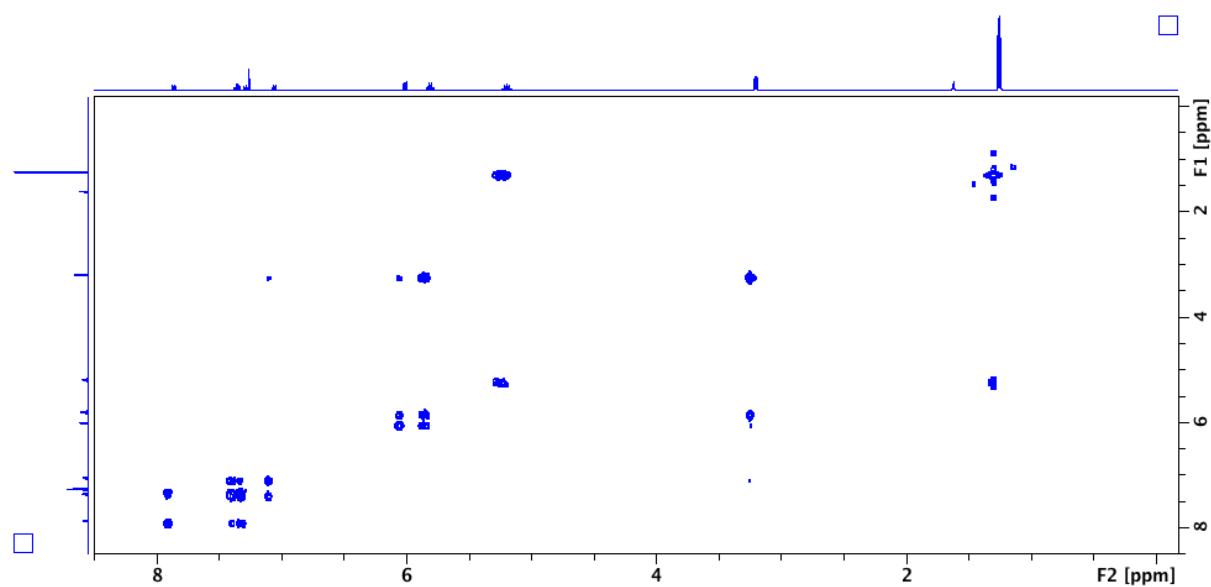
*Figure S54: COSY NMR spectrum of compound **3ab** in CDCl₃ at 298 K.*
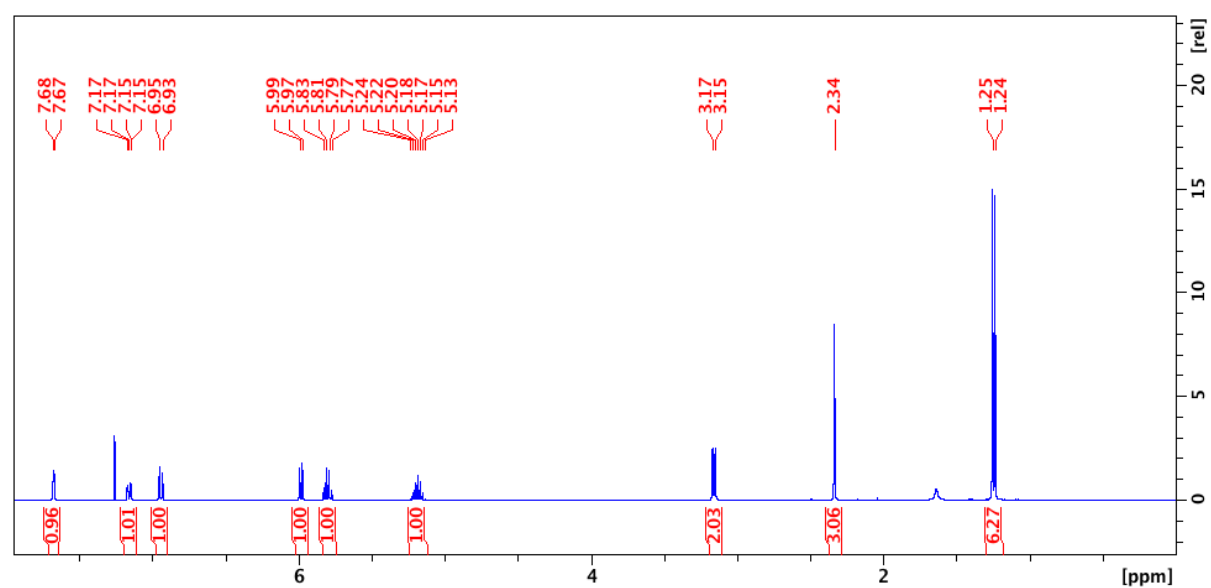


*Figure S55: ¹H NMR spectrum of compound **3cb** in CDCl₃ at 298 K.*
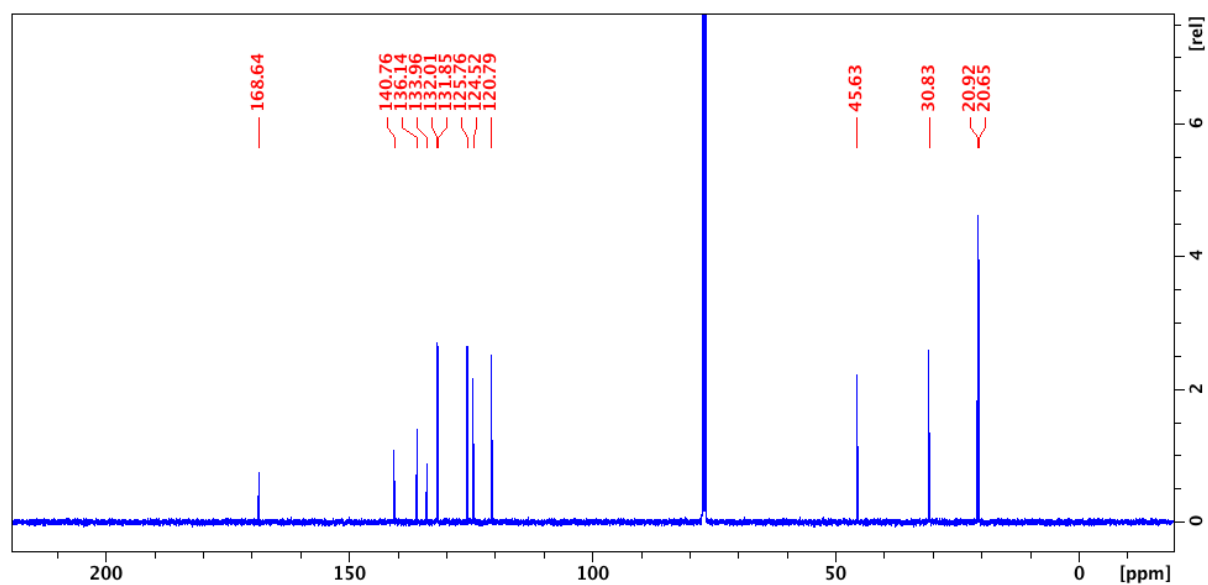
Figure S56: $^{13}C$ {$^{1}H$} NMR spectrum of compound **3cb** in CDCl$_3$ at 298 K.
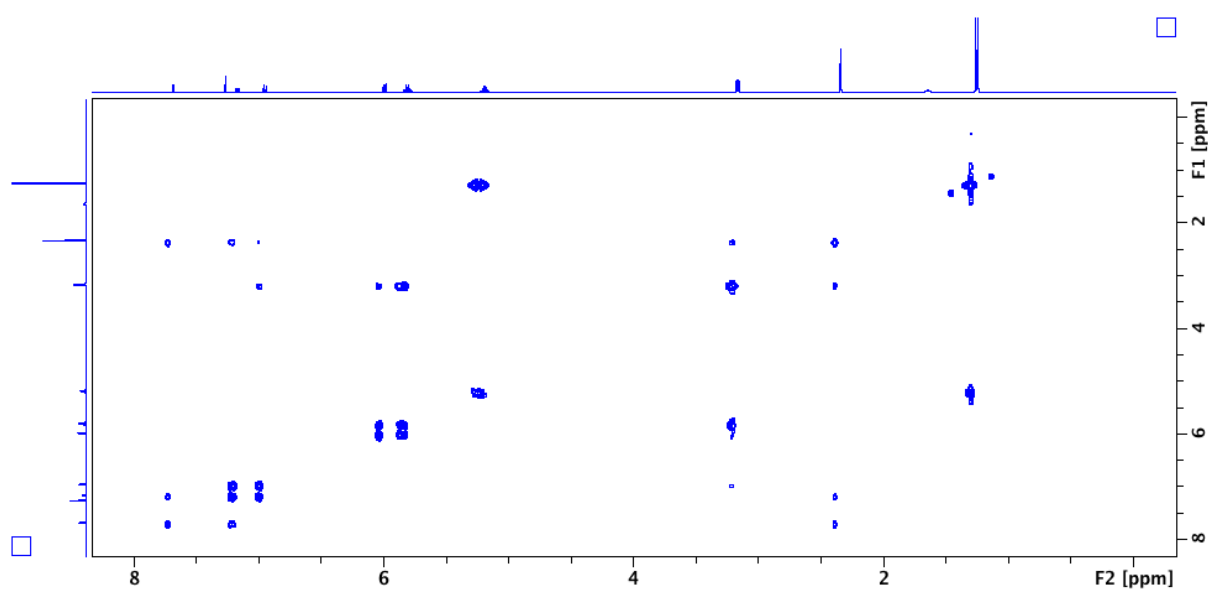


Figure S57: COSY NMR spectrum of compound **3cb** in CDCl$_3$ at 298 K.
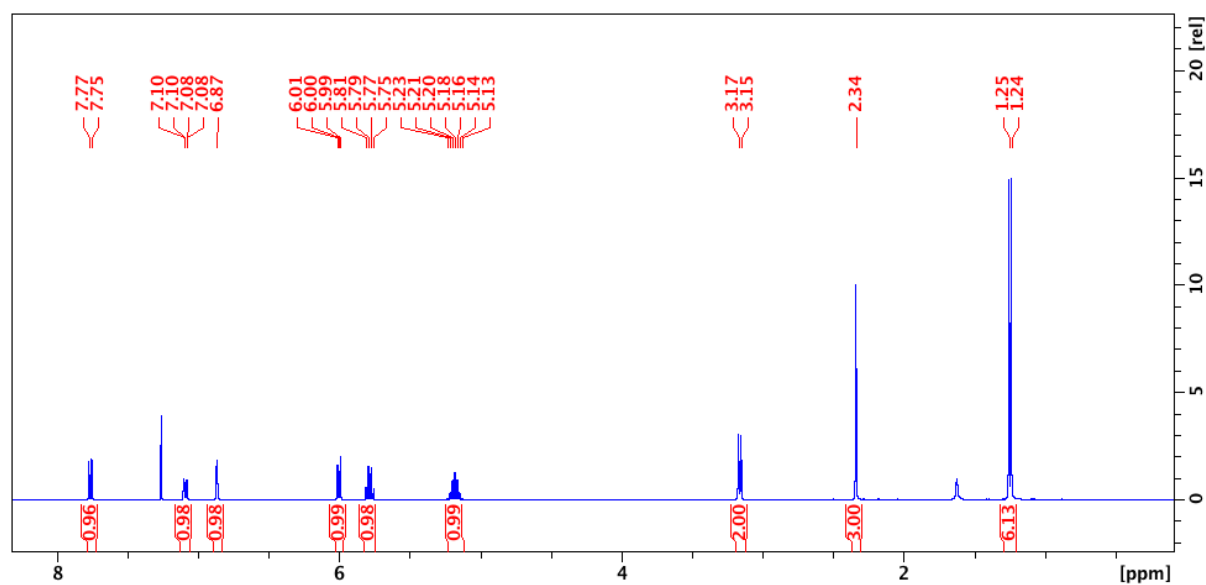
Figure S58: $^1H$ NMR spectrum of compound **3db** in CDCl$_3$ at 298 K.
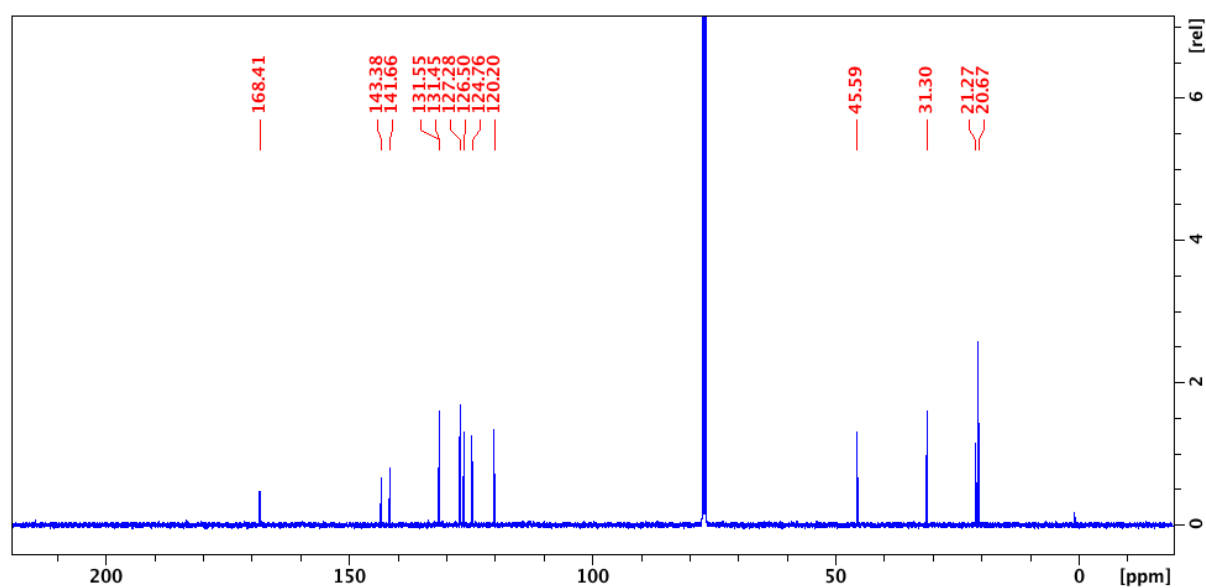


Figure S59: $^{13}C$ {$^1H$} NMR spectrum of compound **3db** in CDCl$_3$ at 298 K.
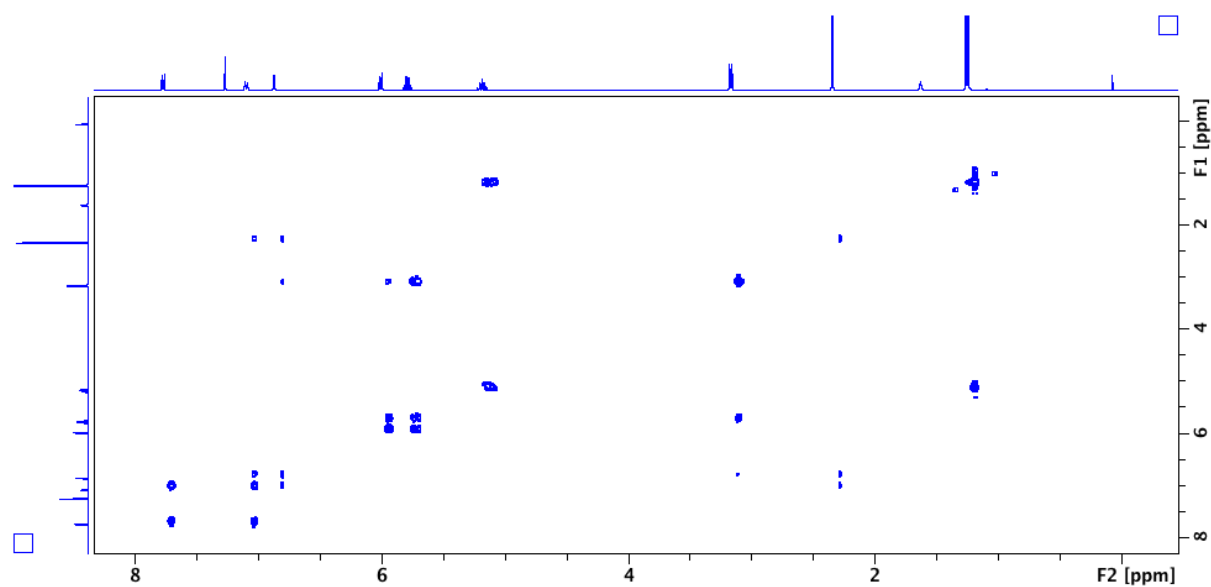
*Figure S60: COSY NMR spectrum of compound **3db** in CDCl₃ at 298 K.*
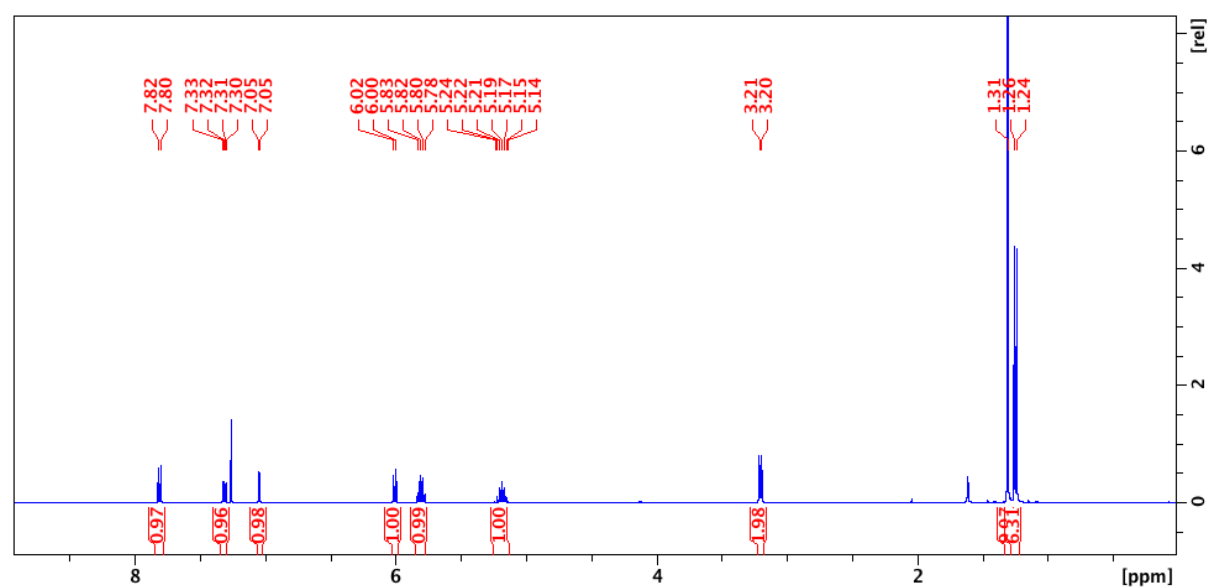


*Figure S61: ¹H NMR spectrum of compound **3eb** in CDCl₃ at 298 K.*
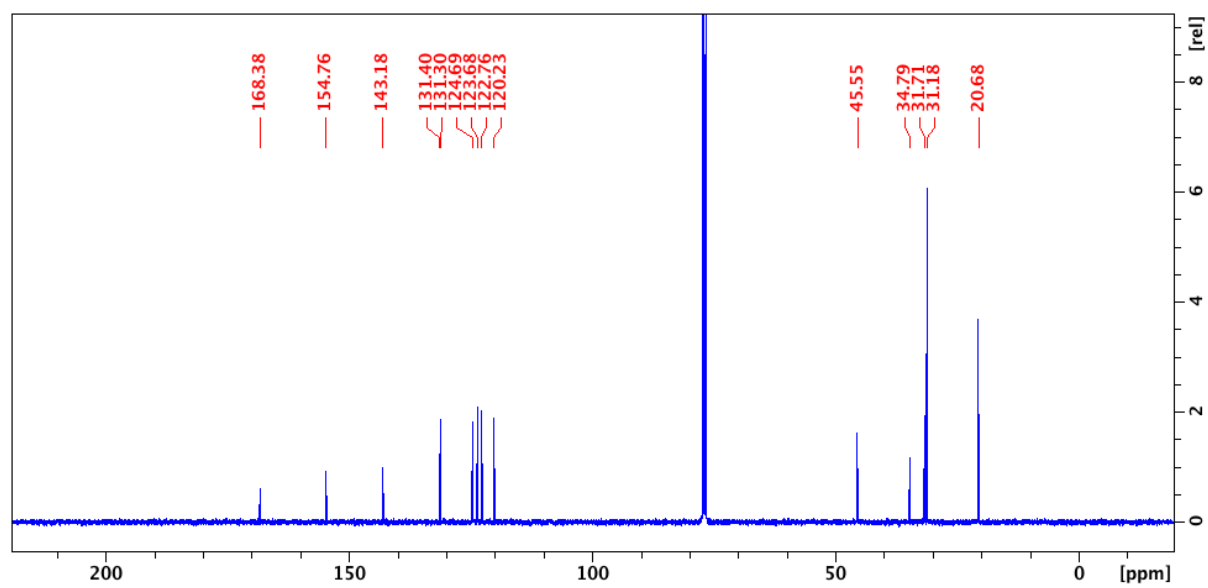
*Figure S62: $^{13}C$ {$^1H$} NMR spectrum of compound **3eb** in CDCl$_3$ at 298 K.*
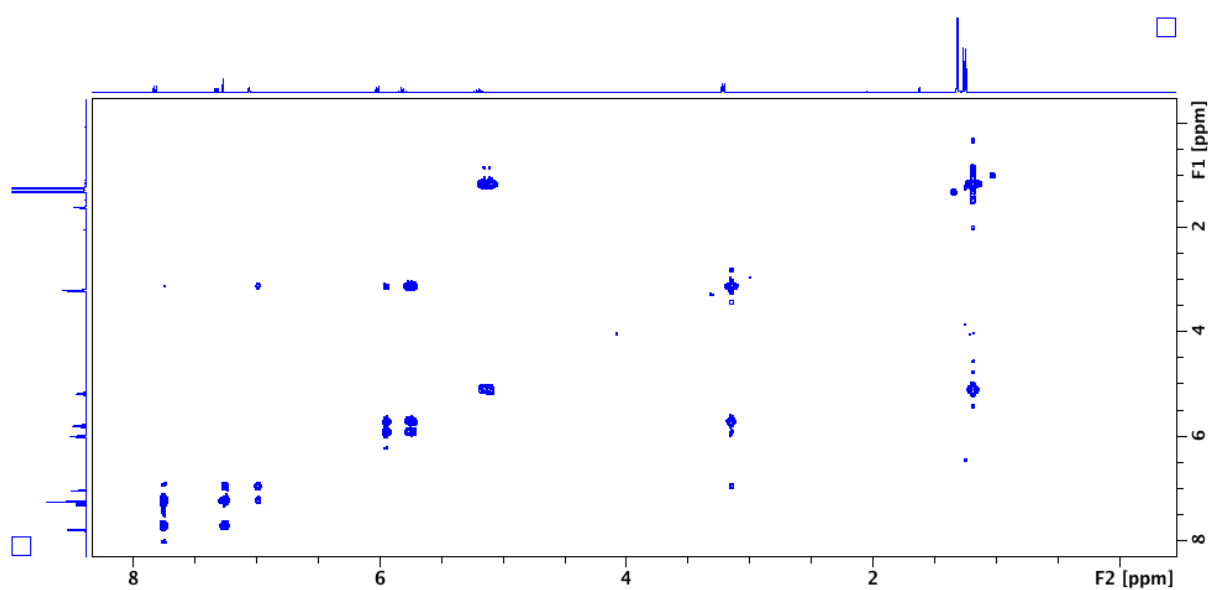


*Figure S63: COSY NMR spectrum of compound **3eb** in CDCl$_3$ at 298 K.*
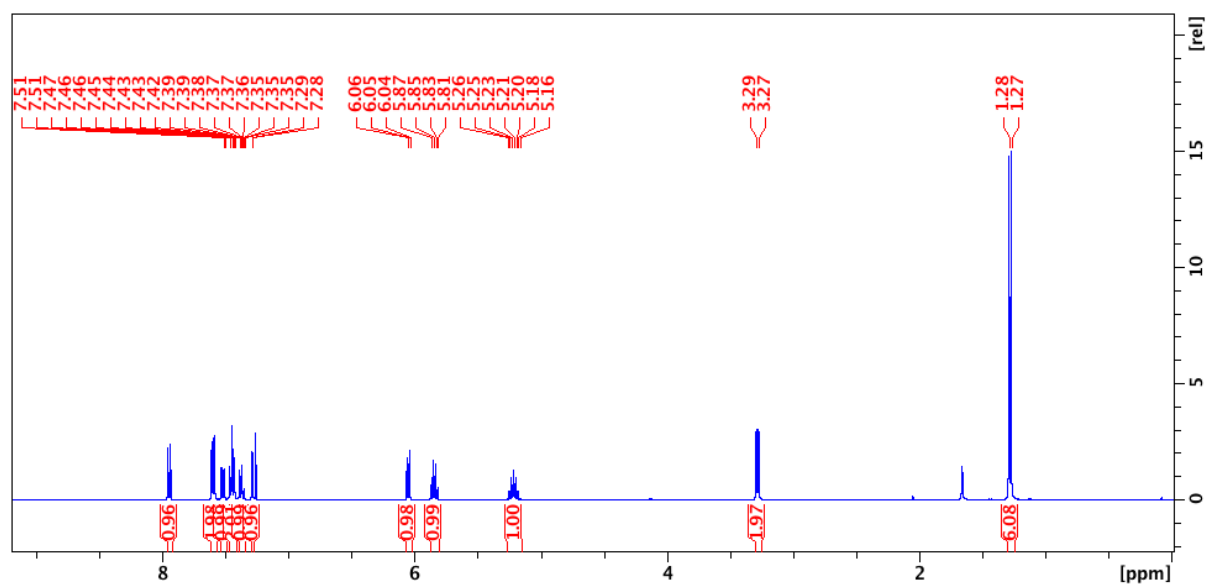
Figure S64: $^1$H NMR spectrum of compound **3fb** in CDCl$_3$ at 298 K.
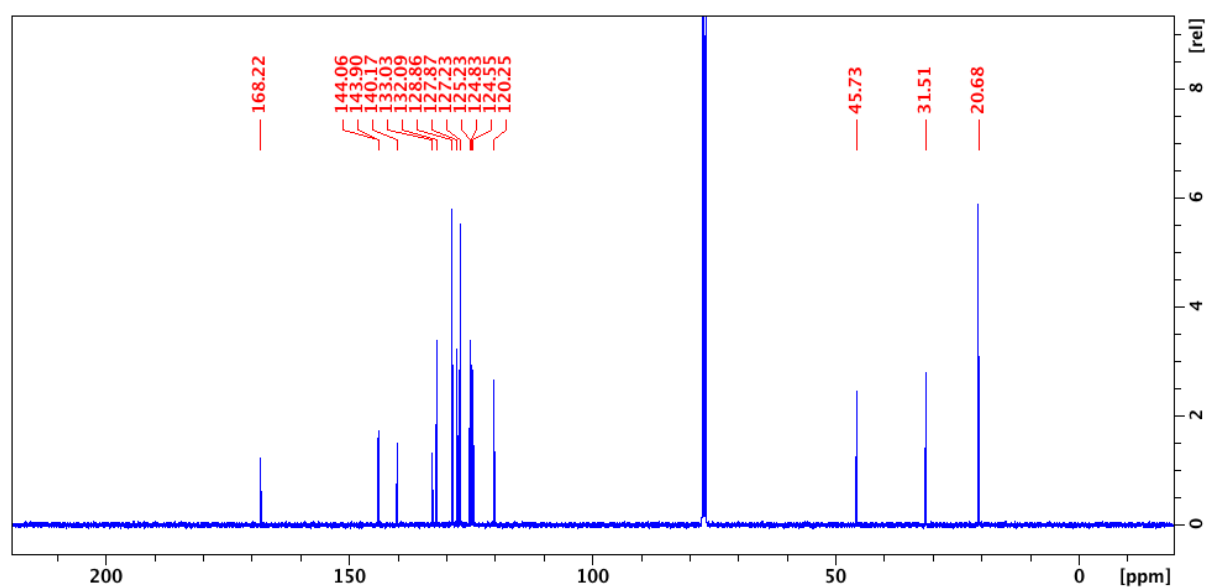


Figure S65: $^{13}$C {$^1$H} NMR spectrum of compound **3fb** in CDCl$_3$ at 298 K.
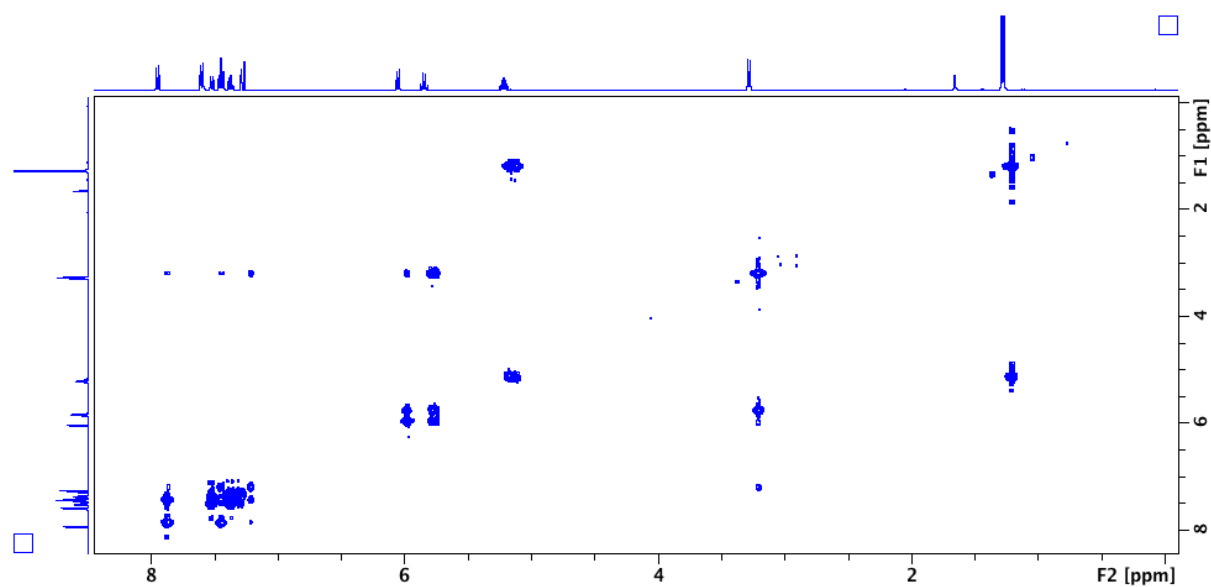
*Figure S66: COSY NMR spectrum of compound **3fb** in CDCl$_3$ at 298 K.*
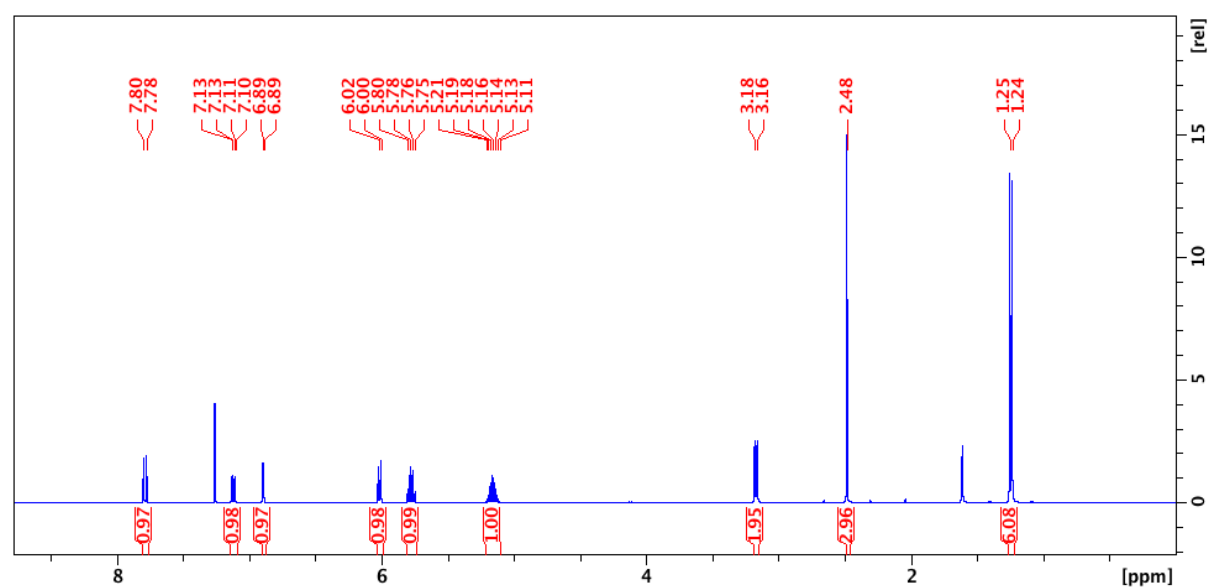


*Figure S67: $^1$H NMR spectrum of compound **3hb** in CDCl$_3$ at 298 K.*
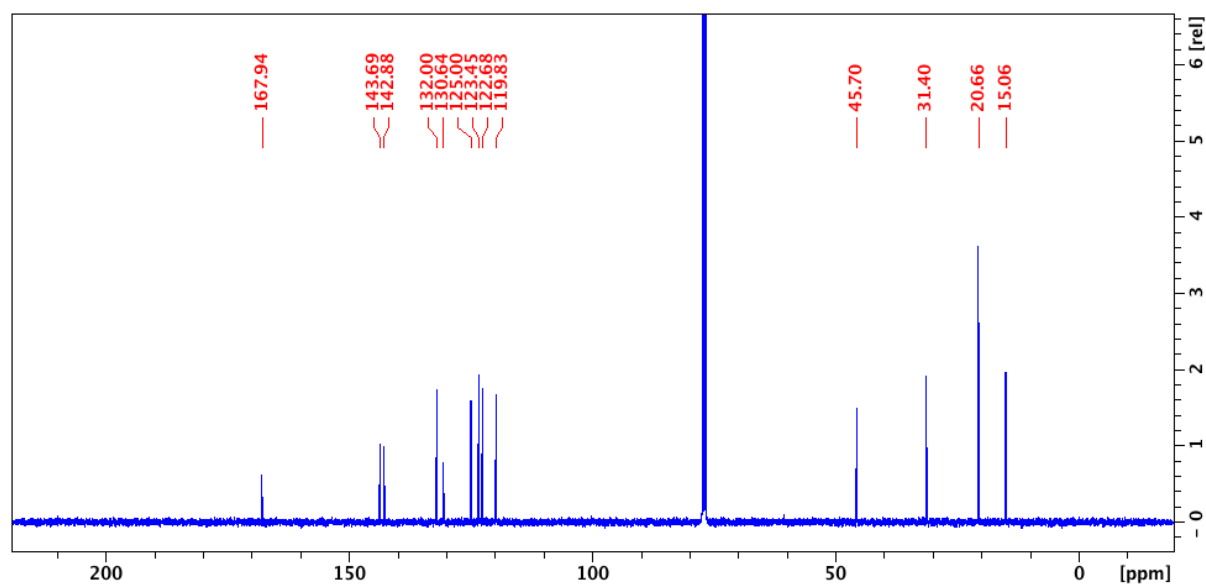
*Figure S68: $^{13}C$ $\{^1H\}$ NMR spectrum of compound **3hb** in CDCl₃ at 298 K.*
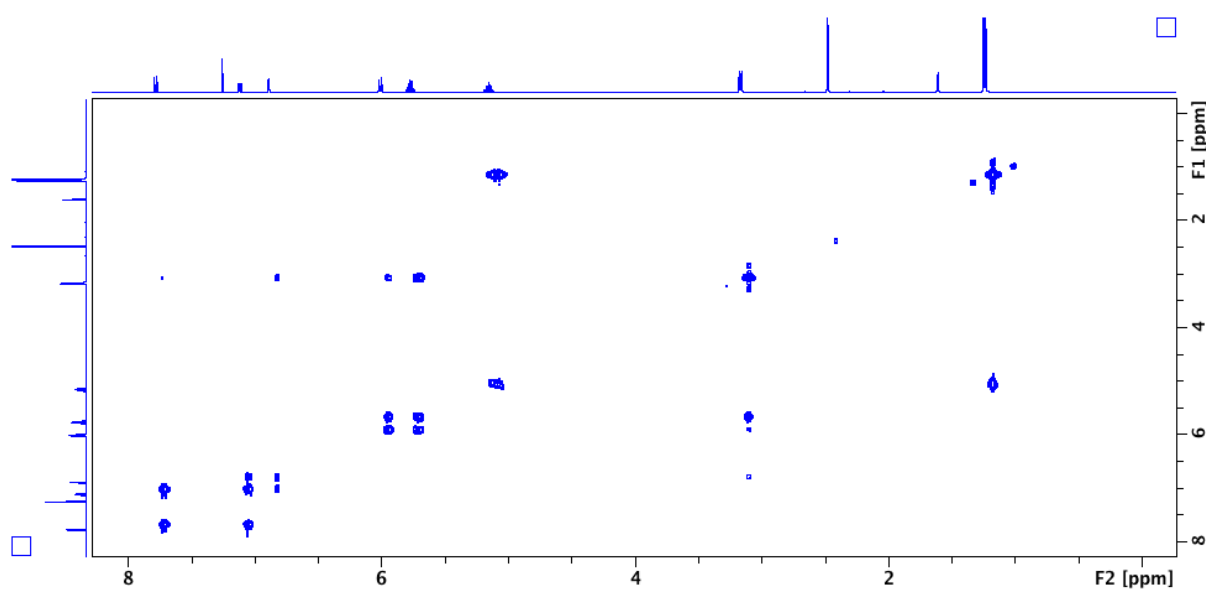


*Figure S69: COSY NMR spectrum of compound **3hb** in CDCl₃ at 298 K.*
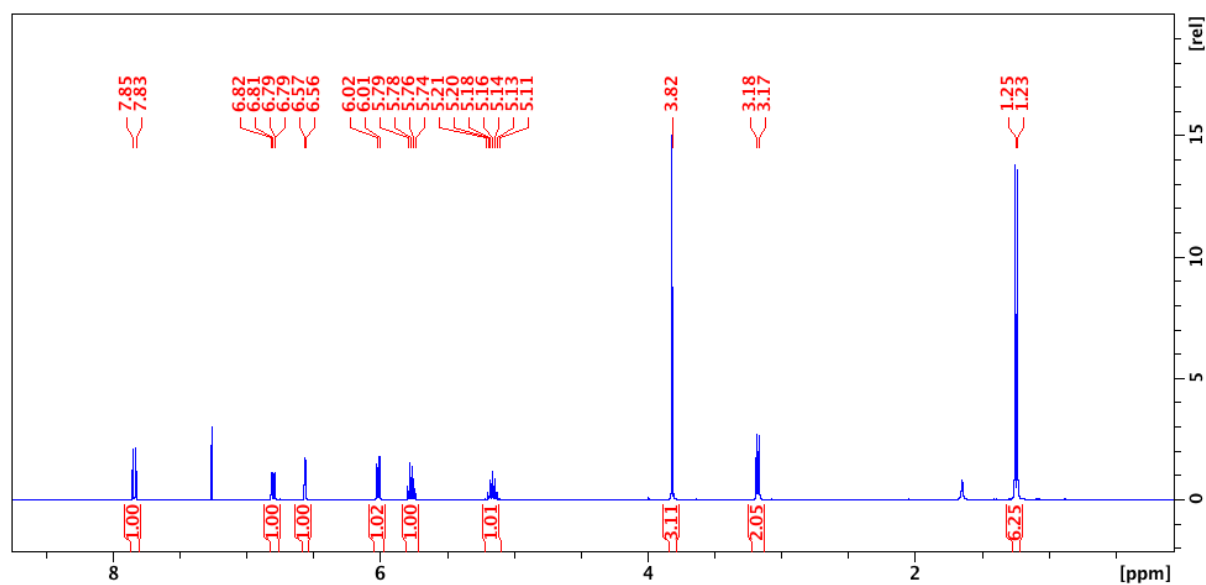
*Figure S70: $^1$H NMR spectrum of compound **3ib** in CDCl$_3$ at 298 K.*
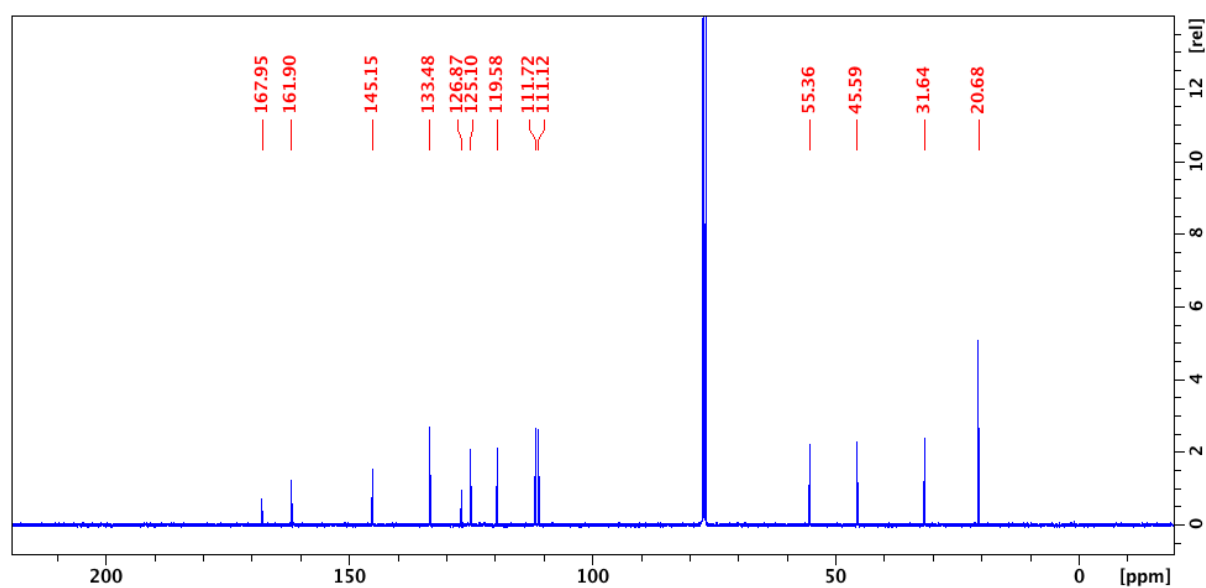


*Figure S71: $^{13}$C {$^1$H} NMR spectrum of compound **3ib** in CDCl$_3$ at 298 K.*
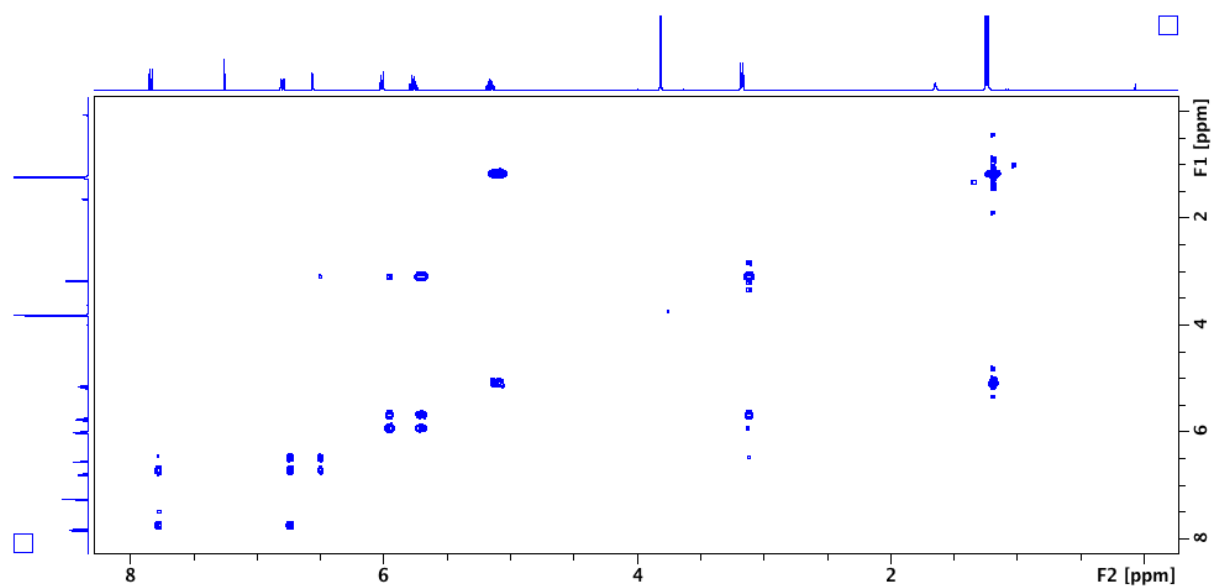
*Figure S72: COSY NMR spectrum of compound **3ib** in CDCl₃ at 298 K.*
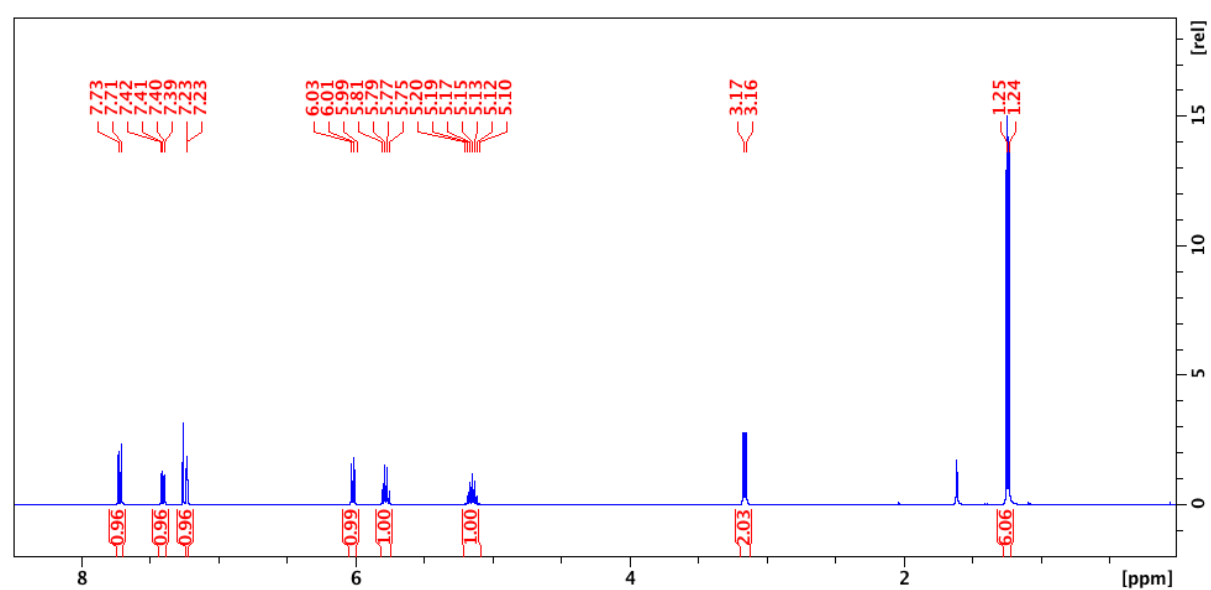


*Figure S73: ¹H NMR spectrum of compound **3jb** in CDCl₃ at 298 K.*
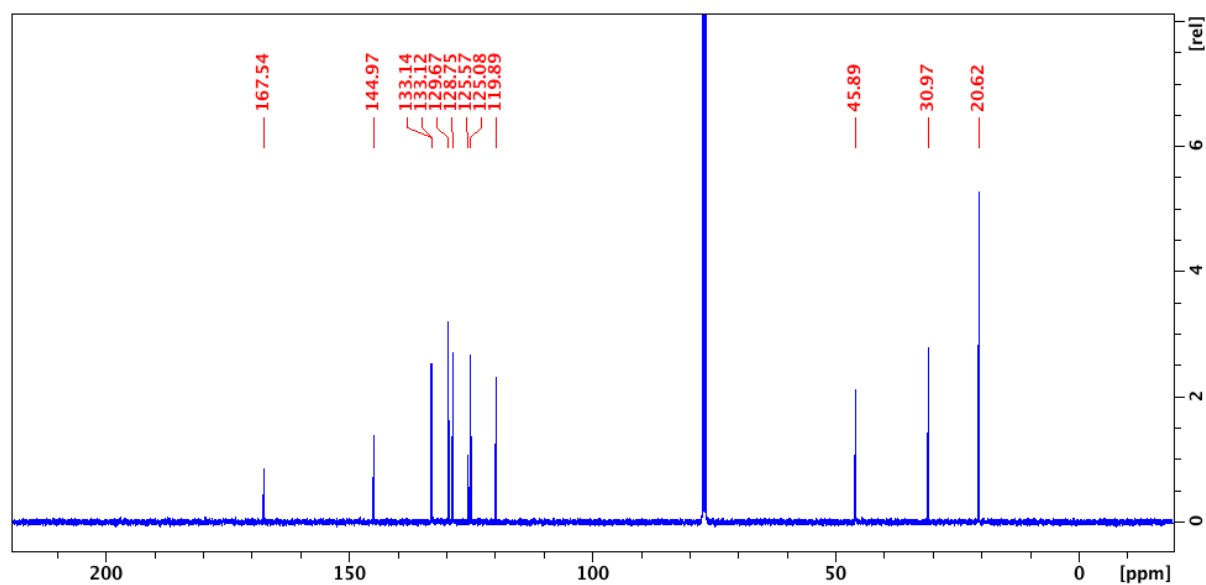
*Figure S74: $^{13}C$ {$^{1}H$} NMR spectrum of compound 3jb in CDCl$_3$ at 298 K.*
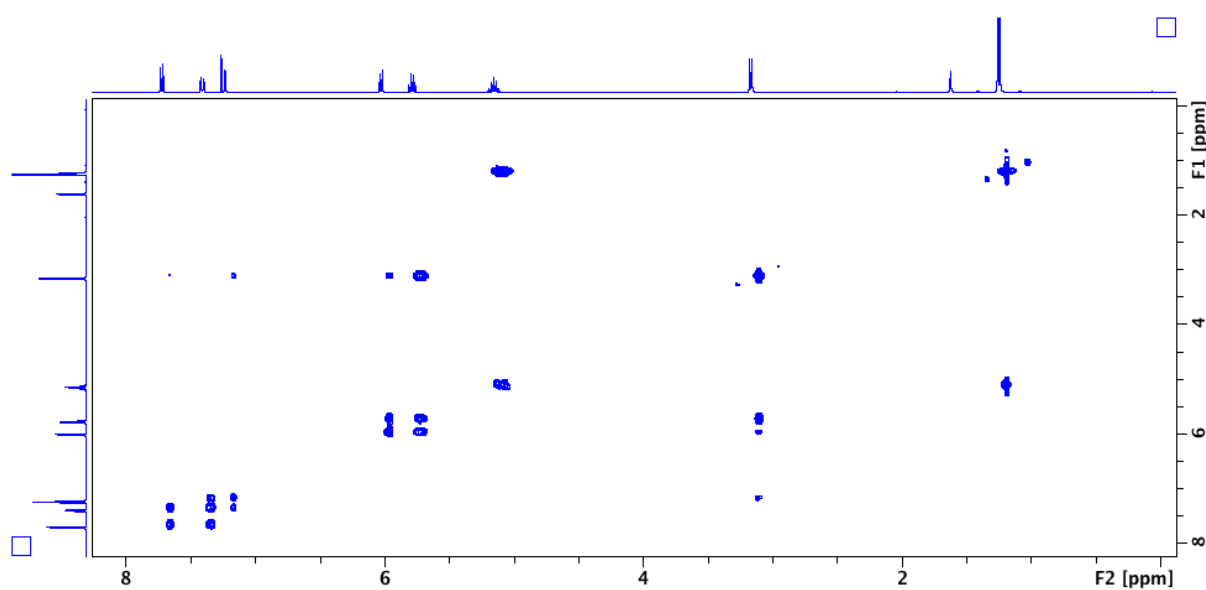


*Figure S75: COSY NMR spectrum of compound 3jb in CDCl$_3$ at 298 K.*
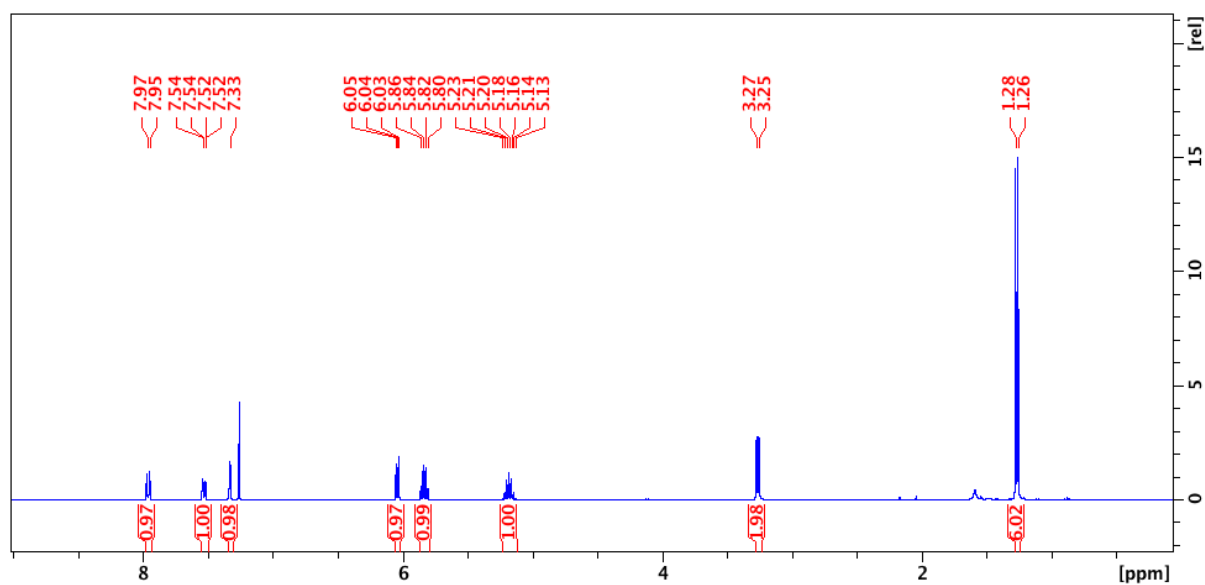
*Figure S76: $^1$H NMR spectrum of compound **3kb** in CDCl$_3$ at 298 K.*
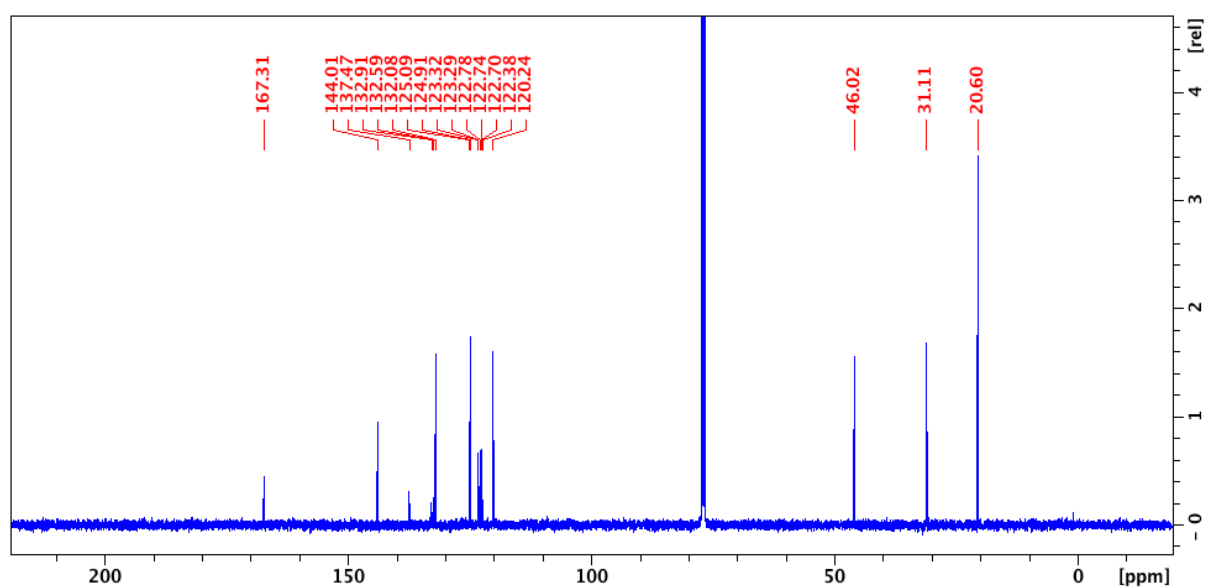


*Figure S77: $^{13}$C {$^1$H} NMR spectrum of compound **3kb** in CDCl$_3$ at 298 K.*
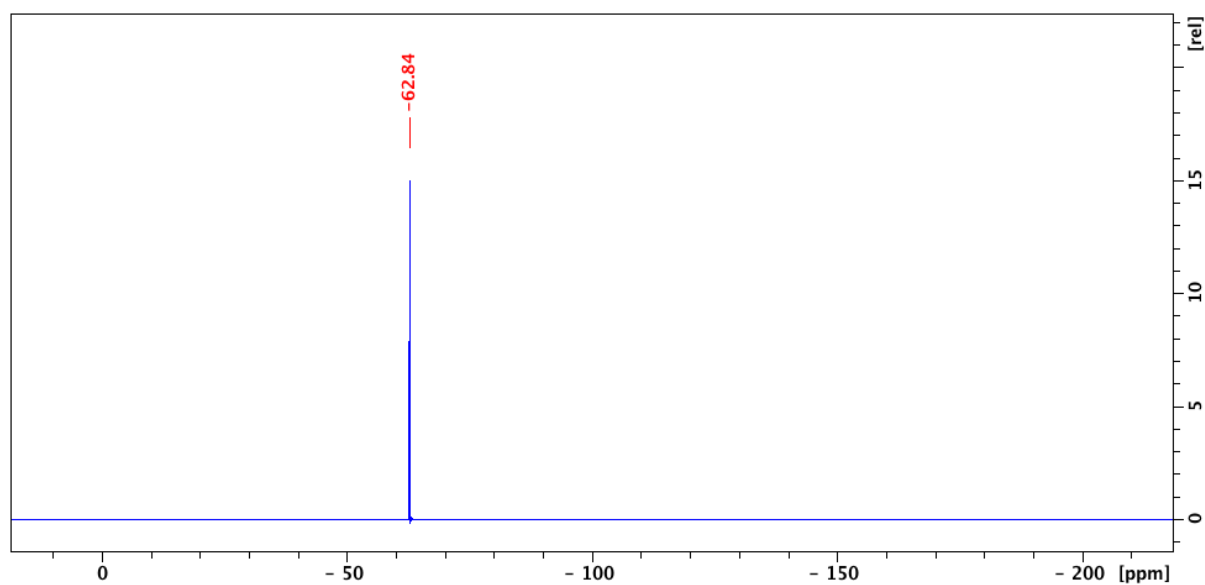
*Figure S78: $^{19}F$ {$^1H$} NMR spectrum of compound **3kb** in CDCl$_3$ at 298 K.*
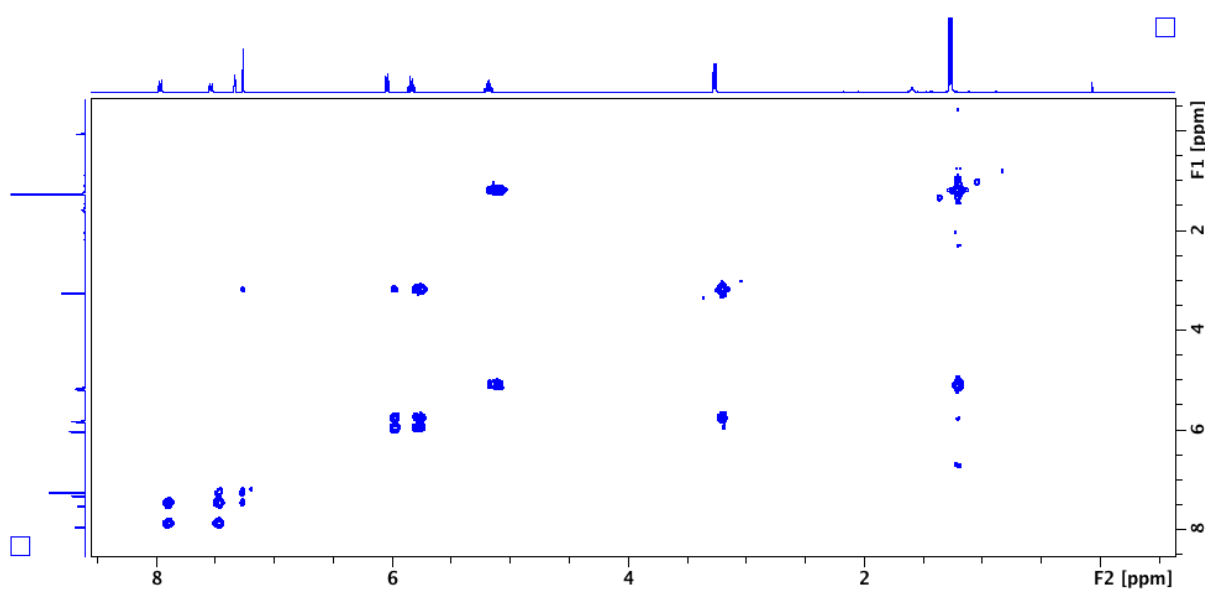


*Figure S79: COSY NMR spectrum of compound **3kb** in CDCl$_3$ at 298 K.*
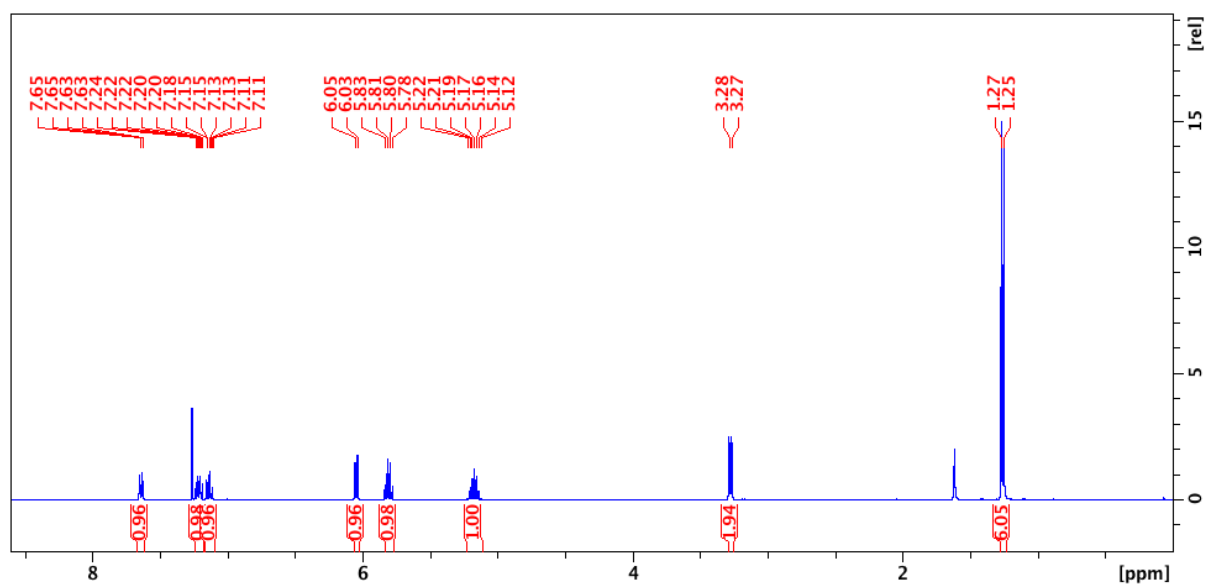
*Figure S80: $^1H$ NMR spectrum of compound **3lb** in CDCl$_3$ at 298 K.*
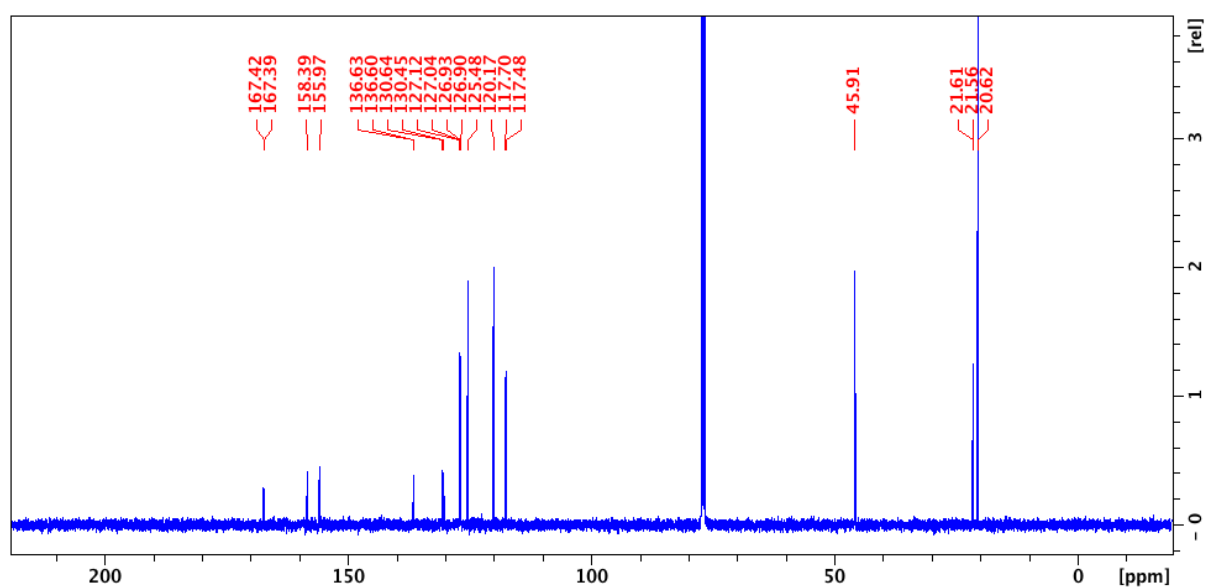


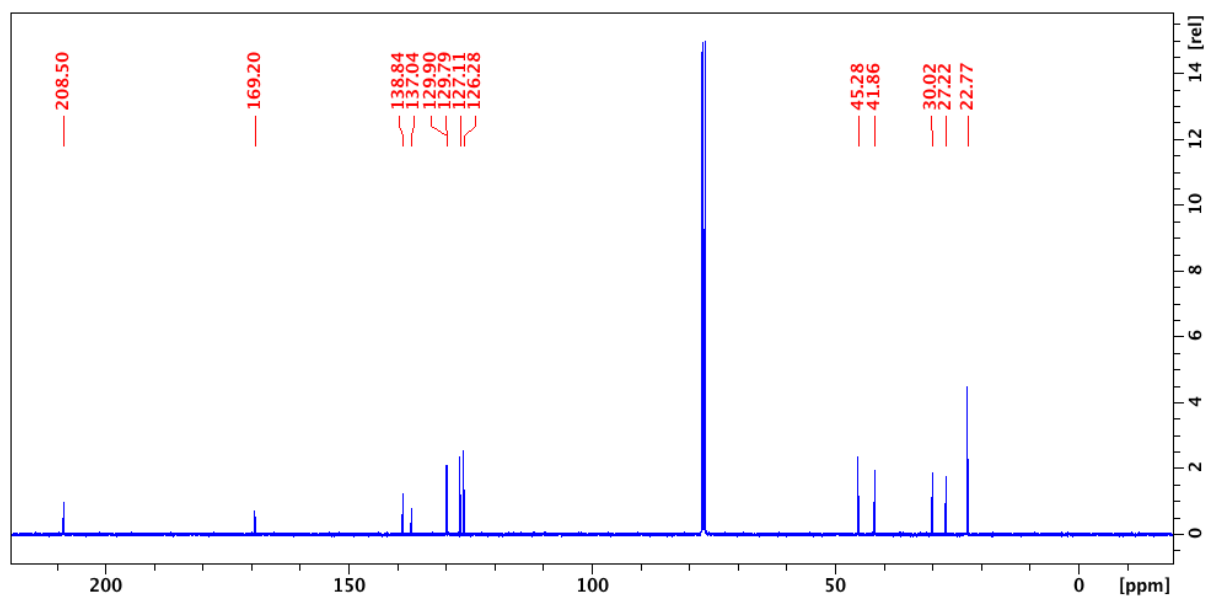*Figure S81: $^{13}C$ {$^1H$} NMR spectrum of compound **3lb** in CDCl$_3$ at 298 K.*
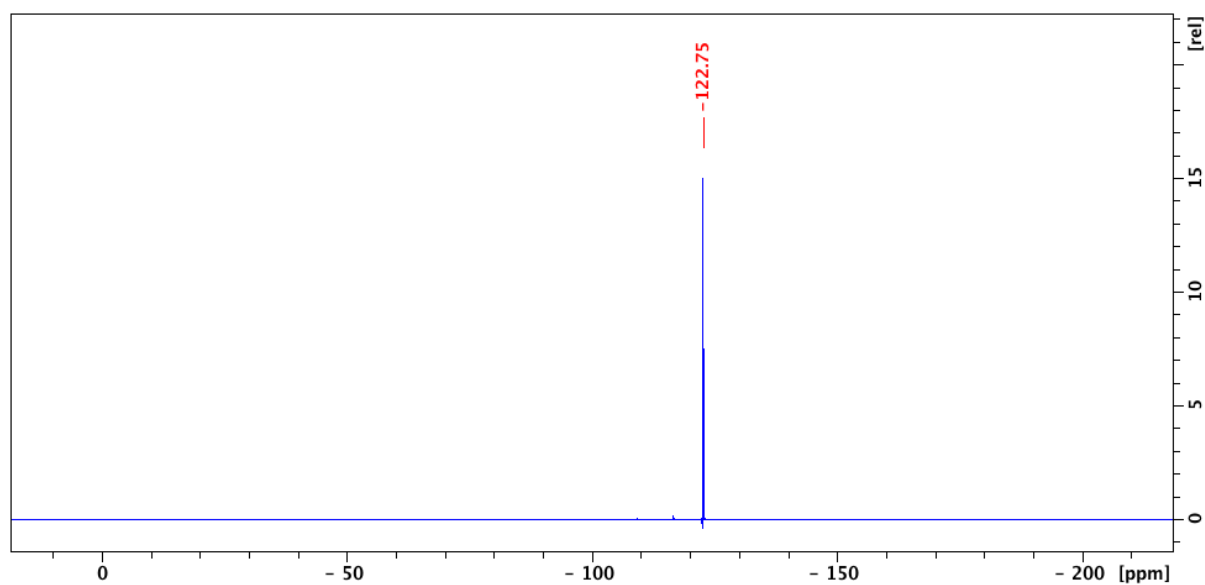
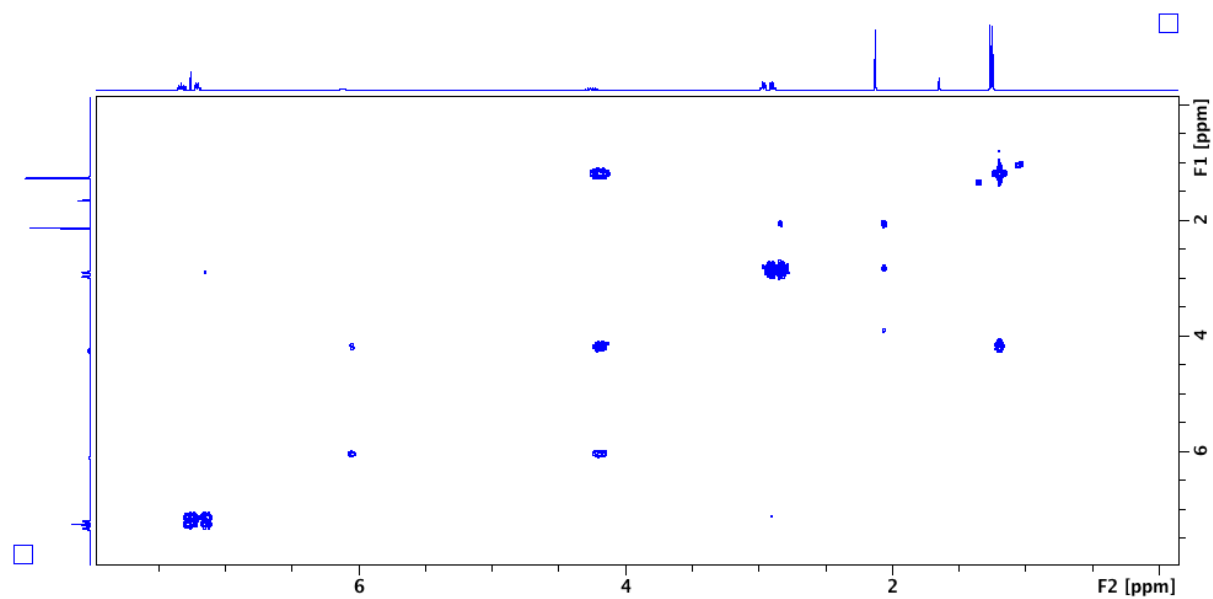*Figure S82: $^{19}F$ {$^1H$} NMR spectrum of compound **3lb** in CDCl$_3$ at 298 K.*
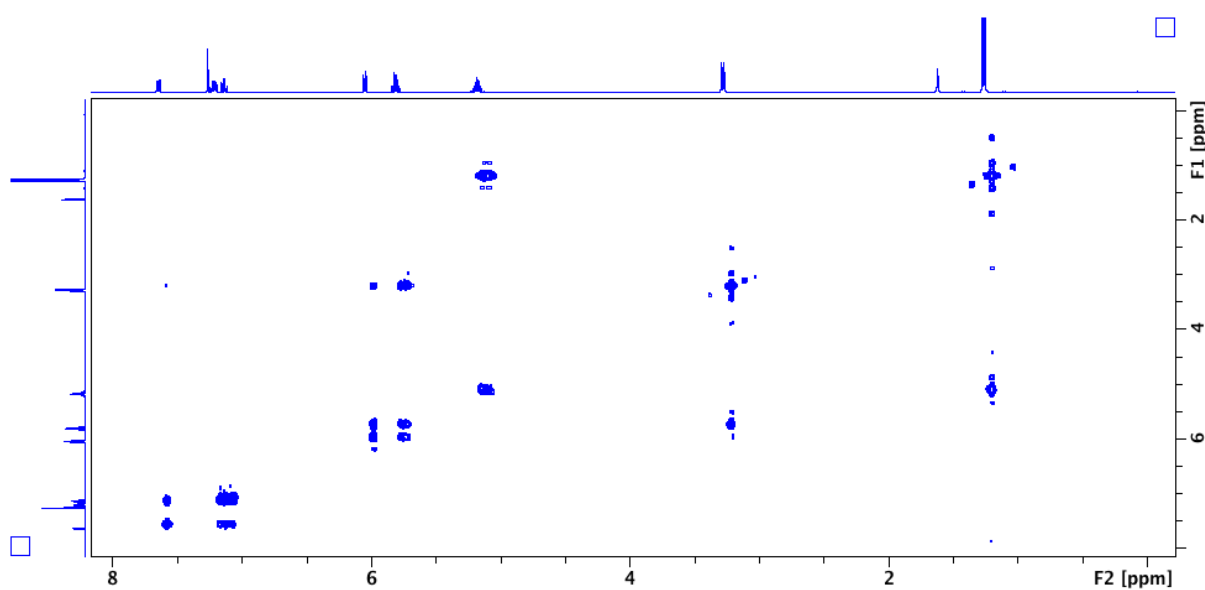


*Figure S83: COSY NMR spectrum of compound **3lb** in CDCl$_3$ at 298 K.*
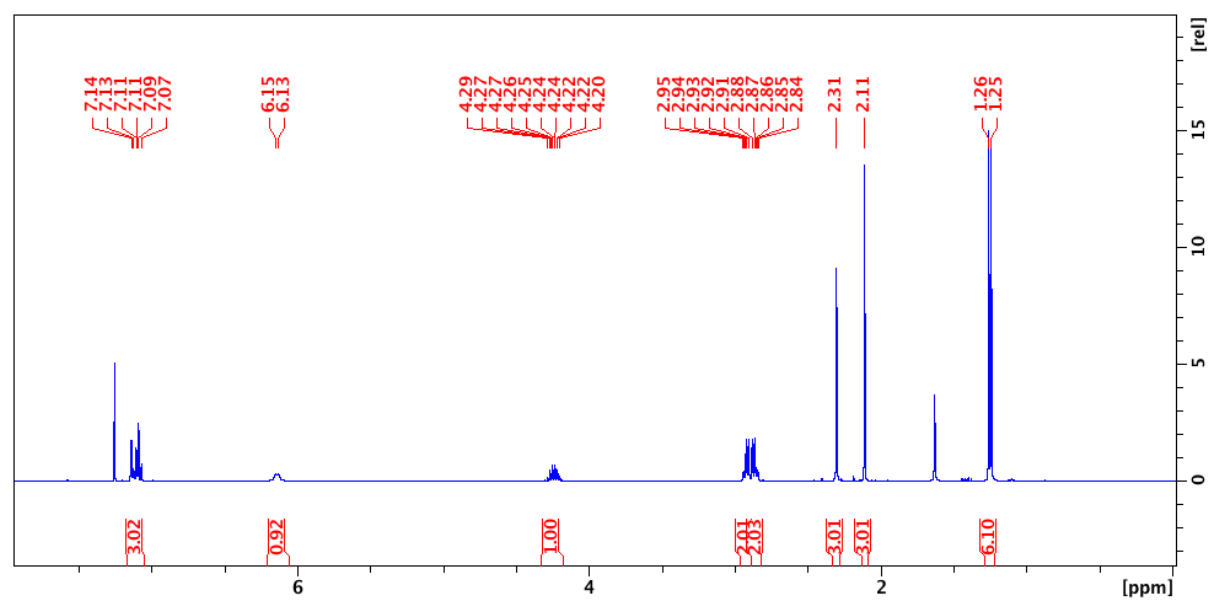
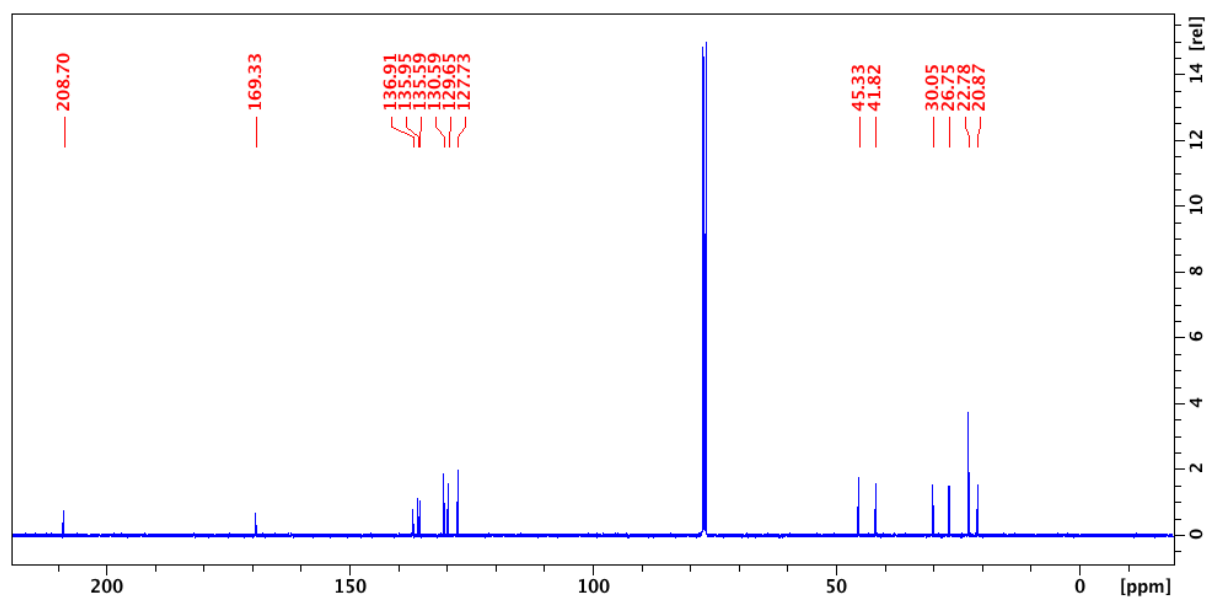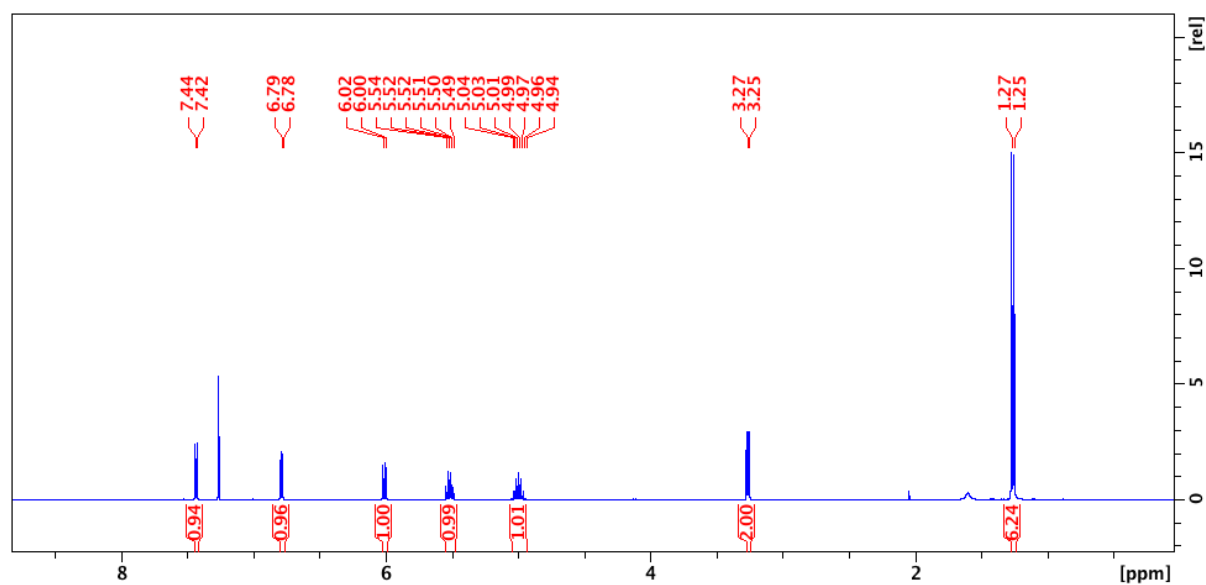Figure S84: $^1$H NMR spectrum of compound **3mb** in CDCl$_3$ at 298 K.
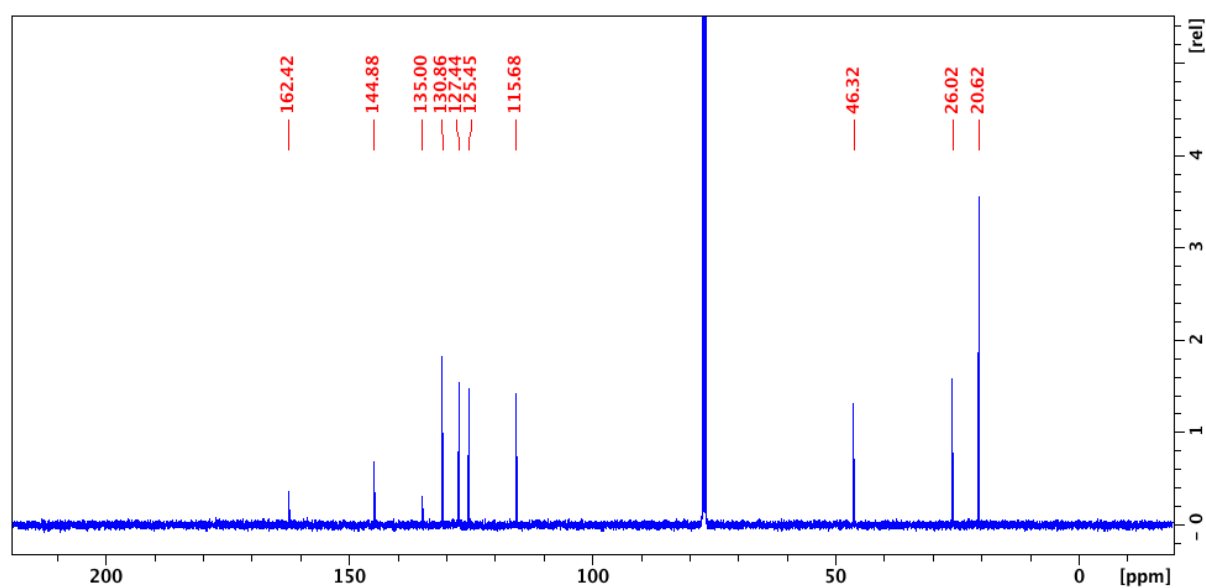


Figure S85: $^{13}$C {$^1$H} NMR spectrum of compound **3mb** in CDCl$_3$ at 298 K.
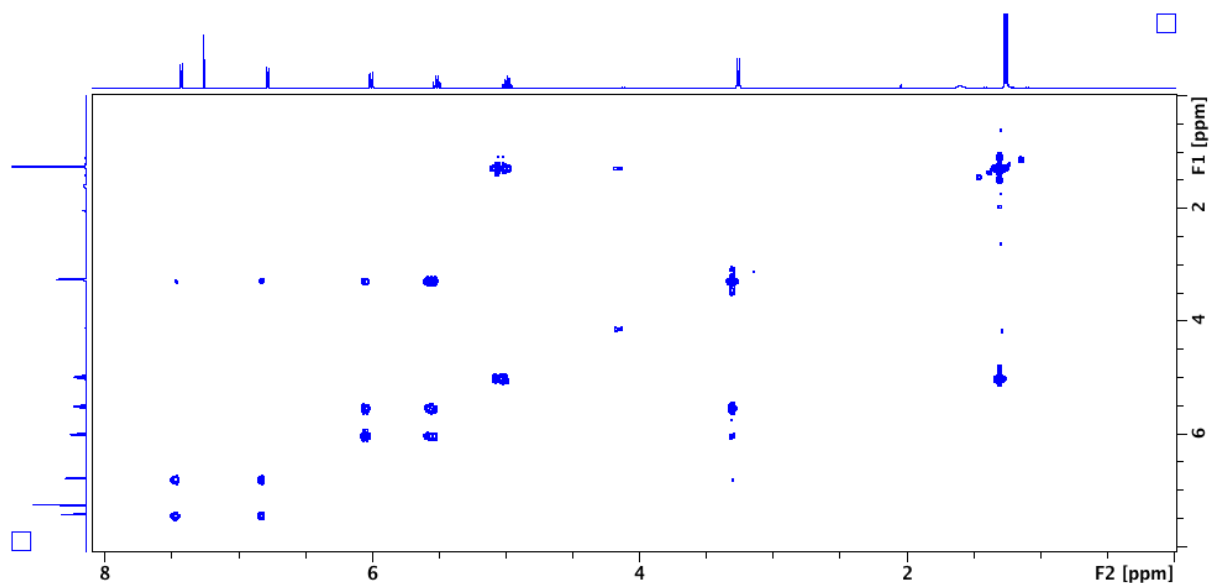
*Figure S86: COSY NMR spectrum of compound **3mb** in CDCl$_3$ at 298 K.*

## [8] $^1$H NMR Spectra for the Conversion of 2oa to 3oa:

The aliphatic ketone product obtained from the coupling of substrate **1o** with MVK was subjected to the standard reaction conditions in order to see if this compound (**2oa**) was an intermediate for the formation of **3oa** or if the product is formed by a different mechanistic pathway. Figure S87 shows the product mixture, which includes both the starting material, **2oa** and the azepinone product, **3oa**. It is observed that the yield of 38 % azepinone **3oa** is obtained.
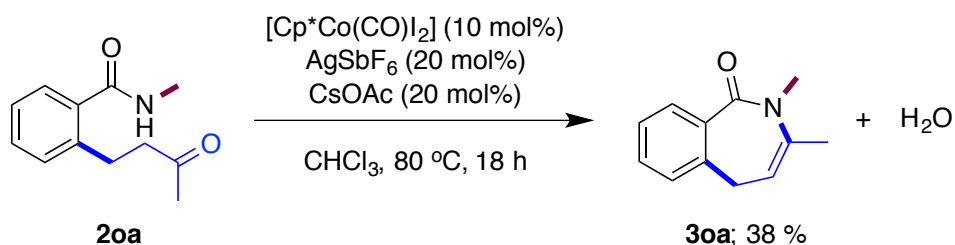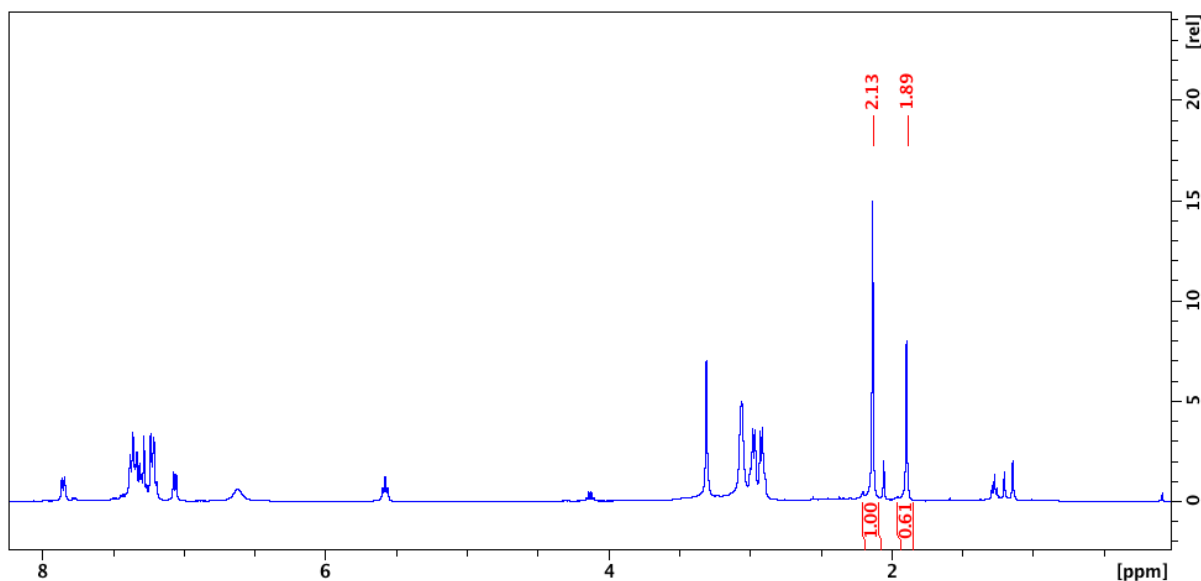
*Figure S87: $^1$H NMR spectrum of the product mixture obtained from **2oa** when subjected to standard coupling conditions in CDCl$_3$ at 298 K. NB.: Traces of ethyl acetate are present. δ 2.13 ppm corresponds to the protons of the CH$_3$ of the aliphatic ketone of **2oa** and δ 1.89 ppm corresponds to the protons of the CH$_3$ of the azepinone product, **3oa**.*

## [9] Computational Details:

**Computational Details:** All DFT calculations undertaken using the ORCA 3.03 computational software.[1] Optimisations were performed at the RI-BP86-D3BJ/def2-TZVP level of theory[2-5] and single point energies and solvation corrections calculated at RIJCOSX-M06/def2-TZVP.[5-7] Frequencies calculations approximated the ZPE correction and entropic contributions to the free energy term as well as confirming all intermediate were true with no imaginary modes and all transition states had the correct critical frequency of decomposition (imaginary mode). Solvation correction was implemented with the COSMO[8] model for CH$_2$Cl$_2$. Graphical visualisation using Gabedit 2.4.8[9] and Avogadro 1.2.0[10] programs.

**Calculated Structures**

**AcOH**

| | | | |
|---|---|---|---|
| C | 0.07314062571764 | 0.39572173448082 | 0.08039171199520 |
| O | 1.24834503036206 | 0.36480072992513 | 0.38251116466215 |
| O | -0.62346203314231 | -0.72539872128957 | -0.27658616421262 |
| H | 0.01984355239347 | -1.46398387771840 | -0.22399919101996 |
| C | -0.78875934242156 | 1.63183919555068 | 0.04978177403677 |
| H | -1.81693483017188 | 1.41431142021261 | -0.25598148763634 |
| H | -0.33864209041947 | 2.35714339224073 | -0.64117089827268 |
| H | -0.78398991231795 | 2.08722812659800 | 1.04910309044746 |

**AcO$^-$**

| | | | |
|---|---|---|---|
| C | 0.03598607385040 | 0.29685776359975 | 0.05511216778790 |
| O | 1.24642324127849 | 0.43030892687872 | 0.39046838938669 |
| O | -0.59263483990739 | -0.74820378331687 | -0.27136091447641 |
| C | -0.79308750064602 | 1.63367755651974 | 0.04924493905048 |
| H | -1.83889776463871 | 1.47018902877139 | -0.25380416156695 |
| H | -0.32228645864540 | 2.35673393006308 | -0.63766940877994 |
| H | -0.77066303692124 | 2.08651073459101 | 1.05467090000639 |

**AgOAc**

| | | | |
|---|---|---|---|
| C | 0.25315202600428 | -0.36464359006794 | -0.11425909200623 |
| O | 1.48496100851511 | -0.32847676045819 | 0.21261970832772 |
| O | -0.37088846693423 | -1.42632533530502 | -0.44172432598208 |
| C | -0.51112232693026 | 0.94982802513432 | -0.10806238149700 |
| H | -1.55371905650363 | 0.80218642391744 | -0.40637819544471 |
| H | -0.02133068597900 | 1.65615131952636 | -0.79189883006478 |
| H | -0.46752523599471 | 1.38785908805536 | 0.89847736908813 |
| Ag | 1.60464873782244 | -2.63719217080232 | -0.11648425242103 |

**AgSbF$_6$**

| | | | |
|---|---|---|---|
| Sb | -0.06067880002312 | 0.08980692244763 | 0.04307952851391 |
| F | -1.74762501280623 | 0.52110203593808 | 0.77506620420186 |
| F | 1.79377738160266 | -0.13816214312118 | -0.57016927416065 |
| F | 0.81003321214130 | 0.41235621731370 | 1.77665724042206 |
| F | -0.69872583809947 | -0.07007024818585 | -1.72745651299273 |
| F | 0.33943391974667 | 1.99469584897506 | -0.23893270102413 |
| F | -0.19528843133265 | -1.75562262791544 | 0.42201883821105 |
| Ag | 2.55667856877085 | 1.76499399454801 | 0.74453467682863 |

**olefin-Me**

| | | | |
|---|---|---|---|
| C | 1.57343543712572 | -2.51205382504275 | 2.46839033020169 |
| C | 0.44820662757486 | -3.17641642674301 | 2.18055536781546 |
| H | 1.56594448953168 | -1.67041172015939 | 3.16699570150053 |
| H | 0.47901991532287 | -4.01464776239209 | 1.48068847940661 |
| H | -0.51052630725876 | -2.90917765286697 | 2.62478734832061 |
| C | 2.88614943442465 | -2.88881012018619 | 1.85507848199699 |
| O | 2.98754548046609 | -3.80553891794395 | 1.04995844810694 |
| C | 4.08148631513075 | -2.06864173830287 | 2.29405211769512 |
| H | 4.98559278502980 | -2.40970484772349 | 1.77966970023948 |
| H | 4.21734535785612 | -2.15442994450205 | 3.38433910664326 |
| H | 3.90908346479622 | -1.00113504413723 | 2.08183391807329 |

**olefin-OMe**

| | | | |
|---|---|---|---|
| C | 1.60265346015314 | -2.46887175436954 | 2.33471172592553 |
| C | 0.48047756401254 | -3.19310512753823 | 2.28057136307336 |
| H | 1.62140413701126 | -1.45621488945349 | 2.73965102076426 |
| H | 0.49804816869616 | -4.20345351128528 | 1.86867527071823 |
| H | -0.46961503082841 | -2.79978949447655 | 2.64182479410113 |
| C | 2.88961234091052 | -3.01867048521641 | 1.84136989852234 |
| O | 3.06327261139218 | -4.12321504635726 | 1.35910387715697 |
| O | 3.88601473118622 | -2.10017223895888 | 2.00264570111412 |
| C | 5.18603622063324 | -2.53934653234678 | 1.55607753036277 |
| H | 5.16240692704310 | -2.77937277791076 | 0.48487680907989 |
| H | 5.50096410853318 | -3.43207683072092 | 2.11226076496671 |
| H | 5.86189176125691 | -1.70076931136588 | 1.75257924421471 |

**Cl-benzamide**

| | | | |
|---|---|---|---|
| Cl | -3.39603322918128 | -2.86984546760100 | -0.55147991861486 |
| H | 0.35193243752740 | 0.58564550759615 | 0.03042362138451 |
| N | -1.71826969250177 | -2.75806248226746 | -0.22977825206422 |
| C | -1.19127952194446 | -1.54104189796442 | 0.19534833673749 |
| O | -1.87799834001245 | -0.58286105046846 | 0.50978209620031 |
| C | 0.30825777919474 | -1.54943946751625 | 0.26041194661648 |
| C | 0.95869126163705 | -0.31159993269823 | 0.15196976376717 |
| C | 2.34937500010311 | -0.24555939448257 | 0.20484063835253 |

```
C    3.10197966389789    -1.41133383238664     0.37992824722166
C    2.45843611967286    -2.64492095385154     0.50585968790727
C    1.06585543432808    -2.71676669763076     0.44506582633183
H    2.84997744629678     0.71925077368498     0.11376774931689
H    4.19063532915164    -1.35668423562206     0.42877358072868
H    3.04122982849860    -3.55289146914185     0.66493469642888
H    0.56878204058409    -3.67748700793466     0.58777957974154
H   -1.16419855725227    -3.34183039171521    -0.85325260005615
```

**Cl-benzamide anion**
```
Cl  -3.41751784405780    -2.85137867657273    -0.30220774574822
H    0.33559109535732     0.58283681636417     0.12104323443079
N   -1.65030275469674    -2.79953327978618    -0.09763083437554
C   -1.20478209223988    -1.53663501631295    -0.04822678279801
O   -1.78864072026019    -0.42774076125666    -0.11915409234831
C    0.31568205794678    -1.54616878848040     0.12887787864473
C    0.96585516392601    -0.30511067265911     0.19882029492613
C    2.35174340532574    -0.22671989210742     0.36077092148403
C    3.11689948179106    -1.39288046867277     0.45727179067265
C    2.47777847275661    -2.63782092378598     0.38674318964425
C    1.09295116771957    -2.71376627132790     0.22502370923240
H    2.83926088597927     0.75074964956612     0.41494946949520
H    4.20074675444627    -1.33484113701559     0.58648926458689
H    3.06625126185575    -3.55631908157425     0.46165392463607
H    0.58114566415024    -3.67453549637835     0.16920777751694
```

**iPr-benzamide**
```
C   -3.13821301815115    -2.97055309700632    -0.55837356922019
N   -2.95182184174973    -1.53029621275897    -0.80613443721635
C   -2.07296955736953    -0.73389365835035    -0.12596036054088
O   -1.32006527642434    -1.15579551098839     0.75644972796873
C   -2.08117755908339     0.71914518645285    -0.52248354943748
C   -1.63777372402852     1.64883454250051     0.42867036701749
C   -1.61848508862599     3.01007344706662     0.12999721615357
C   -2.02474546247545     3.45723017273275    -1.13156509087905
C   -2.44722235592591     2.53576498780364    -2.09303296148590
C   -2.47818064779957     1.17340810457317    -1.78944719564795
H   -1.30798830661809     1.27336614991505     1.39750394243241
H   -1.28133581026148     3.72645525172958     0.88050875446221
H   -2.00275879913083     4.52195414269852    -1.36896021422422
H   -2.74449154259152     2.87790466709601    -3.08513850557296
H   -3.91099759443645    -3.27696197629526    -1.28161302464159
C   -3.66297704060144    -3.24044684322048     0.85764851771093
C   -1.85924426123588    -3.75702958052091    -0.86286441855652
H   -4.59360524165085    -2.68618067879549     1.04333722131947
H   -2.91775809568270    -2.93384933190022     1.60192637753493
H   -3.86959990048660    -4.31271759003693     0.98451768235797
H   -1.06095360200244    -3.46916959876130    -0.16838833593563
H   -1.51808467271752    -3.56398824157205    -1.88959310278355
H   -2.04944911802868    -4.83491633428004    -0.75781552655799
H   -2.77450367597961     0.46239117482073    -2.56293248776979
H   -3.63528980694235    -1.06606717290269    -1.39313002648764
```

**iPr-benzamide anion**
```
H    2.05385570061924     0.00725528193316     1.13777048910020
N   -0.32345738353478    -3.04577663858182     0.26591806445737
C    0.30136972565171    -1.92521259798748     0.61631139948077
O   -0.17195498856739    -0.87776315428220     1.16255853599365
```

```
C   1.79274525210716   -1.93780382245233    0.30997533430384
C   2.57251185291674   -0.82439238864264    0.65585257309110
C   3.94476642246664   -0.79578457163272    0.38982529345857
C   4.56374978132786   -1.88471127753357   -0.23335391971999
C   3.79314623949133   -3.00230815124161   -0.58357804475879
C   2.42356480398521   -3.02693014078938   -0.31330183776298
H   4.53738900129805    0.08055516434421    0.66824940632699
H   5.63567327518831   -1.86402942990419   -0.44671506542488
H   4.26863165776970   -3.85846503927764   -1.07131048500070
H   1.79545019363059   -3.88101492415822   -0.57143808866888
C  -1.74647741314904   -3.05600126295016    0.54963370843078
H  -1.94983415892835   -2.54689969160360    1.51738181341733
C  -2.52965541040141   -2.28264553655338   -0.52713736426209
H  -3.61884302981757   -2.30296485724786   -0.34048178646528
H  -2.33559523173570   -2.72562024559081   -1.51857430641018
H  -2.19039584147930   -1.23813944977794   -0.53511800423532
C  -2.22899429709046   -4.50775650576316    0.63925949989776
H  -3.30919192114854   -4.56691613904634    0.86068165239846
H  -1.67719293494677   -5.04468018301317    1.42523485790112
H  -2.03890329565324   -5.02793343824716   -0.31459672554885
```

**Cp*Co(III)(OAc)₂**

```
Co  1.07615934347659   -1.43758851541960    1.28428257928123
C   0.39082877445472   -0.99738874950653    3.15682503256086
C   0.41213380714687   -2.41214201518510    2.94762687514825
C   1.76370223178281   -2.80319365081618    2.60535340739562
C   2.58530781051292   -1.61901180808370    2.66115547604196
C   1.74425669517078   -0.50121752052151    2.96795415167494
C   2.18650138603048    0.92001589779279    3.03336978576444
H   2.78446552647261    1.15917447622620    2.14236422233080
H   2.80123362364542    1.09299688510355    3.93170289133804
H   1.32985639681623    1.60330869374150    3.07077950625135
C   4.05560504736525   -1.57457785648491    2.42744289675716
H   4.37269082682106   -0.58387771243497    2.08830544434038
H   4.35810740563028   -2.30778344185214    1.66915664433562
H   4.58460057700734   -1.82169908872123    3.36309036180265
C   2.23602896357335   -4.17879526605155    2.27556663339245
H   2.96564142470899   -4.15243754827107    1.45511207909371
H   1.40513915678134   -4.82530143090694    1.96590589667651
H   2.72298427162433   -4.64921651675090    3.14606017300646
C  -0.75777623651138   -3.33581148493537    2.97184776944389
H  -0.77051021486275   -3.98101376712168    2.08300526049626
H  -1.70709686387896   -2.78876646662462    2.99987391340030
H  -0.71198409055904   -3.98402572406697    3.86191386825623
C  -0.80000002681996   -0.15468082877708    3.46968052893250
H  -0.75670598225172    0.80020931443234    2.93074591439664
H  -0.84985412761584    0.06715668094559    4.54753167817328
H  -1.73313260985463   -0.65614431444771    3.18511713562633
C  -0.60863250166111   -0.91162734654151   -0.28259660702422
O   0.08087274520936    0.00053814419816    0.28807975804081
O  -0.41112432104233   -2.11668020375447    0.09752287108441
C  -1.57884211292302   -0.58580849042974   -1.37871854715708
H  -1.06875532990941   -0.70574036763543   -2.34610924446512
H  -1.92010760881888    0.45206207887754   -1.29310257593178
H  -2.43008679848284   -1.27680615939621   -1.35501446267835
C   3.05820915493773   -0.70721846077733   -0.56769353134888
O   2.23134148020894   -1.66636579681457   -0.22475748547588
O   3.28498789143179    0.32970329899755    0.06260557372638
C   3.74823599278465   -0.98095332658904   -1.90097859462008
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| | | | |
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| H | 4.76507709752787 | -0.57137259719138 | -1.88057626085434 |
| H | 3.18996824198886 | -0.45761275994350 | -2.69128994627767 |
| H | 3.76481395208130 | -2.05033125426226 | -2.14141107293609 |

**[Cp*Co(III)OAc]⁺**

| | | | |
|---|---|---|---|
| Co | 0.98417452445472 | -1.55154633671616 | 1.03382410819974 |
| C | 0.38348598124991 | -1.08085806586443 | 2.88984959386938 |
| C | 0.53248269271206 | -2.52652275011278 | 2.76210748463042 |
| C | 1.88000087763379 | -2.78711244999296 | 2.38180959230683 |
| C | 2.57792251781877 | -1.50377148767554 | 2.28675835464876 |
| C | 1.66039233192406 | -0.45886736396026 | 2.62458919237865 |
| C | 1.92896840464291 | 1.00588785751504 | 2.63126032066688 |
| H | 2.84798019889235 | 1.25545955438671 | 2.08883667929965 |
| H | 2.04351253958611 | 1.36008853414174 | 3.66769267660681 |
| H | 1.10367275658335 | 1.57012580462784 | 2.17845364957831 |
| C | 3.98901173016382 | -1.33517118292548 | 1.85679978689079 |
| H | 4.18767835406460 | -0.32698408387611 | 1.47663825803326 |
| H | 4.27388210412669 | -2.06738059527343 | 1.08999084289307 |
| H | 4.65401501467720 | -1.50282609316472 | 2.72181279477845 |
| C | 2.48017744811512 | -4.11342749506034 | 2.08043212592261 |
| H | 3.20439837354852 | -4.05658328547986 | 1.25711770621035 |
| H | 1.71805159685779 | -4.85763257100249 | 1.82321067537163 |
| H | 3.02422858868540 | -4.48335141458388 | 2.96597220022162 |
| C | -0.55578601507655 | -3.52585565261090 | 2.93601916141632 |
| H | -0.34499421329534 | -4.45499259453577 | 2.39518258959504 |
| H | -1.52252358247156 | -3.13817606699802 | 2.59178092715557 |
| H | -0.66244923841387 | -3.77444862336219 | 4.00418547998189 |
| C | -0.87594242099707 | -0.36999143211076 | 3.21984221502902 |
| H | -0.88375864416734 | 0.65497140710560 | 2.83180209519047 |
| H | -0.97334265143006 | -0.30698644129865 | 4.31826915738419 |
| H | -1.76033184221468 | -0.90222566146729 | 2.84884450827216 |
| C | 0.22463019664009 | -1.30938180449407 | -1.11466452675993 |
| O | 0.78220315317825 | -0.34297204011753 | -0.46293683158785 |
| O | 0.10537363830367 | -2.41488916670002 | -0.45374000815906 |
| C | -0.26356882031229 | -1.15755317325534 | -2.50532170576319 |
| H | -0.18484030111324 | -2.10955139319407 | -3.04397559795494 |
| H | 0.28109092633358 | -0.35804050304729 | -3.01955649840599 |
| H | -1.32962822070075 | -0.88039542889658 | -2.46730300790091 |

**Int 1**

| | | | |
|---|---|---|---|
| C | 2.41606806764365 | -3.10531485323142 | 1.15302044585429 |
| Co | -1.61628541008004 | -3.61333269704913 | 2.98018157376544 |
| N | 2.02426506578790 | -4.50129928246893 | 1.40293872138119 |
| C | 0.96540286201419 | -4.87261072620308 | 2.14738288219647 |
| O | 0.30498498608102 | -3.98605365982227 | 2.77200286074543 |
| C | 0.67000312240127 | -6.32699327905938 | 2.22486321344240 |
| C | 0.14034363768257 | -6.85698719161029 | 3.42096019506146 |
| C | -0.12048232855612 | -8.22929525980632 | 3.52450292185442 |
| C | 0.13251823636639 | -9.07990761647062 | 2.43367880656649 |
| C | 0.65084634471886 | -8.55701209264684 | 1.23479089855573 |
| C | 0.92022412711405 | -7.18543711177081 | 1.12920622913957 |
| H | -0.05955894720366 | -6.18276852357498 | 4.26442209112586 |
| H | -0.52726044267805 | -8.63915359685275 | 4.46059215281072 |
| H | -0.07919001139699 | -10.15672217583617 | 2.51611837229037 |
| H | 0.83629687509001 | -9.21963447402187 | 0.37649544275472 |
| H | 1.47583131121413 | -2.52503590604448 | 1.24141479120990 |
| C | 2.96374857442510 | -2.98350387456142 | -0.27110165053313 |
| C | 3.40323361826089 | -2.61552647166389 | 2.22133684995518 |

| H  | 2.21786691278177   | -3.31403500856650   | -1.02032443505914 |
| H  | 3.88584935600499   | -3.58858008812927   | -0.39925623606471 |
| H  | 3.22919838126485   | -1.93106355226562   | -0.49001932101764 |
| H  | 4.35819418652546   | -3.17733354952173   | 2.17215999969940  |
| H  | 2.98107008903907   | -2.74146334583002   | 3.23800518293514  |
| H  | 3.63300830738834   | -1.54220737719992   | 2.07075052567953  |
| C  | -2.45609166389689  | -1.77265331243208   | 2.70212281951817  |
| C  | -3.34033813073529  | -2.68335687812067   | 3.41125601208675  |
| C  | -2.67020918190773  | -3.08144911659761   | 4.64026619116886  |
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| C  | -1.24139389106527  | -1.64525364857093   | 3.46003213302995  |
| C  | -0.03653242568495  | -0.84013961820634   | 3.10957577345774  |
| H  | 0.88958078967814   | -1.41638049128901   | 3.29763568339735  |
| H  | 0.00748164100998   | 0.07692540934241    | 3.73380433973464  |
| H  | -0.04383621610096  | -0.52517982730293   | 2.04982396290448  |
| C  | -0.30238849542455  | -2.64019840265786   | 5.68855524439366  |
| H  | 0.68452572232544   | -2.79784431753831   | 5.21186696280686  |
| H  | -0.50680782100047  | -3.50095674544719   | 6.35117619019751  |
| H  | -0.22728376975885  | -1.73204686890870   | 6.32470792703091  |
| C  | -3.22286127621500  | -4.04976423680115   | 5.63147254522765  |
| H  | -2.49425375464439  | -4.28618653559422   | 6.42756802282238  |
| H  | -3.51180131936460  | -4.99707674092500   | 5.13282828524710  |
| H  | -4.13141788795442  | -3.62868871018062   | 6.11002694999027  |
| C  | -4.70735444595273  | -3.09843783755919   | 2.97673825252623  |
| H  | -4.99029984570627  | -4.07747154523711   | 3.40535691686109  |
| H  | -4.77829022077547  | -3.16647648020083   | 1.87381601428831  |
| H  | -5.46162681760624  | -2.35429543835829   | 3.31225712348773  |
| C  | -2.74821847210623  | -1.16863018329613   | 1.37016757628846  |
| H  | -1.84676149259131  | -0.72053865023537   | 0.91389946884386  |
| H  | -3.51502260700507  | -0.37130973798561   | 1.47276926066262  |
| H  | -3.14432108272758  | -1.93134631280418   | 0.67104807282435  |
| H  | 1.28867039295207   | -6.77312268936903   | 0.17712828228590  |
| H  | 2.65103442827004   | -5.24044513190760   | 1.07296959325300  |
| C  | -2.33019127215758  | -5.44748949869577   | 1.66985634070979  |
| O  | -1.96052815159853  | -4.33939100688142   | 1.13829153642284  |
| O  | -2.31322742207638  | -5.47718235129213   | 2.95421985146698  |
| C  | -2.71943382309808  | -6.64283970727998   | 0.86160300825340  |
| H  | -1.89689416296387  | -7.38669816508319   | 0.91148695820148  |
| H  | -2.89727407229721  | -6.36475529100350   | -0.19203810246529 |
| H  | -3.62001791653152  | -7.11530900759446   | 1.29810779430336  |

**TS 1-2**

| C  | 1.37247423498986   | -2.87590048324255   | 1.63295420233284  |
| Co | -2.46833501193658  | -5.30950886137453   | 3.12780553689065  |
| N  | 1.29195767927932   | -4.28522709350735   | 2.06088180136706  |
| C  | 0.15682689779057   | -4.89410111058190   | 2.41245123719704  |
| O  | -0.94463967171417  | -4.25310429176603   | 2.42554160343270  |
| C  | 0.12985161119315   | -6.31941104144524   | 2.77756562077072  |
| C  | -1.16764139228629  | -6.89459370040520   | 2.71670178691200  |
| C  | -1.28862551538675  | -8.26574808466806   | 2.99981042994522  |
| C  | -0.17814227089683  | -9.01965947190772   | 3.38148439575381  |
| C  | 1.08265074041659   | -8.42018245292390   | 3.48688839563585  |
| C  | 1.24021997173582   | -7.06771476211679   | 3.17560146797015  |
| H  | -1.83671012249835  | -6.59427889313708   | 1.67631965574237  |
| H  | -2.25695093615749  | -8.75432662295751   | 2.88309822825985  |
| H  | -0.29016261717827  | -10.08366342950138  | 3.59458073393484  |
| H  | 1.94332143936829   | -9.00892330439586   | 3.80341220632985  |
| H  | 0.64119560712620   | -2.33701867583475   | 2.25312516660297  |
| C  | 0.97352896420005   | -2.73842127732603   | 0.16106851876834  |

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C    2.77890251240296    -2.35766906555385     1.91940670923430
H   -0.03750319075966    -3.13003928660173    -0.00897628646670
H    1.67542125810048    -3.28299535196382    -0.48669988743703
H    0.98722722366296    -1.68065566851118    -0.13365480733909
H    3.52937136060420    -2.91360007472831     1.33649573625253
H    3.03034493140200    -2.44169326064726     2.98557476150923
H    2.85721535597527    -1.30196177867466     1.63079814828479
C   -4.28591646036609    -4.90964732771729     4.04542415253187
C   -3.74740520254275    -6.15949322230976     4.50430262655377
C   -2.47095627317336    -5.88303003641841     5.14001338311023
C   -2.20816253925464    -4.48828659624212     5.00652304804956
C   -3.32041278802531    -3.87650564006730     4.30495052702624
C   -3.44043616063274    -2.43587967753961     3.94735626022361
H   -2.46971277814055    -2.01812474033364     3.65179936450074
H   -3.80657855153893    -1.85371107105940     4.80856818881546
H   -4.14183798440841    -2.28779750362888     3.11806230150478
C   -0.99649574191113    -3.77709954760623     5.49619447018435
H   -0.73870244475537    -2.92768156245673     4.85238493980413
H   -0.12945465240203    -4.44646169594161     5.56141030279633
H   -1.18240821117040    -3.38124732638037     6.50744168188515
C   -1.62841507439767    -6.85110214253590     5.89501081520596
H   -0.55679093566081    -6.68286152155548     5.72697444669086
H   -1.85268373173748    -7.88804421514194     5.62698895440994
H   -1.81785342189269    -6.73158230463363     6.97434590149103
C   -4.45168018132458    -7.47289432333599     4.46789854326694
H   -3.75522097967675    -8.31286258620456     4.56916084906874
H   -5.01749088244218    -7.60354376467904     3.53625236848253
H   -5.17106404446687    -7.53853909971283     5.30063049886468
C   -5.59408033960545    -4.72272767627999     3.36554796216935
H   -5.52475839962001    -3.98440097937328     2.55782903874643
H   -6.33463427238261    -4.35976201824701     4.09648481179714
H   -5.97036190406450    -5.66114946783111     2.94412604970519
H    2.22525041501983    -6.60547434505135     3.27183231905006
H    2.11827595918508    -4.86507339884235     1.93668643001492
C   -3.09989831695609    -5.57721334863302     0.38596049036745
O   -3.38706637387543    -4.93573385832912     1.46294093202904
O   -2.24145304082443    -6.50125696970198     0.33329081832860
C   -3.86955840975783    -5.20350910674119    -0.85508864205725
H   -3.22686044866453    -5.29804240256660    -1.73743412919744
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**Int 2$_{AcOH}$**

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N    1.34781012869755    -4.37311121363035     1.90317297416855
C    0.23119330227481    -5.00826446912652     2.28467305646614
O   -0.89270590051221    -4.39798422792653     2.28795810149865
C    0.21698126999375    -6.43253801313870     2.66791804542402
C   -1.10179740816719    -6.88918385863800     2.98540969222553
C   -1.26620655817022    -8.27204645468342     3.21470367319098
C   -0.16679854656778    -9.14859572689534     3.18364931105504
C    1.13034115792987    -8.66827338651291     2.91603880457347
C    1.32196007723643    -7.30807002954492     2.64217126587119
H   -1.44522527748439    -7.04459459429678     1.12578895682792
H   -2.26862233782015    -8.68147290597172     3.41303875645106
H   -0.32201547023083   -10.22279072327468     3.36952028185081
H    1.98475951494851    -9.36024767585948     2.90117603744438
H    0.37905508125813    -2.71654217711426     1.14284531761454
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| C | 2.40023718008761 | -2.79333592455533 | 0.35403568863927 |
| C | 1.72284950924870 | -2.06364110825591 | 2.70763594333146 |
| H | 2.13058823740449 | -3.43055742052213 | -0.51087118444423 |
| H | 3.43019600768662 | -3.05651257161404 | 0.67736241090803 |
| H | 2.42300794903653 | -1.74067964190298 | 0.01234485892045 |
| H | 2.72932644798979 | -2.29098065478359 | 3.11618515164592 |
| H | 0.97838162837014 | -2.20480631851801 | 3.51678113075340 |
| H | 1.70988265572848 | -0.99584123236435 | 2.41199481672074 |
| C | -4.12162631495413 | -4.45922158202966 | 3.81650995841551 |
| C | -3.98349650530910 | -5.84406722682942 | 4.27825163115991 |
| C | -2.77258316335482 | -5.93285937008772 | 5.05482279216853 |
| C | -2.09264056246365 | -4.66239184825867 | 4.94546197788576 |
| C | -2.96807450211278 | -3.73911895001179 | 4.21844079380084 |
| C | -2.61717608948051 | -2.32144421499950 | 3.90631355385476 |
| H | -1.64914217747027 | -2.27649476091304 | 3.36743199630112 |
| H | -2.51373937481246 | -1.72921517096184 | 4.83904498497394 |
| H | -3.38142909959262 | -1.83369028392166 | 3.27348931338467 |
| C | -0.77886255697986 | -4.31898897120440 | 5.56744161377669 |
| H | -0.27732309990054 | -3.49568704679996 | 5.02510164992644 |
| H | -0.09830415594547 | -5.19264680950960 | 5.58034117309780 |
| H | -0.91703683031277 | -3.98935916021534 | 6.61971522857847 |
| C | -2.33445155014370 | -7.07304824525054 | 5.91434244016366 |
| H | -1.23706724110827 | -7.20897387662670 | 5.90470567561721 |
| H | -2.80229312608622 | -8.02933516376368 | 5.61940034368177 |
| H | -2.64113085735393 | -6.86730963877436 | 6.96270261111568 |
| C | -5.00233519954817 | -6.91849521916473 | 4.07810076766634 |
| H | -4.57720560285829 | -7.92495812181322 | 4.25407861075704 |
| H | -5.41910944436309 | -6.89433297633131 | 3.05306198570259 |
| H | -5.85222637615596 | -6.78857882262918 | 4.78281504495013 |
| C | -5.26363098131796 | -3.96608382228335 | 2.99217662701286 |
| H | -5.13434343172296 | -2.90955363162668 | 2.69418721164345 |
| H | -6.21517060036956 | -4.05028293208949 | 3.55750431517885 |
| H | -5.36608136431394 | -4.57146053777894 | 2.06961380670620 |
| H | 2.33362966734515 | -6.94436851006786 | 2.39715596621504 |
| H | 2.22915997776317 | -4.89130248442631 | 1.93669876970664 |
| C | -2.89722641392772 | -6.17693096853825 | 0.29520585507719 |
| O | -3.25724751652753 | -5.62488766764527 | 1.35652992786271 |
| O | -1.83738369476689 | -6.95668134470717 | 0.20548894229925 |
| C | -3.65778575670628 | -5.99471172655961 | -0.98266420006588 |
| H | -3.00795020332132 | -5.48675795675375 | -1.72451672370369 |
| H | -4.56597347099984 | -5.39383532407750 | -0.81027161225130 |
| H | -3.92066920154719 | -6.98328202445738 | -1.40803058097739 |

**Int 2<sub>Olefin</sub>**

| C | -3.19276531911706 | -2.72914726122106 | -0.04513249975214 |
| Co | -0.27339259522789 | 1.06168982387514 | 0.16037607051832 |
| N | -1.73079688552745 | -2.68367389294170 | -0.22458775346960 |
| C | -0.98397024350098 | -1.57747875839824 | -0.16109989485181 |
| O | -1.53715056494272 | -0.42114766980914 | -0.09051815672261 |
| C | 0.48082957930037 | -1.61310571635381 | -0.15604608309277 |
| C | 1.06406078466982 | -0.34186066807822 | 0.08762234716588 |
| C | 2.46222486468650 | -0.26691738704107 | 0.20591891113407 |
| C | 3.25754162135429 | -1.41113902387813 | 0.03017148135569 |
| C | 2.67157571195350 | -2.66118404960400 | -0.25227558123884 |
| C | 1.28013195817875 | -2.76417213761839 | -0.33320310752429 |
| H | 2.95265123869024 | 0.68598842317840 | 0.45534728419785 |
| H | 4.35181494871740 | -1.32885057978143 | 0.12225248300198 |
| H | 3.30194402644938 | -3.55055748576926 | -0.39469210116210 |
| H | -3.50834448475892 | -1.66820897834930 | -0.00946297664917 |

| C | -3.51621824752618 | -3.40036661895089 | 1.29587490294017 |
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| C | -3.84949229695653 | -3.41875999695703 | -1.24551376950901 |
| H | -2.98669757501543 | -2.88574877556746 | 2.12173045428200 |
| H | -3.20849056011765 | -4.46735360522549 | 1.29002102314487 |
| H | -4.60719287879583 | -3.37082811694009 | 1.48812295429900 |
| H | -3.51320210822767 | -4.47317964957569 | -1.33442390661999 |
| H | -3.60769270534554 | -2.89863756518882 | -2.19369473344206 |
| H | -4.95084099728488 | -3.43066209684330 | -1.12520920207064 |
| C | -0.59605187015430 | 3.14767491458347 | -0.08727403603345 |
| C | 0.74984655253634 | 2.76929548898976 | -0.48836473761475 |
| C | 0.63927934545623 | 1.84155865110846 | -1.59013876121704 |
| C | -0.75947391359186 | 1.58776498533204 | -1.80537234020154 |
| C | -1.52915779435241 | 2.39799657300153 | -0.87373935065452 |
| C | -3.02117769747589 | 2.44278063061771 | -0.80606916428593 |
| H | -3.45055932967215 | 1.42160955851089 | -0.82778392410035 |
| H | -3.43945594819395 | 2.99570238712646 | -1.67382993973896 |
| H | -3.37767817114588 | 2.94821809565605 | 0.11084545348304 |
| C | -1.32520254493712 | 0.67258734413541 | -2.83799764997036 |
| H | -2.31406542830714 | 0.28305070626910 | -2.53680224521132 |
| H | -0.65353640433836 | -0.18547183758994 | -3.03164660718143 |
| H | -1.45095657510335 | 1.21886734989208 | -3.79740107086939 |
| C | 1.74968513573626 | 1.33006522982887 | -2.44778672456810 |
| H | 1.57699942319981 | 0.28475433833116 | -2.76563516769242 |
| H | 2.72831833171416 | 1.37010152603046 | -1.93732346397880 |
| H | 1.81732821040210 | 1.95525419740809 | -3.36323037832664 |
| C | 2.00695586046848 | 3.40728145942260 | 0.00532004205539 |
| H | 2.88697697875957 | 2.75110494854636 | -0.12487986886374 |
| H | 1.94051299271738 | 3.69441068733873 | 1.07164810165891 |
| H | 2.20593260293393 | 4.33842981587078 | -0.56738774174649 |
| C | -0.91231817835123 | 4.20491392486197 | 0.91969294381555 |
| H | -1.96843558830683 | 4.17274971649752 | 1.24545708550967 |
| H | -0.73715959271870 | 5.20558612150660 | 0.46919841943113 |
| H | -0.26636004852342 | 4.14359866486986 | 1.81803074353894 |
| H | 0.82297848867153 | -3.74471587120286 | -0.54341233830798 |
| H | -1.23664350917320 | -3.57997822737376 | -0.22399367631356 |
| C | 0.41439429249054 | 1.06485650727562 | 2.12365030586054 |
| C | -0.98442656278335 | 1.20254129729343 | 2.12486671711000 |
| H | 1.07261935089772 | 1.93923845457095 | 2.24101715492404 |
| H | 0.82892033737291 | 0.10132092340238 | 2.45368167649866 |
| H | -1.45716592410948 | 2.19040468168482 | 2.21947964745286 |
| C | -1.85412254060695 | 0.02496344007504 | 2.48037069851945 |
| O | -1.37060704751878 | -1.07980437665278 | 2.70918724677089 |
| C | -3.33792969421618 | 0.30439001280982 | 2.54187611337088 |
| H | -3.90336472616835 | -0.61571537547949 | 2.77228778102867 |
| H | -3.67543456772841 | 0.72540727148441 | 1.57260239771372 |
| H | -3.55344651753521 | 1.06960957100542 | 3.31754951219962 |

**TS 2-3**

| C | -3.21114877626006 | -2.78748751248544 | 0.00042822747153 |
|---|---|---|---|
| Co | -0.34794998375009 | 1.05878082455097 | 0.11250709802759 |
| N | -1.73887773996737 | -2.72183898260764 | -0.03921963370173 |
| C | -1.02402892318579 | -1.59803363048403 | -0.04490167587204 |
| O | -1.59289264346666 | -0.45410429326134 | -0.06678386599615 |
| C | 0.44251365895525 | -1.61180861046802 | -0.06398376159447 |
| C | 1.06011370752012 | -0.39304888578734 | 0.34448584437302 |
| C | 2.45908979779428 | -0.30751194723962 | 0.22704777023891 |
| C | 3.20948439662382 | -1.36331213066386 | -0.28417954549131 |
| C | 2.58869080787868 | -2.55410800791642 | -0.67903719055888 |
| C | 1.20373058338351 | -2.67090806354883 | -0.56898928466577 |

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H    2.97351516963164      0.58930653440749      0.57694289256746
H    4.29249636764025     -1.26091533701434     -0.36758970886496
H    3.17865044319017     -3.37808611884276     -1.07859591781849
H   -3.54489399806893     -1.74496983971454     -0.08250730800098
C   -3.66571086161188     -3.36188134427707      1.34303108705064
C   -3.72027669130316     -3.59149145063911     -1.19681515376153
H   -3.28525775155830     -2.75378279755707      2.17344089178947
H   -3.30973068868174     -4.39631326650536      1.46739726554376
H   -4.76319914704132     -3.38160413966418      1.38691586497369
H   -3.36050335637038     -4.63060883848386     -1.15497265111615
H   -3.38986176099975     -3.14945305708334     -2.14660649374242
H   -4.81813058243609     -3.62017021686541     -1.19059031122011
C   -0.75386603988425      3.09223588601043     -0.10716512685803
C    0.62791659019555      2.80894988670488     -0.40566192764432
C    0.66733363981273      1.91338278148167     -1.54512181469337
C   -0.66917995707229      1.57087390016645     -1.87638003615629
C   -1.56155062824778      2.29319980700163     -0.97564004345583
C   -3.04870838507489      2.22317075901065     -1.01761126715226
H   -3.39008885682298      1.17951419366154     -0.98552995938680
H   -3.42745070557352      2.66733831922072     -1.95172434011556
H   -3.50589202972752      2.76527996362668     -0.18227391707137
C   -1.10251627108371      0.64240802379994     -2.95754973539710
H   -2.03752643578005      0.13177379077110     -2.69641914250449
H   -0.33804093762443     -0.11591531226877     -3.16640108613636
H   -1.27798921292912      1.20224344749189     -3.89012728777385
C    1.88395527655813      1.47997953395285     -2.28728032592709
H    1.81694842583586      0.43439778578828     -2.61167859123552
H    2.79442681867214      1.58967567213252     -1.68784427550818
H    2.00099174849550      2.10325694968064     -3.18704142917160
C    1.80671744488510      3.44816065544453      0.24789772025730
H    2.70112148022701      2.81747873801059      0.17843798590252
H    1.61910128043855      3.66726346991854      1.30656280428855
H    2.04388836997025      4.40450030294435     -0.24487832751426
C   -1.24268247420245      4.09846698730456      0.87892052805737
H   -2.23572093520446      3.84708314548179      1.27009505248961
H   -1.31896574290616      5.08128232033196      0.38742992260988
H   -0.55513073748041      4.21677263676102      1.72585129554597
H    0.71316242105065     -3.57885026895232     -0.92482879070136
H   -1.23140273706499     -3.59531442951863      0.08069217098917
C    0.57437680565936      0.39121234359344      1.92896405252918
C   -0.69301262597879      1.09500450080854      2.08117165237294
H    1.46888605500254      0.96816966222662      2.16621785936988
H    0.54546170457691     -0.58296963241371      2.42881530812977
H   -0.67711118890202      2.13907969870455      2.39608906016395
C   -1.85421799786622      0.29674835182693      2.56064015040089
O   -1.75355875577883     -0.91355067710013      2.75621808612587
C   -3.15409429627397      1.03217034120536      2.77516459858838
H   -3.84879911129705      0.41645658696667      3.35645639781138
H   -3.60372475105224      1.24103007443802      1.79156568958059
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**Int 3**

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C   -2.75325230960899     -3.00185393116319      1.13267564470341
Co   0.04348109107988      0.88783061590512      0.83890763535249
N   -1.29544478184621     -2.83969234446186      0.95611047496883
C   -0.66914537625334     -1.66828511352564      0.85436224641533
O   -1.28985565666539     -0.55927854399530      0.84004532862776
C    0.81351473039117     -1.63217068986076      0.63532332132431
C    1.68405386624366     -0.87949224838290      1.48925511235480
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C    3.05502151648944    -0.83867710113657     1.13112879385290
C    3.55394808105564    -1.50569179542952     0.00685809511662
C    2.68435620548783    -2.24556599538861    -0.81578342306256
C    1.32229154499789    -2.30292118838079    -0.50139204997441
H    3.74945015363342    -0.30095734970331     1.79464804177025
H    4.62940427753375    -1.46360303515688    -0.22285035434748
H    3.06911320090717    -2.77493087421556    -1.69985829192130
H   -3.16715458305721    -1.98264113866820     0.99770662814828
C   -3.05661046740131    -3.48163604380249     2.55616160621357
C   -3.29659311592337    -3.92956209829373     0.04119096533375
H   -2.67164089550322    -2.75369036465354     3.29520895005981
H   -2.59708616771386    -4.47382924207720     2.74957647239813
H   -4.15094824279910    -3.58910785939236     2.69078247029120
H   -2.86608336579330    -4.94926871241219     0.12901703163090
H   -3.07082534718530    -3.54186889168518    -0.97248305840545
H   -4.39577431144791    -4.02509424388176     0.13764136061622
C    0.07775135624494     2.92778421716915     0.78497029681533
C    1.25875849880100     2.38694977830659     0.17299523365213
C    0.84719907100372     1.58766425509913    -0.98828986117990
C   -0.57025269030639     1.58054665478475    -1.04543650381085
C   -1.06630720476750     2.36821766182060     0.08446439910095
C   -2.50674560442182     2.63386360353701     0.36192925542886
H   -3.11340794532688     1.71372246507174     0.25541637781284
H   -2.90006522521396     3.37153123417868    -0.37154831077258
H   -2.66887441376149     3.04743544147824     1.37301281751160
C   -1.44028493318722     0.86114945410088    -2.02304059940849
H   -2.25020472493887     0.30981079606680    -1.50614705376893
H   -0.86715745947249     0.13580471820477    -2.63052078674686
H   -1.92038744560539     1.57967518683665    -2.72080619753876
C    1.78489052690039     0.92717673572857    -1.94133914496454
H    1.30424429714009     0.09751614025684    -2.49152023918186
H    2.67831262445599     0.52581721232294    -1.42865586083458
H    2.14093126740051     1.66751292819009    -2.69006221138224
C    2.67169583258522     2.68989758060765     0.55637336873482
H    3.35371557053812     1.86052968963887     0.29006473896248
H    2.77188689211630     2.88677632751836     1.64081155812281
H    3.02760337007617     3.59602134894305     0.01990407134301
C    0.03285092796964     3.94204397075931     1.87921141421465
H   -0.89917613043984     3.87793856158064     2.47132832218676
H    0.07083662957343     4.96090385559834     1.43708858340291
H    0.89132656599652     3.85649596954964     2.57290640720552
H    0.63003334796439    -2.86540780007475    -1.14663767748757
H   -0.70976568989929    -3.67803999137095     1.01893842835862
C    1.26418627431756    -0.32446539316788     2.85287068796038
C    0.16018196546327     0.73265729274328     2.82544711294145
H    2.17245692539794     0.08032961760050     3.33774482010031
H    0.89336604252317    -1.18028211860016     3.46087675909794
H    0.46116280722245     1.71775849919433     3.22385192295721
C   -1.12060898665900     0.25367658593393     3.42455119563882
O   -1.30283666413804    -0.94556027228165     3.65928923478070
C   -2.21612870887937     1.25948541777180     3.71354674260579
H   -3.00367398053177     1.14738605773266     2.94007644869545
H   -1.86044116824805     2.30676166405217     3.71565844413810
H   -2.68454986451477     1.02150884287984     4.68802780384038
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**Int 3<sub>AcOH</sub>**

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C    2.65417046424527     2.62215542158384     1.23662320520779
Co   0.20039890743333    -1.33156250439661     1.16002384115583
N    2.31064661659829     1.97485564711161     2.51280181318068
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C   1.72055503099115    0.77321732002267    2.61409209460159
O   1.44888992976997    0.13045391665266    1.55825475569160
C   1.42071804163435    0.26387051683612    3.96820313115638
C   0.91221083459052    1.12543861044873    4.95461647212612
C   0.60866142285127    0.64064609900011    6.22508620102253
C   0.83237907974439   -0.70813660073688    6.51555384203932
C   1.35808459143746   -1.55777529712925    5.54065018073921
C   1.65931421799572   -1.09594907020758    4.25383175538965
H   0.72295426154391    2.17334465404946    4.71413002639888
H   0.20238665140532    1.30947698312056    6.98350017859802
H   0.60719648675150   -1.09638786877489    7.50907973725983
H   1.55904627981895   -2.60266847523774    5.78457323530098
H   1.94195713244299    2.21290495857391    0.50548487876464
C   4.07596627181514    2.24729367487517    0.80854329880645
C   2.45220353355414    4.12974463168308    1.37080772616224
H   4.19078736632461    1.15764944565716    0.73421880808038
H   4.81346339728657    2.62756505215318    1.52998202619897
H   4.30494805867839    2.69183875763926   -0.16956350649970
H   3.13564563209265    4.55531866722034    2.12157791847186
H   1.42109471809656    4.37251498480458    1.66151277776922
H   2.66524290990272    4.62513533616074    0.41468847957109
C  -1.33706906602685   -0.44116926466135    0.00258608554338
C  -1.45777430435631   -1.88718334795488    0.05603507524178
C  -1.62900584102804   -2.27454271530662    1.42294741793286
C  -1.52345329395215   -1.08632946178754    2.23500267209261
C  -1.38779317578937    0.04201984920538    1.33434906998144
C  -1.30026349927035    1.46976344815441    1.74763568349391
H  -0.95193987014837    1.57558475993679    2.78178925959937
H  -2.29820121172726    1.93300853177578    1.68971463529064
H  -0.63333713561019    2.04293248737580    1.09101570263414
C  -1.76139575722105   -1.02677421465296    3.70386538292852
H  -1.36106038207710   -0.11071642829489    4.15122829748284
H  -1.31182376590612   -1.87959026796702    4.22695113292853
H  -2.84476165382106   -1.05104766899929    3.90752015333905
C  -2.03916811902229   -3.61638159804110    1.92551828314973
H  -1.56325728538199   -3.87254166551488    2.88092990339203
H  -1.82929333763055   -4.41404077197225    1.20559925775835
H  -3.12628004666669   -3.60591002246348    2.10500512786874
C  -1.45169878979436   -2.77967112925319   -1.13432014476707
H  -1.36808637639767   -3.83603733982225   -0.85381437401548
H  -0.62055003450554   -2.52696465434775   -1.80548834676630
H  -2.38899306100051   -2.65765965965286   -1.70129993602324
C  -1.15965140333037    0.35970162252922   -1.24005632949293
H  -0.73993258791851    1.35061020879890   -1.02621797074342
H  -2.12532100780960    0.50900868956196   -1.74848406009698
H  -0.49028897094253   -0.15883232407130   -1.93895965918190
C   1.18367021341373   -2.69530672458421    2.34998870703629
C   2.24759736781246   -2.02634607961489    3.23049325222751
H   0.38743288070489   -3.12504583188347    2.96638758152226
H   2.80633369608341   -2.81561237304614    3.76246183761931
H   2.98439137366819   -1.49981483920282    2.61024335217235
C   1.73898408509091   -3.69263297732452    1.43449410386390
O   2.86793707081954   -3.55846300732163    0.90433974590387
C   0.97918927684323   -4.95169032107914    1.10316494452796
H   0.43972654782647   -4.80380426697988    0.15499714784149
H   0.25968325836006   -5.23288069314971    1.87808106489856
H   1.69668072569470   -5.76420947381642    0.93703513180905
H   2.65082427704403    2.39948365178689    3.37229961781589
C   2.49038407996878   -1.07256094068768   -0.77767343921014
O   1.30852582879733   -1.43362133187693   -0.55242374976792
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| O | 3.51254023383224 | -1.37231249381682 | -0.02601712451989 |
| H | 3.27134167370105 | -2.23687639269786 | 0.55932005628573 |
| C | 2.81053310380568 | -0.27215472220995 | -2.00647046901591 |
| H | 1.96612264227146 | 0.36632449559205 | -2.28601632836812 |
| H | 3.00582777693552 | -0.96993189881172 | -2.83509974902930 |
| H | 3.71952102765600 | 0.32030729703997 | -1.85380788037707 |

**Int 3O$_{AcOH}$**

| C | 4.87694788514831 | 2.54619058019864 | 3.23026938011259 |
| Co | 2.45370408444637 | -0.38752549054018 | 0.16153884462624 |
| N | 3.74623742407862 | 1.69928165974825 | 3.65123099113349 |
| C | 2.95631222692898 | 0.92762588455846 | 2.89923086319478 |
| O | 3.06359251110279 | 0.90934637343174 | 1.62515496110964 |
| C | 1.80427888906332 | 0.33791446720120 | 3.65359303880772 |
| C | 0.81781343433833 | 1.27559391704332 | 4.02229289287850 |
| C | -0.29188248498294 | 0.89231156651342 | 4.76935041129842 |
| C | -0.40403342175274 | -0.43742579225141 | 5.18676556132673 |
| C | 0.58077896242148 | -1.35675145187002 | 4.83901518725686 |
| C | 1.69494724175027 | -1.00254037667444 | 4.05857905900289 |
| H | 0.93562883134852 | 2.31742281106635 | 3.71915635560264 |
| H | -1.04922016064325 | 1.62748164312227 | 5.04121073999127 |
| H | -1.25417699630195 | -0.75282824899269 | 5.79252567211200 |
| H | 0.49456681555755 | -2.39151386400125 | 5.17625390941654 |
| H | 4.62741983081273 | 2.93935236138402 | 2.23588573319807 |
| C | 6.16447694426538 | 1.72631707421428 | 3.14754010613291 |
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**Int 4**

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S73

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| H | -1.31654998151467 | -2.96523945095436 | -2.26790221548290 |
| C | -1.38519735788749 | -1.01250619967211 | 2.09141774227426 |
| O | -1.53042514386245 | -0.52641766434468 | 0.91618569000627 |
| O | -0.18532530396940 | -1.15896322162710 | 2.50957948354865 |
| H | 2.75608486813414 | -3.62619077819389 | -1.66111865078867 |
| C | -2.56402573929312 | -1.42599779963688 | 2.91923501369818 |
| H | -2.29528825110813 | -1.45701799093693 | 3.98132756223847 |
| H | -2.88206396845721 | -2.43281469120578 | 2.61028553291593 |
| H | -3.40542582488490 | -0.74231977317159 | 2.75216849803545 |

## TS 4<sub>alkyl</sub>

| | | | |
|---|---|---|---|
| C | 0.30353930389797 | -6.78067621473248 | 1.56932581849897 |
| Co | 1.90596084251524 | -0.60011049736662 | 1.05340158619551 |
| N | 0.17977216025007 | -5.78586961973650 | 2.65663787519335 |
| C | 0.87542688874795 | -4.62677234299561 | 2.74464217937627 |
| O | 1.61448662854113 | -4.19963044730902 | 1.84218851752503 |
| C | 0.73920756918615 | -3.89839501160323 | 4.05424705559498 |
| C | 0.86928556267823 | -4.62311194163676 | 5.24792194671597 |
| C | 0.85646437145737 | -3.98303020976700 | 6.48822318241231 |
| C | 0.70388859828498 | -2.59795360650556 | 6.54487077721999 |
| C | 0.57364547269945 | -1.86918636307204 | 5.36194385835149 |
| C | 0.59040383102940 | -2.49446645338274 | 4.10789633933272 |
| H | 1.02505370969281 | -5.70243659181808 | 5.20257327539260 |

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H    0.97269847415260    -4.56428873929860     7.40296739454915
H    0.68428169192194    -2.08404654802561     7.50625998330467
H    0.43682414995111    -0.78639144661652     5.40822048655111
H   -0.37258483024247    -7.59570411161224     1.86909397310517
C    1.72831791179027    -7.33712907317034     1.48770496904556
C   -0.18053876987246    -6.21972315742669     0.23061734501374
H    2.04706595211625    -7.75121852348588     2.45383004088461
H    2.43283102233570    -6.54968862205652     1.19269722397668
H    1.77154882557366    -8.14154129797428     0.74044080013488
H    0.47882361512429    -5.40861366441744    -0.10196643328738
H   -1.20570036687116    -5.83554659131837     0.31388077348812
H   -0.17267573218782    -7.01336648287800    -0.52914532793354
C    3.58992052666890     0.14474136230057     1.97020986575825
C    3.73004670099246    -1.28018681032626     1.73086569144649
C    3.56715927082299    -1.52372598774376     0.32552670950572
C    3.33790033924656    -0.24486141875337    -0.31580648923256
C    3.39816624070141     0.78210908702778     0.70396570569094
C    3.21529296414653     2.23728128517965     0.47284753522707
H    2.50377188943167     2.43071629947392    -0.33886142854422
H    4.18136091609967     2.68499855630576     0.18777634397260
H    2.85926023314565     2.74896544090782     1.37355450746655
C    3.10454223873358    -0.03876371159956    -1.76929240301288
H    2.65581434843600     0.93950333461715    -1.97775909235967
H    2.44844862234664    -0.81865093516391    -2.17640120679198
H    4.06195273359303    -0.09294677510390    -2.31259830724620
C    3.61614407926363    -2.84693718906781    -0.35086843380606
H    2.99938523995491    -2.85066216816772    -1.25715278981475
H    3.25947369815748    -3.64482503664518     0.30985824887819
H    4.65322238105731    -3.07208213647135    -0.64765810378088
C    4.00829961304292    -2.31697393917085     2.75893422830694
H    3.42943869010519    -3.22979767872378     2.56186491618180
H    3.78547828689674    -1.96487132139159     3.77307508993273
H    5.07959140650357    -2.57458462442830     2.72286464110475
C    3.64163214525533     0.81139673774095     3.30227999826440
H    3.05025925693903     1.73441007557189     3.30959490180776
H    4.67897563644816     1.07508400079958     3.56231160225052
H    3.26088462682590     0.15408915890977     4.09418999454611
C   -0.63837625251212    -2.02350780302649     1.89034286705034
C    0.43752919981776    -1.63374432531856     2.88165767683030
H   -1.44883094081665    -2.64844867382837     2.27174074532544
H    1.44847959892011    -1.73326140149194     2.34777051251039
H    0.34204428190591    -0.59343628899874     3.22230660362631
C   -0.33078293204274    -2.15773283123797     0.52547897122024
O    0.71886659540136    -1.62911076082711    -0.00817469145033
C   -1.29406574862592    -2.78701514331323    -0.43801395433131
H   -1.64943397376703    -2.03154295268915    -1.15327804770000
H   -2.15434225906986    -3.22751028037110     0.07762862974354
H   -0.77569402156062    -3.56590920189472    -1.01284369265142
C   -0.57231373528027     1.22618800452633     1.33292027683740
O   -1.54258295987500     0.41108935963340     1.53778613013735
O    0.65727066134814     0.92873310837763     1.22413874993229
H   -0.42601045674204    -6.01644755019621     3.43731786673618
C   -0.95616056357458     2.67814796347382     1.20900395340286
H   -0.07134889376882     3.32109727702512     1.21683909179254
H   -1.64486854158043     2.95507634294961     2.01738931126353
H   -1.49823465067056     2.81687099454665     0.26175281814559
H   -1.20098937509458    -0.73247088521035     1.65053781518517
```

**Int 5<sub>alkyl</sub>**

| | | | |
|---|---|---|---|
| C | -0.32426508130166 | -6.66309731895697 | -1.02834496379802 |
| Co | 1.89700024621078 | -0.44204483403111 | 0.89795476325939 |
| N | -0.29477849809080 | -6.37053661380482 | 0.42206684441004 |
| C | 0.35069644322159 | -5.32878252042647 | 1.00648452986624 |
| O | 0.74951458668349 | -4.34481888731282 | 0.35150404116719 |
| C | 0.58283328995463 | -5.44820462770870 | 2.48582423920567 |
| C | 0.77403039586001 | -6.72533590856715 | 3.04524737364820 |
| C | 1.04847052243543 | -6.89937279376390 | 4.39901790681654 |
| C | 1.13500034676773 | -5.77983911506289 | 5.22537318751304 |
| C | 0.96293752893340 | -4.50757861873521 | 4.68045985321731 |
| C | 0.69954541111238 | -4.30654691147729 | 3.31814705265272 |
| H | 0.75809271207835 | -7.60498900722946 | 2.39999515360241 |
| H | 1.20385694697219 | -7.90057211135759 | 4.80069586625012 |
| H | 1.34460927437782 | -5.89372754421526 | 6.28944997078628 |
| H | 1.03619063284092 | -3.63279816027942 | 5.32972102561029 |
| H | -0.83066636187278 | -7.63820645514310 | -1.09267905241879 |
| C | 1.09452788765688 | -6.81539591976956 | -1.58777136208479 |
| C | -1.14942519060265 | -5.64832751142138 | -1.82232503063868 |
| H | 1.65593334416670 | -7.58218389305227 | -1.03751580434730 |
| H | 1.63705699440734 | -5.86429948605153 | -1.52046670338828 |
| H | 1.04863305010393 | -7.11500084049797 | -2.64336927256521 |
| H | -0.64513673437525 | -4.67545404889603 | -1.84563702200997 |
| H | -2.15116708450547 | -5.52608096510124 | -1.38843984495283 |
| H | -1.27148501046896 | -6.00064591752073 | -2.85554854486667 |
| C | 3.80354844953239 | -0.58019616832017 | 1.62455873229980 |
| C | 3.49632899077284 | -1.76298484009252 | 0.86473606826589 |
| C | 3.14106781430770 | -1.34272575679923 | -0.47556576681410 |
| C | 3.23324279441033 | 0.08339078450003 | -0.54070253643902 |
| C | 3.63959975042288 | 0.56598321624872 | 0.77086870108277 |
| C | 3.86169763189738 | 1.99161625454413 | 1.13884328973378 |
| H | 3.15751888728717 | 2.65339373565029 | 0.62030086254497 |
| H | 4.88083557000630 | 2.29874925525989 | 0.85361576302965 |
| H | 3.76003914592427 | 2.15259405951557 | 2.21912324363403 |
| C | 2.91538292722225 | 0.95251291138027 | -1.70577041747103 |
| H | 2.25410164253726 | 1.77956841633920 | -1.41322606986633 |
| H | 2.43061756512892 | 0.39027976645928 | -2.51194916846152 |
| H | 3.84097570765744 | 1.39369210946858 | -2.10787421591619 |
| C | 2.70173408522311 | -2.26262371622104 | -1.55939922866476 |
| H | 2.12835275745551 | -1.73704632103197 | -2.33203105292443 |
| H | 2.08392871599095 | -3.07534382710212 | -1.15506267827876 |
| H | 3.58419614325232 | -2.71333013332750 | -2.04141424082390 |
| C | 3.64798087679893 | -3.17497790703961 | 1.31528719959324 |
| H | 2.84318234213558 | -3.81349182896015 | 0.92732588679898 |
| H | 3.66221211025715 | -3.25678748154985 | 2.40937651506576 |
| H | 4.60789599699606 | -3.57074146655017 | 0.94373659101920 |
| C | 4.16026277997864 | -0.54754268624210 | 3.06883314367490 |
| H | 3.80268442783582 | 0.37030250141580 | 3.55008172252288 |
| H | 5.25515300371872 | -0.58693045814310 | 3.18454070539366 |
| H | 3.73494593150472 | -1.40424302957402 | 3.60538385800442 |
| C | -0.73144326061687 | -2.52801769794524 | 2.11779614183153 |
| C | 0.58140670276971 | -2.88087049830166 | 2.83867912396746 |
| H | -1.45368640154351 | -3.35525134537835 | 2.16446559316014 |
| H | 1.40440670048727 | -2.65430139599462 | 2.14980233825700 |
| H | 0.71101242836380 | -2.21698290388806 | 3.70021499095449 |
| C | -0.60230231733234 | -2.09465960593633 | 0.68317840658777 |
| O | 0.32991969966958 | -1.40540795752532 | 0.23451477115929 |
| C | -1.74300345909982 | -2.41505685677756 | -0.22924230586786 |
| H | -2.65907068579204 | -1.95151426193940 | 0.17176711334008 |

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H  -1.91454511973969    -3.49918943377988    -0.24031943854822
H  -1.55766001790247    -2.04486597566686    -1.24186355967136
C   0.45910894746045     1.06387772985928     2.04361745894136
O   1.01796854163074     0.07029462556383     2.63361285520913
O   0.74262216037112     1.21532575837202     0.80626370786710
H  -0.63880804158020    -7.09786874398198     1.03959328420363
C  -0.49282443642019     1.96952243294110     2.75626917761434
H  -0.46921299220720     2.97196697861553     2.31414506520489
H  -0.25469502847247     2.01133851081875     3.82551461167983
H  -1.51496197019003     1.57580686871426     2.64651915123165
H  -1.21937315067644    -1.68003560721481     2.63136239893896
```

**Vinyl Ester Structures**

**Int 3**

```
C   -2.59787290545138    -3.28053209567230     0.67405461048308
Co  -0.00588179994417     0.73099082380263     0.85023186409561
N   -1.14728966837752    -3.02141304914151     0.53784260124494
C   -0.59267569533236    -1.82010243804540     0.67250018792767
O   -1.28193740927566    -0.77286656689925     0.85772775216035
C    0.88671366235765    -1.65434867432753     0.57607667697888
C    1.57532627669155    -1.01687036886804     1.64946124008100
C    2.96214122531893    -0.82248795818524     1.50499367613881
C    3.64395904479430    -1.25445278188329     0.37161540867227
C    2.95622821941534    -1.91244847860536    -0.65866869219281
C    1.58414772767852    -2.11273353306298    -0.55582094414109
H    3.51196602450852    -0.36261196141229     2.32789069192957
H    4.72201991550055    -1.10630603776054     0.29726733776449
H    3.49432763647611    -2.27068813004646    -1.53640002860285
H   -3.09183120082208    -2.38372557285669     0.27272642051678
C   -2.96559597677476    -3.43547508671116     2.15119751127893
C   -2.95946523310666    -4.49677712909517    -0.17301812681245
H   -2.67613298798760    -2.54507489510158     2.72481279985083
H   -2.46977577651372    -4.31702659789546     2.58360224292860
H   -4.05072419320169    -3.57551554013884     2.24945635268074
H   -2.44756096852122    -5.39957877744583     0.19462849856096
H   -2.69775609741115    -4.34871405862682    -1.22978354669985
H   -4.03866263162714    -4.68558451660496    -0.11077922321471
C    0.08151243218312     2.77828093383571     0.83826701988902
C    1.17342346245580     2.23327949238212     0.09487738289834
C    0.63446541309113     1.48517338237672    -1.03878122197157
C   -0.77290659424245     1.50060021311302    -0.94328317254787
C   -1.13578079779915     2.26533300254933     0.24714658788800
C   -2.52539586101980     2.56071274041408     0.68574754637054
H   -3.17862034949864     1.68677501065123     0.56348643610062
H   -2.94627282293772     3.37340229722423     0.07043887021362
H   -2.55343385729740     2.87661543032321     1.73329682041889
C   -1.74645358383444     0.82062164961487    -1.84353707446734
H   -2.56389881382376     0.36597159382269    -1.26899906762048
H   -1.26625573114469     0.03557417036687    -2.44015848173300
H   -2.19600910489780     1.54483577035369    -2.54105323942378
C    1.46076994490474     0.86837858852715    -2.11154444689686
H    0.92075741980261     0.08087456843009    -2.65132244323561
H    2.38803677686289     0.43767194761773    -1.71460076547143
H    1.74730012663000     1.63885431665304    -2.84544170379375
C    2.62232660692351     2.47827198528239     0.34347135844351
H    3.23386288840599     1.60989628407484     0.06706241582550
H    2.81727532472429     2.71484666925815     1.39616862336966
H    2.97001957874990     3.33293028642268    -0.25951722227336
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C    0.16598952826557     3.74718216600223     1.96511013713345
H   -0.58817910801196     3.54425131358429     2.73459511405263
H   -0.00322038489776     4.76545701204873     1.57910303414735
H    1.15507362297940     3.73989783791358     2.43911390198113
H    1.03728484262829    -2.61090411195505    -1.35757990664369
H   -0.52069831473206    -3.82125525904166     0.47776115016609
C    0.87371545025492    -0.69850794906302     2.96193274398693
C    0.09732033993636     0.60873227640770     2.85848358425047
H    1.62262878424860    -0.66188727931525     3.76755122251077
H    0.16666446277848    -1.50469071290272     3.20756123251153
H    0.66016528023233     1.48141699500226     3.20263052668712
C   -1.24845035966951     0.54150087681827     3.48141680155149
O   -1.88475380963359    -0.47855942740519     3.69943716923512
O   -1.72363510318017     1.78181508295797     3.80705133408800
C   -3.02815232372877     1.78524359916068     4.43546206809578
H   -3.25190789127726     2.83687888749410     4.63768447279964
H   -3.00177396898176     1.20976220697449     5.36857234903364
H   -3.77902669384360     1.34661057660887     3.76611053080012
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**Int3<sub>AcOH</sub>**

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C    2.68573017819439     2.63887069788350     1.26964169743118
Co   0.21699241146424    -1.31490387330676     1.15368586745247
N    2.33019338427246     1.97974382143400     2.53620298125611
C    1.73293541412268     0.77989763574857     2.61998591522263
O    1.45687984013461     0.15264320233314     1.55672089459941
C    1.43096070137345     0.25386836582629     3.96759646246418
C    0.91600961136956     1.10537266306611     4.95934967380046
C    0.60932786964389     0.60902100992843     6.22448960404497
C    0.83576913614361    -0.74132572884887     6.50408237105121
C    1.36692942060980    -1.58129268023488     5.52358690399842
C    1.67157555211061    -1.10805810966028     4.24199028904644
H    0.72344430377481     2.15426145517400     4.72564377387044
H    0.19732504164977     1.26986848448496     6.98683109676662
H    0.60751452462080    -1.13903315355854     7.49316755207890
H    1.56737864890928    -2.62829122555049     5.75865199681465
H    1.97731698176008     2.23963838540817     0.52986363827961
C    4.10938074371971     2.26198389907333     0.84904289771566
C    2.48998426793498     4.14591590789028     1.41717014160167
H    4.22009863286688     1.17282801603240     0.76352324120736
H    4.84302490126003     2.63003359669167     1.58083399012725
H    4.34861669830415     2.71575179148511    -0.12239742396150
H    3.16889797947889     4.56038469393268     2.17821664031358
H    1.45765082875361     4.39056593333226     1.70156982855583
H    2.71374768568822     4.65013736079258     0.46808751538197
C   -1.34540689854231    -0.50693811940009    -0.03936024302150
C   -1.40556713826359    -1.95705472298664     0.06816385416592
C   -1.57700977665593    -2.30132721548673     1.44562145893195
C   -1.51430214538910    -1.08218346053692     2.21333653982258
C   -1.40959568262781     0.02043764757034     1.27229016731423
C   -1.34504601085857     1.46136446999045     1.64594140562991
H   -0.96838614328688     1.59873852395788     2.66718687601279
H   -2.35279607298093     1.90462181135421     1.60844338352706
H   -0.70721284076238     2.03109945229985     0.95821816122698
C   -1.75224961753795    -0.97726822414233     3.67948156130627
H   -1.38229909684649    -0.03319509379082     4.09300022697379
H   -1.27185602874036    -1.79503414465357     4.23006346391391
H   -2.83360279205208    -1.03101481609613     3.88703141395922
C   -1.90216541691553    -3.65244278061353     1.98231403012163
H   -1.67915577879633    -3.73649041975843     3.05391288835460
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H   -1.36016586971101    -4.44689357427978     1.45816033548081
H   -2.98214257976550    -3.83337488742772     1.85956427831257
C   -1.35432110670047    -2.90552132019691    -1.07721737105979
H   -1.09849784977799    -3.91849344933078    -0.74643076186244
H   -0.61725356560634    -2.58235472972834    -1.82256373011986
H   -2.33720832720760    -2.95131052507947    -1.57444941368635
C   -1.20353988841726     0.24956189966474    -1.31361337271034
H   -0.89561204322061     1.28820870431267    -1.13994784629838
H   -2.16086233878704     0.27253320503689    -1.85829348347720
H   -0.46101849028735    -0.22945395079017    -1.96601021082020
C    1.19084648782618    -2.67447954238922     2.31828494858743
C    2.26079192964545    -2.03297566782762     3.21185493795224
H    0.41090634667945    -3.13988779321796     2.92815642627437
H    2.80986999035701    -2.83134417276000     3.74026007009178
H    3.00479767561244    -1.50423235243083     2.60083156266706
C    1.76347755850448    -3.66667786378350     1.39960597990973
O    2.88360823870273    -3.58742958994721     0.86431850739425
H    2.67084839596624     2.39038390282583     3.40225876642145
C    2.51971398946253    -1.01371012757431    -0.78462676350777
O    1.34799780452679    -1.39540859779088    -0.56393597989884
O    3.56096330624973    -1.37305317289399    -0.07833731411585
H    3.31549616664572    -2.22753369114831     0.48048840697711
C    2.81632977109442    -0.10937743573187    -1.94556092168122
H    2.08420639264163     0.70666380761738    -1.98373854143923
H    2.71223640574996    -0.68881518278205    -2.87533780712317
H    3.83639967424660     0.28330822014481    -1.89312074356887
O    0.97452835268294    -4.73346083680419     1.16469195559726
C    1.47914288859876    -5.69415249985494     0.20094943825021
H    0.71503495558898    -6.47516828756147     0.14759172554726
H    2.43495135487536    -6.10934168160671     0.54081040520177
H    1.61718105591950    -5.21350186372924    -0.77574322065460
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**Int3O$_{AcOH}$**

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C    4.86885381713972     2.54627883724560     3.19733307134987
Co   2.39915601343497    -0.30404178809608     0.09489010830576
N    3.74117243605540     1.69227639561306     3.61547557062555
C    2.94123637187993     0.93034575764329     2.86459907063243
O    3.00342966823433     0.96266624150706     1.58273576178342
C    1.80137372036326     0.32505432267592     3.62691880442931
C    0.79780960503745     1.24266442572425     3.99828779054316
C   -0.29773794057357     0.83674904057184     4.75472369612843
C   -0.38169836217886    -0.49510769354722     5.17303079950272
C    0.62059305412072    -1.39467415600876     4.82255386010765
C    1.72422975667731    -1.01333085954786     4.04111130685682
H    0.89358552479718     2.28657621696694     3.69491680953046
H   -1.06726196802786     1.55680300044649     5.03295925045964
H   -1.22252143486645    -0.82630603887960     5.78342220953555
H    0.55876584078149    -2.43047955928467     5.16209934848103
H    4.59828107284048     2.97337393545074     2.22274205527146
C    6.15278601958568     1.72710322919634     3.06421398121376
C    4.99724859070141     3.68531191716821     4.20738168999846
H    6.02421173240154     0.88005841849015     2.37910758195546
H    6.45925029073945     1.33295357532416     4.04396753604890
H    6.96129208479155     2.36728833220406     2.68681929887415
H    5.24012571113695     3.29645206659234     5.20824515975290
H    4.07274193419999     4.27493477046187     4.27399269048557
H    5.81222064059785     4.35696543118413     3.90932635900654
C    1.26283537875651     0.48664137106391    -1.43053342580034
C    1.57220428975570    -0.91839684489611    -1.66120364139715
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C    1.00356752494691    -1.68272383340076    -0.59076920885215
C    0.40883296814181    -0.76727536693829     0.34301970632268
C    0.55767022937907     0.57487958680621    -0.19763231010831
C    0.03932459032816     1.82325112868477     0.42732692838046
H   -0.05925177061463     1.71754958965027     1.51374719100940
H   -0.95999292151883     2.05178899145369     0.02336830304662
H    0.68574169856840     2.68378938974960     0.21477504679103
C   -0.39221279186682    -1.16074390371603     1.53246321733962
H   -0.49786128314093    -0.34414022268753     2.25482928403160
H    0.04587228659536    -2.02186853767428     2.04838686122359
H   -1.40562978116649    -1.44946999291246     1.20723435886900
C    1.10338798626652    -3.15637363365609    -0.42073242451587
H    0.25963410044225    -3.54566340416301     0.16226792553999
H    2.03394830573237    -3.40399242886091     0.11819646621970
H    1.12241867893630    -3.66703573185996    -1.39114642829024
C    2.31507749709574    -1.46679108816767    -2.82694526107279
H    2.71446190562320    -2.46481863168616    -2.61286653819934
H    3.15273440898158    -0.81652196419681    -3.10772668597419
H    1.64389377418440    -1.54738123352597    -3.69749199588470
C    1.61495196190770     1.61733721539848    -2.33455543705064
H    1.77742756100466     2.54886717302899    -1.77769321501911
H    0.79510034640447     1.79938799580525    -3.04818566417276
H    2.51511265746184     1.39925234620320    -2.92139246181182
C    4.06113131020753    -1.60594052478450     3.13542373809382
C    2.74007755765217    -2.07025665366526     3.65666830207708
H    4.89771016042425    -1.45799362574391     3.81692594693083
H    2.26743207201396    -2.70108977769697     2.88285556590080
H    2.89171028631993    -2.72315633289655     4.53088338278238
C    4.28863010509491    -1.52592199128912     1.79318770195037
O    3.38197813295481    -1.77900770654144     0.88544186903265
H    3.57955296463454     1.61782504644063     4.61805845593005
C    4.82272090148359     1.18955651457189    -0.91189798359042
O    4.07751753737287     0.19431671881590    -0.98335810558595
O    4.71340045306544     2.10123045979044     0.03177444814352
H    4.03453551686876     1.75057742469692     0.71544728790977
C    5.91619923260427     1.42820677883851    -1.90380513151132
H    5.87765576837709     0.68605526893609    -2.70594787040775
H    6.88594494615180     1.36782524838735    -1.38919208647656
H    5.83335544173884     2.44341479893333    -2.31485587386820
O    5.54294128138457    -1.11861954887765     1.37729019431150
C    6.08164937220693    -1.85752452901502     0.26322037403179
H    7.02550413723031    -1.36557353260671     0.00474328283045
H    5.39676533106019    -1.84111934712095    -0.59288944217007
H    6.28252870907804    -2.89728547777758     0.56273054218196
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**Int4C**

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C   -4.07242055917192    -0.63592876254153    -4.59430526536495
Co  -1.47465482724551     1.15903430212473     1.04655173491723
N   -4.69243045388360    -0.02529338905176    -3.40929962040901
C   -4.52703619457179    -0.52708766994553    -2.15756235895917
O   -3.84951030116519    -1.53386230432871    -1.91893075939490
C   -5.22195101980358     0.22035744623556    -1.05110188658342
C   -4.58425441145212     0.37305261098293     0.19847362220794
C   -5.30243731468220     0.92812601831625     1.26135990268764
C   -6.62149296704433     1.35572271313515     1.10328461930495
C   -7.24205071322307     1.23188600834103    -0.13983219619826
C   -6.54344494499752     0.66183595200639    -1.20483897968524
H   -4.82272674473143     1.01061747823223     2.23892739430040
H   -7.16417677079158     1.77440992053551     1.95091240890574
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| H | -8.27467204781243 | 1.55288609271775 | -0.27500121098618 |
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| H | -4.12088404431172 | -1.72256365607806 | -4.42872294037998 |
| C | -2.60015061253984 | -0.22633708099303 | -4.70474402943370 |
| C | -4.88303407341376 | -0.26246136087668 | -5.83200375515873 |
| H | -2.05083928299563 | -0.51259236797205 | -3.79791784926375 |
| H | -2.50971674941451 | 0.86081706382399 | -4.85218736280558 |
| H | -2.12780769963922 | -0.72668483762241 | -5.56125731468249 |
| H | -4.87317179997482 | 0.82681177398830 | -5.99741408414091 |
| H | -5.92649483245805 | -0.59349439044154 | -5.74191413466148 |
| H | -4.45218685408386 | -0.73445212653834 | -6.72401001631285 |
| C | -2.04117142648178 | 3.10382429496295 | 1.24981488211404 |
| C | -1.74022429964867 | 2.55256953460243 | 2.56947302181745 |
| C | -0.40021144102903 | 2.08146298300756 | 2.56602245126480 |
| C | 0.14987991692131 | 2.34752042627096 | 1.24426475373478 |
| C | -0.85306093039961 | 3.00759605802899 | 0.44847709798580 |
| C | -0.67651908840186 | 3.50627659749938 | -0.94633730909125 |
| H | -0.02427377127463 | 2.84845157923353 | -1.53417706779998 |
| H | -0.21241714469164 | 4.50507651588136 | -0.93125536238840 |
| H | -1.63610479348102 | 3.59641609635780 | -1.46843764793093 |
| C | 1.53962768747184 | 2.02925088718416 | 0.81866215356201 |
| H | 1.63097850098181 | 1.97563773085392 | -0.27311754372269 |
| H | 1.88847792797131 | 1.08575034058799 | 1.25576138681257 |
| H | 2.22130794427481 | 2.82281646800076 | 1.16706395197920 |
| C | 0.33551795117076 | 1.43704436183865 | 3.69123388749872 |
| H | 1.01551751903673 | 0.65406696179344 | 3.33180375465654 |
| H | -0.34863210891908 | 0.98458189042864 | 4.41867766205564 |
| H | 0.94456621030494 | 2.18422287389747 | 4.22580033443194 |
| C | -2.67906108798532 | 2.53232043246899 | 3.72710299962517 |
| H | -2.47990074602446 | 1.69244767722952 | 4.40373322276107 |
| H | -3.72635771450189 | 2.48730246994749 | 3.40574009261172 |
| H | -2.56099340036907 | 3.46132175574317 | 4.30897336345684 |
| C | -3.31936210323688 | 3.75352835644101 | 0.84469319570996 |
| H | -3.52302553400827 | 3.62048073499229 | -0.22526438688759 |
| H | -3.26434664370880 | 4.83703056563039 | 1.04111345384260 |
| H | -4.17769310408586 | 3.35839250506549 | 1.39884546928023 |
| H | -7.04959505492781 | 0.51068470804178 | -2.15987208778191 |
| H | -5.20083605240770 | 0.84680656611967 | -3.52509584698350 |
| C | -3.17093847271790 | -0.09642847715409 | 0.41386693001814 |
| C | -2.14985637767400 | 0.31982045347539 | -0.59265073427510 |
| H | -3.11227264559557 | -1.18191234006009 | 0.59605128082200 |
| H | -2.86429869948709 | 0.26751823124733 | 1.50638443991151 |
| H | -2.42318812936021 | 0.83761760970705 | -1.50845817866679 |
| C | -0.87527062345309 | -0.33568624521390 | -0.45692352695458 |
| O | -0.52322868766006 | -0.63924362787708 | 0.73447589095575 |
| O | -0.09554334071490 | -0.48274594450087 | -1.51999160298378 |
| C | 1.20356482649187 | -1.10363312603744 | -1.29434555331172 |
| H | 1.66432348091297 | -1.15752233728671 | -2.28366672414533 |
| H | 1.06760634147162 | -2.10596461976751 | -0.87233650624480 |
| H | 1.80657133464392 | -0.49191038269203 | -0.61424951564343 |

**Int 4C<sub>AcO</sub>**

| C | 4.87045526780905 | -3.73257668977807 | -2.21735102722688 |
|---|---|---|---|
| Co | 0.50106521515076 | -0.39724599540550 | 0.75527656700848 |
| N | 3.68473120673761 | -4.14336886160241 | -1.45495693045485 |
| C | 3.65749551800574 | -5.19859035045649 | -0.60275095494950 |
| O | 4.64408153074473 | -5.90474057267936 | -0.35146450421146 |
| C | 2.31621401548319 | -5.53416805027427 | 0.01529744426741 |
| C | 2.01035957223105 | -6.90711740054930 | 0.02268017357462 |
| C | 0.83691911432237 | -7.38703849842839 | 0.59299832964663 |

| C | -0.03970735999517 | -6.49007938309968 | 1.21168937016635 |
| C | 0.26866129717708 | -5.13354894863513 | 1.23288951447571 |
| C | 1.43077033498591 | -4.62236877332072 | 0.62740515484344 |
| H | 2.73314439098266 | -7.59039573583862 | -0.42386220910360 |
| H | 0.61294936935553 | -8.45465178792387 | 0.57084124818101 |
| H | -0.95409054114269 | -6.85024065190032 | 1.68608629551289 |
| H | -0.40014960907276 | -4.43888055698599 | 1.74522979726651 |
| H | 4.54257967847712 | -2.83623109980884 | -2.76762265123469 |
| C | 5.28203355643543 | -4.80193024246403 | -3.23806293538832 |
| C | 6.03750164674054 | -3.33754215457164 | -1.30478500702527 |
| H | 4.44256319001294 | -5.04569758005111 | -3.90394821927833 |
| H | 5.59611892473444 | -5.71648489951289 | -2.71923919868878 |
| H | 6.11919232926118 | -4.41135053469557 | -3.85410992495912 |
| H | 6.39539347767883 | -4.21010637215776 | -0.74561819560074 |
| H | 5.72950674510454 | -2.56675896791630 | -0.58457878209133 |
| H | 6.86471315168077 | -2.93399434192731 | -1.90640272791634 |
| C | 1.06685869714417 | 1.44155036973784 | 1.54539945976615 |
| C | 2.19407876521850 | 0.53871865976828 | 1.37918667541676 |
| C | 2.31659858688035 | 0.21523488443113 | -0.01207132187642 |
| C | 1.21496028900174 | 0.83687177300727 | -0.70452992661433 |
| C | 0.47025201835666 | 1.61497890396352 | 0.26602722131008 |
| C | -0.76913925427865 | 2.38384234510839 | -0.04466515394407 |
| H | -1.41799269643250 | 1.82176295576954 | -0.72880350772248 |
| H | -0.51481932175668 | 3.33991388394450 | -0.52963656786935 |
| H | -1.34643791091402 | 2.60486885437596 | 0.86097328739791 |
| C | 0.98088632483185 | 0.82004666245507 | -2.17662895086963 |
| H | -0.09083407165120 | 0.85871549461415 | -2.41170381603702 |
| H | 1.40273023702837 | -0.08341288098333 | -2.63389831108468 |
| H | 1.45863818636194 | 1.69164774013433 | -2.65489256837693 |
| C | 3.43088592419108 | -0.53258906502029 | -0.65769530805769 |
| H | 3.06827638172781 | -1.20885793986326 | -1.44169059750581 |
| H | 3.99913940567353 | -1.12465635040458 | 0.06837541962138 |
| H | 4.13113757602100 | 0.18185402209991 | -1.12129681828242 |
| C | 3.05717938870369 | 0.04856659099490 | 2.49197051037923 |
| H | 3.70908978260983 | -0.77288640077368 | 2.17067671396898 |
| H | 2.44655025740244 | -0.31180427646391 | 3.33176282515411 |
| H | 3.69815162796741 | 0.86118968722169 | 2.87099670568954 |
| C | 0.60884915500828 | 2.00938048163234 | 2.84733842218492 |
| H | -0.42475351877877 | 2.37256396389083 | 2.78649859839885 |
| H | 1.24254709254982 | 2.85678863698839 | 3.15437381251329 |
| H | 0.65440746487671 | 1.25305185153885 | 3.64283544122762 |
| C | 0.53976314021462 | -2.31350039649125 | 0.08322268028002 |
| C | 1.66312453590062 | -3.12245609385981 | 0.73334533510390 |
| H | -0.44076544562398 | -2.63050641356411 | 0.45368766613107 |
| H | 2.63654700020361 | -2.85593456042663 | 0.31312865632189 |
| H | 1.68676145112463 | -2.85960827929602 | 1.80078117764213 |
| C | 0.49359700727599 | -2.34076586800501 | -1.38331865795723 |
| O | 1.43263475610304 | -2.55765362647953 | -2.15959548634436 |
| C | -1.34375527518660 | -1.01485917857194 | 2.11284161066389 |
| O | -1.50651388653457 | -0.51481266610617 | 0.94882103816764 |
| O | -0.13615914266224 | -1.17057460645348 | 2.51221343155172 |
| H | 2.80425286368063 | -3.66450913714456 | -1.68073408397862 |
| C | -2.50989044330750 | -1.43738930166166 | 2.95532709469524 |
| H | -2.21987856531330 | -1.50001818316808 | 4.01029274566072 |
| H | -2.84832628824629 | -2.43050458667851 | 2.62498202363409 |
| H | -3.34581670386621 | -0.73898384282560 | 2.82432954283029 |
| O | -0.75750012277311 | -2.08680006726328 | -1.86576938277973 |
| C | -0.89705928702693 | -2.16380247364931 | -3.29560210129730 |
| H | -1.95096845909861 | -1.94476311264108 | -3.49541723345011 |
| H | -0.63616507875940 | -3.16833011248160 | -3.65533396287125 |

H    -0.25099046674861       -1.43190289141659      -3.79807596560573

**Int 4O<sub>AcOH</sub>**

| | | | |
|---|---|---|---|
| C | -4.18255036753871 | -2.40013628289245 | 5.13701141537214 |
| Co | -2.06391083831784 | 0.92839441165212 | 0.24181193830166 |
| N | -2.97585800107226 | -2.82010937237218 | 4.41137389690746 |
| C | -2.74527254389169 | -2.51169973498132 | 3.11448402239327 |
| O | -3.54942892894814 | -1.87235278699831 | 2.41805783785933 |
| C | -1.47010836062009 | -3.06374831660286 | 2.53739722758499 |
| C | -0.55392005629404 | -2.23526739504047 | 1.85456300098534 |
| C | 0.55618581552463 | -2.82575115471032 | 1.23582391884605 |
| C | 0.77331838598803 | -4.20301568553596 | 1.29345032541885 |
| C | -0.12948079616973 | -5.01635893465224 | 1.97960442928259 |
| C | -1.24285012333476 | -4.44439219201407 | 2.59960611609261 |
| H | 1.27268261542261 | -2.18462130447401 | 0.71728834835281 |
| H | 1.64824543124968 | -4.63837758435157 | 0.81015964165874 |
| H | 0.02670379985547 | -6.09452729439081 | 2.02831160429073 |
| H | -5.00115522773987 | -2.45422458343709 | 4.40369763866949 |
| C | -4.04930450111045 | -0.95210829469634 | 5.61605951825889 |
| C | -4.44265559427583 | -3.37856683112150 | 6.27839533637220 |
| H | -3.83321423130582 | -0.29059068377256 | 4.76873359147748 |
| H | -3.23480063872671 | -0.85424216585059 | 6.34913325731363 |
| H | -4.98223602903007 | -0.61996856867992 | 6.09268878262969 |
| H | -3.61573100346048 | -3.36245400454321 | 7.00628207796534 |
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| H | -5.35912331453694 | -3.10115788593883 | 6.81566770737735 |
| C | -2.11214700669087 | 0.29763733143675 | -1.69654045689879 |
| C | -3.07771708194758 | -0.43985989434787 | -0.91951161538546 |
| C | -3.97619034572355 | 0.50747416980914 | -0.30539927630865 |
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| C | -2.45777308417104 | 1.69780197401921 | -1.61836618124894 |
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| H | -4.55425195459022 | 3.06816709604648 | 0.71261970454009 |
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| C | -3.13683626858877 | -1.91654844791431 | -0.75682056228461 |
| H | -3.45977405654752 | -2.18852345384107 | 0.25745123402850 |
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| C | -0.96592975706153 | -0.27755887865030 | -2.45634134449747 |
| H | -0.09538362549037 | 0.39076950779771 | -2.43462819005391 |
| H | -1.24178543359689 | -0.43279731953785 | -3.51163233544229 |
| H | -0.66248637509748 | -1.24863951611686 | -2.04725195978117 |
| H | -1.96513293832267 | -5.08073928464040 | 3.11397136716992 |
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| C | -0.71202161735655 | -0.74299359216943 | 1.78680128058732 |
| C | -1.06784519900716 | -0.05352709717822 | 3.04350247846474 |
| H | -1.59133947782841 | -0.56326628232183 | 1.03173083215837 |
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| C | -1.83443905239363 | 1.07912981129849 | 3.05846801316198 |

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| O | -0.22548886661375 | 1.72931764139153 | 0.23880340283047 |
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| H | -1.59572399987022 | 2.94302256415584 | 1.65575157022130 |
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| H | 1.92710472751302 | 3.49424793154001 | 1.46467447091137 |
| H | 1.26070486058325 | 4.53278727795872 | 0.20007005721568 |
| H | 1.96116548444195 | 2.92856386782677 | -0.23603622636767 |
| O | -2.03827441761860 | 1.70722567289533 | 4.24208251685604 |
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| H | -3.18993288374843 | 2.92293781204409 | 5.37523925144236 |
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**TS 4**<sub>alkene</sub>

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| O | 2.85667869391159 | -4.72510143629133 | 3.09964879930410 |
| C | 1.16115957324763 | -4.93382130846304 | 1.42324391042291 |
| C | 0.48785741840186 | -5.98420604668492 | 2.06055545946728 |
| C | -0.81815564634789 | -6.32072097376487 | 1.71438495921515 |
| C | -1.47035073577576 | -5.59215377242734 | 0.71773909305539 |
| C | -0.82322893710192 | -4.52362864784037 | 0.10284352915780 |
| C | 0.49030987224295 | -4.16239875505932 | 0.44389480995249 |
| H | 1.01450581946674 | -6.52988342444137 | 2.84374278105916 |
| H | -1.32112626114734 | -7.14756967582831 | 2.21675778354362 |
| H | -2.48901786720430 | -5.84809079671252 | 0.42367995699103 |
| H | -1.35521723510547 | -3.94064943543370 | -0.64708984745755 |
| H | 5.43651793219560 | -4.59382746576803 | 0.16294815559391 |
| C | 5.32294089180438 | -6.18668466781953 | 1.61324358106592 |
| C | 5.53588986669805 | -3.71026533724576 | 2.11426998218831 |
| H | 4.95388942821961 | -6.93300165467297 | 0.89572474604671 |
| H | 4.86749288341439 | -6.38594614363954 | 2.59218009057641 |
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| H | 6.63065532561552 | -3.80070220673184 | 2.16193226052774 |
| C | 0.78693447574657 | 0.52313631858348 | 1.77157173059948 |
| C | 2.02648243374524 | -0.19185094219663 | 1.77060594179068 |
| C | 2.56957819323491 | -0.12442880455267 | 0.43476906071730 |
| C | 1.67500015199272 | 0.67492243555516 | -0.37276716385043 |
| C | 0.55985469620718 | 1.04497098145380 | 0.43489542328606 |
| C | -0.63766799922841 | 1.83167212176282 | 0.01799880242335 |
| H | -0.69144186623842 | 1.92986992672704 | -1.07295499916510 |
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| C | 1.92626339537157 | 1.11479417345031 | -1.77568521201440 |
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H    0.14145973281701     1.70496149975739    3.42889940683374
H   -0.00649672832713    -0.05493544426292    3.68221082428830
C    0.50053661222902    -2.18880391716611   -1.21714695201468
C    1.11654553973289    -2.94868118267520   -0.15778282432199
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C    1.28906220300260    -1.87075591477396   -2.41025681712369
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**TS4<sub>alkyl</sub>**

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C   -1.40078701054641    -2.97530859050558    2.61946364582555
C   -0.47542142160851    -2.21578100838278    1.87115277296197
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C    0.81341165588861    -4.24457113812539    1.45553190323797
C   -0.10116865610013    -4.98825142778293    2.20237961739131
C   -1.20075505030290    -4.35106278112122    2.78315728667317
H    1.35037231103456    -2.28322140766701    0.73336454695502
H    1.67915438669035    -4.73013685658096    1.00476304176837
H    0.03681592465441    -6.06206498322835    2.33234200199039
H   -4.40257833854817    -1.18068391749508    4.57283724433765
C   -3.53702909222599    -1.34703886728150    6.54689507270506
C   -5.05387620204118    -3.05539613872373    5.41264092589314
H   -2.80640744647184    -0.54641608165904    6.36970855328286
H   -3.08007520067957    -2.10540290966816    7.20205833599057
H   -4.39500691961182    -0.92431813486418    7.08659574214520
H   -4.66695348828761    -3.87625151717670    6.03453488565802
H   -5.36055299371550    -3.46659929383742    4.44188317655836
H   -5.94387598478181    -2.64449462975251    5.90877755771589
C   -2.10072612143293     0.29581099133107   -1.68740707105749
C   -3.06174848067309    -0.48178388947202   -0.92709149266860
C   -4.03464860632532     0.42211592177939   -0.37611704191800
C   -3.68496554481707     1.76104663423468   -0.80290571505871
C   -2.51669027377282     1.66775576098821   -1.64328289379390
C   -1.81732291385570     2.80723541498789   -2.29625542586598
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H   -2.26022831293267     2.98232664824801   -3.29009786985526
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| C | -0.91878591737503 | 0.05731385357213 | 2.94410126111093 |
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| C | 0.36106578045070 | 2.52300998825299 | 1.07371126163070 |
| O | -0.51158618943953 | 2.02728849872418 | 0.30828274323609 |
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| H | -0.07079429142843 | 1.36175449549875 | 2.64904421795552 |
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| H | 1.09855145993343 | 3.76155353772909 | -0.52486301364120 |
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**Int 5<sub>alkene</sub>**

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| O | 4.22346564657904 | -4.29119805368486 | 1.19154965625744 |
| C | 1.94257961187305 | -4.61639196200613 | 0.53192250401761 |
| C | 1.76419066321750 | -5.66479726747574 | 1.45694971070141 |
| C | 0.49092277221558 | -6.14408996430199 | 1.78916662829260 |
| C | -0.63255216221184 | -5.55891682668549 | 1.18065295930048 |
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| H | 0.37720441963518 | -6.97670541029786 | 2.49975409355409 |
| H | -1.64358817663138 | -5.93907424912011 | 1.39608646105256 |
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C   2.23287525391450     0.05370754265013   -0.63387431066319
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C  -0.79809572906006     1.86363360444284    0.76236500686440
H  -1.42610469186092     1.97504832019555   -0.14276307276027
H  -0.57140454029171     2.88480915746425    1.14173162286402
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C  -0.18980062433331    -1.48915344756869   -2.74211220467965
O   0.76610828809634    -1.48465448312995   -3.51583016550535
C  -0.43131943348826    -2.27043338370313    2.34244074039631
O  -0.78904908738916    -1.62755259266130    1.33123760620195
O   0.83804249788486    -2.52309508373501    2.59493877280004
H   3.01462767879523    -4.18886482680340   -1.73225676924130
C  -1.40429693770133    -2.78223329805354    3.35834049084794
H  -1.21402963909683    -2.29321933863389    4.33516801644953
H  -1.24650315039214    -3.87013211193517    3.49226847667575
H  -2.43781690209792    -2.57744706440693    3.03063382425898
O  -1.41284541281918    -0.98916185484697   -3.11245953457842
C  -1.50226515969730    -0.52401964892813   -4.46170686712529
H  -2.56966004041692    -0.29838142877792   -4.63898633480286
H  -1.14399939526832    -1.29371125919917   -5.17494248443504
H  -0.89523235089821     0.39236596005627   -4.61269535092344
```

**Int5<sub>alkyl</sub>**

```
C  -0.09795402162831    -6.48048489853235   -0.68171944237490
Co  2.34241808848532    -0.32130496235962    1.20962615264100
N   0.10984324210862    -6.23526665144832    0.76044199981114
C   0.85408679734955    -5.23747251096369    1.29754707818907
O   1.31659386922106    -4.29924742476279    0.61950217008015
C   1.10725621414744    -5.35321064120947    2.77417008981342
C   1.35846591055384    -6.62352477295596    3.32121181772353
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C   1.65686245353318    -6.78815134008464    4.67231134671644
C   1.69918848850081    -5.66860851520975    5.50217769991722
C   1.45679844414746    -4.40287888774037    4.96663101966577
C   1.17095371835697    -4.21204322115288    3.60821446755062
H   1.36591239570261    -7.49723100770053    2.66733490296816
H   1.86207492818506    -7.78215681046007    5.06952339700129
H   1.92441066743012    -5.77698052268995    6.56360532794442
H   1.48781786829195    -3.52866718780697    5.62030207904571
H  -0.71011852515638    -7.39457653259509   -0.71562185249401
C   1.22963928262449    -6.76194793165456   -1.39100678750461
C  -0.88562459560919    -5.35076477991580   -1.34837042572674
H   1.76286392141860    -7.59490033278364   -0.91318624064186
H   1.87308335155204    -5.87359440114605   -1.36997282583000
H   1.04267746202501    -7.03177509154806   -2.43931157573558
H  -0.28404100461980    -4.43561105804319   -1.36796366860183
H  -1.81938791571809    -5.14619900588164   -0.80857760741001
H  -1.13575676794589    -5.63191942715948   -2.38012863217728
C   4.20462966440119    -0.42481451866744    2.03608889183526
C   3.95994449585635    -1.62042145503691    1.27589019849683
C   3.66865529353852    -1.22155111074798   -0.08637984430250
C   3.74104412006445     0.20473961765924   -0.16583198932964
C   4.06592655621044     0.70988647494123    1.15991886432225
C   4.24464041195280     2.14288541488371    1.52185453842710
H   3.56069576689134     2.78669908218748    0.95587376036617
H   5.27363678843920     2.46254271401995    1.29028471283001
H   4.07959051904477     2.31494882281707    2.59245172416191
C   3.47375809818459     1.05375676802650   -1.35812050282830
H   2.80073149493292     1.88568936928789   -1.11007034917185
H   3.02536652296683     0.47726595634130   -2.17552080294284
H   4.41598262484744     1.48805543220914   -1.72785079863416
C   3.30440223306577    -2.16634779664750   -1.17645577630272
H   2.81628482365418    -1.65463762423047   -2.01415823372055
H   2.63885977360863    -2.95622018704552   -0.80305529779137
H   4.21593695166590    -2.64998741982997   -1.56338672422175
C   4.10552505645134    -3.02535358610488    1.74841831878885
H   3.32143481622307    -3.67616474849468    1.33663585298604
H   4.08139594776583    -3.09530983842325    2.84309343897484
H   5.08147820191158    -3.41593182378175    1.41456704661998
C   4.48415757278151    -0.37045242469134    3.49627603984520
H   4.09005409279888     0.54704422664736    3.94869747577127
H   5.71190556356899    -0.39269484421187    3.66889347218733
H   4.04411977985969    -1.22795493233671    4.01970785544200
C  -0.32732745062924    -2.51875626142758    2.35112298934349
C   0.97490394133272    -2.79731059243862    3.12087921548621
H  -0.97830699243673    -3.40080817578547    2.29327781595997
H   1.81094151090709    -2.52328233885503    2.46546389457315
H   1.03624460638717    -2.12519549072114    3.98395374316615
C  -0.13784219073695    -2.00908889628785    0.95180894455190
O   0.80657077754844    -1.33578720731964    0.51046035121683
C   0.80530166488158     1.15681627504905    2.25502799838007
O   1.36023167940456     0.18747567795910    2.88709266663505
O   1.15635900056992     1.30610259409503    1.03423483059412
H  -0.27954780903944    -6.91288835747306    1.40721211828364
C  -0.21683654381450     2.03602476934167    2.89975302326747
H  -0.19572939347386     3.03654475287072    2.45337613818894
H  -0.04878301764444     2.09007366864044    3.98167530059573
H  -1.21707885787867     1.60967751557766    2.72797734178166
H  -0.91763496333330    -1.74692663716501    2.87273859566194
O  -1.17361838022359    -2.28439188884513    0.16679140226126
C  -1.13354898668302    -1.73370213450909   -1.17740383528105
```

```
H   -2.06959081358514    -2.05366882575050    -1.64228505576299
H   -0.26997939585009    -2.13710181519629    -1.71903117777666
H   -1.06594182934522    -0.64022728472502    -1.13141366350736
```

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