Green alternative solvents for the copper-catalysed arylation of phenols and amides

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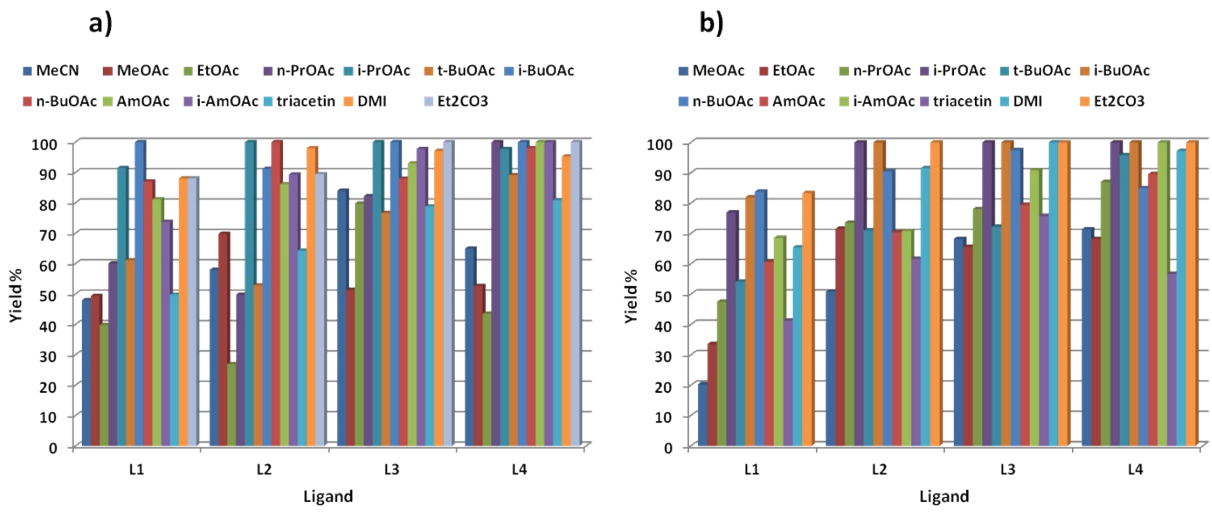


Figure S1: Synthesis of aryl ether **1**. Catalytic results ordered according to the ligand: a) base = Cs_2CO_3; b) base = K_3PO_4

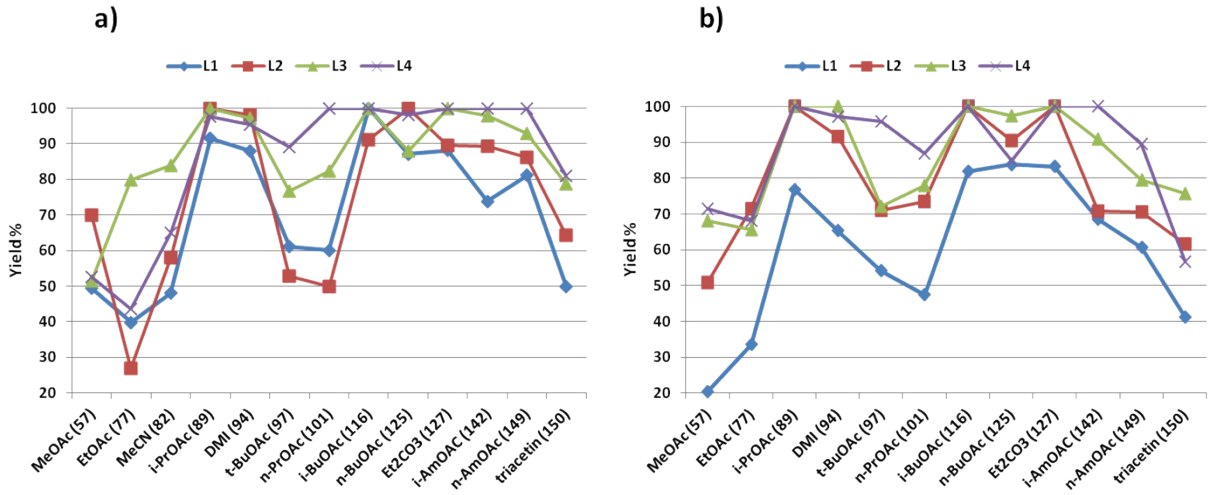


Figure S2: Synthesis of aryl ether **1**. Correlation with boiling points (°C); boiling points are reported in parentheses (temp. for triacetin is the reaction temperature, not the boiling point); a) base = Cs_2CO_3; b) base = K_3PO_4

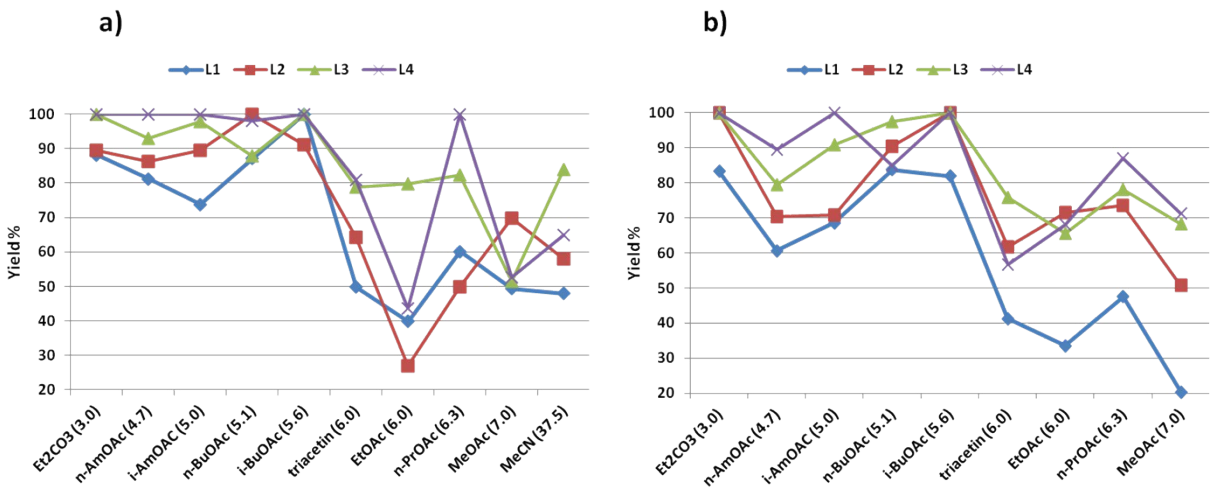


Figure S3: Synthesis of aryl ether **1**. Correlation with dielectric constants (dielectric constants values at room temperature are reported in parentheses)[1]: a) base = Cs_2CO_3; b) base = K_3PO_4

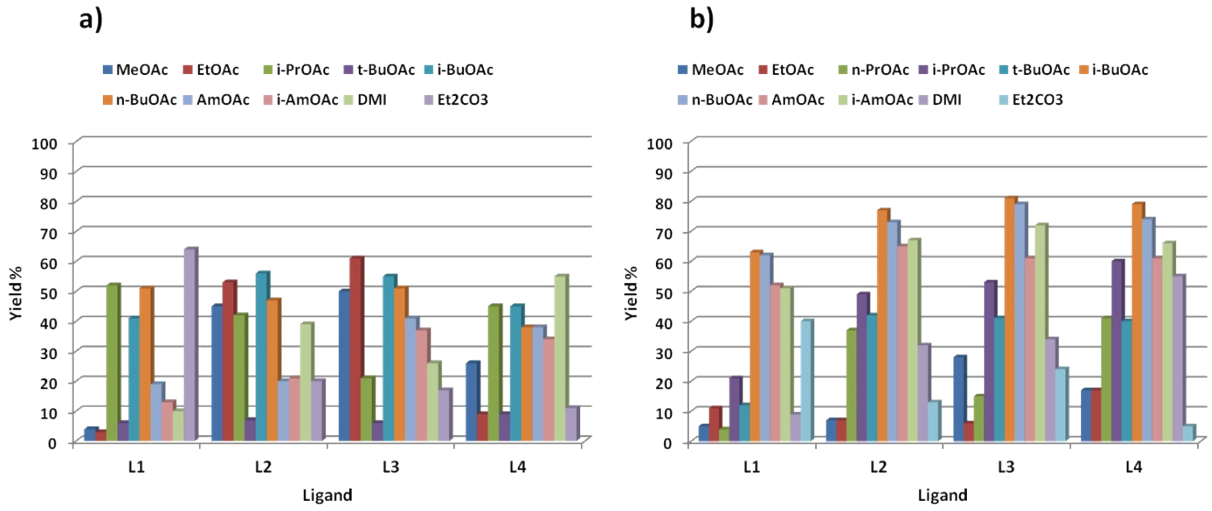


Figure S4: Synthesis of amide **25**. Catalytic results ordered according to the ligand: a) base = Cs_2CO_3; b) base = K_3PO_4

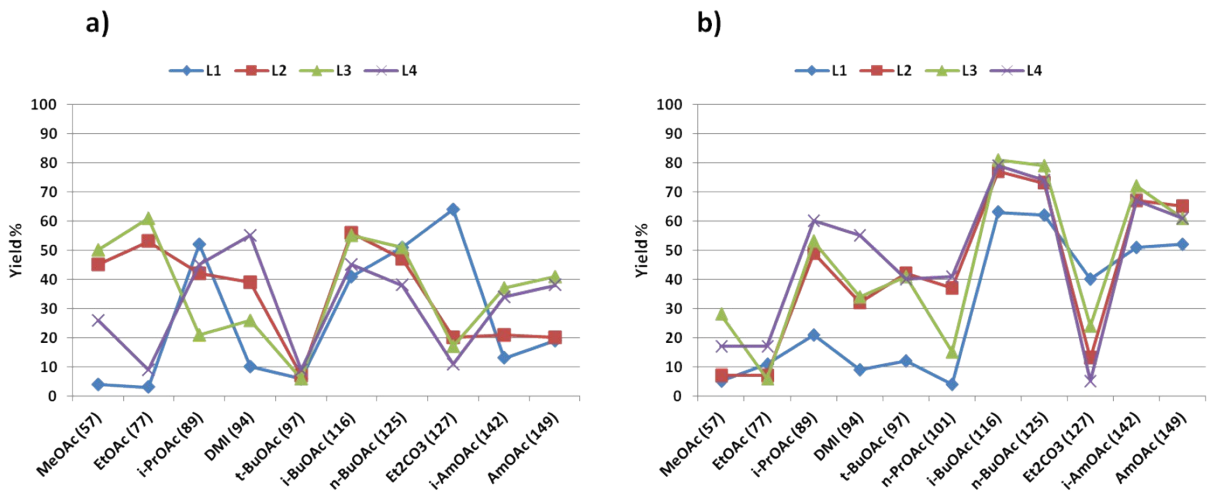


Figure S5: Synthesis of amide **25**. Correlation with boiling points (°C); boiling points are reported in parentheses; a) base = Cs_2CO_3; b) base = K_3PO_4

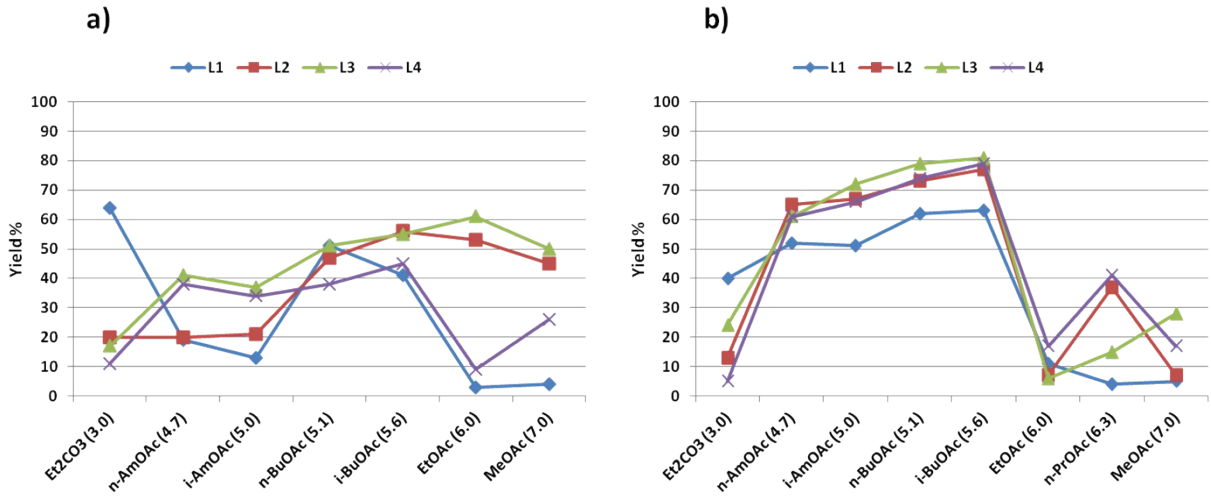


Figure S6: Synthesis of amide **25**. Correlation with dielectric constants (dielectric constants values at room temperature are reported in parentheses):[1] a) base = Cs_2CO_3; b) base = K_3PO_4

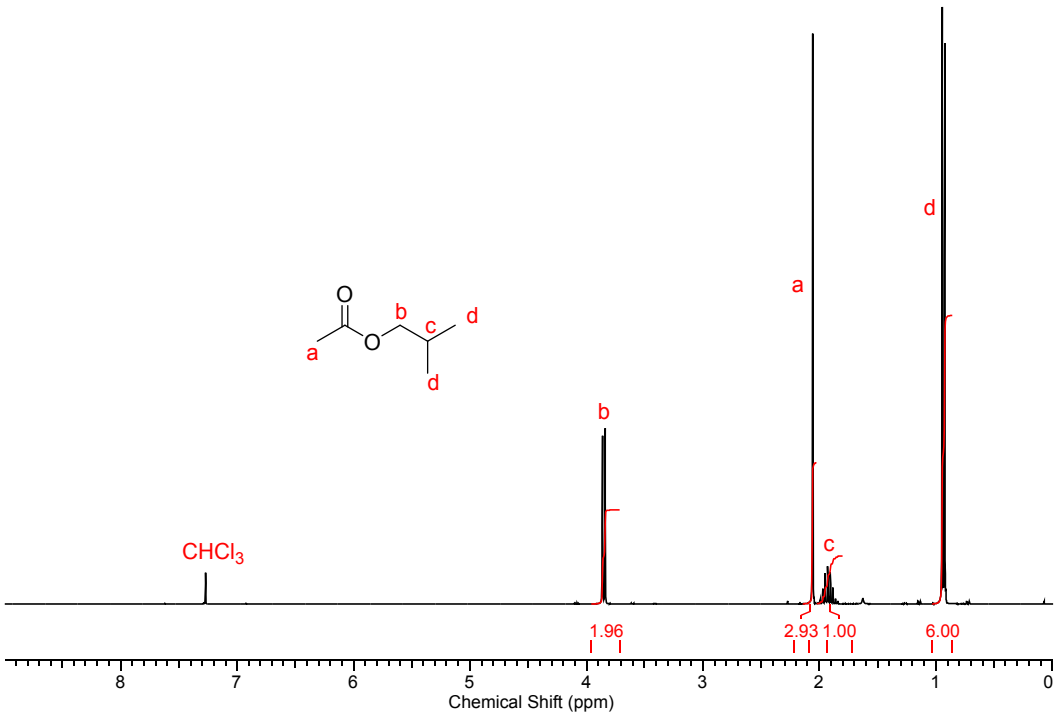


Figure S7: ^{1}H-NMR spectrum (300 MHz) of the Isobutyl acetate used for the arylation of amides, showing that no free isobutyl alcohol is present in the solvent

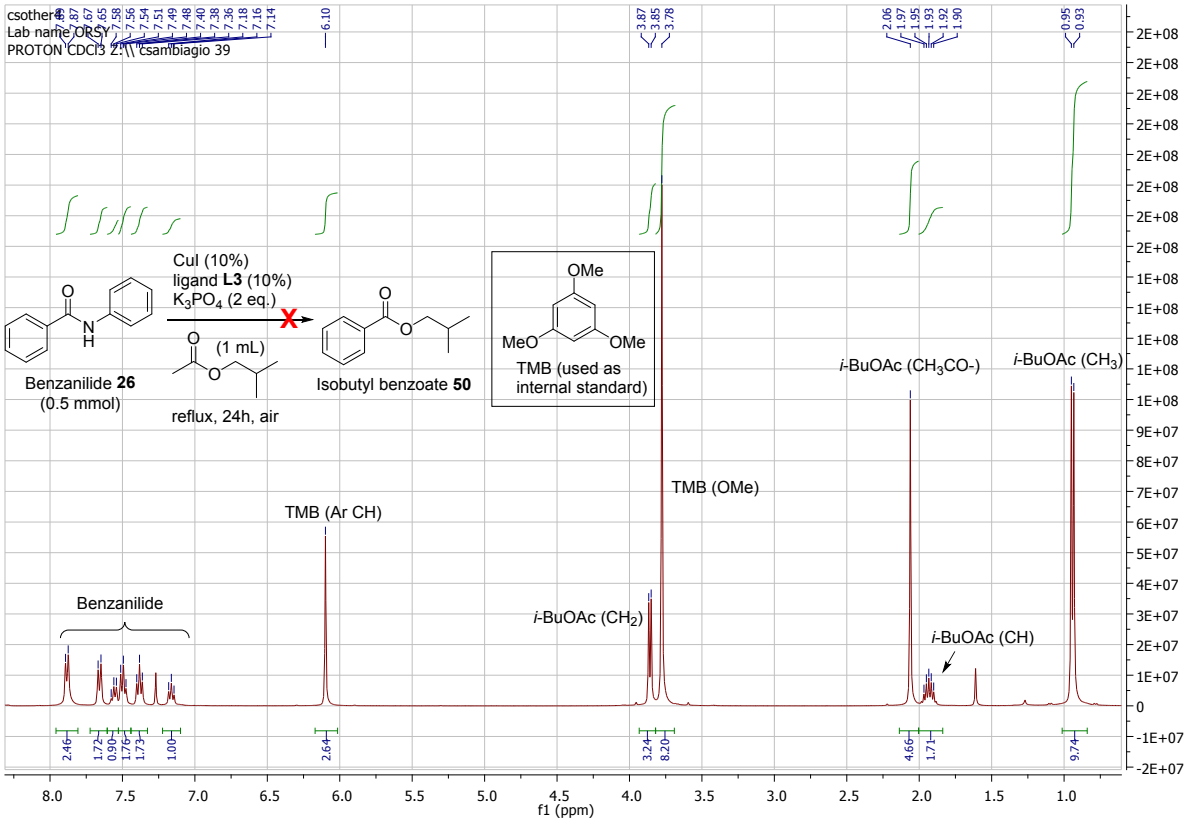


Figure S8: Crude ^{1}H-NMR spectrum (400 MHz) of the reaction between benzanilide **26** and isobutyl acetate in the catalytic conditions. No isobutyl benzoate **50** is observed (cf. chemical shifts/spectrum at pag. S68)

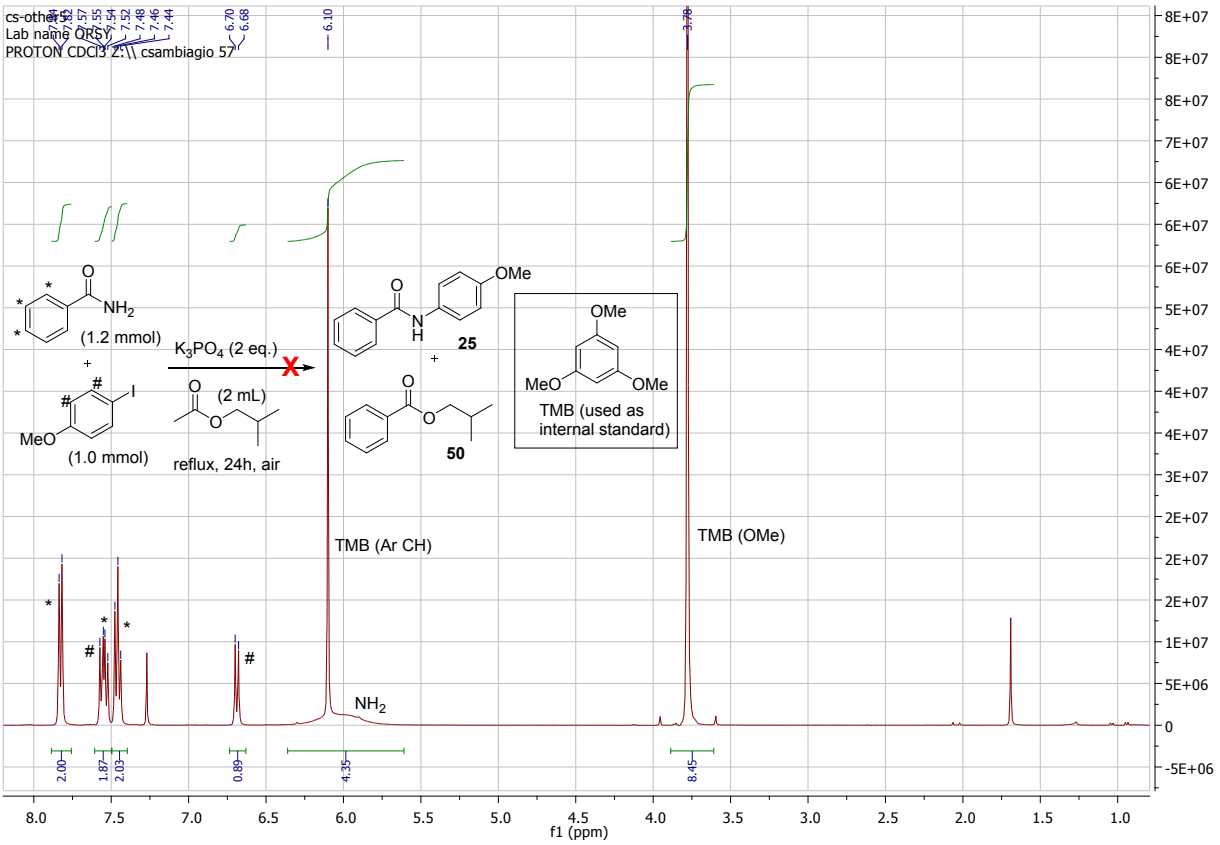
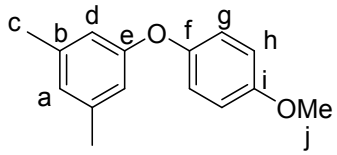


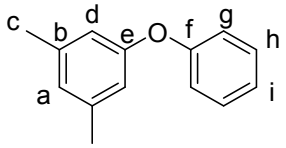
Figure S9: Crude ^{1}H-NMR spectrum (400 MHz) of the reaction between benzamide and 4-iodoanisole in isobutyl acetate in the absence of catalyst. No coupling product **25** nor isobutyl benzoate **50** are observed

Characterisation data for aryl ethers 1-24



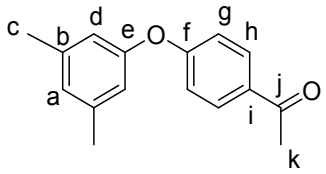
5-(4-Methoxyphenoxy)-1,3-dimethylbenzene (1)

Purified by column chromatography (Hexane/EtOAc : 100/0 to 95/5); white solid, yield 90% (205 mg). **^{1}H-NMR (500MHz) δ:** 6.98 (d, 2H, H_g, J_{g-h} = 9.2 Hz); 6.89 (d, 2H, H_h, J_{h-g} = 8.9 Hz); 6.70 (s, 1H, H_a); 6.58 (s, 2H, H_d); 3.82 (s, 1H, H_j); 2.28 (s, 6H, H_c). **^{13}C{^{1}H}-NMR (125MHz) δ:** 158.5; 155.7; 150.3; 139.4; 124.2; 120.8; 115.3; 114.8; 55.6; 21.3. **M/z (HR-APCI+):** calcd. for $C_{15}H_{17}O_2$ $[M+H]^+$: 229.1223. Found: 229.1227. **M.p.:** 72-74°C.



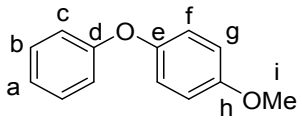
1,3-Dimethyl-5-phenoxybenzene (2)

Purified by column chromatography (Hexane); colourless oil, yield 99% (197 mg). **^{1}H-NMR (500MHz) δ:** 7.34 (t, 2H, H_h, J_{h-g} = J_{h-i} = 8.0 Hz); 7.10 (t, 1H, H_i, J_{i-h} = 7.4 Hz); 7.01 (d, 2H, H_g, J_{g-h} = 7.7 Hz); 6.76 (s, 1H, H_a); 6.65 (s, 2H, H_d); 2.30 (s, 6H, H_c). **^{13}C{^{1}H}-NMR (125MHz) δ:** 157.4; 157.1; 139.6; 129.6; 125.0; 122.9; 118.8; 116.6; 21.3. **M/z (HR-APCI+):** calcd. for $C_{14}H_{15}O$ $[M+H]^+$: 199.1117. Found: 199.1120.



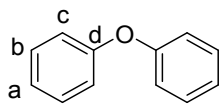
5-(4-Acetylphenoxy)-1,3-dimethylbenzene (3)

Purified by column chromatography (Hexane/EtOAc : 100/0 to 95/5); yellow solid, yield 93% (222 mg). **^{1}H-NMR (500MHz) δ:** 7.94 (d, 2H, H_h, J_{h-g} = 8.8 Hz); 7.00 (d, 2H, H_g, J_{g-h} = 8.8 Hz); 6.85 (s, 1H, H_a); 6.69 (s, 2H, H_d); 2.58 (s, 3H, H_k); 2.32 (s, 6H, H_c). **^{13}C{^{1}H}-NMR (125MHz) δ:** 196.8; 162.2; 155.4; 139.9; 131.7; 130.5; 126.3; 117.8; 117.2; 26.4; 21.3. **M/z (HR-ESI+):** calcd. for $C_{16}H_{17}O_2$ $[M+H]^+$: 241.1223. Found: 241.1228. **M.p.:** 84-86°C.



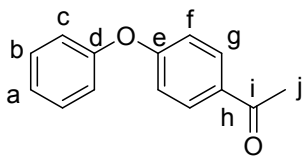
4-Phenoxyanisol (4)

Purified by column chromatography (Hexane/EtOAc : 100/0 to 95/5); colourless oil, yield 79% (158 mg). **^{1}H-NMR (500MHz) δ (ppm):** 7.31 (t, 2H, H_b, J_{b-a} = J_{b-c} = 8.0 Hz); 7.05 (t, 1H, H_a, J_{a-b} = 7.4 Hz); 7.00 (d, 2H, H_f, J_{f-g} = 9.0 Hz); 6.96 (d, 2H, H_c, J_{c-b} = 8.5 Hz); 6.90 (d, 2H, H_g, J_{g-f} = 9.2 Hz); 3.82 (s, 3H, H_i). **^{13}C{^{1}H}-NMR (125MHz) δ (ppm):** 158.5; 155.9; 150.1; 129.6; 122.4; 120.8; 117.6; 114.9; 55.6. **M/z (HR-APCI+):** calcd. for $C_{13}H_{13}O_2$ $[M+H]^+$: 201.0910. Found: 201.0916.



Diphenylether (5)

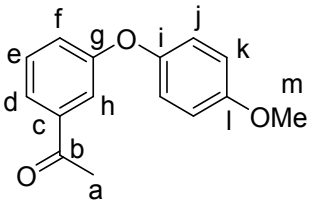
Purified by column chromatography (Hexane); white solid, yield 39% (67 mg). **^{1}H-NMR (500MHz):** 7.35 (t, 4H, H_b, J_{b-a} = J_{b-c} = 8.0 Hz); 7.11 (t, 2H, H_a, J_{a-b} = 7.3 Hz); 7.03 (d, 4H, H_c, J_{c-b} = 7.8 Hz). **^{13}C{^{1}H}-NMR (125MHz):** 157.2; 129.7; 123.2; 118.9. **M/z (HR-APCI+):** calcd. for $C_{12}H_{11}O$ $[M+H]^+$: 171.0804. Found: 171.0806. **M.p.:** 33-35°C.



4'-Phenoxyacetophenone (6)

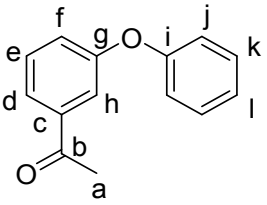
Purified by column chromatography (Hexane/AcOEt : 100/0 to 95/5); brown oil, yield 97% (205 mg). **^{1}H-NMR (500MHz):** 7.95 (d, 2H, H_g, J_{g-f} = 8.5 Hz); 7.41 (t, 2H, H_b, J_{b-a} = J_{b-c} = 7.9 Hz); 7.22 (t, 1H, H_a, J_{a-b} = 7.4 Hz);

7.08 (d, 2H, H_c, J_{c-b} = 7.7 Hz); 7.01 (d, 2H, H_f, J_{f-g} = 8.8 Hz); 2.58 (s, 3H, H_j). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 196.8; 162.0; 155.5; 131.9; 130.6; 130.0; 124.6; 120.1; 117.3; 26.4. **M/z (HR-ESI+):** calcd. for $C_{14}H_{12}NaO_2$ $[M+Na]^+$: 235.0729. Found: 235.0730.



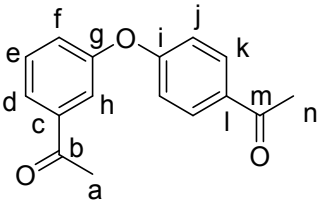
3'-(4-Methoxyphenoxy)acetophenone (7)

Purified by column chromatography (Hexane/AcOEt : 100/0 to 90/10); yellow oil, yield 59% (143 mg). **^{1}H-NMR (500MHz) δ:** 7.63 (dd, 1H, H_d, J_{d-h} = 1.1 Hz, J_{d-e} = 7.8 Hz); 7.49-7.53 (m, 1H, H_h); 7.39 (t, 1H, H_e, J_{e-d} = J_{e-f} = 7.9 Hz); 7.15 (ddd, 1H, H_f, J_{f-d} = 0.9 Hz, J_{f-h} = 2.4 Hz, J_{f-e} = 8.1 Hz); 7.00 (d, 2H, H_j, J_{j-k} = 8.9 Hz); 6.91 (d, 2H, H_k, J_{k-j} = 9.1 Hz); 3.83 (s, 3H, H_m); 2.57 (s, 3H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 197.5; 159.0; 156.3; 149.5; 138.8; 129.8; 122.4; 122.1; 121.0; 116.8; 115.1; 55.6; 26.7. **M/z (HR-ESI+):** calcd. for $C_{15}H_{15}O_3$ $[M+H]^+$: 243.1016. Found: 243.1016.



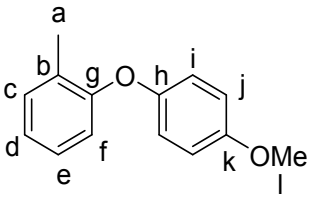
3'-Phenoxyacetophenone (8)

Purified by column chromatography (Hexane/AcOEt : 100/0 to 95/5); yellow oil, yield 84% (179 mg). **^{1}H-NMR (500MHz) δ:** 7.69 (d, 1H, H_d, J_{d-e} = 7.7 Hz); 7.58-7.60 (m, 1H, H_h); 7.44 (t, 1H, H_e, J_{e-d} = J_{e-f} = 7.9 Hz); 7.37 (t, 2H, H_k, J_{k-j} = J_{k-l} = 8.0 Hz); 7.22 (ddd, 1H, H_f, J_{f-d} = 0.9 Hz, J_{f-h} = 2.4 Hz, J_{f-e} = 8.1 Hz); 7.15 (t, 1H, H_l, J_{l-k} = 7.4 Hz); 7.03 (d, 2H, H_j, J_{j-k} = 7.7 Hz); 2.59 (s, 3H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 197.4; 157.8; 156.6; 138.9; 129.9; 123.8; 123.3; 123.1; 119.1; 118.1; 26.7. **M/z (HR-ESI+):** calcd. for $C_{14}H_{12}NaO_2$ $[M+Na]^+$: 235.0729. Found: 235.0732.



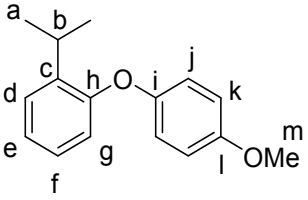
3'-(4-Acetylphenoxy)acetophenone (9)

Purified by column chromatography (Hexane/AcOEt : 100/0 to 90/10); white solid, yield 90% (230 mg). **^{1}H-NMR (500MHz) δ:** 7.97 (d, 2H, H_k, J_{k-j} = 9.0 Hz); 7.79 (dd, 1H, H_d, J_{d-h} = 0.9 Hz, J_{d-e} = 7.7 Hz);7.67-7.64 (m, 1H, H_h); 7.50 (t, 1H, H_e, J_{e-d} = J_{e-f} = 7.9 Hz); 7.26-7.30 (m, 1H, H_f); 7.03 (d, 2H, H_j, J_{j-k} = 9.0 Hz); 2.60 (s, 3H, H_a); 2.59 (s, 3H, H_n). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 197.1; 196.7; 161.3; 156.1; 139.2; 132.5; 130.7; 130.3; 124.6; 124.4; 119.3; 117.7; 26.7; 26.6. **M/z (HR-ESI+):** calcd. for $C_{16}H_{14}NaO_3$ $[M+Na]^+$: 277.0835. Found: 277.0846. **M.p.:** 78-80°C.



4-(*o*-Tolyloxy)anisol (10)

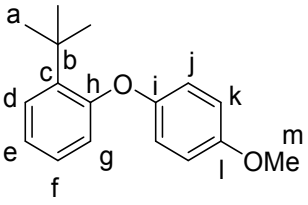
Purified by column chromatography (Hexane/ AcOEt : 100/0 to 95/5); colourless oil, yield 85% (183 mg). **^{1}H-NMR (500MHz) δ:** 7.24 (d, 1H, H_c, J_{c-d} = 7.5 Hz); 7.13 (t, 1H, H_e, J_{e-d} = J_{e-f} = 7.5 Hz); 7.02 (t, 1H, H_d, J_{d-c} = J_{d-e} = 7.3 Hz); 6.91-6.86 (m, 4H, $H_{i,j}$); 6.81 (d, 1H, H_f, J_{f-e} = 7.9 Hz); 3.81 (s, 3H, H_l); 2.29 (s, 3H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 155.8; 155.3; 151.1; 131.3; 129.1; 126.9; 123.1; 119.3; 118.0; 114.8; 55.7; 16.2. **M/z (HR-APCI+):** calcd. for $C_{14}H_{15}O_2$ $[M+H]^+$: 215.1067. Found: 215.1070.



1-Isopropyl-2-(4-methoxyphenoxy)benzene (11)

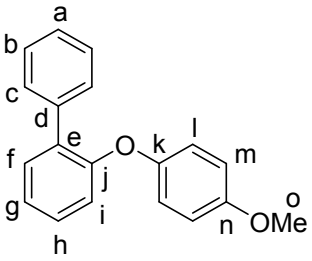
Purified by column chromatography (Hexane/AcOEt : 100/0 to 95/5); yellow oil, yield 72% (175 mg). **^{1}H-NMR (500MHz) δ:** 7.33 (dd, 1H, H_d, J_{d-f} = 1.6 Hz, J_{d-e} = 7.6 Hz); 7.12 (dt, 1H, H_f, J_{f-d} = 1.8 Hz, J_{f-e} = J_{f-g} = 7.8 Hz); 7.08 (dt, 1H, H_e, J_{e-g} = 1.3 Hz, J_{e-d} = J_{e-f} = 7.4 Hz); 6.91 (d, 2H, H_j, J_{j-k} = 9.4

Hz); 6.87 (d, 2H, H_k, J_{k-j} = 9.2 Hz); 6.79 (dd, 1H, H_g, J_{g-e} = 1.3 Hz, J_{g-f} = 7.9 Hz); 3.81 (s, 3H, H_m); 3.37 (sept, 1H, H_b, J_{b-a} = 6.9 Hz); 1.27 (d, 6H, H_a, J_{a-b} = 6.9 Hz). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 155.3; 154.9; 151.5; 139.4; 126.8; 126.7; 123.3; 119.4; 118.2; 114.8; 55.7; 27.1; 22.9. **M/z (HR-APCI+):** calcd. for $C_{16}H_{19}O_2$ $[M+H]^+$: 243.1380. Found: 243.1388.



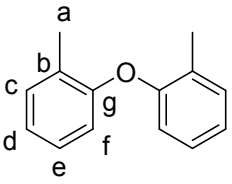
1-(*Tert*-butyl)-2-(4-methoxyphenoxy)benzene (12)

Purified by column chromatography (Hexane/AcOEt : 100/0 to 95/5); brown oil, yield 75% (192 mg). **^{1}H-NMR (500MHz) δ:** 7.39 (dd, 1H, H_d, J_{d-f} = 1.6 Hz, J_{d-e} = 7.8 Hz); 7.11 (dt, 1H, H_f, J_{f-d} = 1.6 Hz, J_{f-e} = J_{f-g} = 7.7 Hz); 7.01 (dt, 1H, H_e, J_{e-g} = 1.1 Hz, J_{e-d} = J_{e-f} = 7.6 Hz); 6.95 (d, 2H, H_j, J_{j-k} = 9.2 Hz); 6.89 (d, 2H, H_k, J_{k-j} = 9.1 Hz); 6.76 (dd, 1H, H_g, J_{g-e} = 1.1 Hz; J_{g-f} = 8.0 Hz); 3.81 (s, 3H, H_m); 1.45 (s, 9H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 157.0; 155.4; 151.0; 140.2; 127.0; 127.0; 122.5; 120.2; 118.8; 114.8; 55.7; 34.8; 30.0. **M/z (HR-APCI+):** calcd. for $C_{17}H_{21}O_2$ $[M+H]^+$: 257.1536. Found: 257.1544.



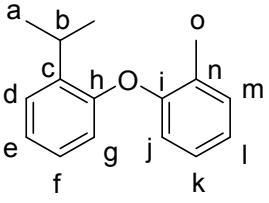
2-(4-Methoxyphenoxy)-1,1'-biphenyl (13)

Purified by column chromatography (Hexane/AcOEt : 100/0 to 95/5); yellow oil, yield 69% (190 mg). **^{1}H-NMR (500MHz) δ:** 7.59 (d, 2H, H_c, J_{c-b} = 8.5 Hz); 7.44 (dd, 1H, H_f, J_{f-h} = 1.6 Hz, J_{f-g} = 7.6 Hz); 7.40 (t, 2H, H_b, J_{b-a} = J_{b-c} = 7.5 Hz); 7.32 (t, 1H, H_a, J_{a-b} = 7.5 Hz); 7.28-7.25 (m, 1H, H_h); 7.17 (dt, 1H, H_g, J_{g-i} = 1.1 Hz, J_{g-f} = J_{g-h} =7.3 Hz); 6.93-6.91 (m, 3H, $H_{i,l}$); 6.84 (d, 2H, H_m, J_{m-l} = 9.2 Hz); 3.79 (s, 3H, H_o). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 155.5; 154.8; 150.9; 137.9; 132.8; 131.2; 129.3; 128.6; 128.1; 127.1; 123.2; 120.0; 118.6; 114.8; 55.6. **M/z (HR-APCI+):** calcd. for $C_{19}H_{17}O_2$ $[M+H]^+$: 277.1223. Found: 277.1219.



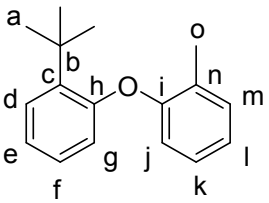
Di-(*o*-tolyl)ether (14)

Purified by chromatography (Hexane); colourless oil, yield 24% (48 mg). **^{1}H-NMR (500MHz) δ:** 7.26 (d, 2H, H_c, J_{c-d} = 6.8 Hz); 7.13 (t, 2H, H_e, J_{e-d} = J_{e-f} = 7.3 Hz); 7.02 (t, 2H, H_d, J_{d-c} = J_{d-e} = 7.4 Hz); 6.73 (d, 2H, H_f, J_{f-e} = 8.1 Hz); 2.30 (s, 6H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 155.2; 131.3; 128.8; 127.0; 123.0; 117.6; 16.1. **M/z (HR-APCI+):** calcd. for $C_{14}H_{15}O$ $[M+H]^+$: 199.1117. Found: 119.1124.



1-Isopropyl-2-(*o*-tolyloxy)benzene (15)

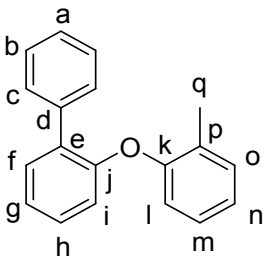
Purified by column chromatography (Hexane); colourless oil, yield 15% (33 mg). **^{1}H-NMR (500MHz) δ:** 7.34 (dd, 1H, H_d, J_{d-f} = 1.8 Hz, J_{d-e} = 7.3 Hz); 7.27-7.25 (m, 1H, H_m); 7.15-7.06 (m, 3H, $H_{e,f,k}$); 7.02 (t, 1H, H_l, J_{l-k} = J_{l-m} = 7.4 Hz); 6.76 (d, 1H, H_j, J_{j-k} = 8.0 Hz); 6.71 (dd, 1H, H_g, J_{g-e} = 1.6 Hz, J_{g-f} = 7.8 Hz); 3.36 (sept, 1H, H_b, J_{b-a} = 6.9 Hz); 2.32 (s, 3H, H_o); 1.29 (d, 6H, H_a, J_{a-b} = 7.1 Hz). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 155.5; 154.3; 139.0; 131.2; 129.0; 127.0; 126.8; 126.7; 123.1; 123.0; 117.8; 117.6; 27.2; 22.9; 16.2. **M/z (HR-APCI+):** calcd. for $C_{16}H_{19}O$ $[M+H]^+$: 227.1430. Found: 227.1436.



1-(*Tert*-butyl)-2-(*o*-tolyloxy)benzene (16)

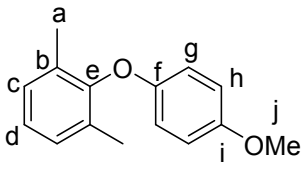
Purified by column chromatography (Hexane); colourless oil, yield 17% (41 mg). **^{1}H-NMR (500MHz) δ:** 7.41 (dd, 1H, H_d, J_{d-f} = 1.4 Hz, J_{d-e} = 7.8 Hz); 7.28-7.26 (m, 1H, H_m); 7.15 (t, 1H, H_k, J_{k-j} = J_{k-l} = 7.3 Hz); 7.10 (t, 1H, H_f, J_{f-e} = J_{f-g} = 7.7 Hz); 7.05-7.00 (m, 2H, $H_{e,l}$); 6.82 (d, 1H, H_j, J_{j-k} = 8.0 Hz); 6.66 (dd, 1H, H_g,

$J_{g\text{-}e}$ = 0.9 Hz, $J_{g\text{-}f}$ = 8.0 Hz); 2.33 (s, 3H, H_o); 1.48 (s, 9H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 155.3; 155.1; 139.8; 131.2; 129.6; 127.1; 127.1; 127.0; 123.2; 122.4; 118.7; 118.0; 34.8; 30.1; 16.4. **M/z (HR-APCI+):** calcd. for $C_{17}H_{21}O$ $[M+H]^+$: 241.1587. Found: 241.1591.



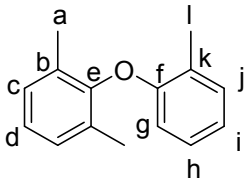
2-(*o*-Tolyloxy)-1,1'-biphenyl (17)

Purified by column chromatography (Hexane); colourless oil, yield 13% (35 mg). **^1H-NMR (500MHz) δ:** 7.61 (d, 2H, H_c, $J_{c\text{-}b}$ = 7.1 Hz); 7.46 (dd, 1H, H_f, $J_{f\text{-}h}$ = 1.5 Hz, $J_{f\text{-}g}$ = 7.7 Hz); 7.39 (t, 2H, H_b, $J_{b\text{-}c}$ = 7.6 Hz); 7.32 (t, 1H, H_a, $J_{a\text{-}b}$ = 7.3 Hz); 7.29-7.24 (m, 1H, H_h); 7.22-7.15 (m, 2H, $H_{g,o}$); 7.11 (t, 1H, H_m, $J_{m\text{-}l}$ = $J_{m\text{-}n}$ = 7.6 Hz); 7.00 (t, 1H, H_n, $J_{n\text{-}m}$ = $J_{n\text{-}o}$ = 7.4 Hz); 6.85 (d, 1H, H_i, $J_{i\text{-}h}$ = 8.1 Hz); 6.82 (d, 1H, H_l, $J_{l\text{-}m}$ = 8.1 Hz); 2.24 (s, 3H, H_q). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 155.1; 154.1; 138.0; 132.7; 131.2; 129.3; 129.2; 128.5; 128.0; 127.1, 127.0; 123.2; 123.1; 118.3; 118.1; 16.3. **M/z (HR-APCI+):** calcd. for $C_{19}H_{17}O$ $[M+H]^+$: 261.1274. Found: 261.1272.



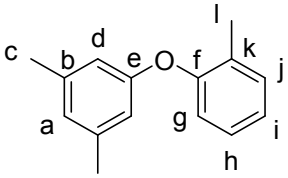
2-(4-Methoxyphenoxy)-1,3-dimethylbenzene (18)

Purified by chromatography (Hexane/AcOEt : 100/0 to 95/5); yellow oil, yield 37% (85 mg). **^1H-NMR (500MHz) δ:** 7.12-7.02 (m, 3H, $H_{c,d}$); 6.80 (d, 2H, H_g, $J_{g\text{-}h}$ = 9.1 Hz); 6.69 (d, 2H, H_h, $J_{h\text{-}g}$ = 9.2 Hz); 3.77 (s, 3H, H_m); 2.14 (s, 6H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 154.1; 152.0; 151.5; 131.6; 128.9; 124.9; 115.2; 114.7; 55.7; 16.3. **M/z (HR-APCI+):** calcd. for $C_{15}H_{17}O_2$ $[M+H]^+$: 229.1223. Found: 229.1229.



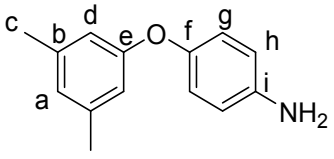
1,3-Dimethyl-2-(*o*-tolyloxy)benzene (19)

Purified by chromatography (Hexane); colourless oil, yield 22% (46 mg). **^1H-NMR (500MHz) δ:** 7.24-7.21 (m, 1H, H_j); 7.12-7.04 (m, 3H, $H_{c,d}$); 6.98 (dt, 1H, H_h, $J_{h\text{-}j}$ = 1.2 Hz, $J_{h\text{-}g}$ = $J_{h\text{-}i}$ = 6.9 Hz); 6.88 (t, 1H, H_i, $J_{i\text{-}h}$ = $J_{i\text{-}j}$ = 7.1 Hz); 6.27 (d, 1H, H_g, $J_{g\text{-}h}$ = 8.1 Hz); 2.44 (s, 3H, H_l); 2.12 (s, 6H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 155.7; 151.5; 131.4; 131.0; 128.9; 126.7; 126.0; 124.8; 120.9; 111.8; 16.2; 16.1. **M/z (HR-APCI+):** calcd. for $C_{15}H_{17}O$ $[M+H]^+$: 213.1274. Found: 213.1274.



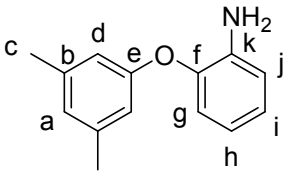
1,3-Dimethyl-5-(*o*-tolyloxy)benzene (20)

Purified by chromatography (Hexane); colourless oil, yield 45% (95 mg). **^1H-NMR (300MHz) δ:** 7.27-7.25 (m, 1H, H_j); 7.17 (dt, 1H, H_h, $J_{h\text{-}j}$ = 1.7 Hz, $J_{h\text{-}g}$ = $J_{h\text{-}i}$ = 7.7 Hz); 7.07 (dt, 1H, H_i, $J_{i\text{-}g}$ = 1.2 Hz, $J_{i\text{-}h}$ = $J_{i\text{-}j}$ = 7.4 Hz); 6.91 (d, 1H, H_g, $J_{g\text{-}h}$ = 8.1 Hz); 6.70 (s, 1H, H_a); 6.55 (s, 2H, H_d); 2.28 (s, 6H, H_c); 2.26 (s, 3H, H_l). **$^{13}C\{^1H\}$-NMR (75MHz) δ:** 157.9; 154.6; 139.5; 131.3; 129.9; 127.0; 124.1; 123.7; 119.7; 115.0; 21.3; 16.2. **M/z (HR-ESI+):** calcd. for $C_{15}H_{17}O$ $[M+H]^+$: 213.1274. Found: 213.1270.



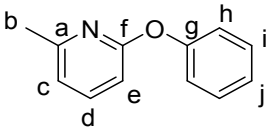
4-(3,5-Dimethylphenoxy)aniline (21)

Purified by column chromatography (Hexane/AcOEt : 100/0 to 90/10); brown oil, yield 79% (168 mg). **^1H-NMR (500MHz) δ:** 6.88 (d, 2H, H_g, $J_{g\text{-}h}$ = 8.8 Hz); 6.70 (d, 2H, H_h, $J_{h\text{-}g}$ = 8.8 Hz); 6.68 (s, 1H, H_a); 6.57 (s, 2H, H_d); 3.58 (broad s, 2H, NH_2); 2.27 (s, 6H, H_c). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 158.8; 148.9; 142.3; 139.3; 123.8; 121.1; 116.3; 114.9; 21.3. **M/z (HR-ESI+):** calcd. for $C_{14}H_{15}NNaO$ $[M+Na]^+$: 236.1046. Found: 236.1048.



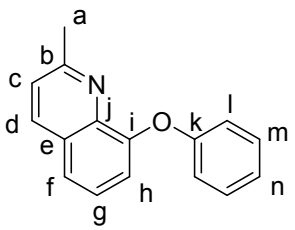
2-(3,5-Dimethylphenoxy)aniline (22)

Purified by chromatography (Hexane/ AcOEt : 100/0 to 90/10); brown oil, yield 71% (151 mg). **^{1}H-NMR (500MHz) δ:** 7.00 (dt, 1H, H_i, J_{i-g} = 1.3 Hz, J_{i-h} = J_{i-j} = 7.6 Hz); 6.89 (dd, 1H, H_g, J_{g-i} = 1.3 Hz, J_{g-h} = 7.9 Hz); 6.84 (dd, 1H, H_j, J_{j-h} = 1.3 Hz, J_{j-i} = 7.9 Hz); 6.76-6.71 (m, 2H, $H_{a,h}$); 6.61 (s, 2H, H_d); 3.73 (broad s, 2H, NH_2); 2.29 (s, 6H, H_c). **^{13}C{^{1}H}-NMR (125MHz) δ:** 157.5; 143.3; 139.5; 138.5; 124.6; 124.4; 120.2; 118.8; 116.5; 114.8; 21.3. **M/z (HR-ESI+):** calcd. for $C_{14}H_{15}NNaO$ $[M+Na]^+$: 236.1046. Found: 236.1043.



2-Methyl-6-phenoxypyridine (23)

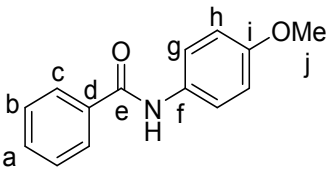
Purified by column chromatography (Hexane/AcOEt : 100/0 to 95/5); yellow oil, yield 17% (31 mg). **^{1}H-NMR (500MHz) δ:** 7.54 (t, 1H, H_d, J_{d-c} = J_{d-e} = 7.7 Hz); 7.38 (t, 2H, H_i, J_{i-h} = J_{i-j} = 8.1 Hz); 7.18 (t, 1H, H_j, J_{j-i} = 7.4 Hz); 7.13 (d, 2H, H_h, J_{h-i} = 7.5 Hz); 6.88 (d, 1H, H_c, J_{c-d} = 7.5 Hz); 6.58 (d, 1H, H_e = 8.1 Hz); 2.47 (s, 3H, H_b). **^{13}C{^{1}H}-NMR (125MHz) δ:** 163.1; 157.6; 154.7; 139.5; 129.6; 124.3; 120.7; 118.0; 107.5; 24.1. **M/z (HR-ESI+):** calcd. for $C_{12}H_{12}NNaO$ $[M+Na]^+$: 208.0733. Found: 208.0733.



2-Methyl-8-phenoxyquinoline (24)

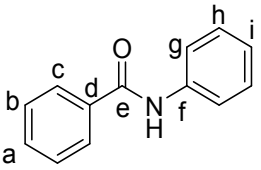
Purified by column chromatography (Hexane/AcOEt : 100/0 to 95/5); white solid, yield 21% (50 mg). **^{1}H-NMR (500MHz) δ:** 8.08 (d, 1H, H_d, J_{d-c} = 8.5 Hz); 7.49 (dd, 1H, H_f, J_{f-h} = 1.1 Hz, J_{f-g} = 8.3 Hz); 7.40-7.32 (m, 4H, $H_{c,g,m}$); 7.18-7.13 (m, 3H, $H_{l,n}$); 7.01 (dd, 1H, H_h, J_{h-f} = 1.1 Hz; J_{h-g} = 7.6 Hz); 2.79 (s, 3H, H_a). **^{13}C{^{1}H}-NMR (125MHz) δ:** 159.0; 157.1; 153.6; 140.0; 136.4; 129.7; 128.0; 125.6; 123.8; 122.9; 121.9; 120.4; 115.5; 25.6. **M/z (HR-ESI+):** calcd. for $C_{16}H_{13}NNaO$ $[M+Na]^+$: 258.0889. Found: 258.0889. **M.p.:** 97-99°C.

Characterisation data for amides 25-49



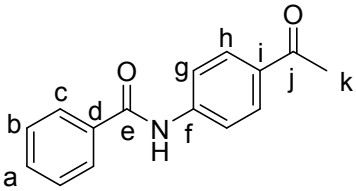
***N*-(4-Methoxyphenyl)benzamide (25)**

Purified by column chromatography (Hexane/EtOAc: 95/5 to 80/20). White solid, yield 83% (189 mg, 0.83 mmols).**^{1}H-NMR (300MHz) δ:** 7.87 (d, 2H, H_c, $J_{c\text{-}b}$ = 6.8 Hz); 7.78 (broad s, 1H, NH); 7.59-7.44 (m, 5H, $H_{a,b,g}$); 6.92 (d, 2H, H_h, $J_{h\text{-}g}$ = 9.1 Hz); 3.82 (s, 3H, H_j). **^{13}C{^{1}H}-NMR (75MHz) δ:** 165.6; 156.6; 135.0; 131.7; 131.0; 128.7; 127.0; 122.1; 114.2; 55.5. **M/z (HR-ESI+):** calcd. for $C_{14}H_{13}NNaO_2$ $[M+Na]^+$: 250.0838. Found: 250.0837.



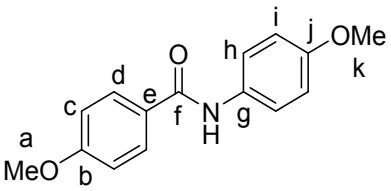
***N*-Phenylbenzamide (26)**

Purified by column chromatography (Hexane/EtOAc: 90/10 to 80/20). White solid, yield 85% (167 mg, 0.85 mmols). **^{1}H-NMR (500MHz) δ:** 7.89 (d, 2H, H_c, $J_{c\text{-}b}$ = 7.1 Hz); 7.81 (broad s, 1H, NH); 7.66 (d, 2H, H_g, $J_{g\text{-}h}$ = 7.7 Hz); 7.60-7.54 (m, 1H, H_a); 7.51 (t, 2H, H_b, $J_{b\text{-}a}$ = $J_{b\text{-}c}$ = 7.5 Hz); 7.39 (t, 2H, H_h, $J_{h\text{-}g}$ = $J_{h\text{-}i}$ = 7.9 Hz); 7.17 (t, 1H, H_i, $J_{i\text{-}h}$ = 7.3 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 165.6; 138.1; 135.3; 131.8; 129.1; 128.8; 127.0; 124.6; 120.3. **M/z (HR-ESI+):** calcd. for $C_{13}H_{12}NO$ $[M+H]^+$: 198.0913. Found: 198.0918.



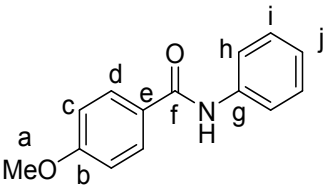
***N*-(4-Acetylphenyl)benzamide (27)**

Purified by column chromatography (Hexane/EtOAc: 85/15 to 65/35). Yellow solid, yield 59% (141 mg, 0.59 mmols). **^{1}H-NMR (500MHz) δ:** 8.03-7.99 [(d, 2H, H_h, $J_{h\text{-}g}$ = 8.8 Hz), and (broad s, 1H, NH)]; 7.90 (d, 2H, H_c, $J_{c\text{-}b}$ = 7.1 Hz); 7.78 (d, 2H, H_g, $J_{g\text{-}h}$ = 8.8 Hz); 7.60 (t, 1H, H_a, $J_{a\text{-}b}$ = 7.5 Hz); 7.53 (t, 2H, H_b, $J_{b\text{-}a}$ = $J_{b\text{-}c}$ = 7.6 Hz); 2.61 (s, 3H, H_k). **^{13}C{^{1}H}-NMR (125MHz) δ:** 196.6; 165.7; 142.3; 134.7; 133.5; 132.2; 129.8; 129.0; 127.1; 119.4; 26.3. **M/z (HR-ESI+):** calcd. for $C_{15}H_{14}NO_2$ $[M+H]^+$: 240.1019. Found: 240.1020.



4-Methoxy-*N*-(4-methoxyphenyl)benzamide (28)

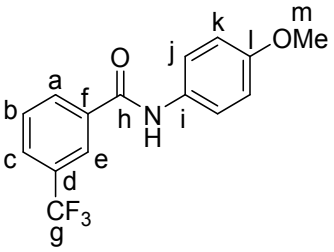
Purified by column chromatography (Hexane/EtOAc: 90/10 to 20/80). Yellow solid, yield 67% (173 mg, 0.67 mmols). **^{1}H-NMR (500MHz) δ:** 7.84 (d, 2H, H_d, $J_{d\text{-}c}$ = 9.0 Hz); 7.65 (broad s, 1H, NH); 7.53 (d, 2H, H_h, $J_{h\text{-}i}$ = 9.0 Hz); 6.98 (d, 2H, H_c, $J_{c\text{-}d}$ = 8.8 Hz); 6.92 (d, 2H, H_i, $J_{i\text{-}h}$ = 9.0 Hz); 3.88 (s, 3H, H_a); 3.82 (s, 3H, H_k). **^{13}C{^{1}H}-NMR (125MHz) δ:** 165.1; 162.6; 156.8; 131.4; 128.8; 127.5; 122.2; 114.5; 114.1; 55.6; 55.5. **M/z (HR-ESI+):** calcd. for $C_{15}H_{15}NNaO_3$ $[M+Na]^+$: 280.0944. Found: 280.0948.



4-Methoxy-*N*-phenylbenzamide (29)

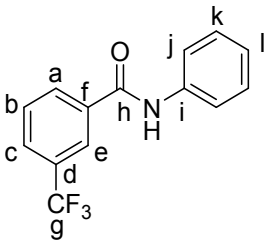
Purified by column chromatography (Hexane/EtOAc: 95/5 to 70/30). White solid, yield 88% (200 mg, 0.88 mmols). **^{1}H-NMR (500MHz) δ:** 7.85 (d, 2H, H_d, $J_{d\text{-}c}$ = 8.8 Hz); 7.74 (broad s, 1H, NH); 7.64 (d, 2H, H_h, $J_{h\text{-}i}$ = 8.5 Hz); 7.38 (t, 2H, H_i, $J_{i\text{-}h}$ = $J_{i\text{-}j}$ = 7.9 Hz); 7.15 (t, 1H, H_j, $J_{j\text{-}i}$ = 7.4 Hz);

6.99 (d, 2H, H_c, J_{c-d} = 8.8 Hz); 3.89 (s, 3H, H_a). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 165.1; 162.7; 138.3; 129.1; 128.9; 127.5; 124.4; 120.3; 114.1; 55.5. **M/z (HR-ESI+):** calcd. for $C_{14}H_{13}NNaO_2$ $[M+Na]^+$: 250.0838. Found: 250.0837.



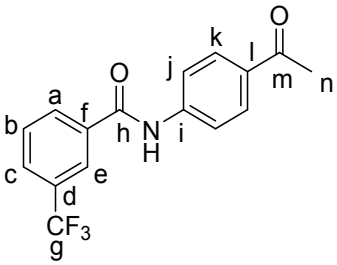
***N*-(4-Methoxyphenyl)-3-(trifluoromethyl)benzamide (30)**

Purified by column chromatography (Hexane/EtOAc: 90/10 to 60/40). Orange solid, yield 66% (195 mg, 0.66 mmols). **^1H-NMR (500MHz) δ:** 8.12 (s, 1H, H_e); 8.04 (d, 1H, H_a, J_{a-b} = 7.5 Hz); 7.90 (broad s, 1H, NH); 7.79 (d, 1H, H_c, J_{c-b} = 7.7 Hz); 7.60 (t, 1H, H_b, J_{b-a} = J_{b-c} = 7.7 Hz); 7.53 (d, 2H, H_j, J_{j-k} = 8.8 Hz); 6.91 (d, 2H, H_k, J_{k-j} = 9.0 Hz); 3.82 (s, 3H, H_m). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 164.3; 157.0; 135.9; 131.3(q, J_{C-F} = 32 Hz); 130.5; 130.3; 129.4; 128.2 (q, J_{C-F} = 3 Hz); 124.0 (q, J_{C-F} = 3 Hz); 123.7 (q, J_{C-F} = 272 Hz); 122.4; 114.3; 55.5. **M/z (HR-ESI+):** calcd. for $C_{15}H_{12}F_3NNaO_2$ $[M+Na]^+$: 318.0712. Found: 318.0713.



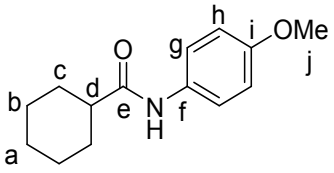
***N*-Phenyl-3-(trifluoromethyl)benzamide (31)**

Purified by column chromatography (Hexane/EtOAc: 95/5 to 80/20). Off-white solid, yield 81% (216 mg, 0.81 mmols). **^1H-NMR (500MHz) δ:** 8.12 (s, 1H, H_e); 8.07 (broad s, 1H, NH); 8.04 (d, 1H, H_a, J_{a-b} = 8.0 Hz); 7.79 (d, 1H, H_c, J_{c-b} = 7.8 Hz); 7.64 (d, 2H, H_j, J_{j-k} = 8.0 Hz); 7.60 (t, 1H, H_b, J_{b-a} = J_{b-c} = 7.8 Hz); 7.37 (t, 2H, H_k, J_{k-j} = J_{k-l} = 7.9 Hz); 7.18 (t, 1H, H_l, J_{l-k} = 7.3 Hz). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 164.4; 137.5; 135.8; 131.3(q, J_{C-F} = 33 Hz); 130.4; 129.4; 129.1; 128.3 (q, J_{C-F} = 4 Hz); 125.0; 124.1 (q, J_{C-F} = 4 Hz); 123.6 (q, J_{C-F} = 273 Hz); 120.5. **M/z (HR-ESI+):** calcd. for $C_{14}H_{10}F_3NNaO$ $[M+Na]^+$: 288.0607. Found: 288.0604.



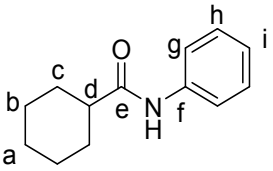
***N*-(4-Acetylphenyl)-3-(trifluoromethyl)benzamide (32)**

Purified by column chromatography (Hexane/EtOAc: 85/15 to 60/40). White solid, yield 56% (173 mg, 0.56 mmols). **^1H-NMR (500MHz) δ:** 8.45 (broad s, 1H, NH); 8.15 (s, 1H, H_e); 8.09 (d, 1H, H_a, J_{a-b} = 7.8 Hz); 7.97 (d, 2H, H_k, J_{k-j} = 8.5 Hz); 7.83-7.77 (m, 3H, $H_{c,j}$); 7.63 (t, 1H, H_b, J_{b-a} = J_{b-c} = 7.8 Hz); 2.59 (s, 3H, H_n). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 197.2; 164.5; 142.0; 135.3; 133.4; 131.4 (q, J_{C-F} = 33 Hz); 130.5; 129.8; 129.5; 128.7 (q, J_{C-F} = 4 Hz); 124.1 (q, J_{C-F} = 4 Hz); 123.5 (q, J_{C-F} = 273 Hz): 119.6; 26.4. **M/z (HR-ESI+):** calcd. for $C_{16}H_{13}F_3NO_2$ $[M+H]^+$: 308.0898. Found: 308.0909.



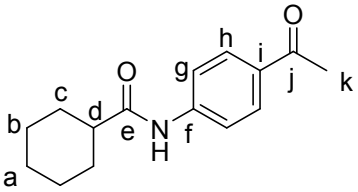
***N*-(4-Methoxyphenyl)cyclohexanecarboxamide (33)**

Purified by column chromatography (Hexane/EtOAc: 85/15 to 70/30). White solid, yield 71% (165 mg, 0.71 mmols). **^1H-NMR (500MHz) δ:** 7.43 (d, 2H, H_g, J_{g-h} = 9.0 Hz); 7.04 (broad s, 1H, NH); 6.86 (d, 2H, H_h, J_{h-g} = 9.0 Hz); 3.80 (s, 3H, H_j); 2.25-1.21 (6 multiplets, 11H, H_{a-d}). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 174.1; 156.3; 131.2; 121.6; 114.1; 55.5; 46.4; 29.7; 25.7. **M/z (HR-ESI+):** calcd. for $C_{14}H_{19}NNaO_2$ $[M+Na]^+$: 256.1308. Found: 256.1305.



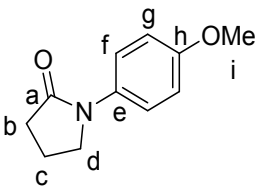
***N*-Phenylcyclohexanecarboxamide (34)**

Purified by column chromatography (Hexane/EtOAc: 95/5 to 70/30). White solid, yield 78% (159 mg, 0.78 mmols). **^{1}H-NMR (500MHz) δ:** 7.53 (d, 2H, H_g, $J_{g\text{-}h}$ = 7.9 Hz); 7.32 (t, 2H, H_h, $J_{h\text{-}g}$ = $J_{h\text{-}i}$ = 7.9 Hz); 7.16 (broad s, 1H, NH); 7.10 (t, 1H, H_i, $J_{i\text{-}h}$ = 7.4 Hz); 2.28-1.24 (6 multiplets, 11H, $H_{a\text{-}d}$). **^{13}C{^{1}H}-NMR (125MHz) δ:** 174.1; 138.3; 129.0; 124.1; 119.9; 46.6; 29.8; 25.8; 25.7. **M/z (HR-ESI+):** calcd. for $C_{13}H_{18}NO$ $[M+H]^+$: 204.1383. Found: 204.1384.



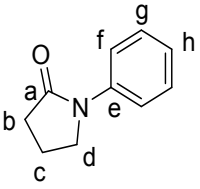
***N*-(4-Acetylphenyl)cyclohexanecarboxamide (35)**

Purified by column chromatography (Hexane/EtOAc: 85/15 to 65/35). White solid, yield 72% (177 mg, 0.72 mmols). **^{1}H-NMR (500MHz) δ:** 7.94 (d, 2H, H_h, $J_{h\text{-}g}$ = 8.8 Hz); 7.64 (d, 2H, H_g, $J_{g\text{-}h}$ = 8.8 Hz); 7.35 (broad s, 1H, NH); 2.58 (s, 3H, H_k); 2.31-1.22 (6 multiplets, 11H, $H_{a\text{-}d}$). **^{13}C{^{1}H}-NMR (125MHz) δ:** 196.6; 174.3; 142.5; 133.1; 129.7; 119.0; 46.7; 29.7; 26.2; 25.7; 25.7. **M/z (HR-ESI+):** calcd. for $C_{15}H_{20}NO_2$ $[M+H]^+$: 246.1489. Found: 246.1489.



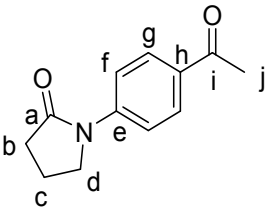
1-(4-Methoxyphenyl)pyrrolidin-2-one (36)

Purified by column chromatography (Hexane/EtOAc: 85/15 to 55/45). White solid, yield 97% (185 mg, 0.97 mmols). **^{1}H-NMR (500MHz) δ:** 7.50 (d, 2H, H_f, $J_{f\text{-}g}$ = 8.9 Hz); 6.91 (d, 2H, H_g, $J_{g\text{-}f}$ = 8.9 Hz); 3.83 (t, 2H, H_b, $J_{b\text{-}c}$ = 7.1 Hz); 3.81 (s, 3H, H_i); 2.60 (t, 2H, H_d, $J_{d\text{-}c}$ = 8.0 Hz); 2.16 (quint, 2H, H_c, $J_{c\text{-}b}$ = $J_{c\text{-}d}$ = 7.8 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 173.9; 156.6; 132.6; 121.8; 114.0; 55.5; 49.2; 32.4; 18.0. **M/z (HR-ESI+):** calcd. for $C_{11}H_{13}NNaO_2$ $[M+Na]^+$: 214.0838. Found: 214.0842.



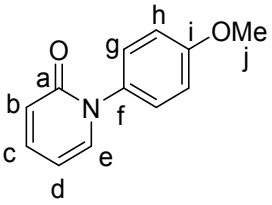
1-Phenylpyrrolidin-2-one (37)

Purified by column chromatography (Hexane/EtOAc: 90/10 to 60/40). White solid, yield 97% (157 mg, 0.97 mmols). **^{1}H-NMR (500MHz) δ:** 7.62 (d, 2H, H_f, $J_{f\text{-}g}$ = 8.0 Hz); 7.38 (t, 2H, H_g, $J_{g\text{-}f}$ = $J_{g\text{-}h}$ = 7.8 Hz); 7.15 (t, 1H, H_h, $J_{h\text{-}g}$ = 7.2 Hz); 3.87 (t, 2H, H_b, $J_{b\text{-}c}$ = 7.0 Hz); 2.62 (t, 2H, H_d, $J_{d\text{-}c}$ = 8.0 Hz); 2.17 (quint, 2H, H_c, $J_{c\text{-}b}$ = $J_{c\text{-}d}$ = 7.5 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 174.1; 139.4; 128.8; 124.5; 119.9; 48.7; 32.7; 18.0. **M/z (HR-ESI+):** calcd. for $C_{10}H_{12}NO$ $[M+H]^+$: 162.0913. Found: 162.0911.



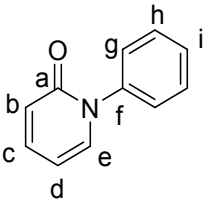
1-(4-Acetylphenyl)pyrrolidin-2-one (38)

Purified by column chromatography (Hexane/EtOAc: 85/15 to 50/50). White solid, yield 87% (176 mg, 0.87 mmols). **^{1}H-NMR (500MHz) δ:** 7.98 (d, 2H, H_g, $J_{g\text{-}f}$ = 8.8 Hz); 7.76 (d, 2H, H_f, $J_{f\text{-}g}$ = 8.8 Hz); 3.92 (t, 2H, H_b, $J_{b\text{-}c}$ = 7.1 Hz); 2.66 (t, 2H, H_d, $J_{d\text{-}c}$ = 8.1 Hz); 2.59 (s, 3H, H_j); 2.21 (quint, 2H, H_c, $J_{c\text{-}b}$ = $J_{c\text{-}d}$ = 7.6 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 196.7; 174.5; 143.7; 133.1; 129.3; 118.8; 48.5; 32.8; 26.3; 17.9. **M/z (HR-ESI+):** calcd. for $C_{12}H_{13}NNaO_2$ $[M+Na]^+$: 226.0838. Found: 226.0842.



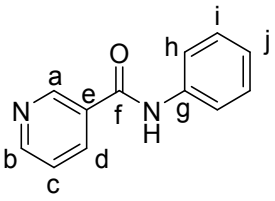
1-(4-Methoxyphenyl)pyridin-2(1*H*)-one (39)

Purified by column chromatography (Hexane/EtOAc: 90/10 to 40/60). Yellow solid, yield 95% (192 mg, 0.95 mmols). **^{1}H-NMR (500MHz) δ:** 7.38 (ddd, 1H, H_c, $J_{c\text{-}e}$ = 2.1 Hz, $J_{c\text{-}d}$ = 6.7 Hz, $J_{c\text{-}b}$ = 9.1 Hz); 7.34-7.27 (m, 3H, $H_{e,g}$); 6.99 (d, 2H, H_h, $J_{h\text{-}g}$ = 9.0 Hz); 6.65 (d, 1H, H_b, $J_{b\text{-}c}$ = 9.3 Hz); 6.22 (dt, 1H, H_d, $J_{d\text{-}b}$ = 1.4 Hz, $J_{d\text{-}c}$ = $J_{d\text{-}e}$ = 6.7 Hz); 3.84 (s, 1H, H_j). **^{13}C{^{1}H}-NMR (125MHz) δ:** 162.6; 159.4; 139.7; 138.3; 133.8; 127.5; 121.7; 114.5; 105.7; 55.5. **M/z (HR-ESI+):** calcd. for $C_{12}H_{11}NNaO_2$ $[M+Na]^+$: 224.0682. Found: 224.0679.



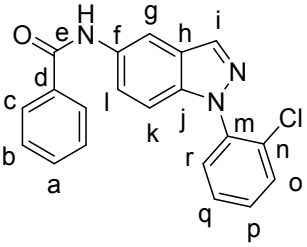
1-Phenylpyridin-2(1*H*)-one (40)

Purified by column chromatography (Hexane/EtOAc: 85/15 to 50/50). Off-white solid, yield 98% (167 mg, 0.98 mmols). **^{1}H-NMR (500MHz) δ:** 7.50 (t, 2H, H_h, $J_{h\text{-}g}$ = $J_{h\text{-}i}$ = 7.6 Hz); 7.45-7.37 (m, 4H, $H_{c,g,i}$); 7.34 (dd, 1H, H_e, $J_{e\text{-}c}$ = 2.1 Hz, $J_{e\text{-}d}$ = 6.9 Hz); 6.68 (d, 1H, H_b, $J_{b\text{-}c}$ = 9.2 Hz); 6.25 (t, 1H, H_d, $J_{d\text{-}c}$ = $J_{d\text{-}e}$ = 6.5 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 162.4; 140.9; 139.8; 138.0; 129.3; 128.5; 126.5; 121.9; 105.9. **M/z (HR-ESI+):** calcd. for $C_{11}H_9NNaO$ $[M+Na]^+$: 194.0576. Found: 194.0574.



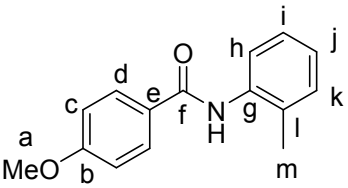
***N*-Phenylnicotinamide (41)**

Purified by column chromatography (Hexane/EtOAc: 85/15 to 20/80). Yellow solid, yield 61% (121 mg, 0.61 mmols). **^{1}H-NMR (500MHz) δ:** 9.08 (s, 1H, H_a); 8.72 (d, 1H, H_b, $J_{b\text{-}c}$ = 3.9 Hz); 8.42 (broad s, 1H, NH); 8.20 (d, 1H, H_d, $J_{d\text{-}c}$ = 7.9 Hz); 7.66 (d, 2H, H_h, $J_{h\text{-}i}$ = 7.9 Hz); 7.43-7.33 (m, 3H, $H_{c,i}$); 7.17 (t, 1H, H_j, $J_{j\text{-}i}$ = 7.5 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 164.0; 152.2; 147.9; 137.5; 135.5; 130.9; 129.1; 125.0; 123.7; 120.6. **M/z (HR-ESI+):** calcd. for $C_{12}H_{10}N_2NaO$ $[M+Na]^+$: 221.0685. Found: 221.0683.



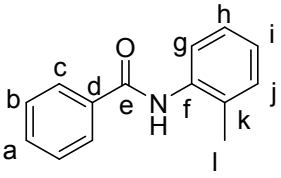
***N*-(1-(2-Chlorophenyl)-1*H*-indazol-5-yl)benzamide (42)**

Purified by column chromatography (Hexane/EtOAc: 90/10 to 30/70). Yellow solid, yield 31% (109 mg, 0.31 mmols). **^{1}H-NMR (500MHz) δ:** 8.22 (d, 1H, H_g, $J_{g\text{-}l}$ = 1.1 Hz); 8.19 (s, 1H, H_i); 8.14 (broad s, 1H, NH); 7.91 (d, 2H, H_c, $J_{c\text{-}b}$ = 7.0 Hz); 7.62-7.58 (m, 1H, H_r); 7.58-7.53 (m, 1H, H_a); 7.53-7.50 (m, 2H, $H_{l,o}$); 7.50-7.47 (m, 2H, H_b); 7.46-7.41 (m, 2H, $H_{p,q}$); 7.22 (d, 1H, H_k, $J_{k\text{-}l}$ = 8.9 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 165.9; 138.2; 137.2; 135.7; 135.1; 132.1; 131.8; 131.7; 130.8; 129.9; 129.5; 128.8; 127.7; 127.1; 124.7; 122.0; 112.5; 110.9. **M/z (HR-ESI+):** calcd. for $C_{20}H_{14}ClN_3NaO$ $[M+Na]^+$: 370.0718. Found: 370.0720.



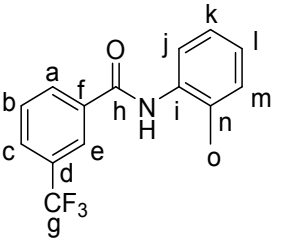
4-Methoxy-*N*-(*o*-tolyl)benzamide (43)

Purified by column chromatography (Hexane/EtOAc: 95/5 to 70/30). White solid, yield 55% (133 mg, 0.55 mmols). **^{1}H-NMR (500MHz) δ:** 7.96 (d, 1H, H_h, $J_{h\text{-}i}$ = 8.0 Hz); 7.87 (d, 2H, H_d, $J_{d\text{-}c}$ = 8.5 Hz); 7.60 (broad s, 1H, NH); 7.29-7.22 (m, 2H, $H_{i,k}$); 7.12 (t, 1H, H_j, $J_{j\text{-}i}$ = $J_{j\text{-}k}$ = 7.3 Hz); 7.00 (d, 2H, H_c, $J_{c\text{-}d}$ = 8.7 Hz); 3.89 (s, 3H, H_a); 2.35 (s, 3H, H_m). **^{13}C{^{1}H}-NMR (125MHz) δ:** 165.1; 162.5; 136.0; 130.5; 129.0; 128.9; 127.3; 126.9; 125.1; 123.0; 114.0; 55.5; 17.8. **M/z (HR-ESI+):** calcd. for $C_{15}H_{15}NNaO_2$ $[M+Na]^+$: 264.0995. Found: 254.0997.



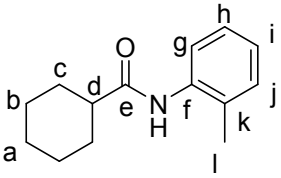
***N*-(*o*-Tolyl)benzamide (44)**

Purified by column chromatography (Hexane/EtOAc: 90/10 to 80/20). White solid, yield 57% (121 mg, 0.57 mmols). **^{1}H-NMR (500MHz) δ:** 7.97 (d, 1H, H_g, $J_{g\text{-}h}$ = 7.9 Hz); 7.90 (d, 2H, H_c, $H_{c\text{-}b}$ = 7.3 Hz); 7.69 (broad s, 1H, NH); 7.58 (t, 1H, H_a, $J_{a\text{-}b}$ = 7.5 Hz); 7.54-7.49 (m, 2H, H_b); 7.30-7.23 (m, 2H, $H_{j,h}$); 7.14 (dt, 1H, H_i, $J_{i\text{-}g}$ = 1.1 Hz, $J_{i\text{-}j}$ = $J_{i\text{-}j}$ = 7.5 Hz); 2.36 (s, 3H, H_l). **^{13}C{^{1}H}-NMR (125MHz) δ:** 165.6; 136.0; 135.3; 131.8; 130.6; 129.3; 128.9; 127.1; 127.0; 125.4; 123.3; 17.7. **M/z (HR-ESI+):** calcd. for $C_{14}H_{13}NNaO$ $[M+Na]^+$: 234.0889. Found: 234.0893.



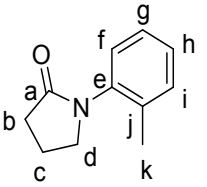
***N*-(*o*-Tolyl)-3-(trifluoromethyl)benzamide (45)**

Purified by column chromatography (Hexane/EtOAc: 95/5 to 70/30). Off-white solid, yield 36% (101 mg, 0.36 mmols) **^{1}H-NMR (500MHz) δ:** 8.16 (s, 1H, H_e); 8.07 (d, 1H, H_a, $J_{a\text{-}b}$ = 7.6 Hz); 7.87-7.81 (m, 2H, $H_{c,j}$); 7.70 (broad s, 1H, NH); 7.65 (t, 1H, H_b, $J_{b\text{-}a}$ = $J_{b\text{-}c}$ = 7.8 Hz); 7.30-7.22 (m, 2H, $H_{k,m}$); 7.16 (t, 1H, H_l, $J_{l\text{-}k}$ = $J_{l\text{-}m}$ = 7.5 Hz); 2.35 (s, 3H, H_o). **^{13}C{^{1}H}-NMR (125MHz) δ:** 164.3; 135.8; 135.2; 131.4 (q, $J_{C\text{-}F}$ = 33 Hz); 130.7; 130.2; 129.9; 129.5; 128.4 (q, $J_{C\text{-}F}$ = 4 Hz); 126.9; 125.9; 124.2 (q, $J_{C\text{-}F}$ = 4 Hz); 123.6; 123.6 (q, $J_{C\text{-}F}$ = 273 Hz); 17.8. **M/z (HR-ESI+):** calcd. for $C_{15}H_{12}F_3NNaO$ $[M+Na]^+$: 302.0763. Found: 302.0760.



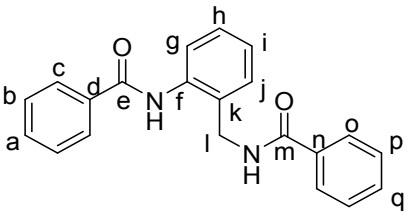
***N*-(*o*-Tolyl)cyclohexanecarboxamide (46)**

Purified by column chromatography (Hexane/EtOAc: 95/5 to 70/30). White solid, yield 63% (138 mg, 0.63 mmols). **^{1}H-NMR (500MHz) δ:** 7.90-7.84 (m, 1H, H_g); 7.24-7.17 (m, 2H, $H_{h,j}$); 7.09-7.05 (m, 1H, H_i); 6.98 (broad s, 1H, NH); 2.33-1.22 (6 multiplets, 14H, $H_{a\text{-}d,l}$). **^{13}C{^{1}H}-NMR (125MHz) δ:** 174.1; 135.8; 130.4; 128.7; 126.8; 124.9; 123.0; 122.8; 46.4; 29.9; 25.7; 17.7. **M/z (HR-ESI+):** calcd. for $C_{14}H_{19}NNaO$ $[M+Na]^+$: 240.1359. Found: 240.1357.



1-(*o*-Tolyl)pyrrolidin-2-one (47)

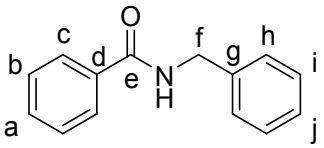
Purified by column chromatography (Hexane/EtOAc: 90/10 to 50/50). Yellow oil, yield 81% (141 mg, 0.81 mmols). **^{1}H-NMR (500MHz) δ:** 7.31-7.20 (m, 3H, $H_{f,h,i}$); 7.19-7.11 (m, 1H, H_g); 3.73 (t, 2H, H_b, $J_{b\text{-}c}$ = 7.0 Hz); 2.59 (t, 2H, H_d, $J_{d\text{-}c}$ = 8.0 Hz); 2.29-2.19 (m, 5H, $H_{c,k}$). **^{13}C{^{1}H}-NMR (125MHz) δ:** 174.3; 137.4; 135.5; 131.1; 127.8; 126.8; 126.6; 50.7; 31.2; 19.1; 17.9. **M/z (HR-ESI+):** calcd. for $C_{11}H_{13}NNaO$ $[M+Na]^+$: 198.0889. Found: 198.0885.c



***N*-(2-Benzamidobenzyl)benzamide (48)**

Purified by column chromatography (Hexane/EtOAc: 85/15 to 65/35). Off-white solid, yield 30% (59 mg, 0.18 mmols). **^{1}H-NMR (500MHz) δ:** 10.44 (broad s, 1H, NH); 8.22 (dd, 2H, H_c, $J_{c\text{-}a}$ = 1.5 Hz, $J_{c\text{-}b}$ = 8.1 Hz); 8.01 (d, 1H, H_g, $J_{g\text{-}h}$ = 7.3 Hz); 7.76 (dd, 2H, H_o, $J_{o\text{-}q}$ = 1.3 Hz, $J_{o\text{-}p}$ = 8.3 Hz); 7.60-1.49 (m, 4H, $H_{a,b,q}$); 7.43 (t, 2H, H_p, $J_{p\text{-}o}$ = $J_{p\text{-}q}$ = 7.6 Hz); 7.38 (dt, 1H, H_h, $J_{h\text{-}j}$ = 1.5 Hz, $J_{h\text{-}g}$ = $J_{h\text{-}i}$ = 8.1 Hz); 7.33 (dd, 1H, H_j, $J_{j\text{-}h}$ = 1.4 Hz, $J_{j\text{-}i}$ = 7.6 Hz); 7.17 (dt, 1H, H_i, $J_{i\text{-}g}$ = 1.3 Hz, $J_{i\text{-}h}$ = $J_{i\text{-}j}$ = 7.5 Hz); 6.93 (broad s, 1H, benzyl. NH); 4.59 (d,

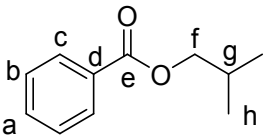
2H, H_l, $J_{l\text{-}NH}$ = 6.4 Hz). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 168.3; 166.6; 136.8; 134.9; 133.7; 131.9; 131.7; 130.6; 130.1; 128.9; 128.7; 128.5; 127.9; 127.1; 125.5; 125.3; 41.1. **M/z (HR-ESI+):** calcd. for $C_{21}H_{18}N_2NaO_2$ $[M+Na]^+$: 353.1260. Found: 353.1263.



***N*-Benzylbenzamide (49)**

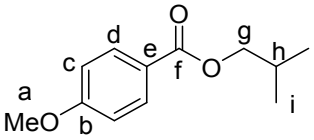
Purified by column chromatography (Hexane/EtOAc: 90/10 to 70/30). Yellow solid, different yields. **^1H-NMR (500MHz) δ:** 7.82-7.78 (m, 2H, H_c); 7.51 (tt, 1H, H_a, $J_{a\text{-}c}$ = 1.2 Hz, $J_{a\text{-}b}$ = 7.3 Hz); 7.46-7.41 (m, 2H, H_b); 7.38-7.34 (m, 4H, $H_{h,i}$); 7.34-7.28 (m, 1H, H_j); 6.46 (broad s, 1H, NH); 4.66 (d, 2H, H_f, $J_{f\text{-}f(gem)}$ = 5.6 Hz). **$^{13}C\{^1H\}$-NMR (125MHz) δ:** 167.3; 138.4; 134.7; 131.5; 128.8; 128.6; 127.9; 127.6; 127.0; 44.3. **M/z (HR-ESI+):** calcd. for $C_{14}H_{13}NNaO$ $[M+Na]^+$: 234.0889. Found: 234.0889.

Characterisation data for ester side-products 50-53



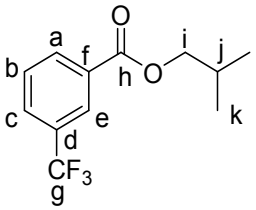
Isobutyl benzoate (50)

Yellow oil. **^{1}H-NMR (500MHz) δ:** 8.07 (d, 2H, H_c, J_{c-b} = 8.3 Hz); 7.57 (t, 1H, H_a, J_{a-b} = 7.5 Hz); 7.45 (t, 2H, $H_{b,}$, J_{b-a} = J_{b-c} = 7.7 Hz); 4.12 (d, 2H, H_f, J_{f-g} = 6.6 Hz); 2.10 (sept, 1H, H_g, J_{g-h} = J_{g-h} = 6.7 Hz); 1.04 (d, 6H, H_h, J_{h-g} = 6.8 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 166.6; 132.7; 130.8; 129.6; 128.3; 71.0; 28.0; 19.2. These data correspond to those previously reported.[2]



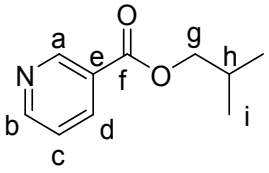
Isobutyl 4-methoxybenzoate (51)

Yellow oil. **^{1}H-NMR (500MHz) δ:** 8.02 (d, 2H, H_d, J_{d-c} = 8.7 Hz); 6.93 (d, 2H, H_c, J_{c-d} = 8.9 Hz); 4.08 (d, 2H, H_g, J_{g-h} = 6.4 Hz); 3.87 (s, 3H, H_a); 2.08 (sept, 1H, H_h, J_{h-g} = J_{h-i} = 6.7 Hz); 1.03 (d, 6H, H_i, J_{i-h} = 6.6 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 166.4; 163.3; 131.5; 123.0; 113.5; 70.7; 55.4; 27.9; 19.2. These data correspond to those previously reported.[3]



Isobutyl 3-(trifluoromethyl)benzoate (52)

Yellow oil. **^{1}H-NMR (500MHz) δ:** 8.31 (s, 1H, H_e); 8.25 (d, 1H, H_a, J_{a-b} = 7.8 Hz); 7.82 (d, 1H, H_c, J_{c-b} = 7.8 Hz); 7.60 (t, 1H, H_b, J_{b-a} = J_{b-c} = 7.8 Hz); 4.16 (d, 2H, H_i, J_{i-j} = 6.6 Hz); 2.12 (sept, 1H, H_j, J_{j-i} = J_{j-k} = 6.7 Hz); 1.04 (d, 6H, H_k, J_{k-j} = 6.6 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 165.3; 132.7; 131.4; 131.0 (q, J_{C-F} = 33 Hz); 129.3 (q, J_{C-F} = 4 Hz); 129.0; 126.4 (q, J_{C-F} = 4 Hz); 124.7 (q, J_{C-F} = 272 Hz); 71.5; 27.9; 19.1.



Isobutyl nicotinate (53)

Orange oil. **^{1}H-NMR (500MHz) δ:** 9.25 (s, 1H, H_a); 8.78 (d, 1H, H_b, J_{b-c} = 4.1 Hz); 8.32 (dt, 1H, $H_{d,}$, J_{d-a} = J_{d-b} = 1.9 Hz, J_{d-c} = 8.0 Hz); 7.41 (dd, 1H, H_c, J_{c-b} = 4.9 Hz, J_{c-d} = 7.9 Hz); 4.15 (d, 2H, H_g, J_{g-h} = 6.6 Hz); 2.11 (sept, 1H, H_h, J_{h-g} = J_{h-i} = 6.7 Hz); 1.04 (d, 6H, H_i, J_{i-h} = 6.8 Hz). **^{13}C{^{1}H}-NMR (125MHz) δ:** 165.2; 153.2; 150.8; 137.1; 126.5; 123.3; 71.4; 27.9; 19.1.

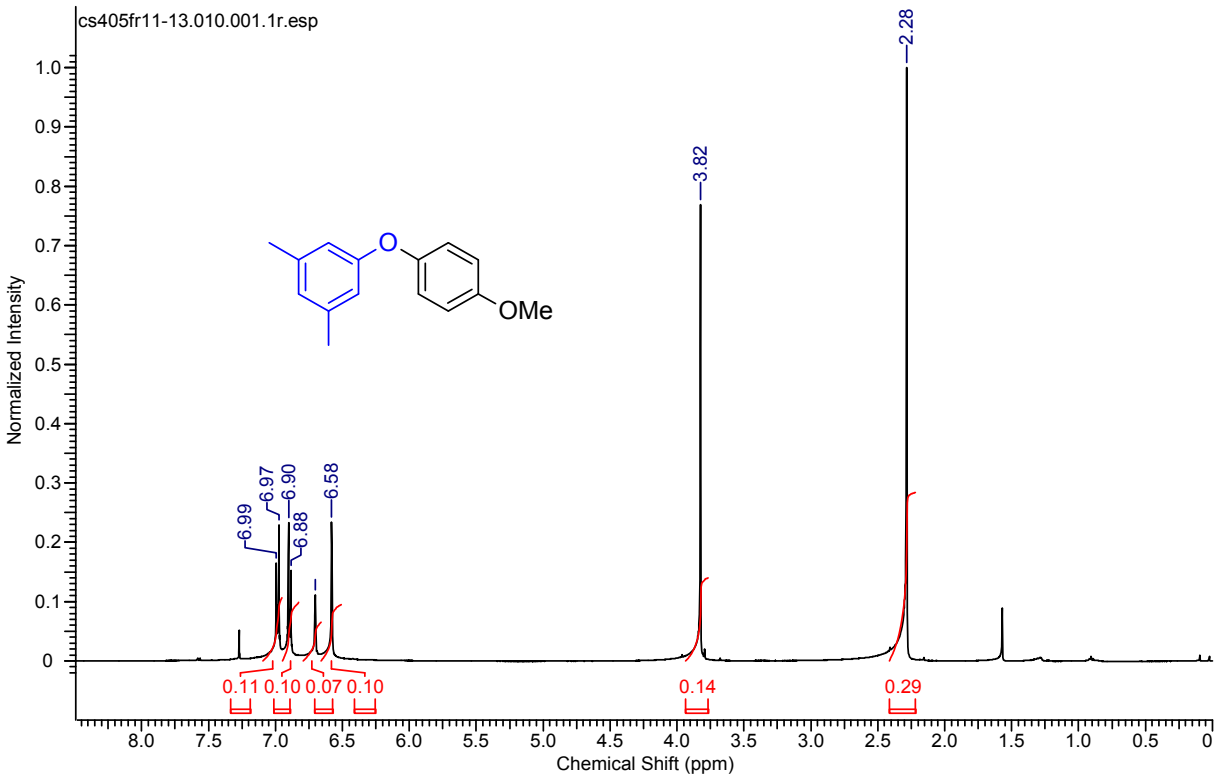
References

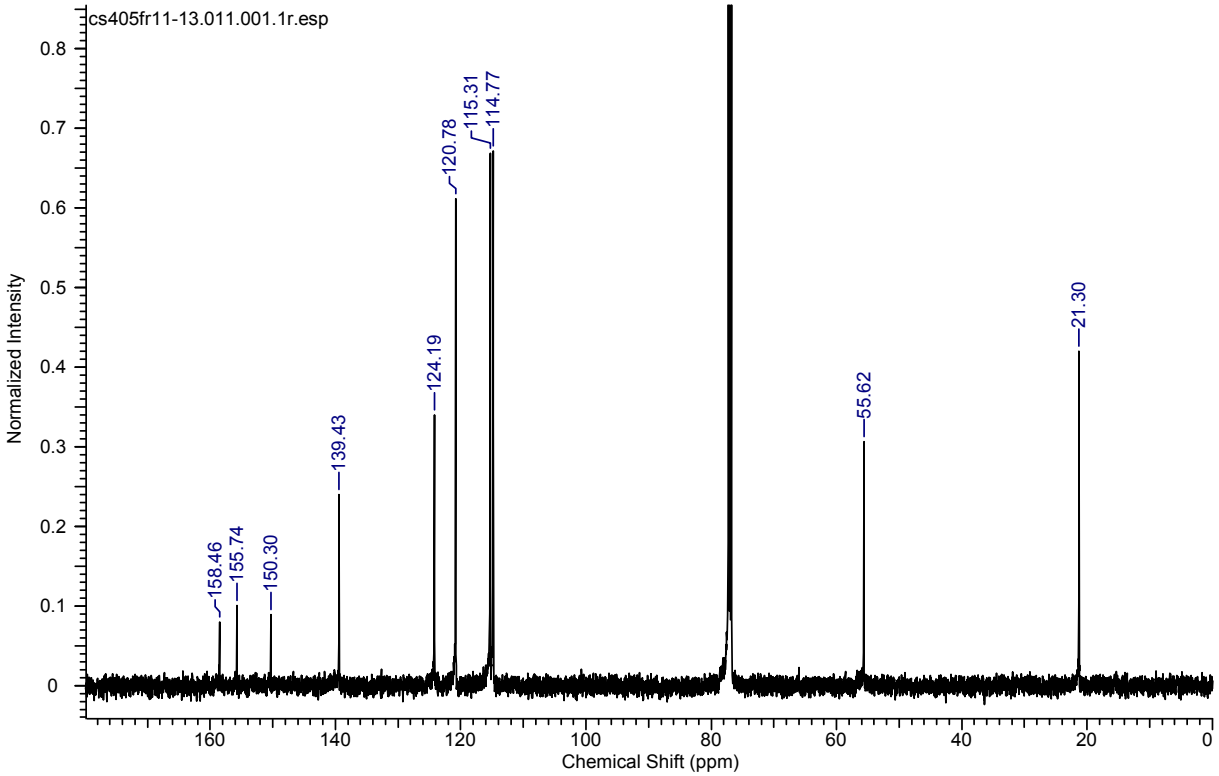
[1] Values of dielectric constants were obtained from: http://macro.lsu.edu/HowTo/solvents/Dielectric%20Constant%20.htm; http://deltacnt.com/99-00032.htm

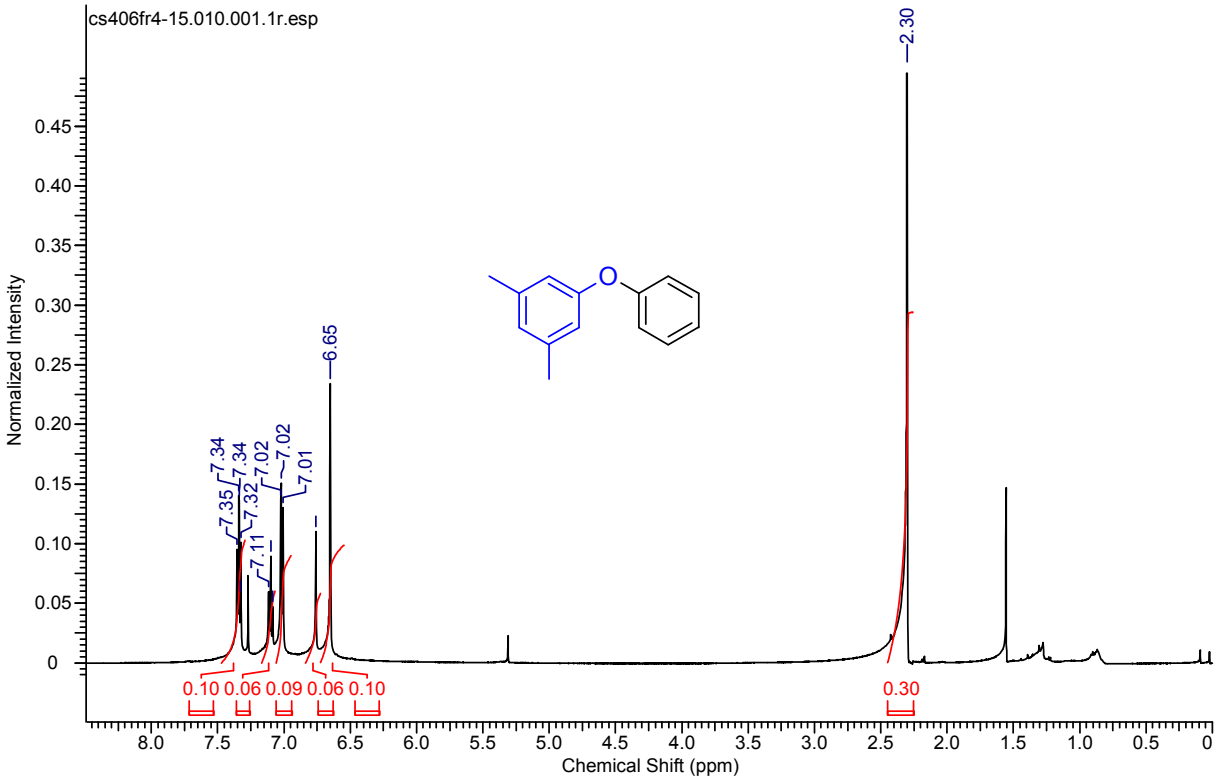
[2] S. M. A. H. Siddiki, A. S. Touchy, M. Tamura and K.-I. Shimizu, *RSC Advances*, 2014, **4**, 35803-35807

[3] J. Xia, A. Shao, S. Tang, X. Gao, M. Gao and A. Lei, *Org. Biomol. Chem.*, 2015, **13**, 6154-6157

^{1}H- and ^{13}C-NMR spectra



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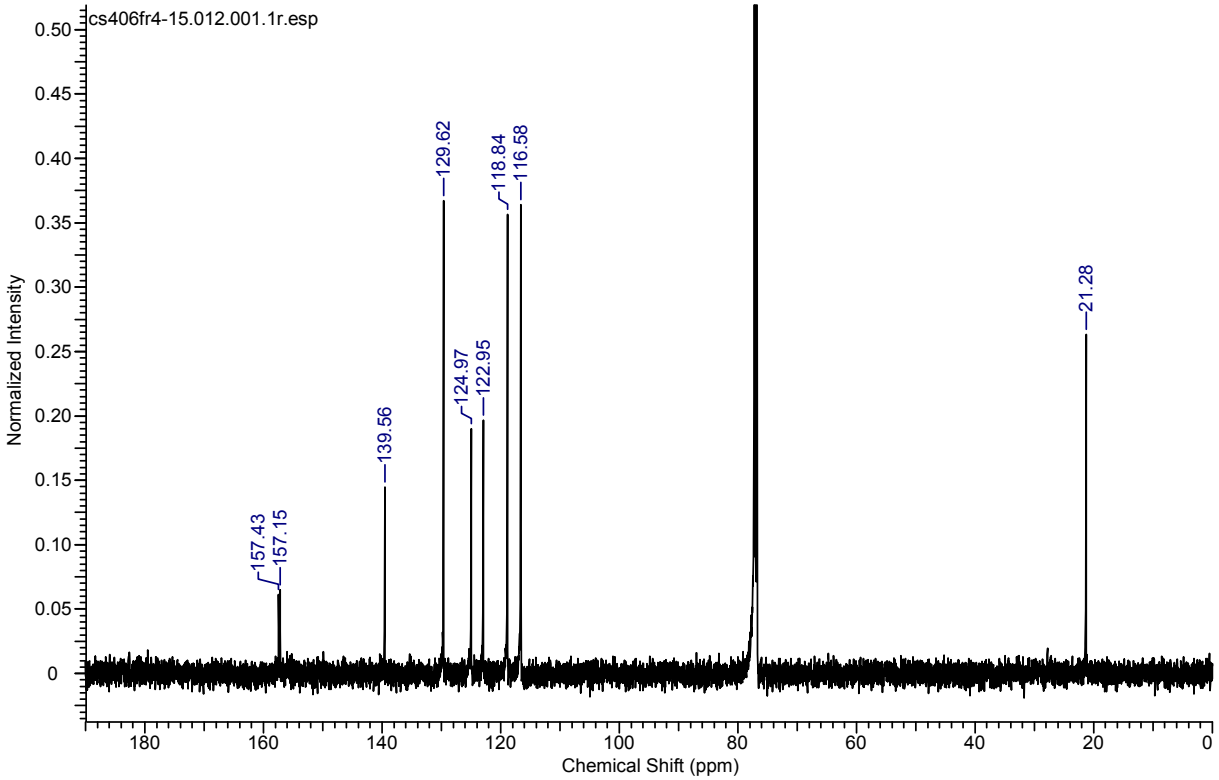
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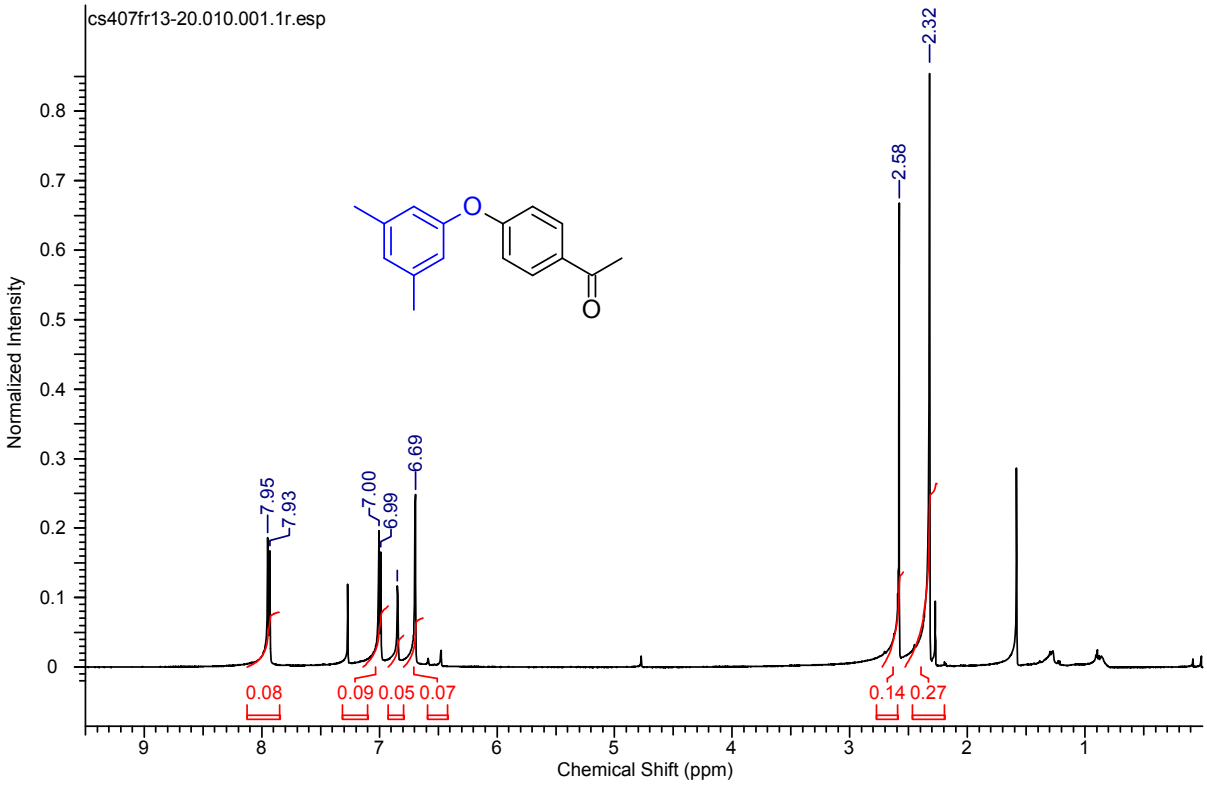
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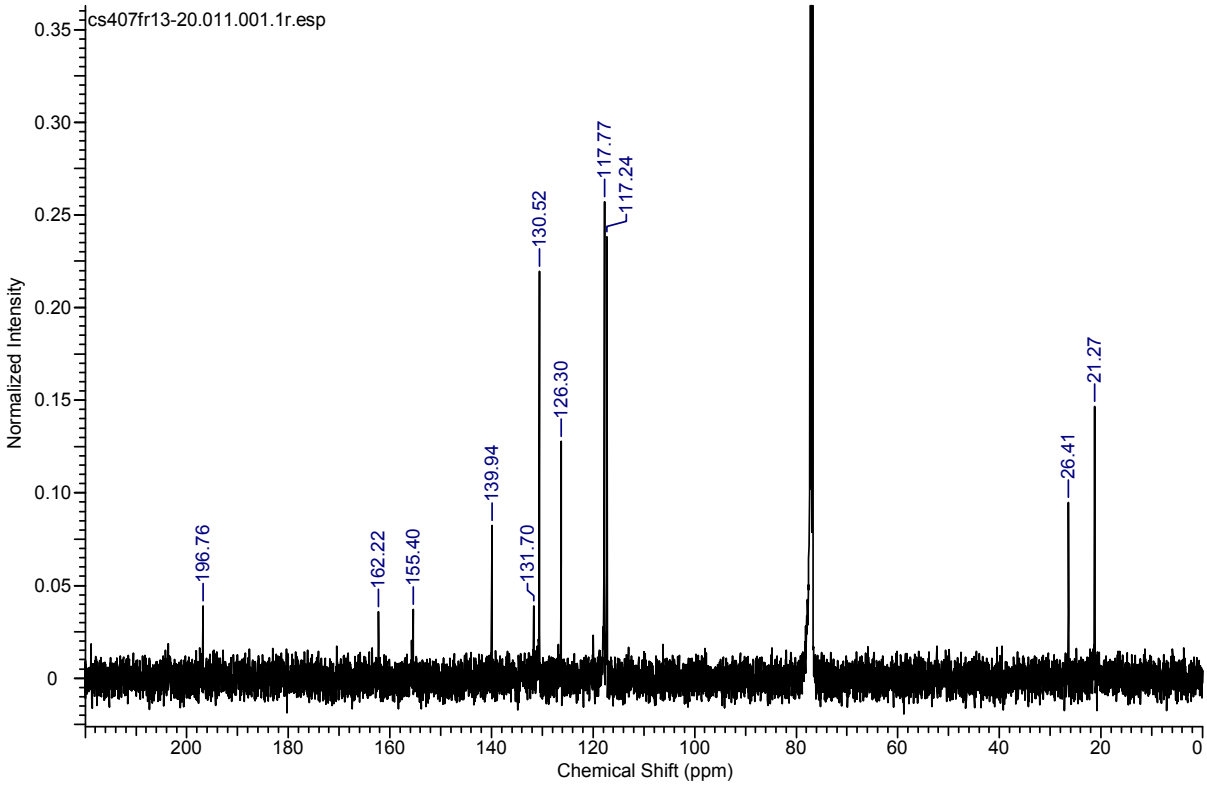
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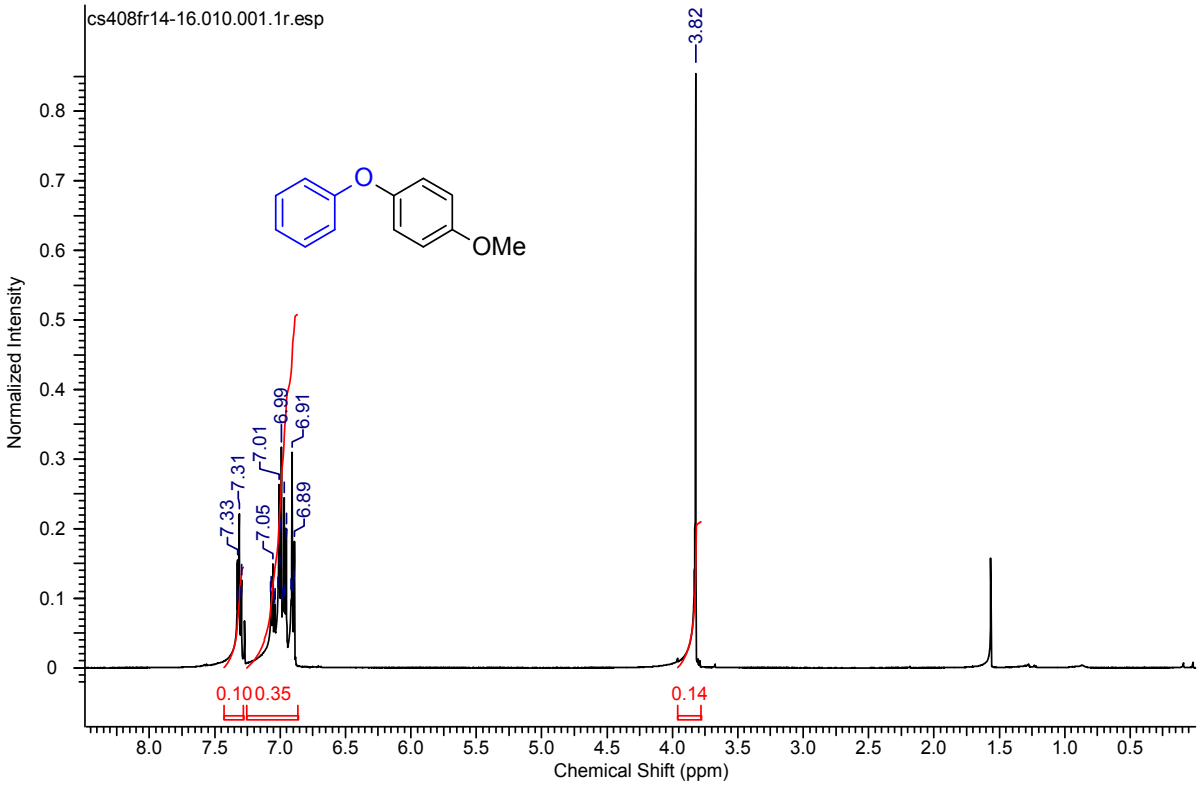
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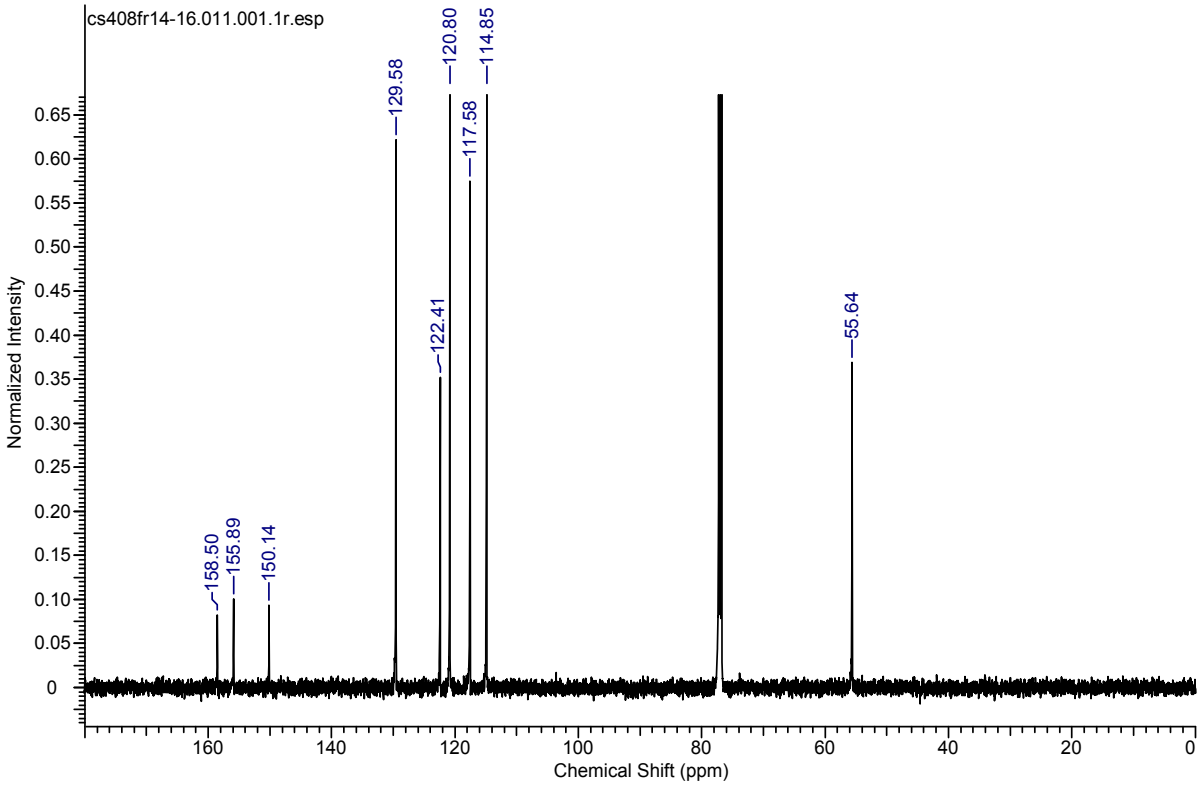
Normalized Intensity
Chemical Shift (ppm)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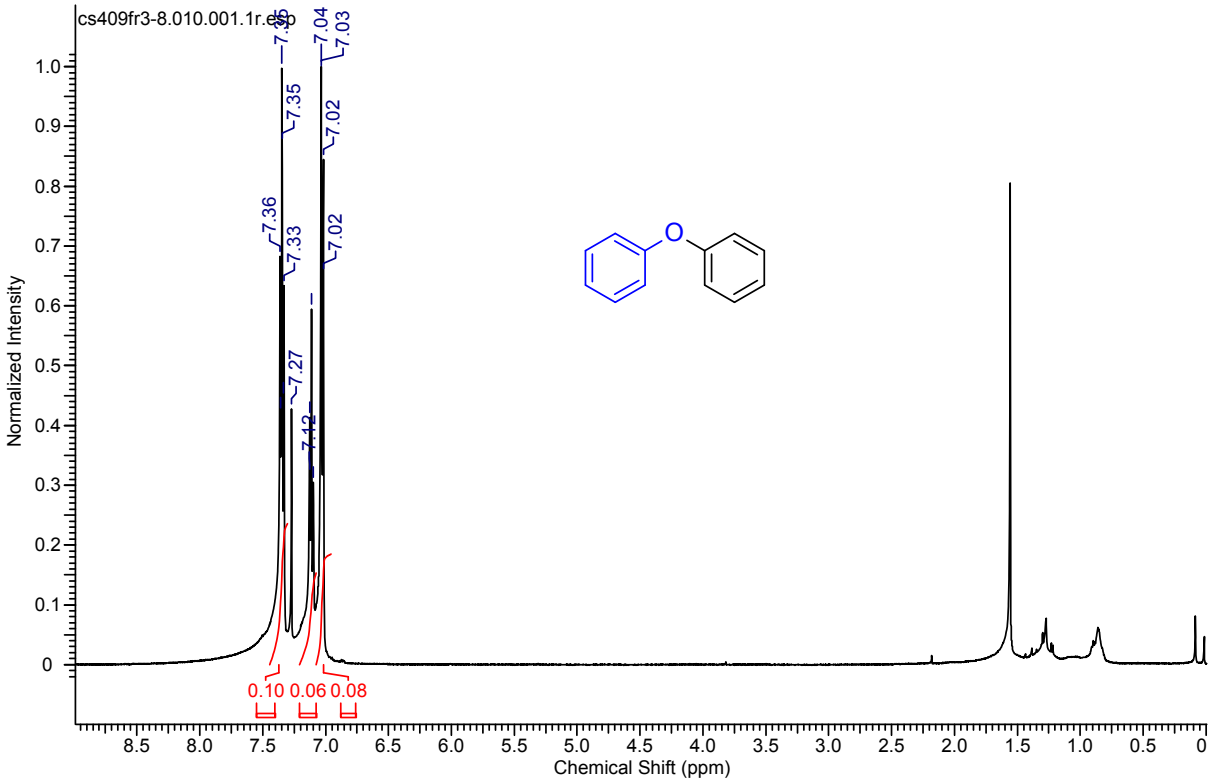
Chemical Shift (ppm)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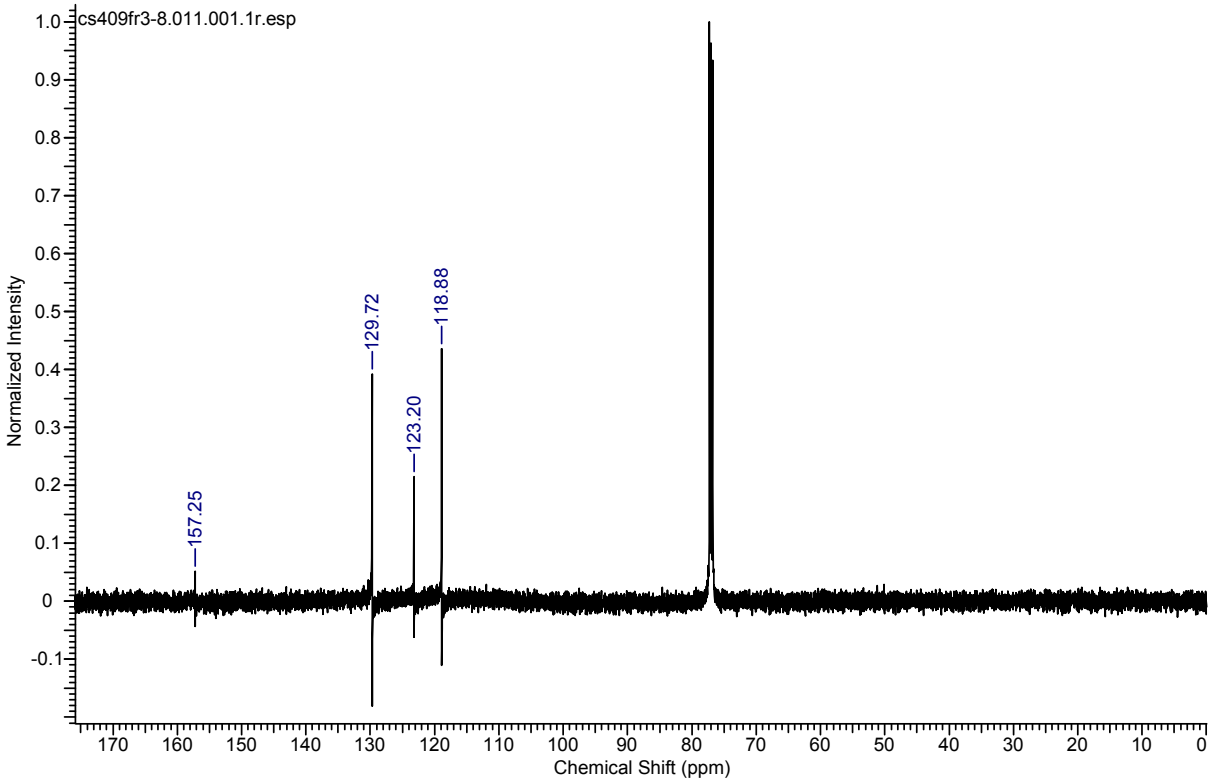
Normalized Intensity
Chemical Shift (ppm)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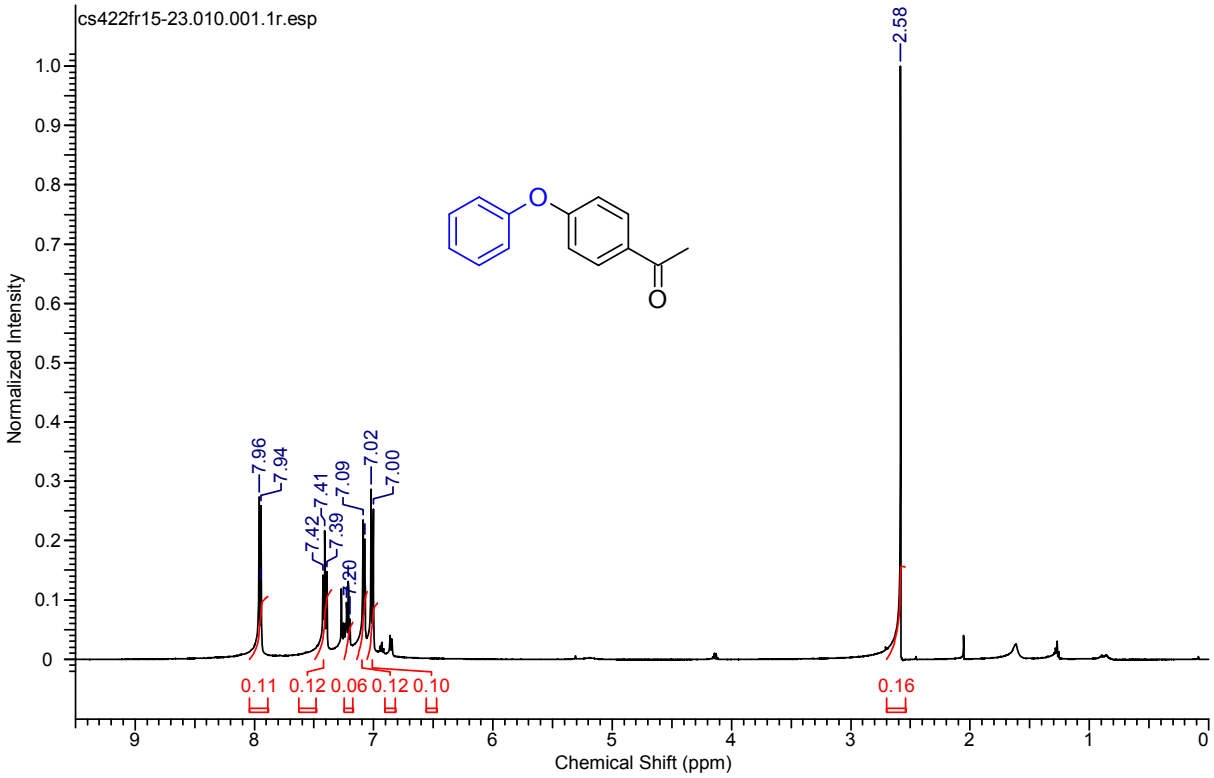
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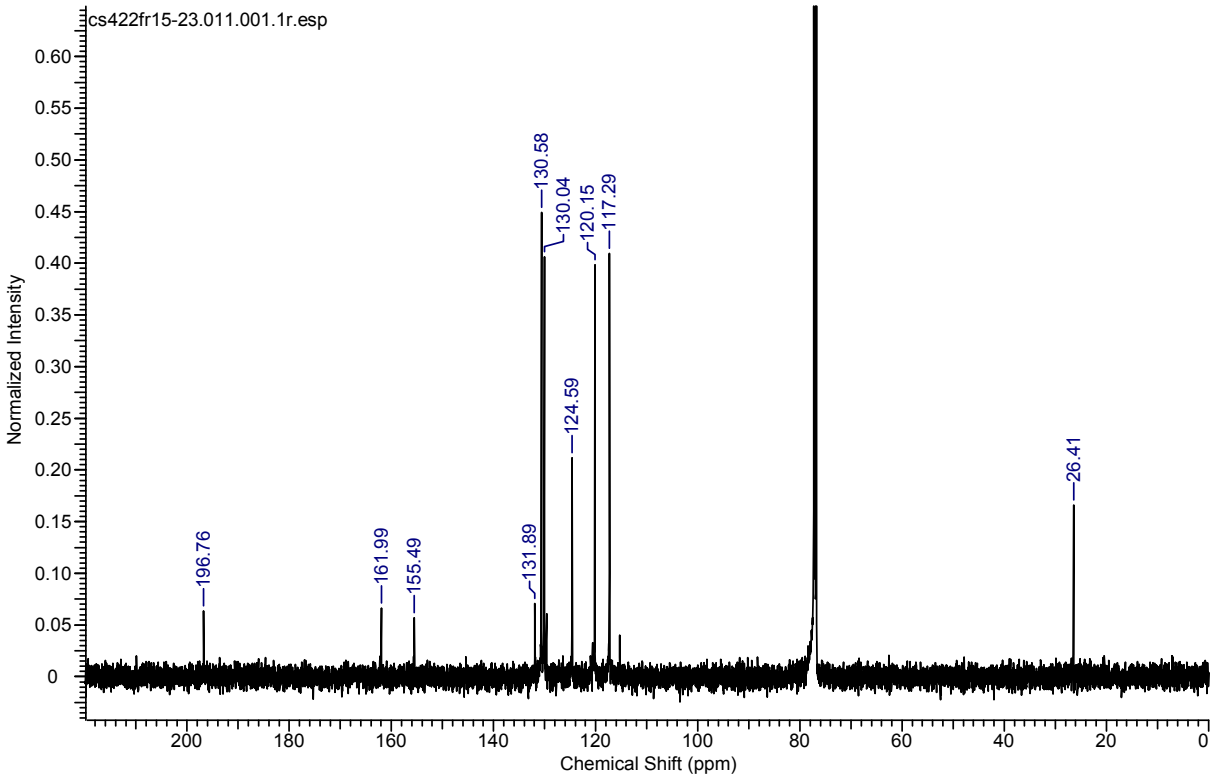
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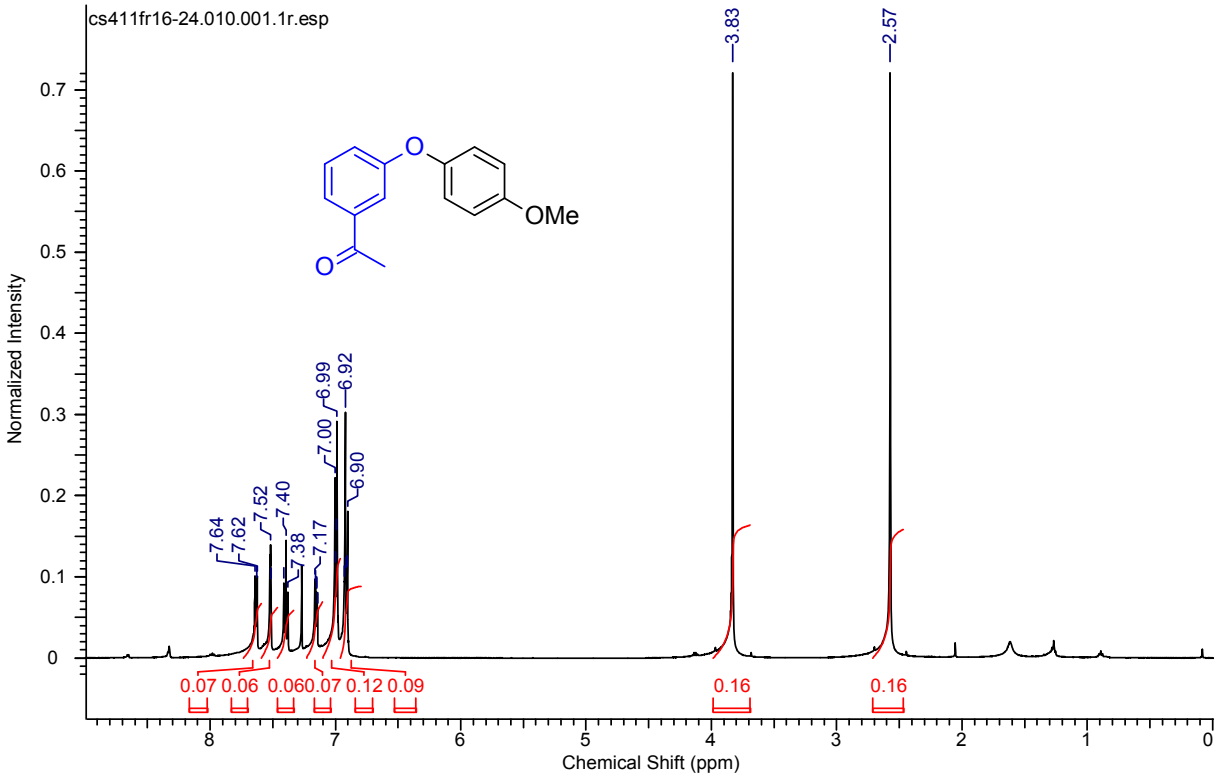
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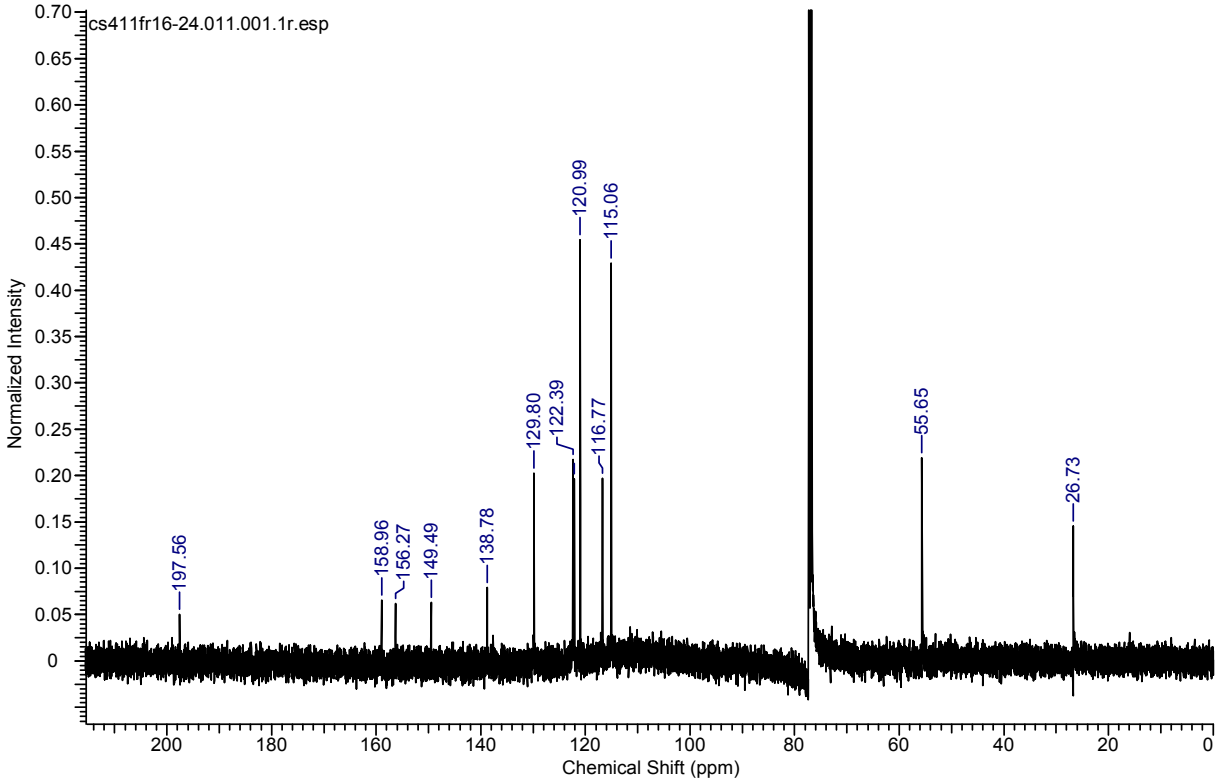
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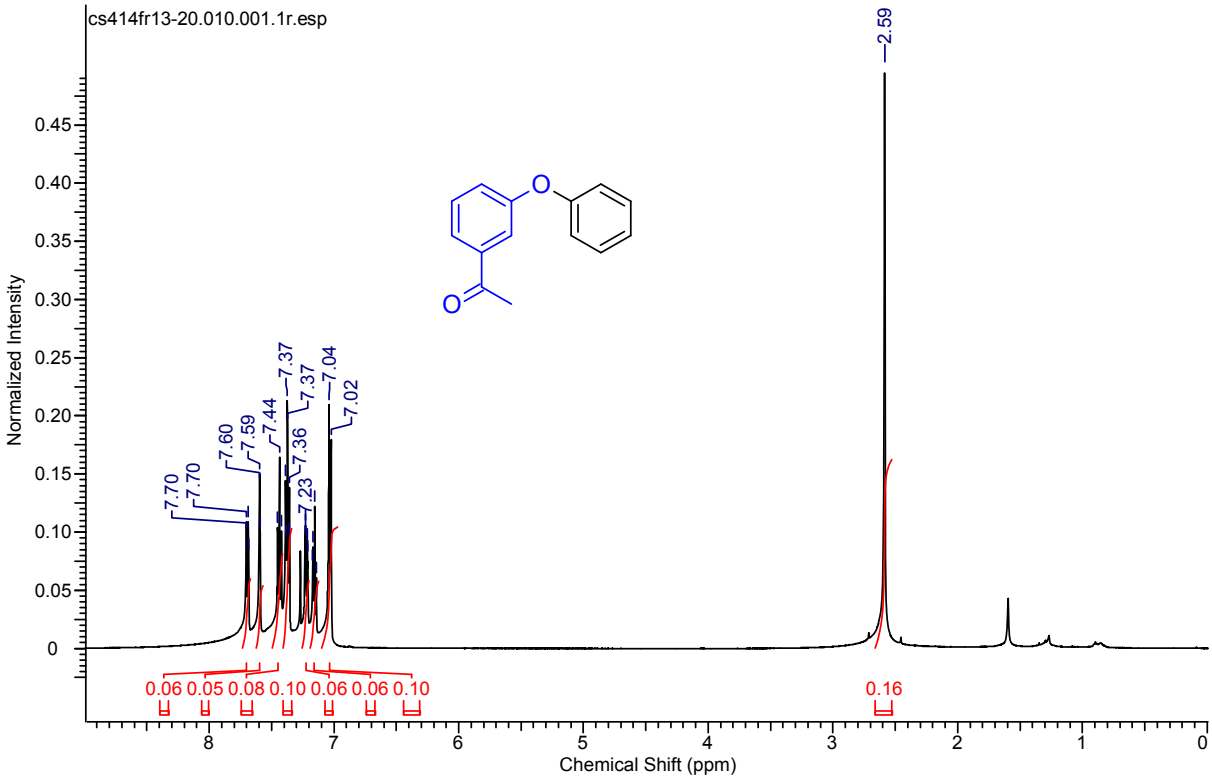
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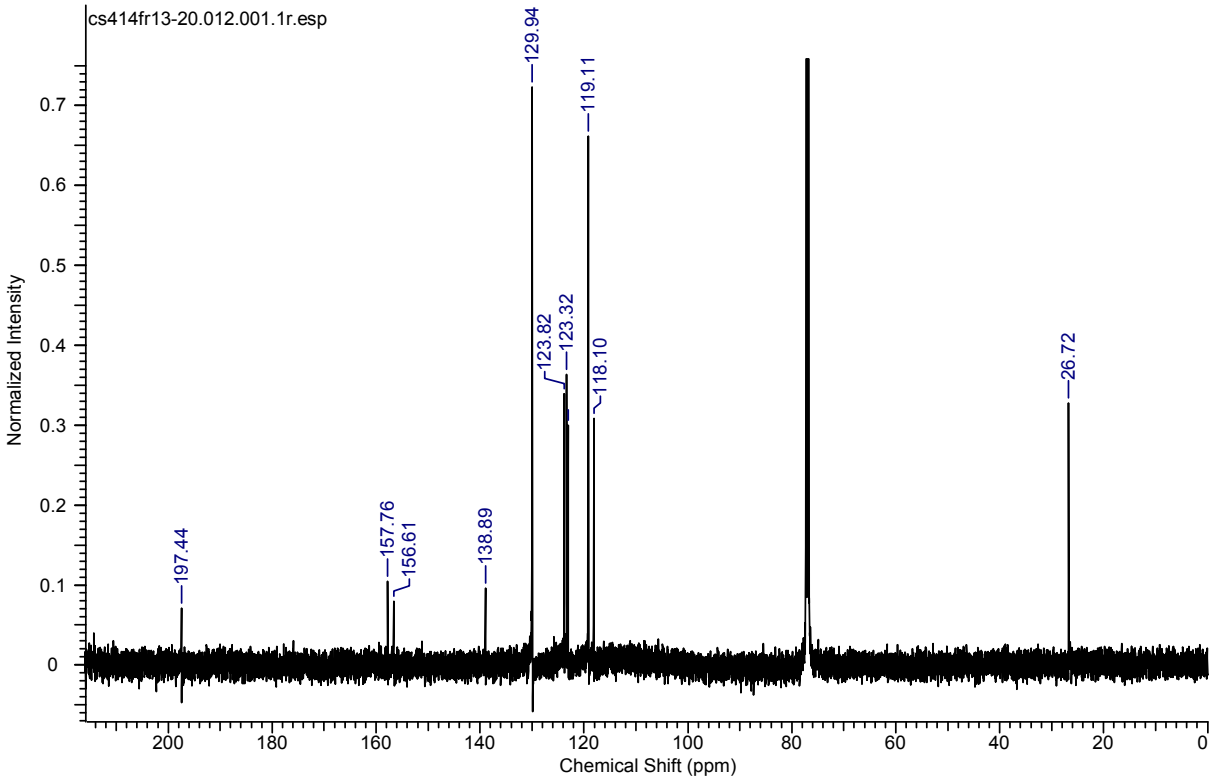
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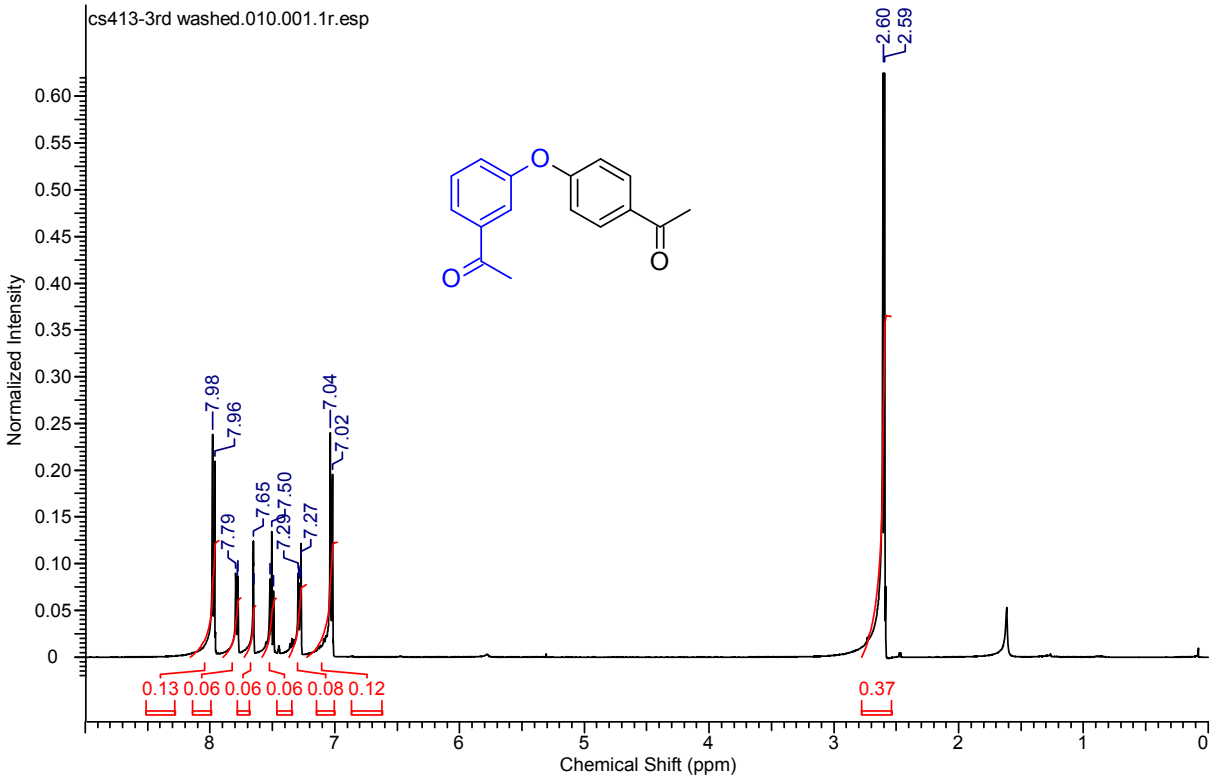
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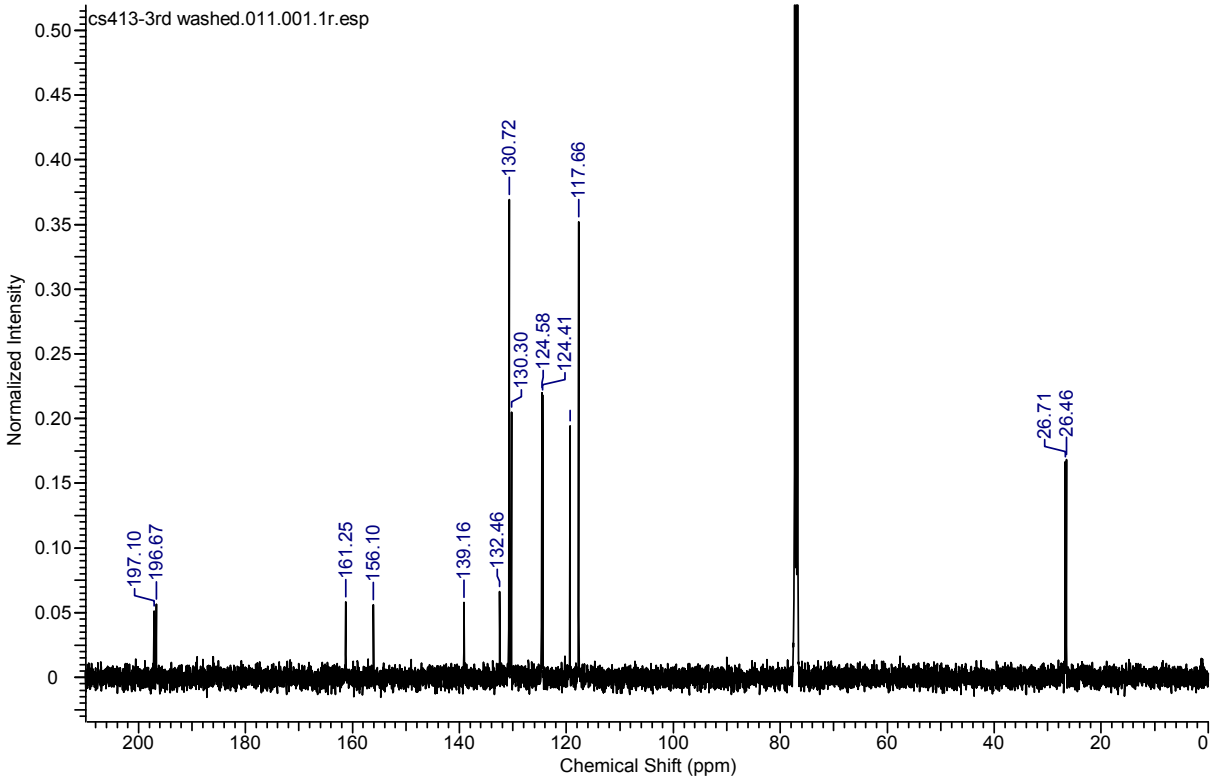
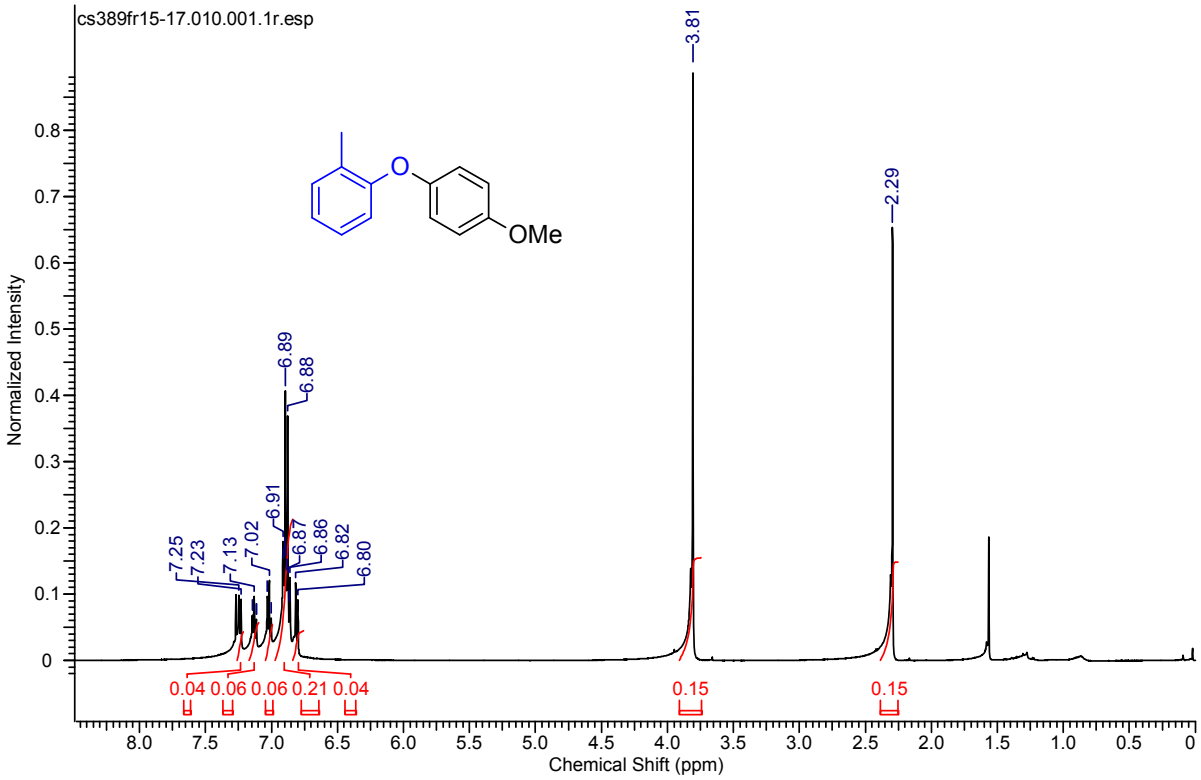
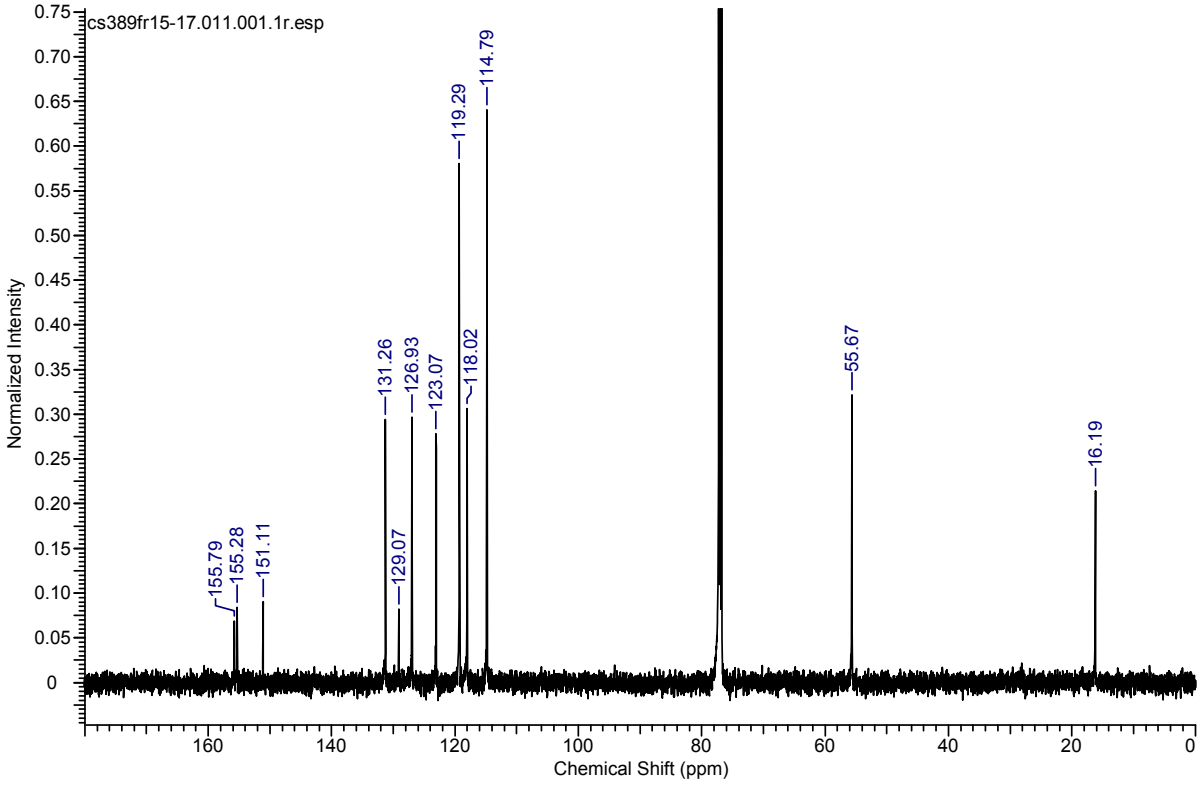
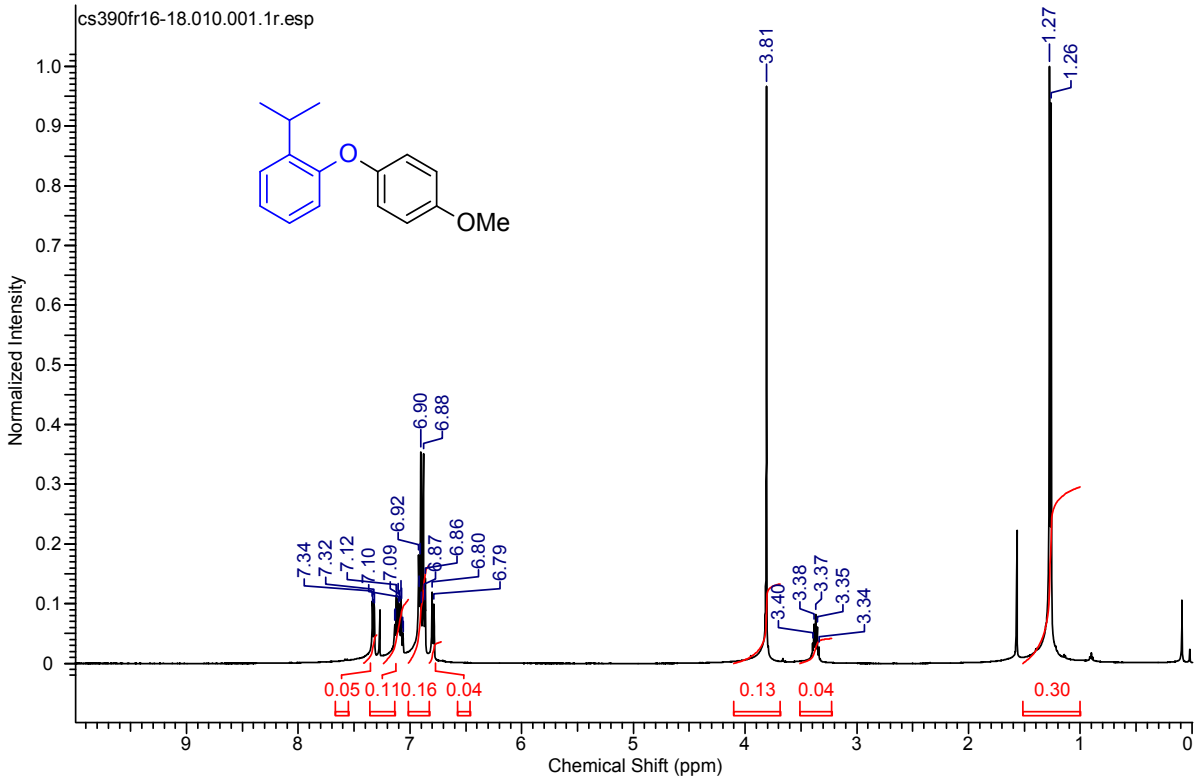
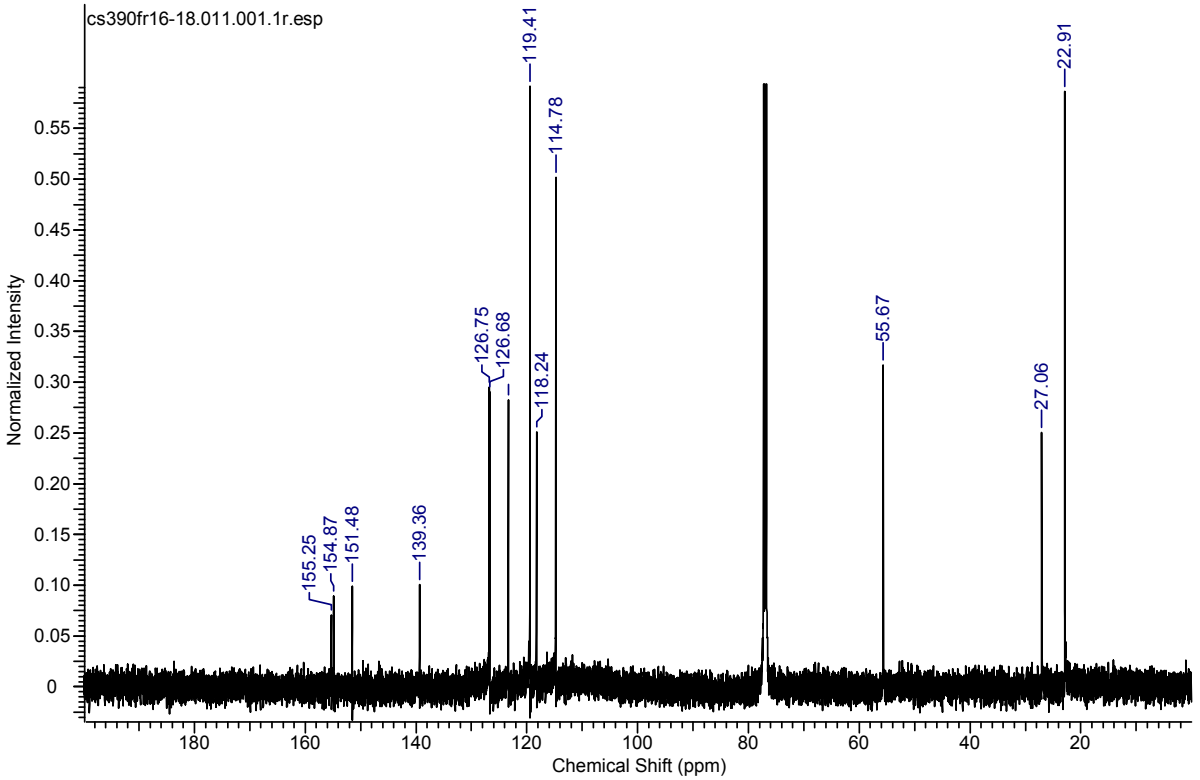
0.13 0.06 0.06 0.06 0.06 0.08 0.12
0.37

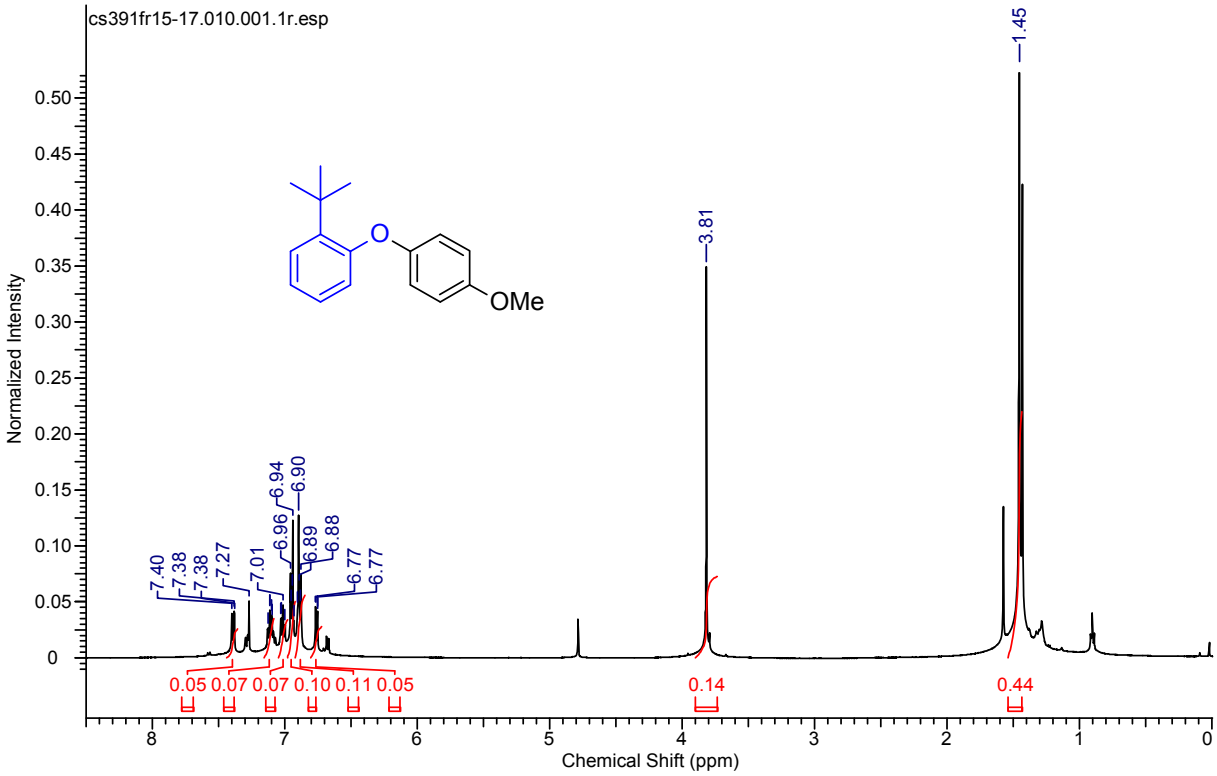

cs413-3rd washed.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
197.10
196.67
161.25
156.10
139.16
132.46
130.72
130.30
124.58
124.41
117.66
26.71
26.46

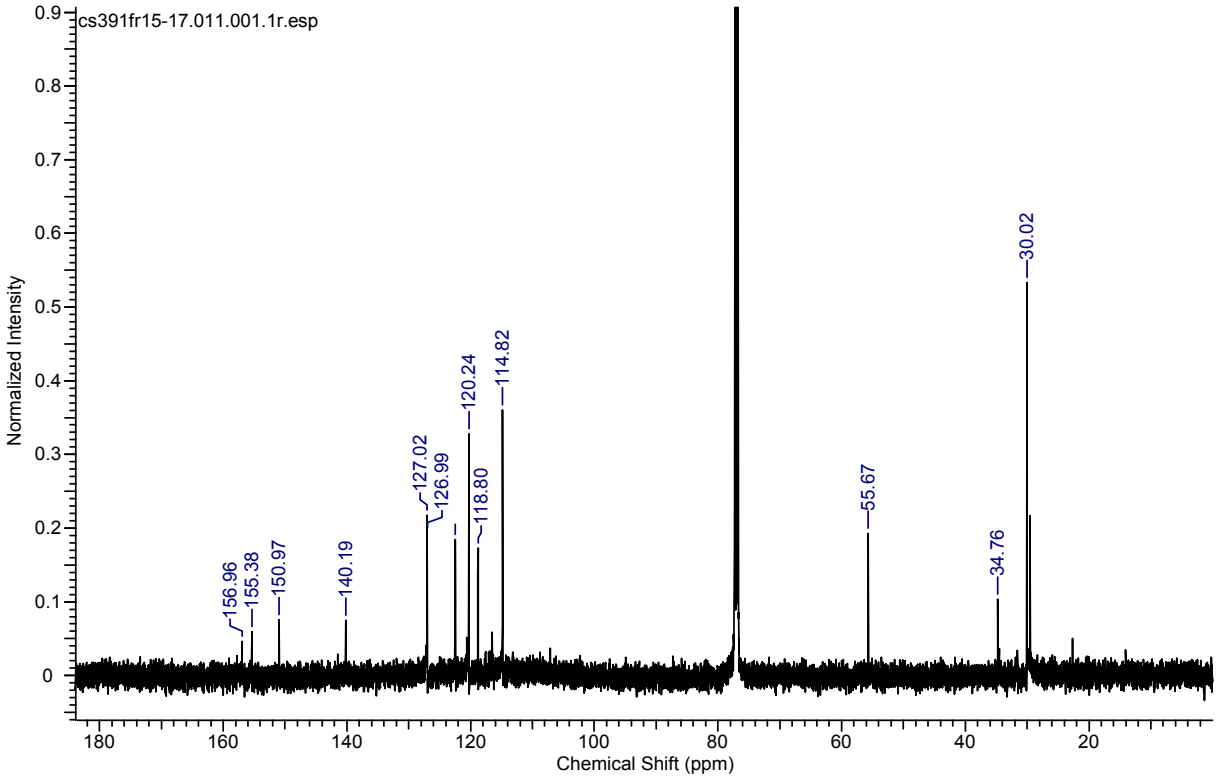

cs389fr15-17.010.001.1r.esp
O
OMe
3.81
2.29
6.89
6.88
6.91
7.25
7.23
7.13
7.02
6.87
6.86
6.82
6.80
0.04 0.06 0.06 0.21 0.04
0.15
0.15
Normalized Intensity
Chemical Shift (ppm)

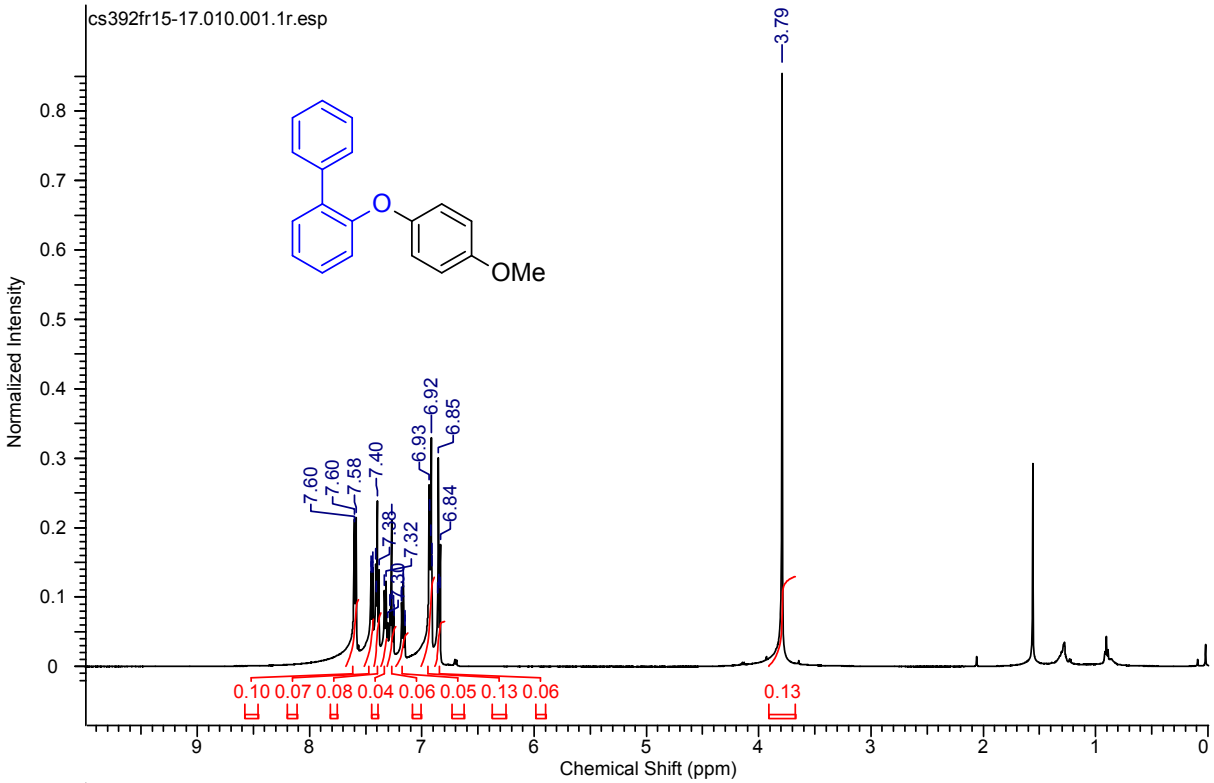

cs389fr15-17.011.001.1r.esp
114.79
119.29
131.26
126.93
123.07
118.02
55.67
16.19
155.79
155.28
151.11
129.07
Normalized Intensity
Chemical Shift (ppm)

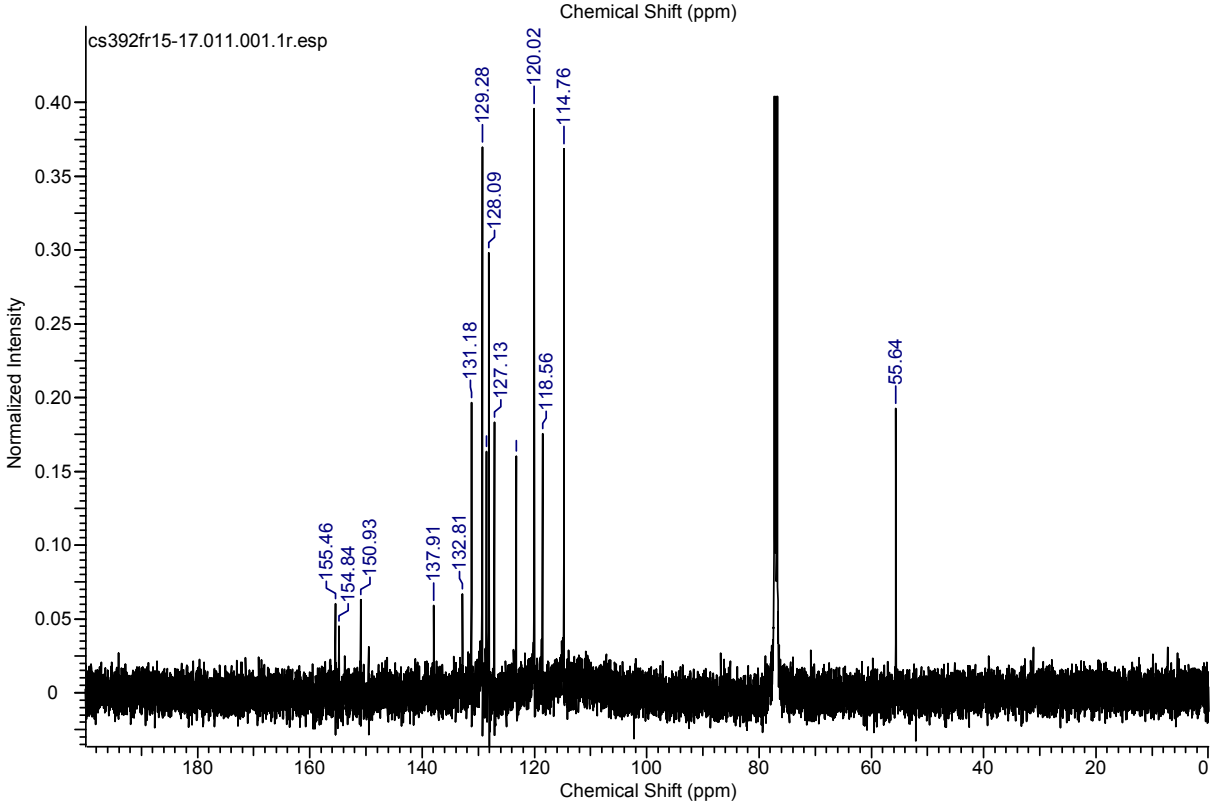

cs390fr16-18.010.001.1r.esp
OMe
Normalized Intensity
Chemical Shift (ppm)
3.81
1.27
1.26
6.90
6.88
6.92
7.34
7.32
7.12
7.10
7.09
6.87
6.86
6.80
6.79
3.40
3.38
3.37
3.35
3.34
0.05
0.11
0.16
0.04
0.13
0.04
0.30

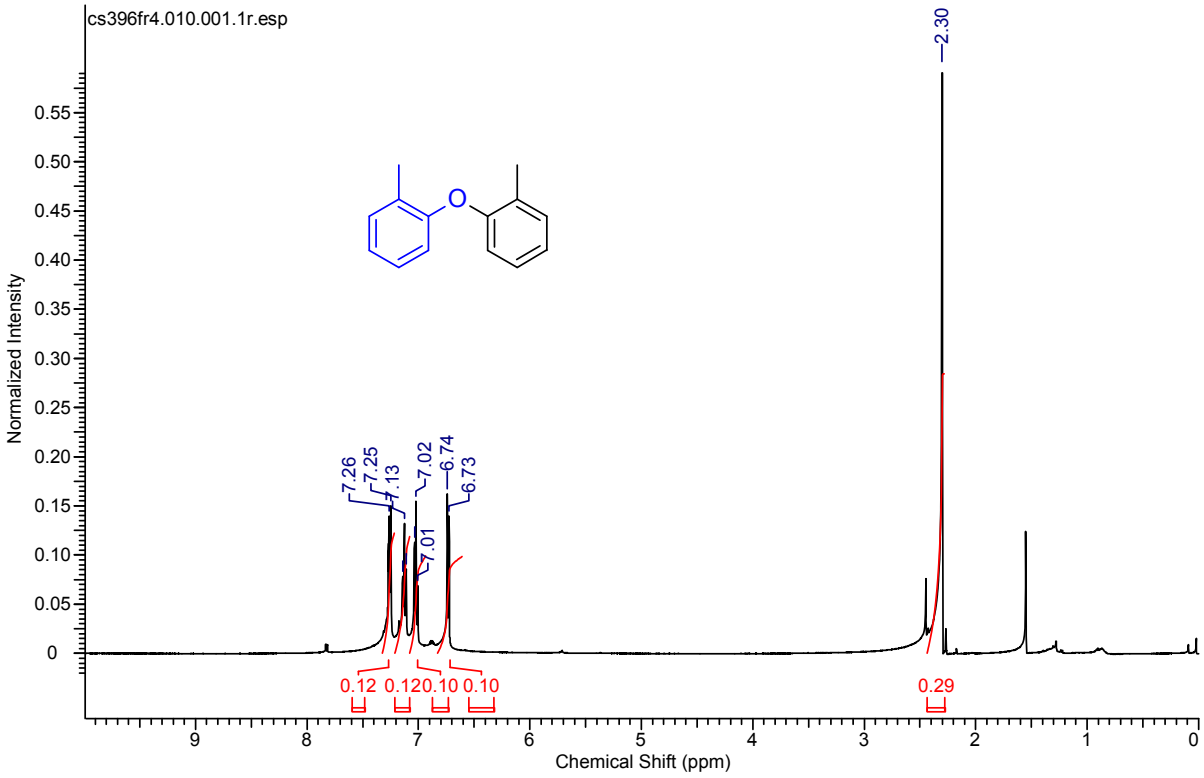

cs390fr16-18.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
119.41
114.78
22.91
126.75
126.68
118.24
55.67
27.06
155.25
154.87
151.48
139.36

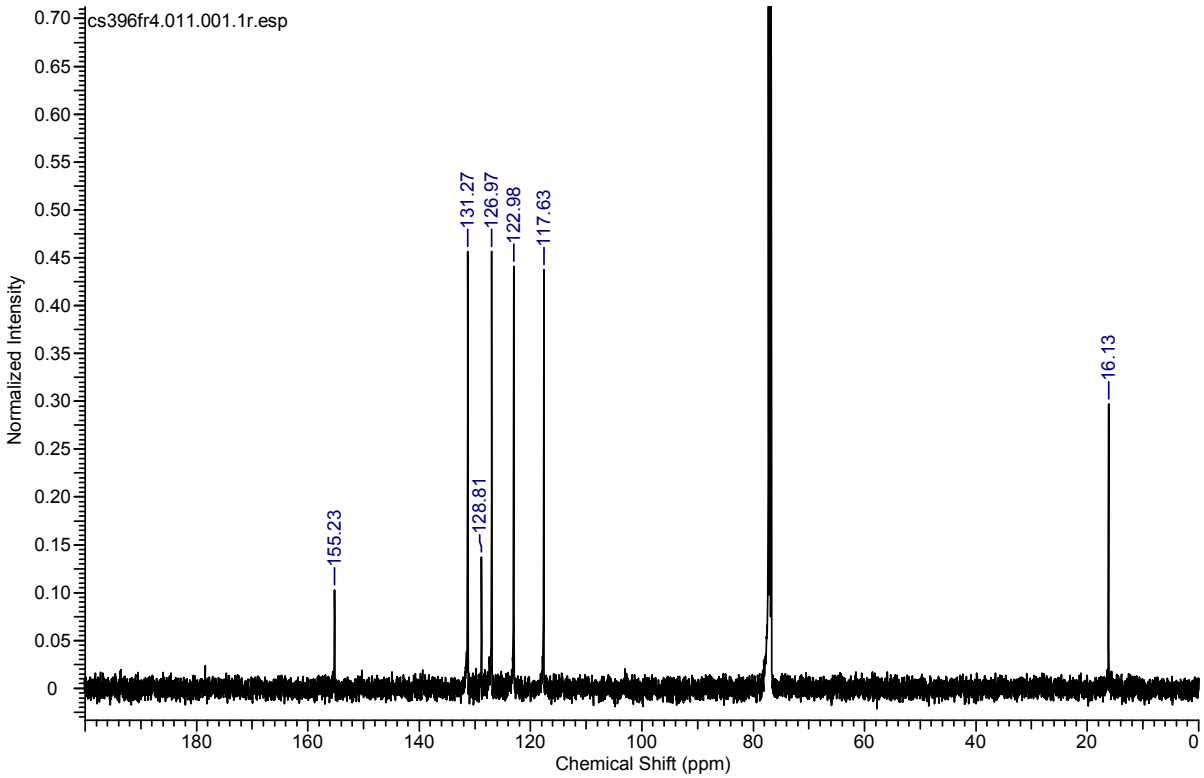

cs391fr15-17.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
OMe
1.45
3.81
7.40
7.38
7.38
7.27
7.01
6.96
6.94
6.90
6.89
6.88
6.77
6.77
0.05 0.07 0.07 0.10 0.11 0.05
0.14
0.44

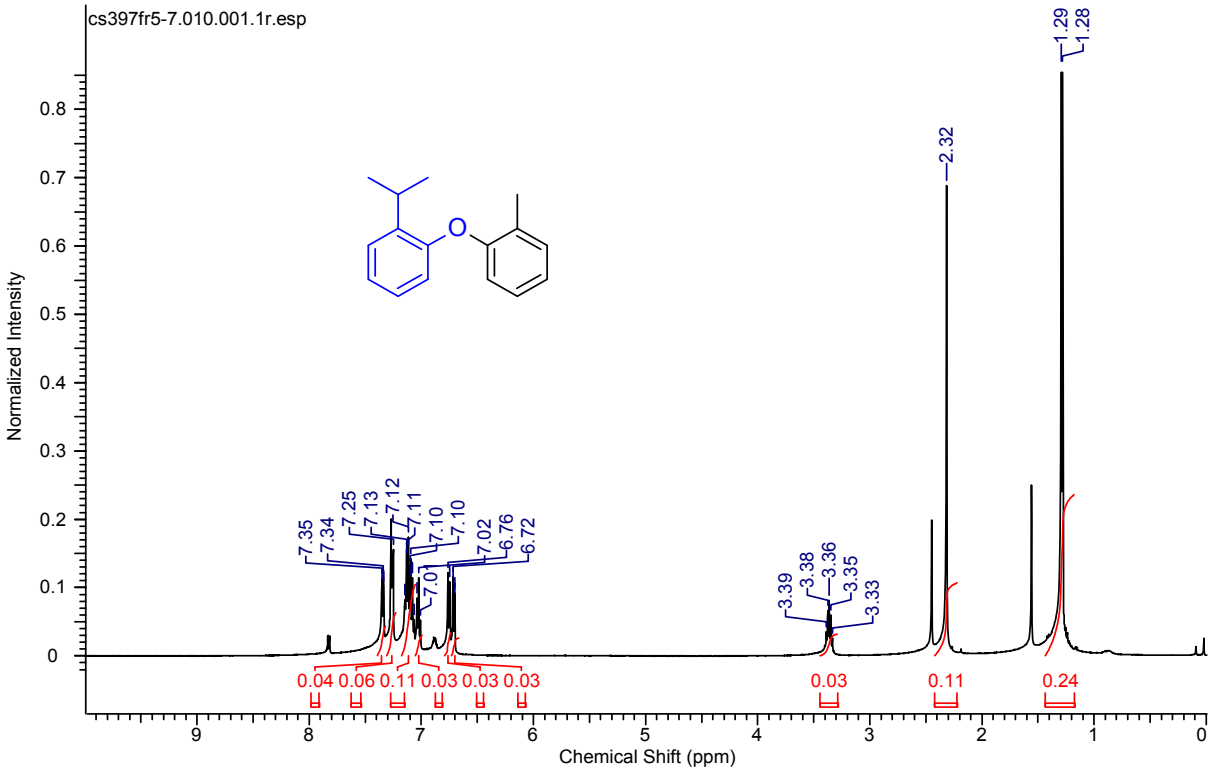

cs391fr15-17.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
156.96
155.38
150.97
140.19
127.02
126.99
120.24
118.80
114.82
55.67
34.76
30.02

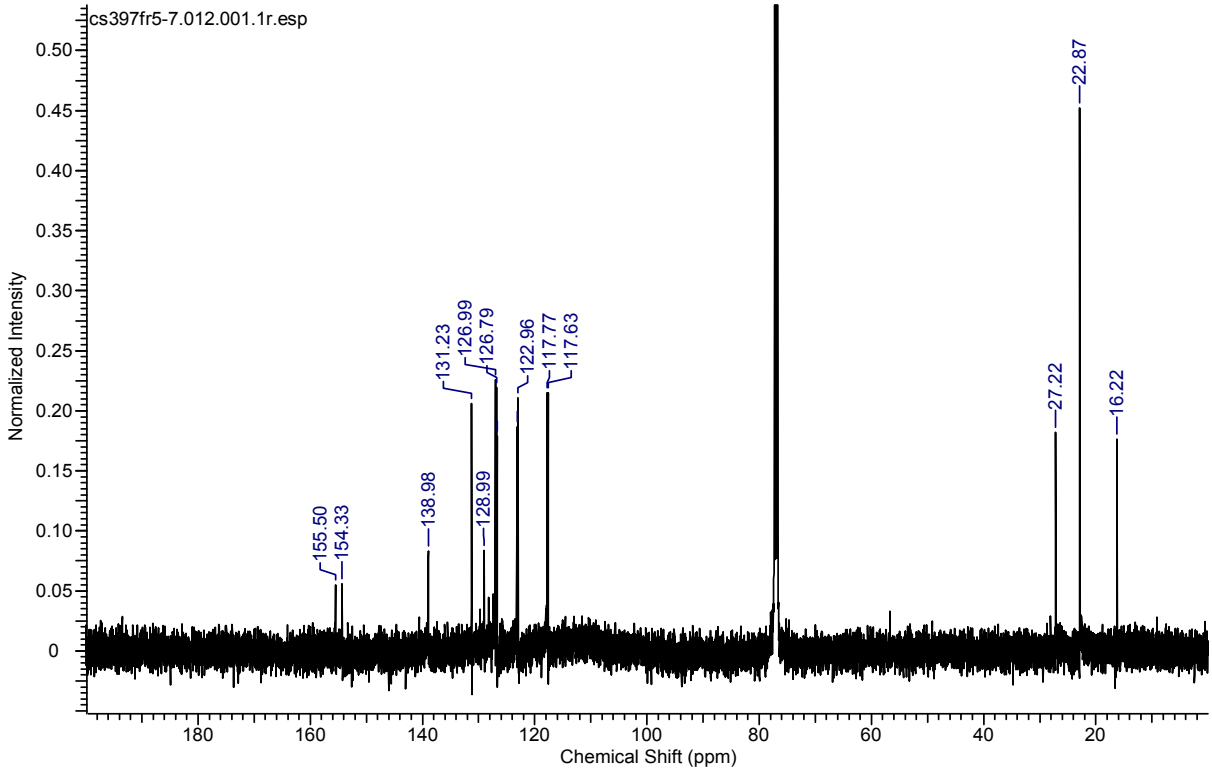

cs392fr15-17.010.001.1r.esp
O
OMe
3.79
6.92
6.85
6.93
6.84
7.60
7.60
7.58
7.40
7.38
7.32
0.10 0.07 0.08 0.04 0.06 0.05 0.13 0.06
0.13
Normalized Intensity
Chemical Shift (ppm)

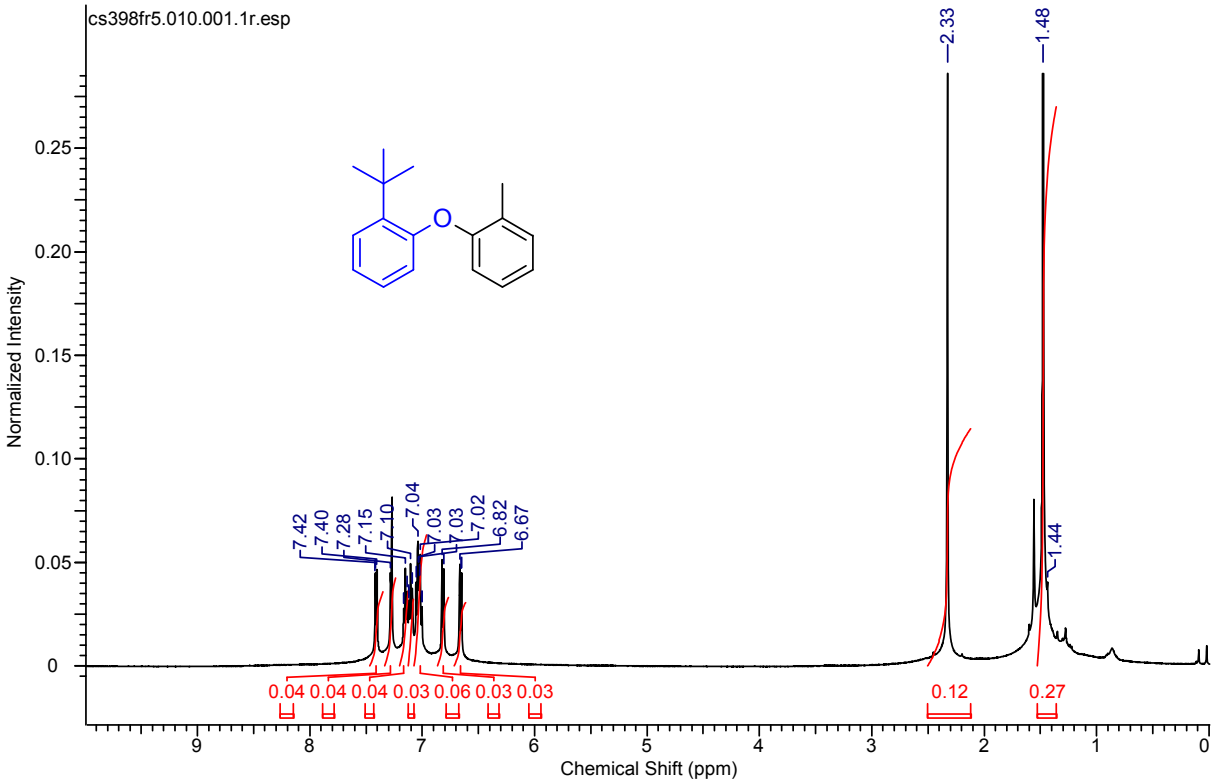

cs392fr15-17.011.001.1r.esp
129.28
120.02
114.76
128.09
131.18
127.13
118.56
55.64
155.46
154.84
150.93
137.91
132.81
Normalized Intensity
Chemical Shift (ppm)

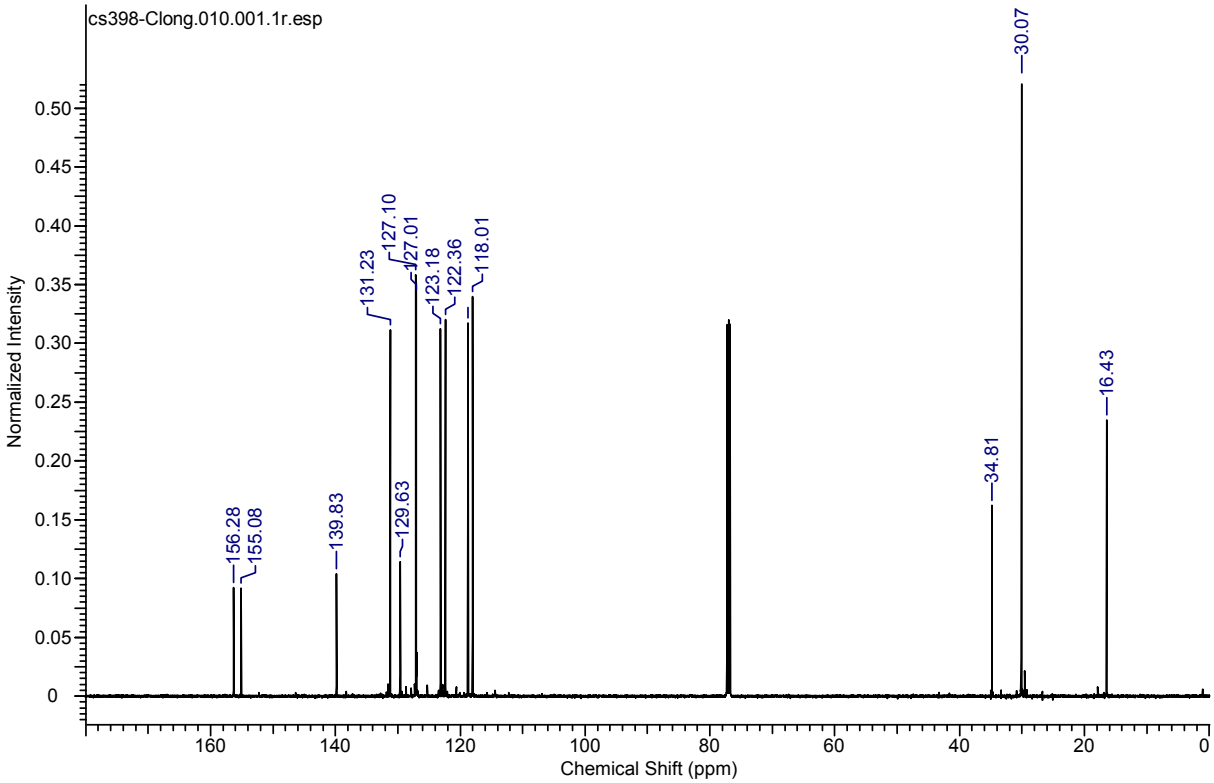

cs396fr4.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
2.30
7.26
7.25
7.13
7.02
6.74
6.73
7.01
0.12
0.12
0.10
0.10
0.29

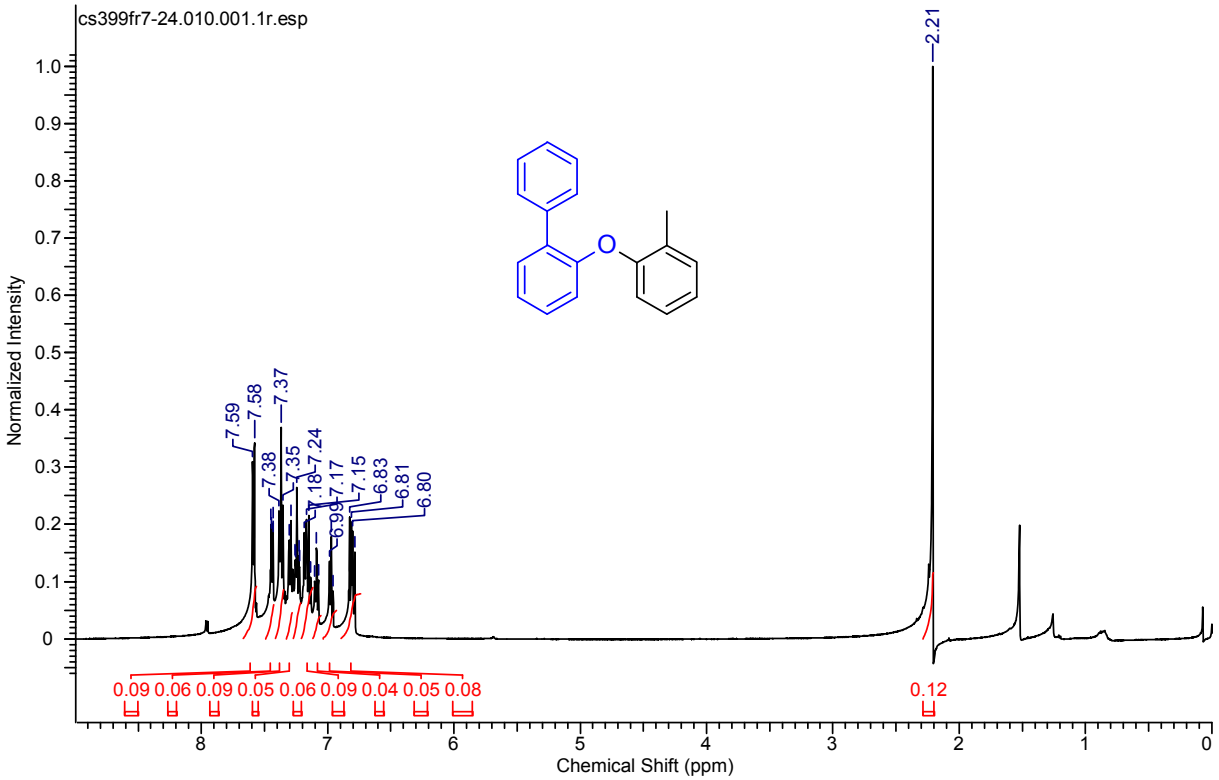

cs396fr4.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
131.27
126.97
122.98
117.63
155.23
128.81
16.13

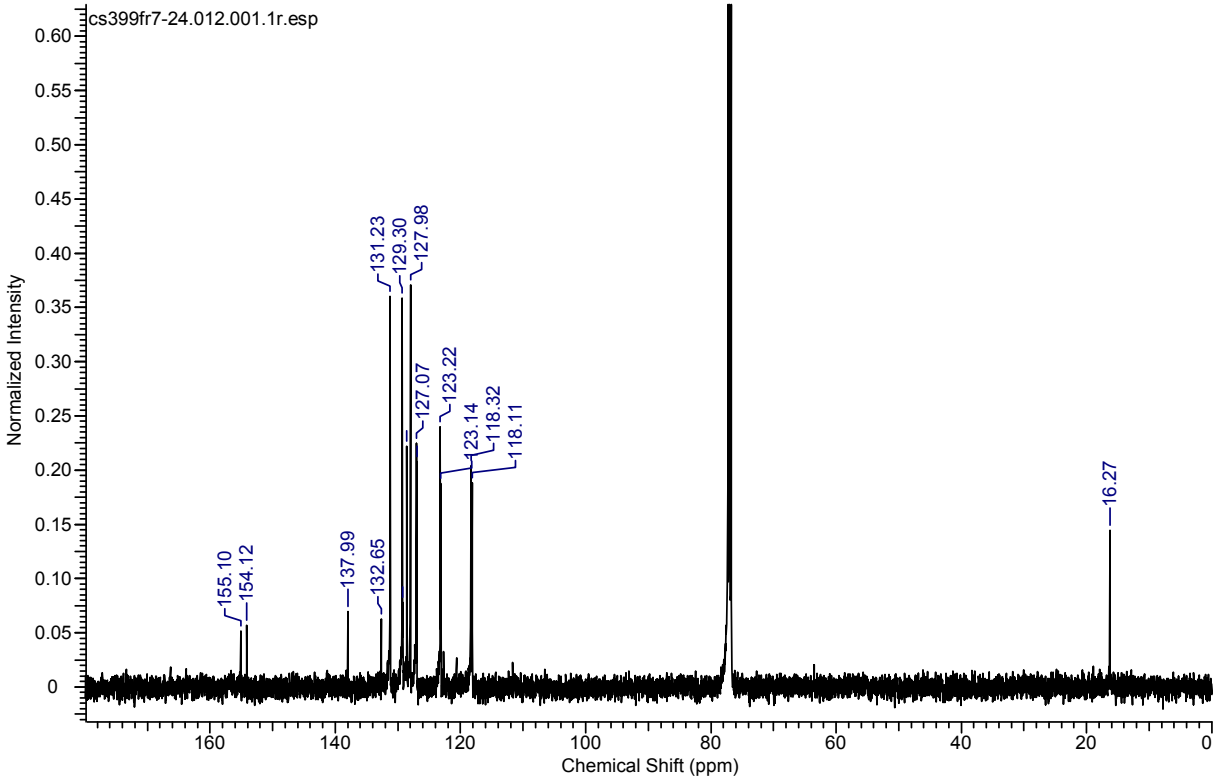

cs397fr5-7.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
1.29
1.28
2.32
7.35
7.34
7.25
7.13
7.12
7.11
7.10
7.10
7.02
6.76
6.72
7.01
3.39
3.38
3.36
3.35
3.33
0.04 0.06 0.11 0.03 0.03 0.03
0.03
0.11
0.24

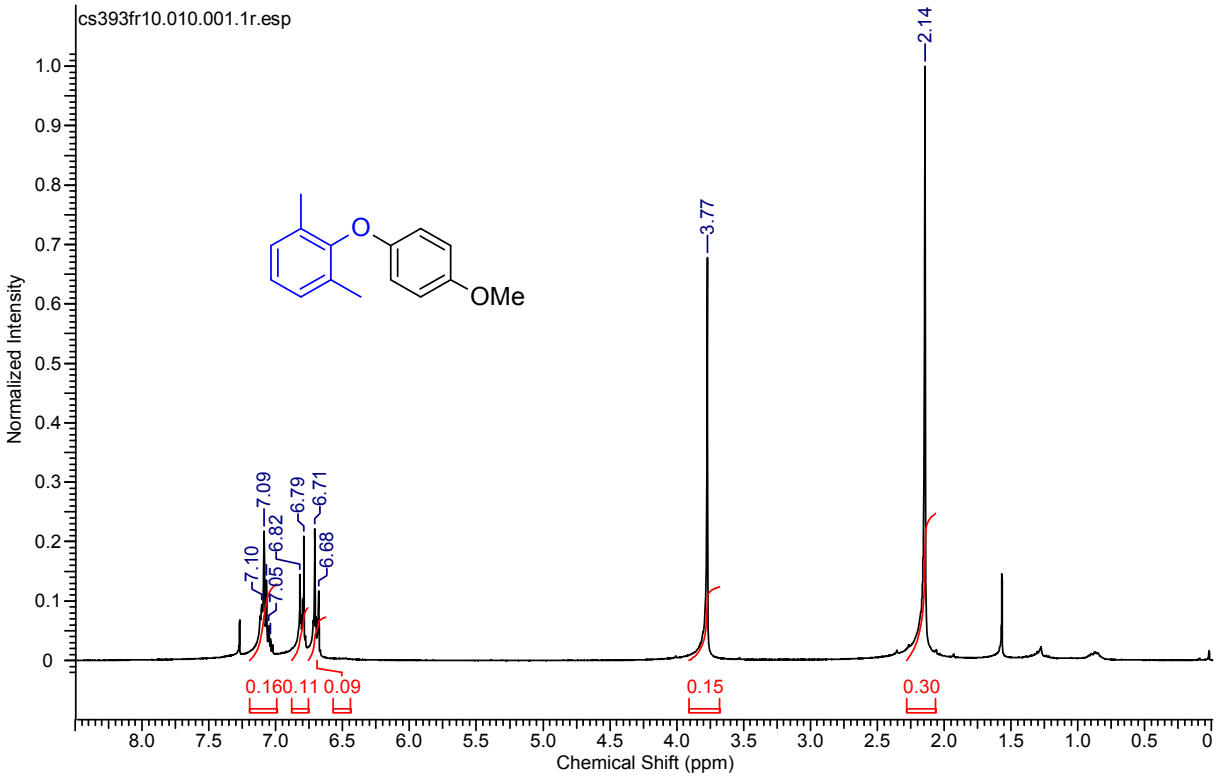

cs397fr5-7.012.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
22.87
27.22
16.22
131.23
126.99
126.79
122.96
117.77
117.63
155.50
154.33
138.98
128.99

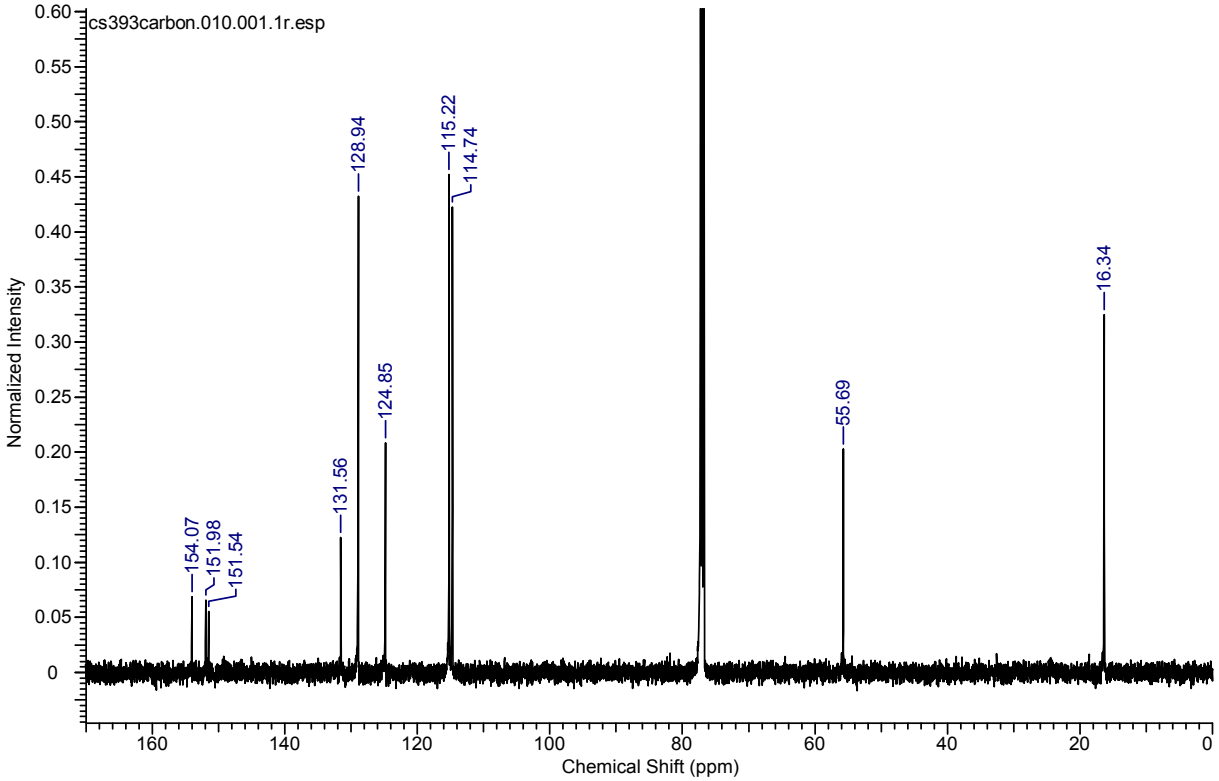

cs398fr5.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
2.33
1.48
1.44
7.42
7.40
7.28
7.15
7.10
7.04
7.03
7.03
7.02
6.82
6.67
0.04 0.04 0.04 0.03 0.06 0.03 0.03
0.12
0.27

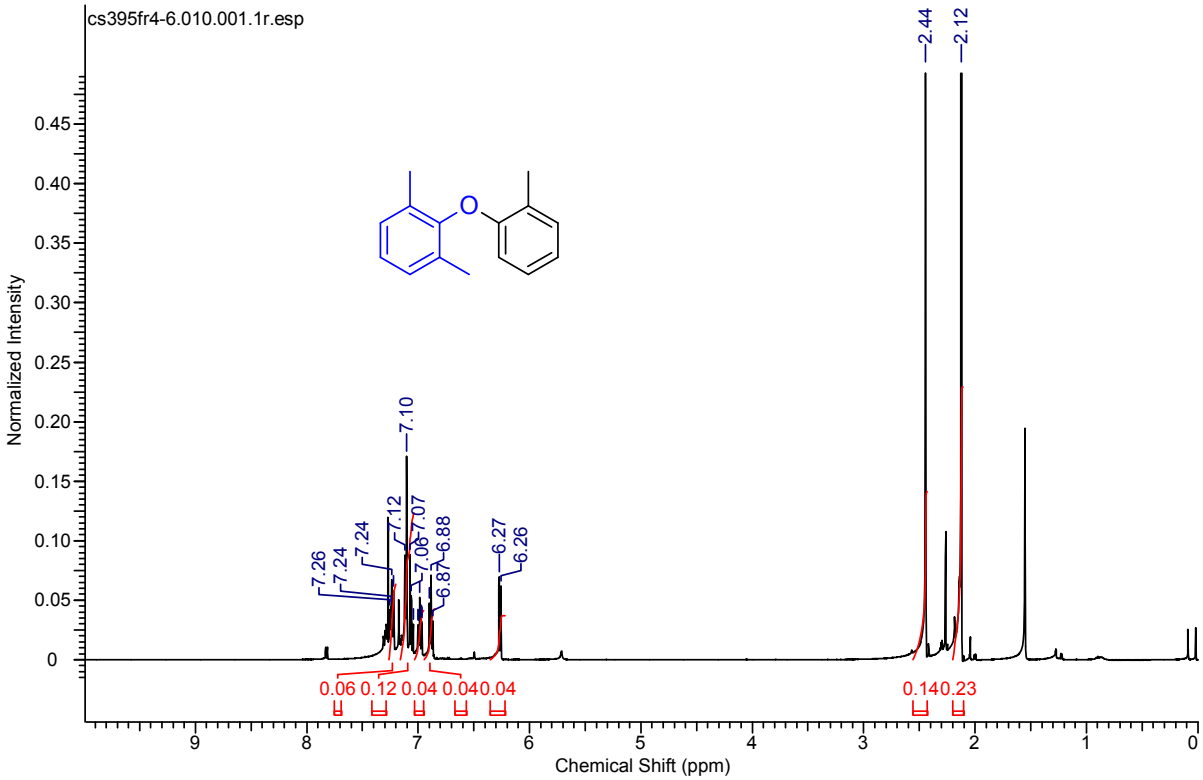

cs398-Clong.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
30.07
16.43
34.81
156.28
155.08
139.83
131.23
129.63
127.10
127.01
123.18
122.36
118.01

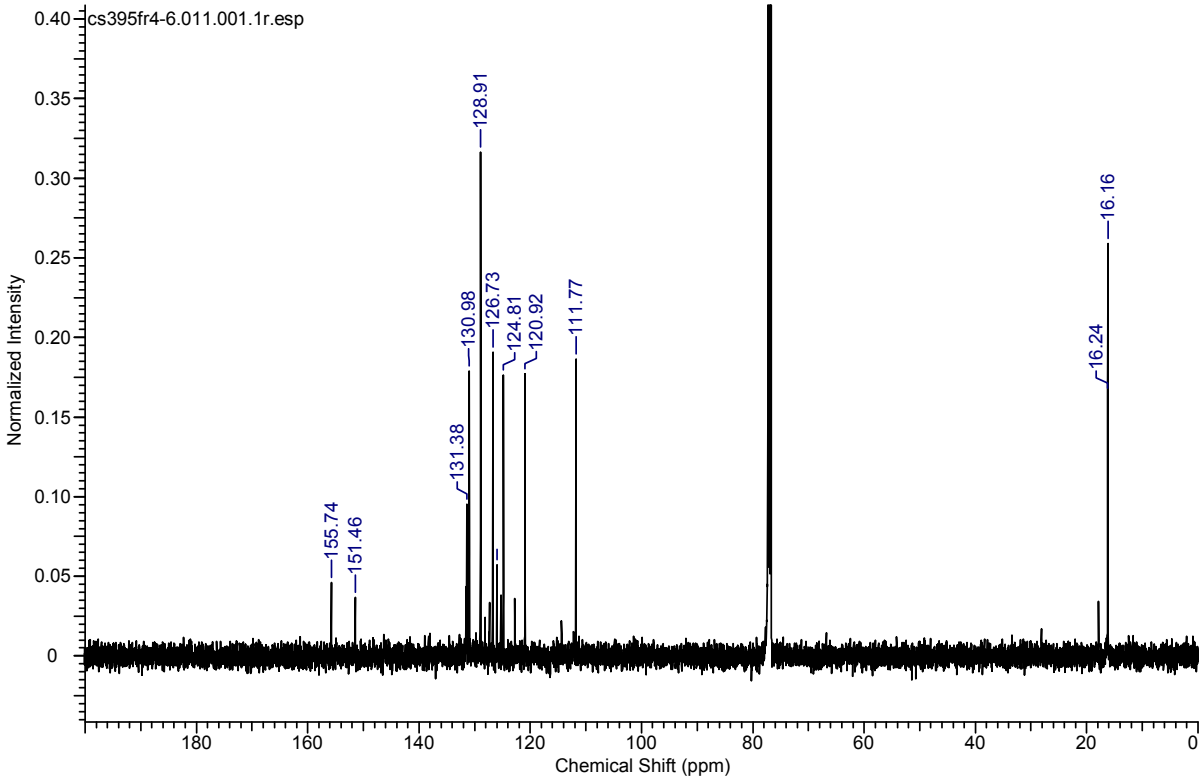

cs399fr7-24.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
2.21
7.59
7.58
7.37
7.38
7.35
7.24
7.18
7.17
7.15
6.83
6.81
6.80
0.09 0.06 0.09 0.05 0.06 0.09 0.04 0.05 0.08
0.12
O

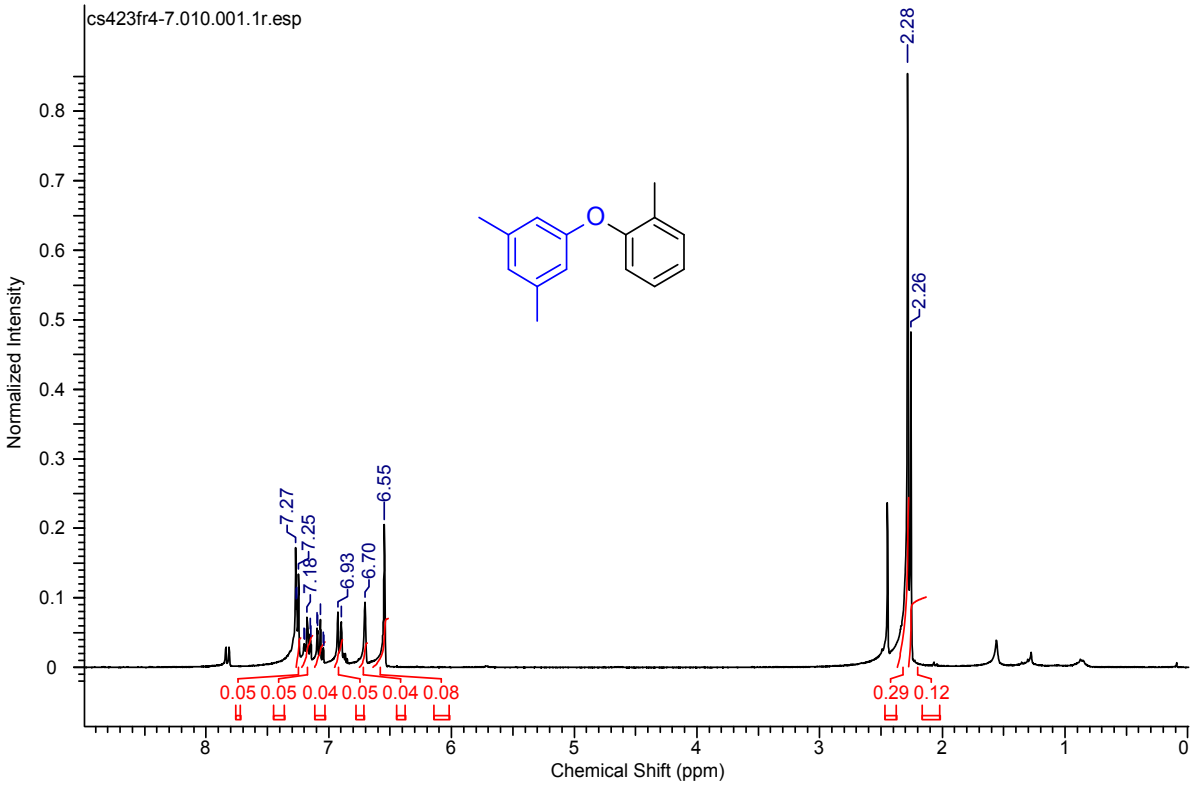

cs399fr7-24.012.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
131.23
129.30
127.98
127.07
123.22
123.14
118.32
118.11
155.10
154.12
137.99
132.65
16.27

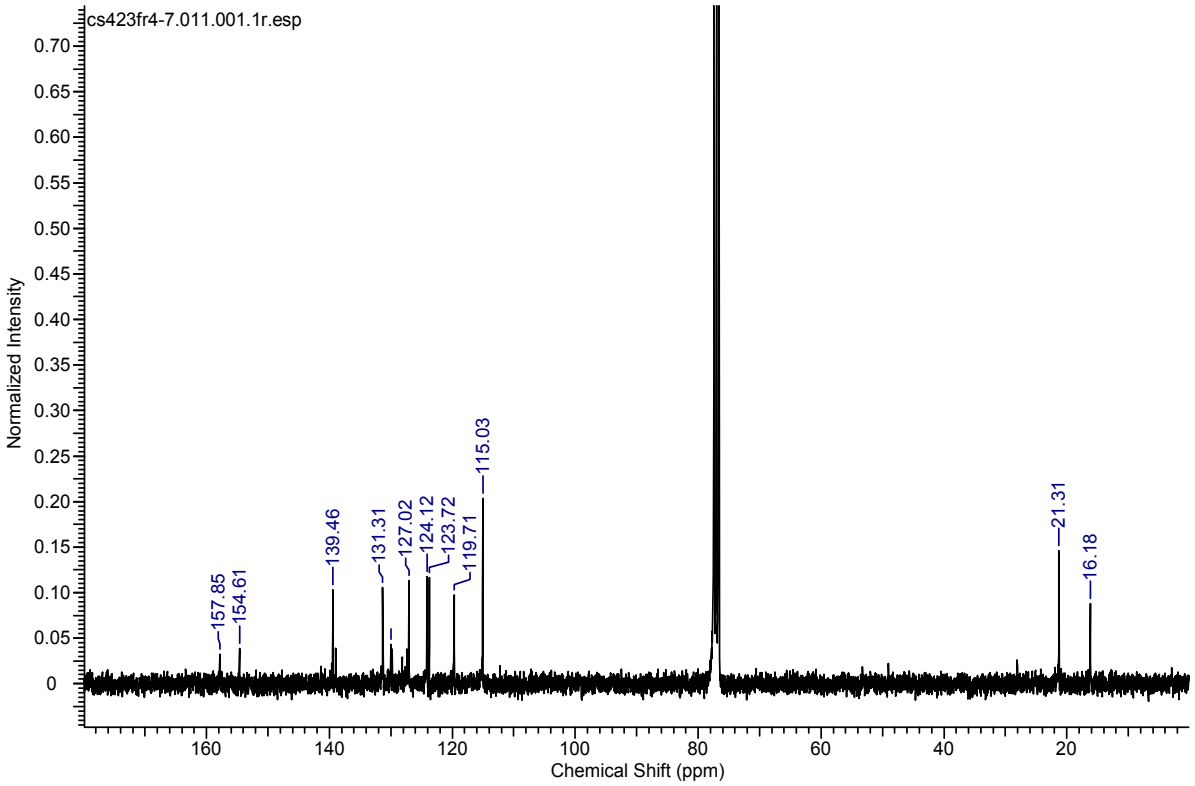

cs393fr10.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
O
OMe
2.14
3.77
7.09
6.79
6.71
6.82
7.10
7.05
6.68
0.16
0.11
0.09
0.15
0.30

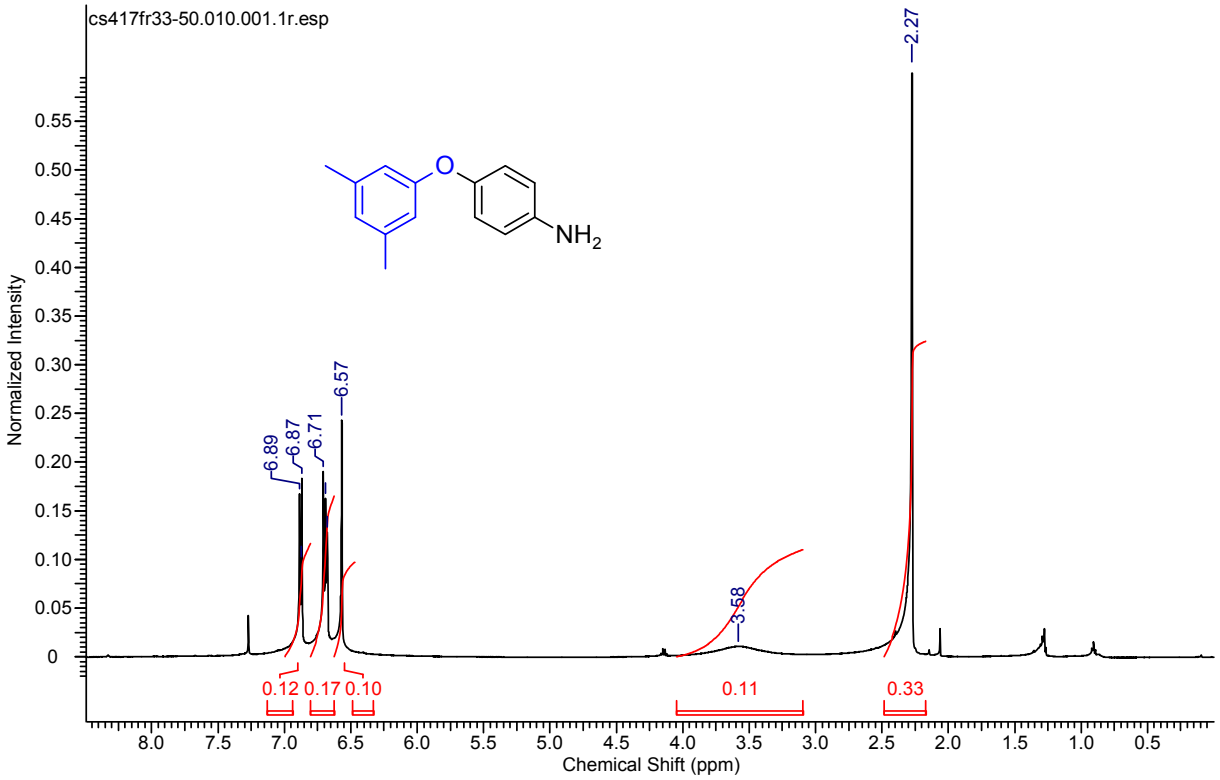

cs393carbon.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
128.94
115.22
114.74
124.85
131.56
154.07
151.98
151.54
55.69
16.34

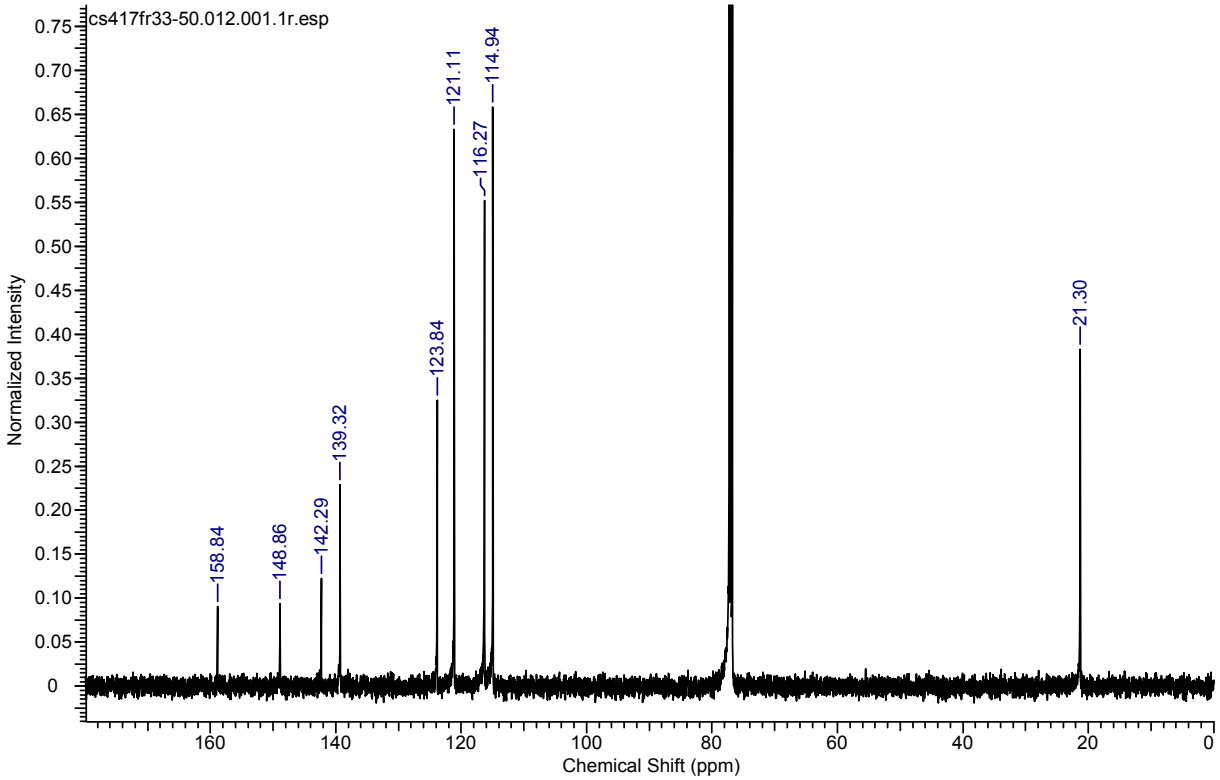

cs395fr4-6.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
2.44
2.12
7.10
7.26
7.24
7.24
7.12
7.07
7.06
6.88
6.87
6.27
6.26
0.06 0.12 0.04 0.04 0.04
0.14 0.23

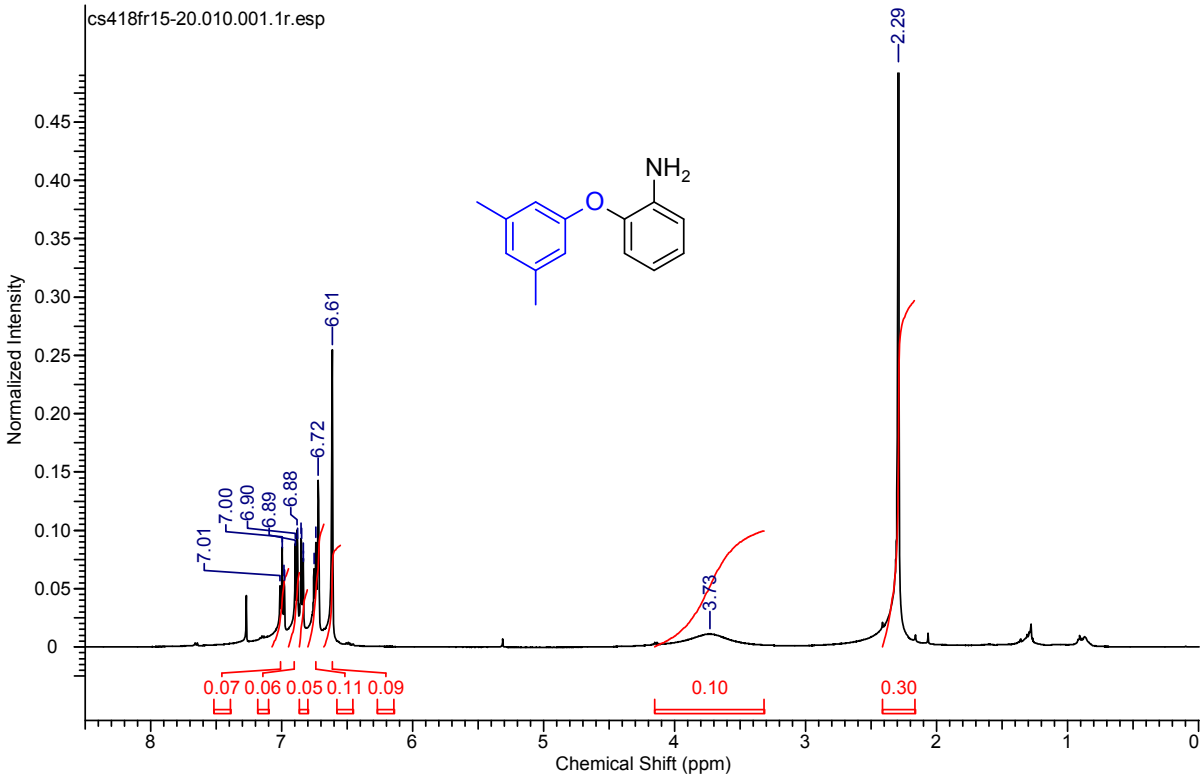

cs395fr4-6.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
128.91
130.98
126.73
124.81
120.92
111.77
131.38
155.74
151.46
16.16
16.24

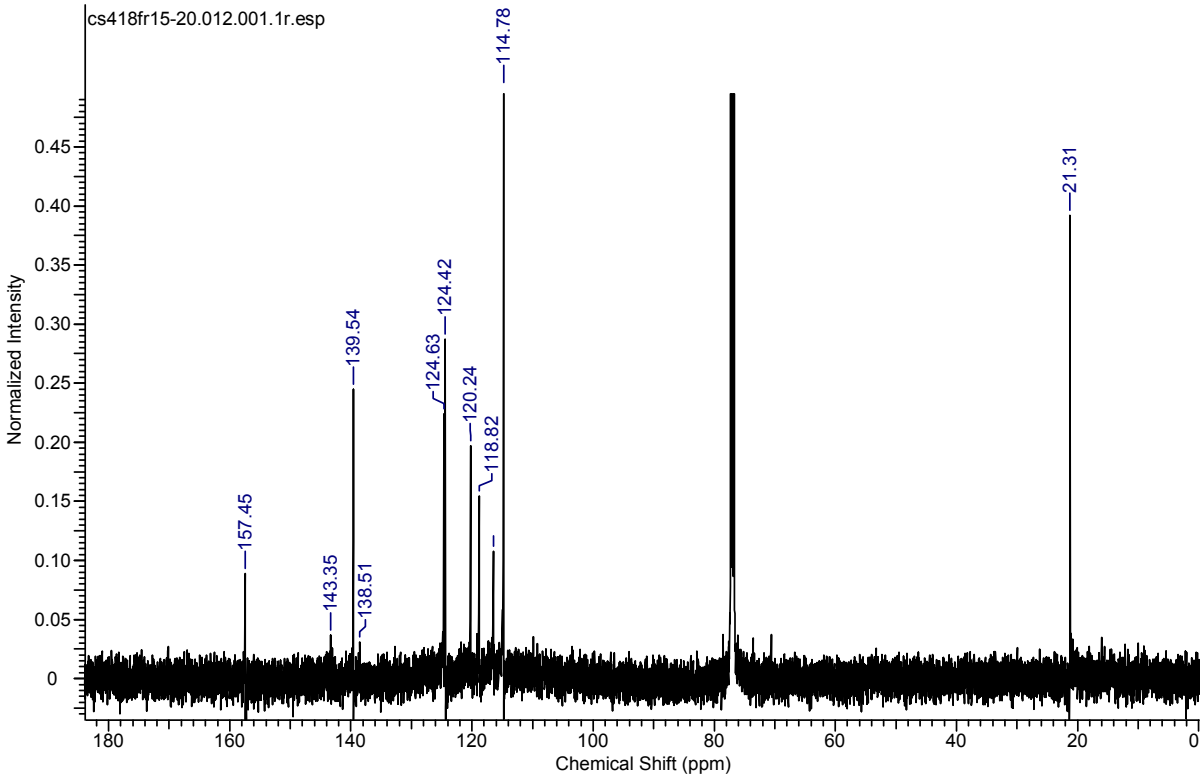

cs423fr4-7.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
2.28
2.26
7.27
7.25
7.18
6.93
6.70
6.55
0.05 0.05 0.04 0.05 0.04 0.08
0.29 0.12
O

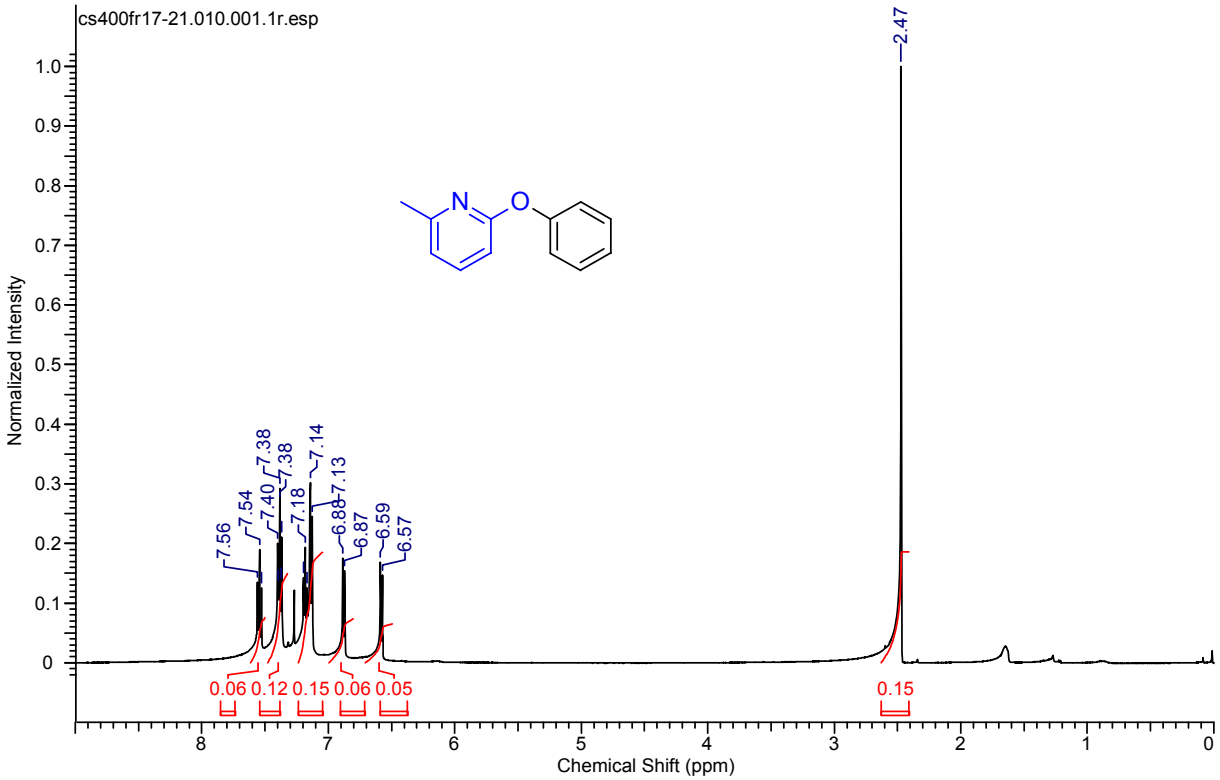

cs423fr4-7.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
157.85
154.61
139.46
131.31
127.02
124.12
123.72
119.71
115.03
21.31
16.18

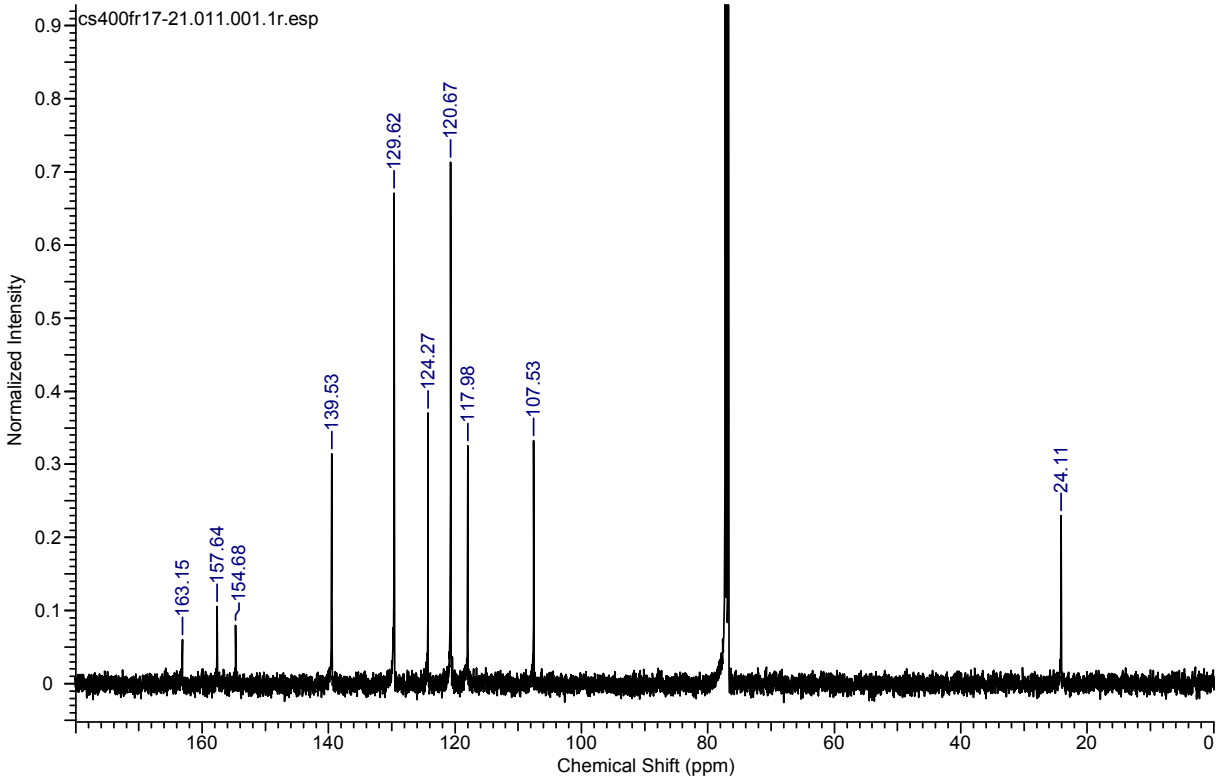

cs417fr33-50.010.001.1r.esp
O
NH2
2.27
6.89
6.87
6.71
6.57
3.58
0.12
0.17
0.10
0.11
0.33
Normalized Intensity
Chemical Shift (ppm)

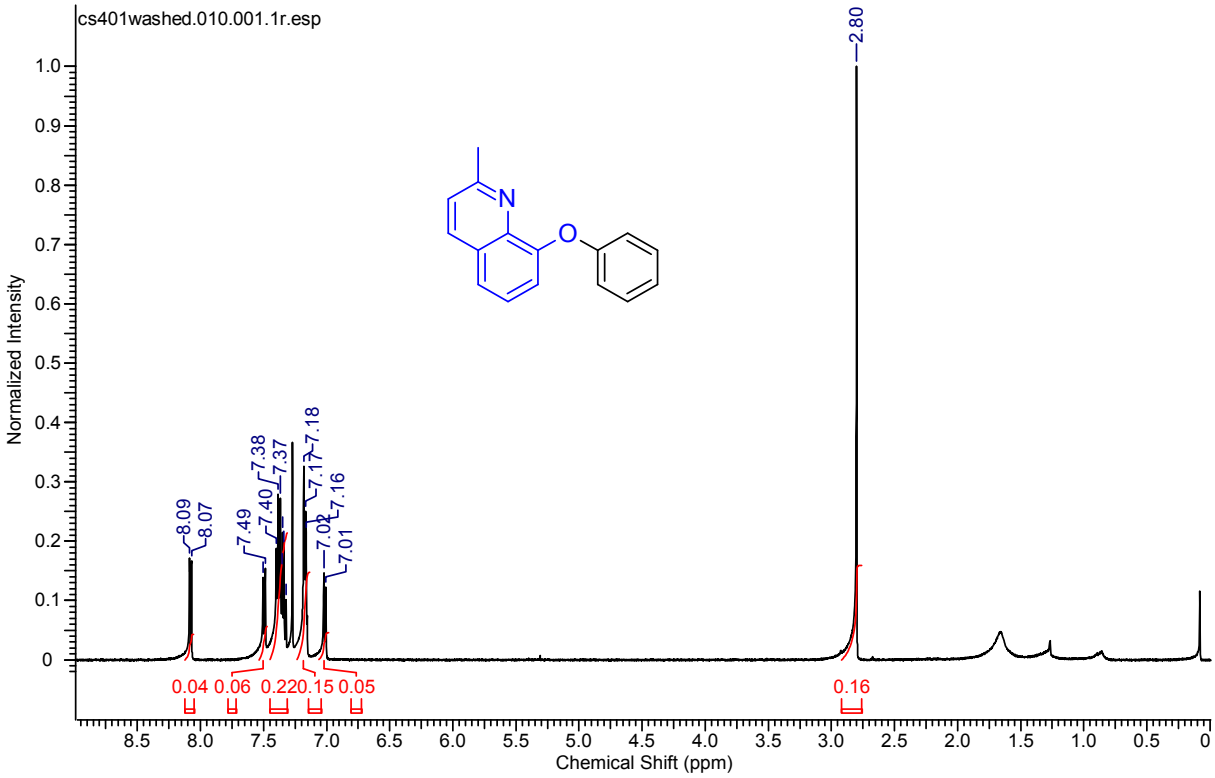

cs417fr33-50.012.001.1r.esp
158.84
148.86
142.29
139.32
123.84
121.11
116.27
114.94
21.30
Normalized Intensity
Chemical Shift (ppm)

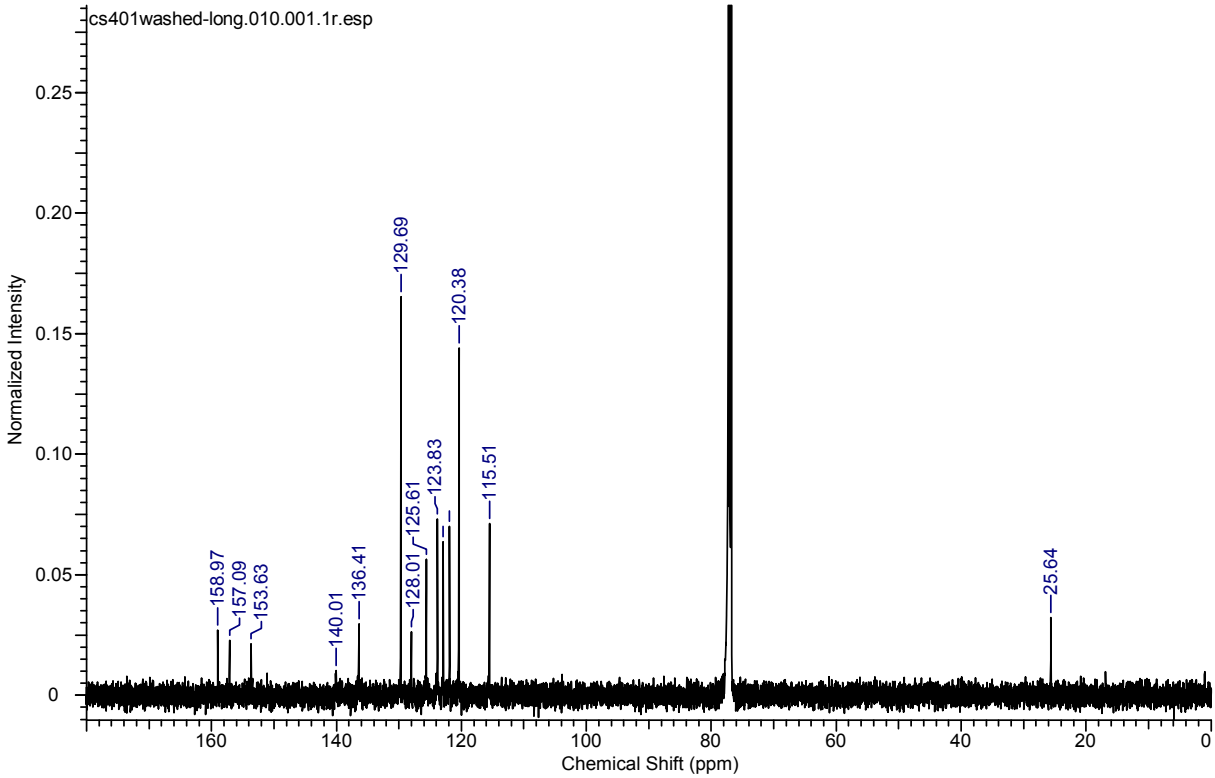

cs418fr15-20.010.001.1r.esp
NH2
O
2.29
6.61
6.72
6.88
6.89
6.90
7.00
7.01
3.73
0.07 0.06 0.05 0.11 0.09
0.10
0.30
Normalized Intensity
Chemical Shift (ppm)

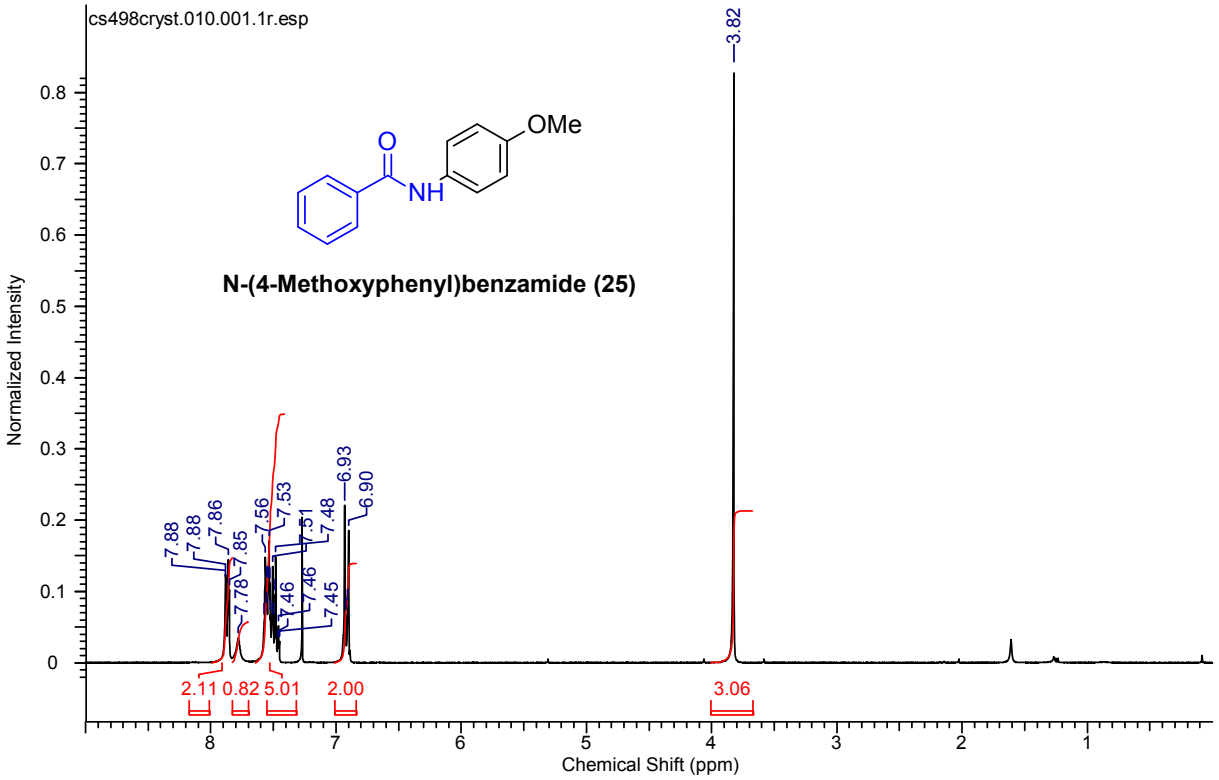

cs418fr15-20.012.001.1r.esp
114.78
21.31
124.42
139.54
124.63
120.24
118.82
157.45
143.35
138.51
Normalized Intensity
Chemical Shift (ppm)

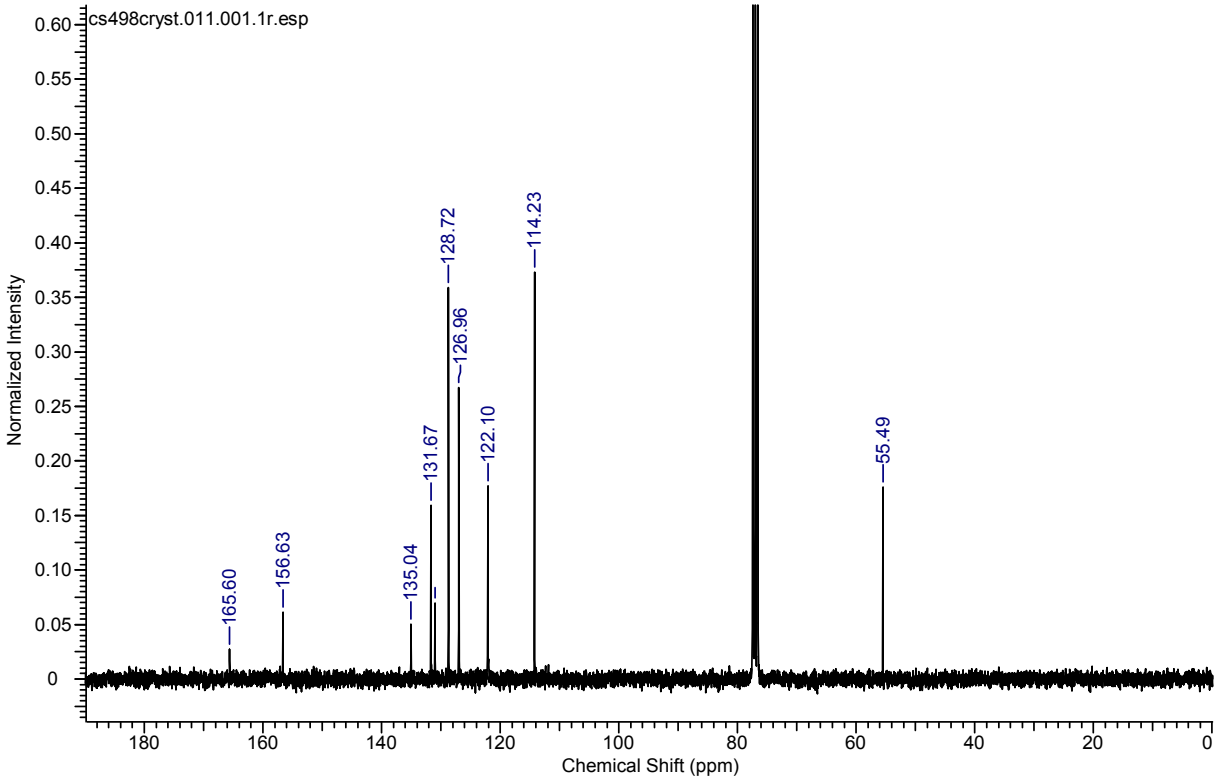

cs400fr17-21.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
2.47
7.56
7.54
7.40
7.38
7.38
7.18
7.14
7.13
6.88
6.87
6.59
6.57
0.06 0.12 0.15 0.06 0.05
0.15
N
O

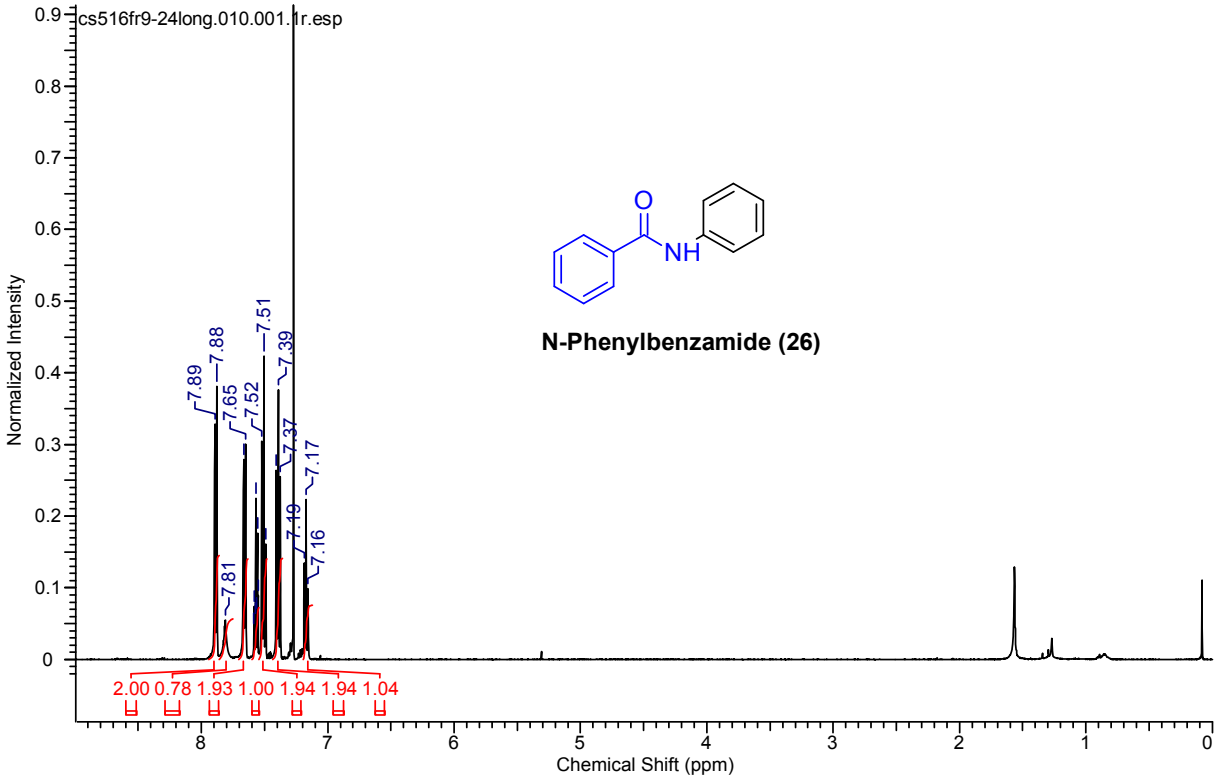

cs400fr17-21.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
163.15
157.64
154.68
139.53
129.62
124.27
120.67
117.98
107.53
24.11


cs401washed.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
2.80
8.09
8.07
7.49
7.40
7.38
7.37
7.18
7.17
7.16
7.02
7.01
0.04 0.06 0.22 0.15 0.05
0.16
N
O

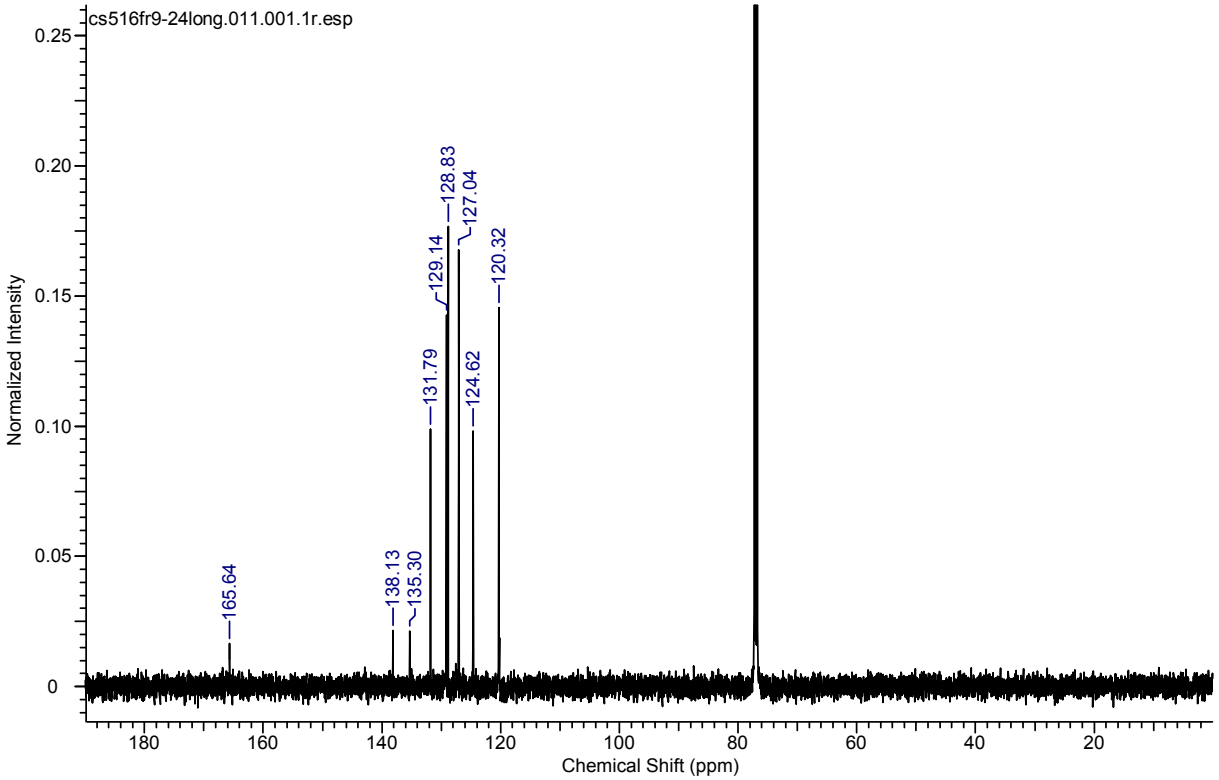

cs401washed-long.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
158.97
157.09
153.63
140.01
136.41
129.69
128.01
125.61
123.83
120.38
115.51
25.64

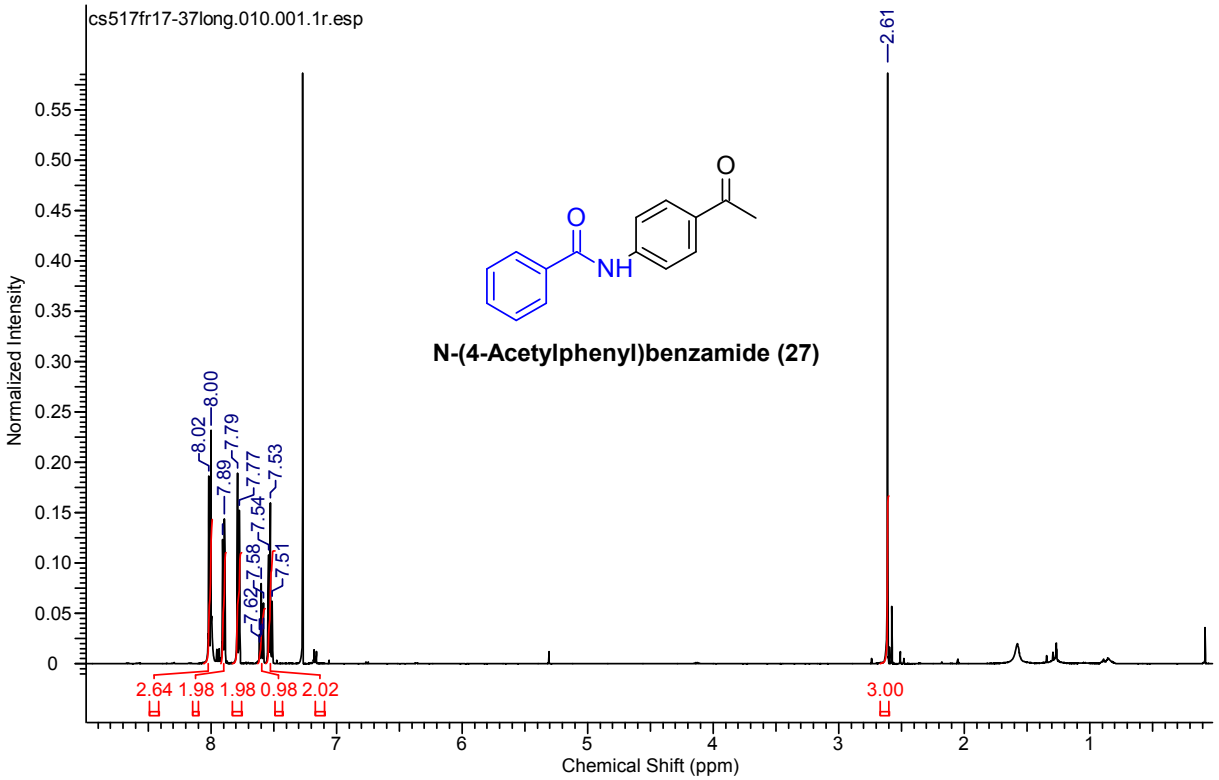

cs498cryst.010.001.1r.esp
OMe
O
NH
N-(4-Methoxyphenyl)benzamide (25)
Normalized Intensity
Chemical Shift (ppm)
3.82
7.88
7.88
7.86
7.85
7.78
7.56
7.53
7.51
7.48
7.46
7.46
7.45
6.93
6.90
2.11
0.82
5.01
2.00
3.06


cs498cryst.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
165.60
156.63
135.04
131.67
128.72
126.96
122.10
114.23
55.49

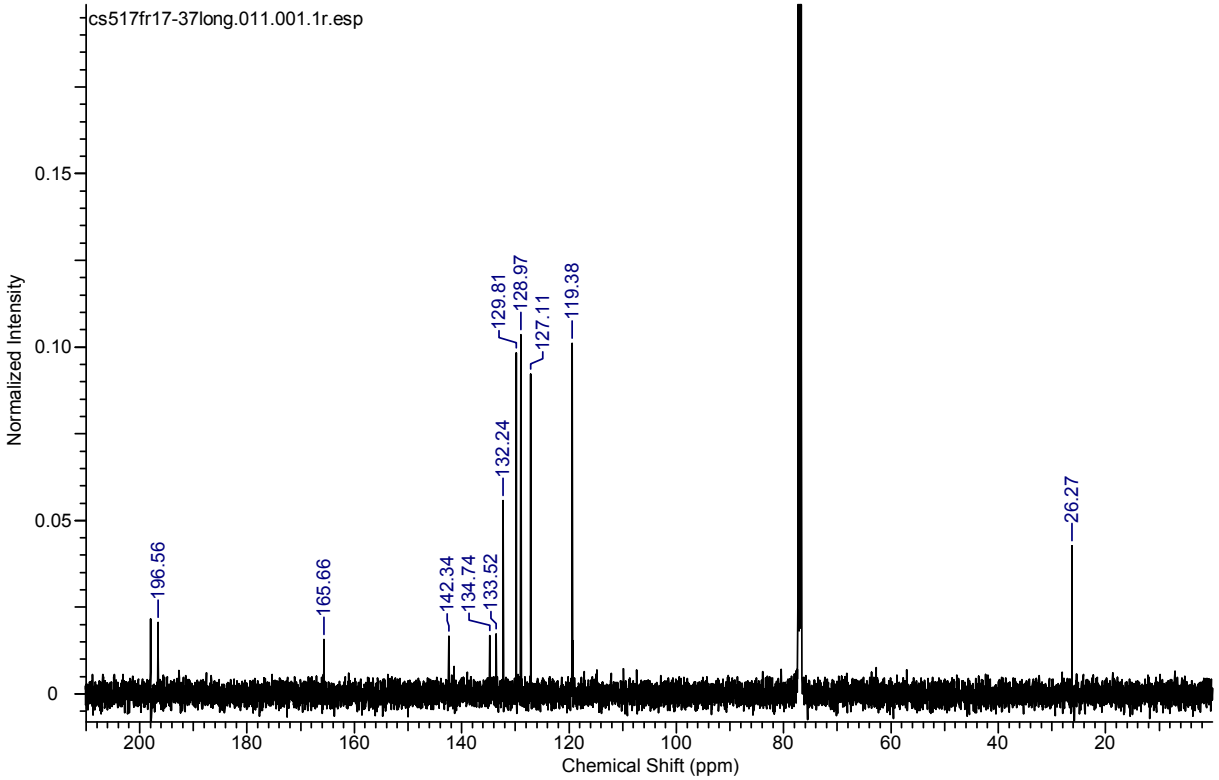


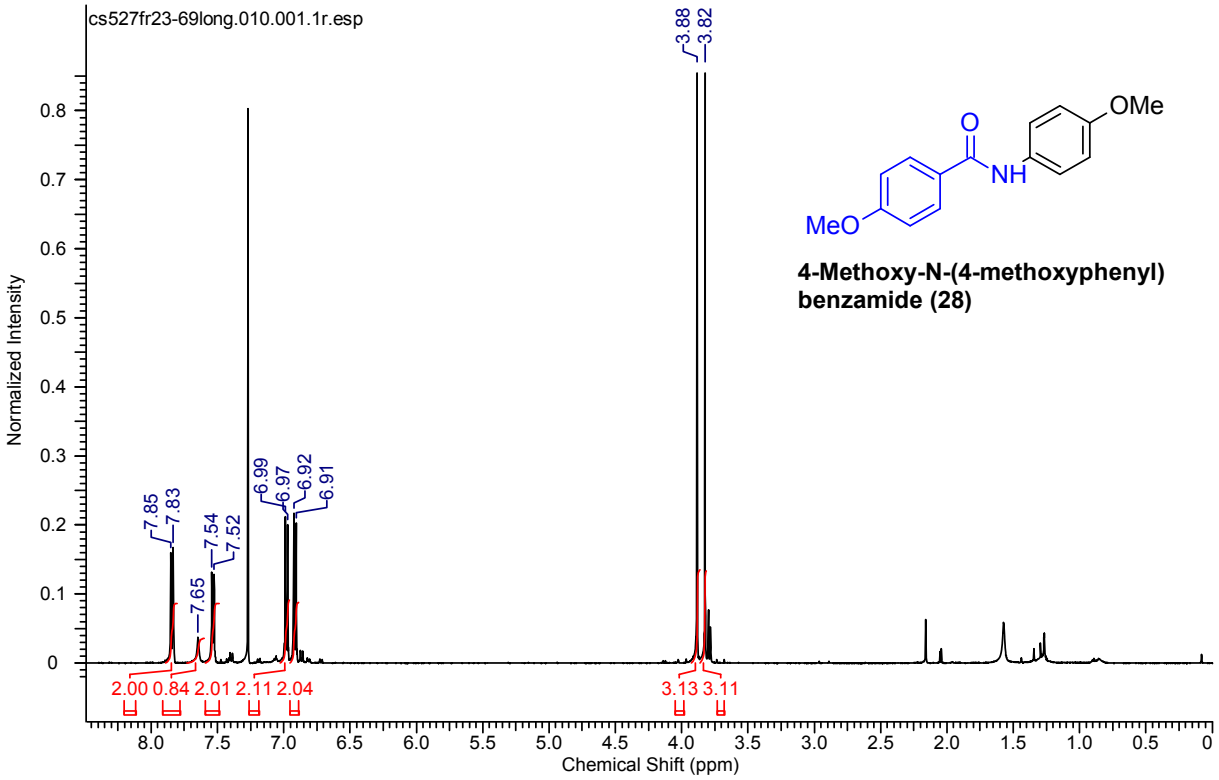
N-Phenylbenzamide (26)



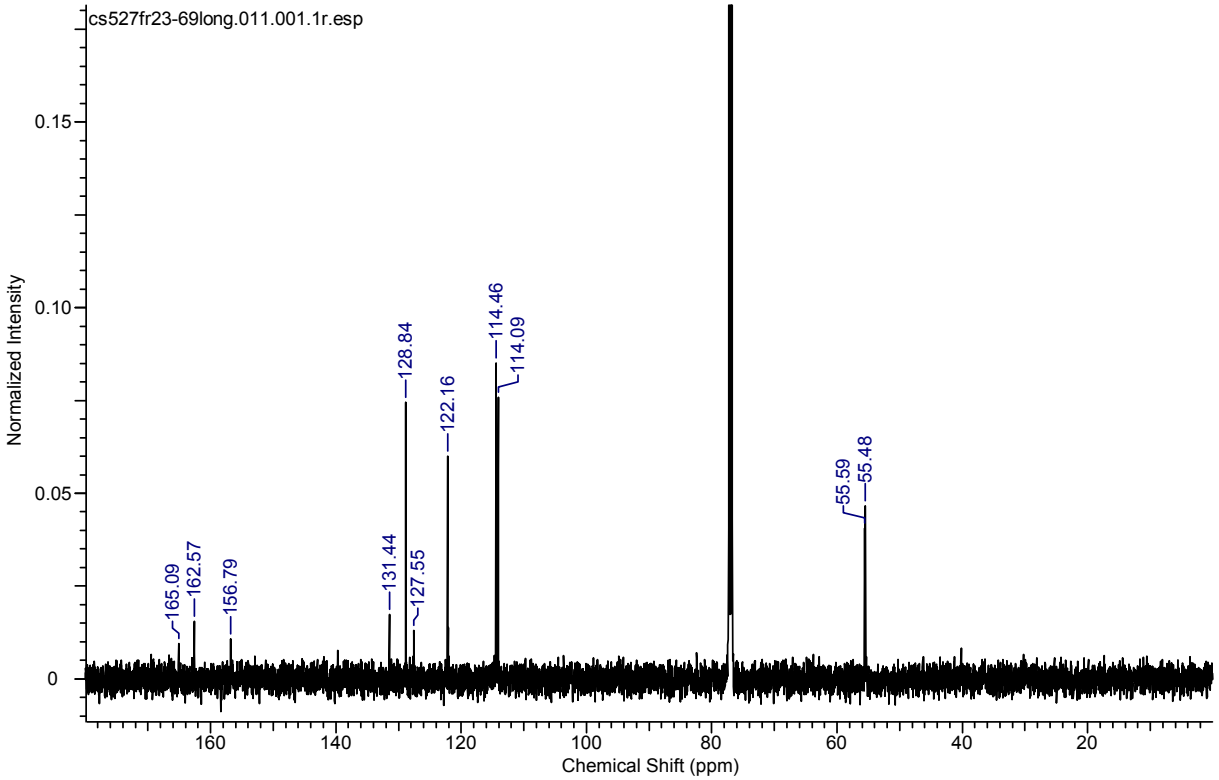


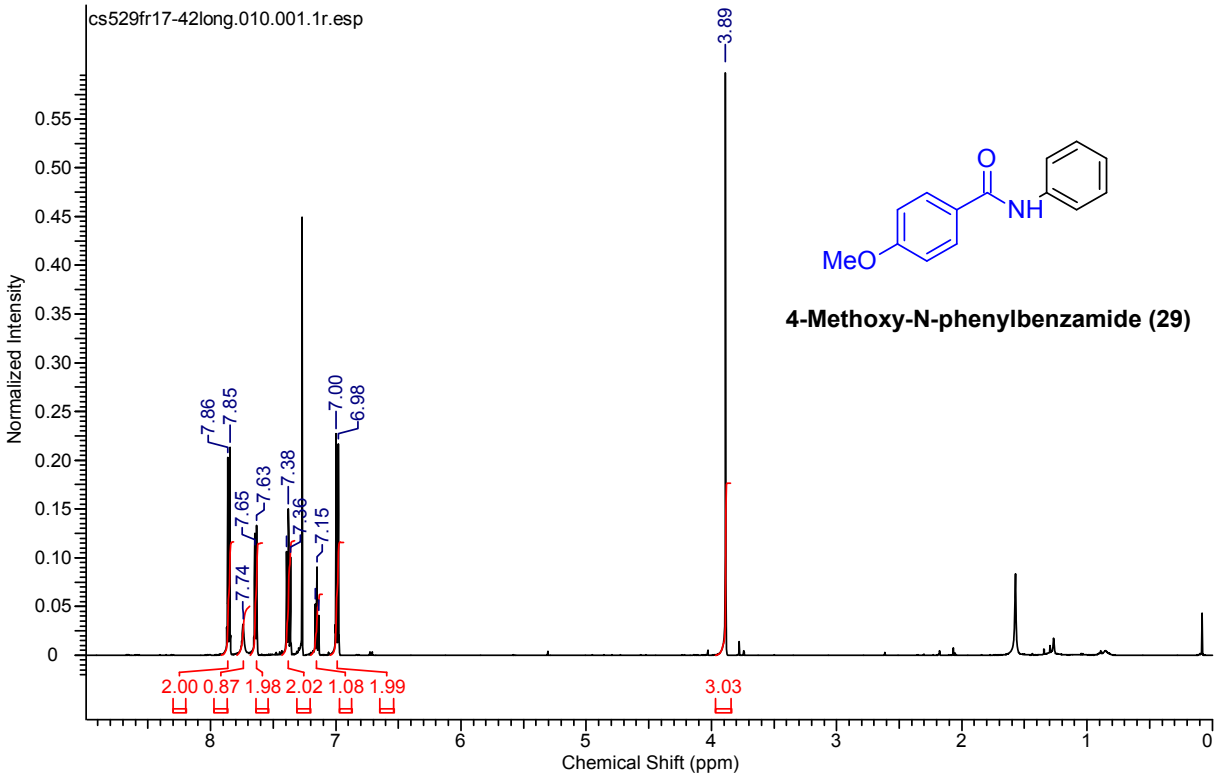
N-(4-Acetylphenyl)benzamide (27)

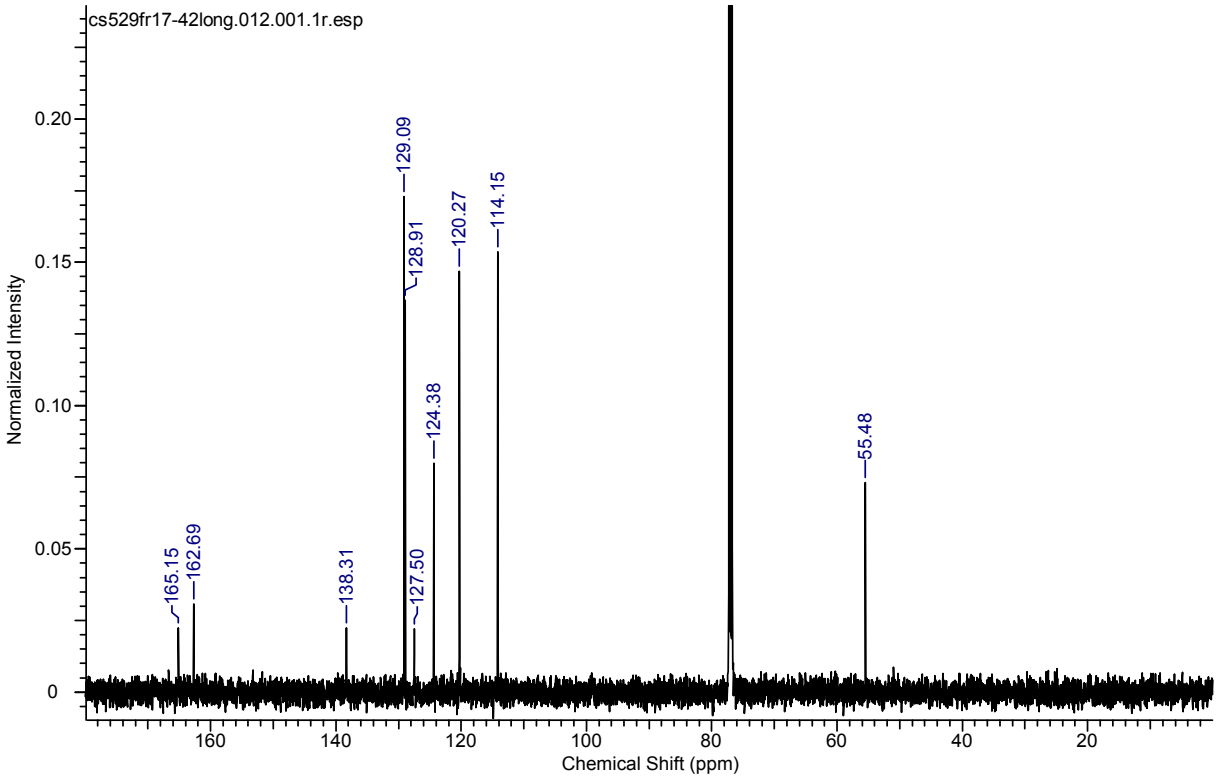


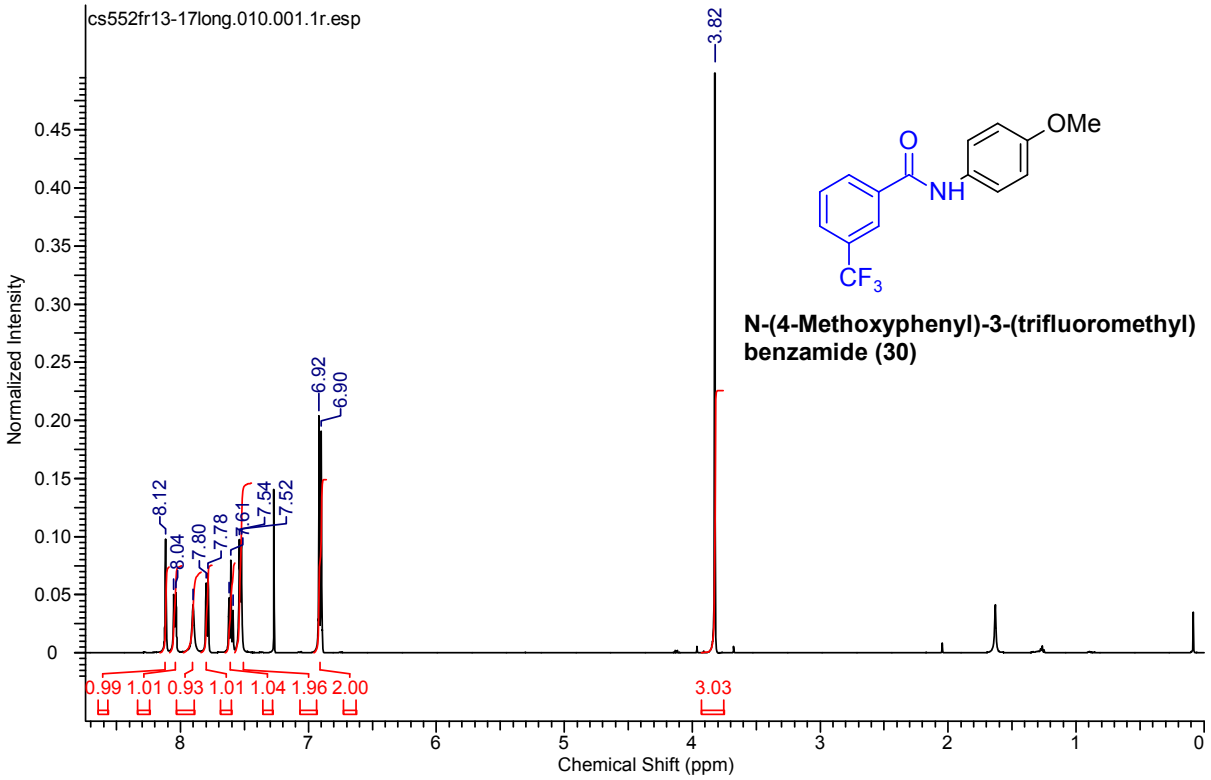


4-Methoxy-N-(4-methoxyphenyl) benzamide (28)

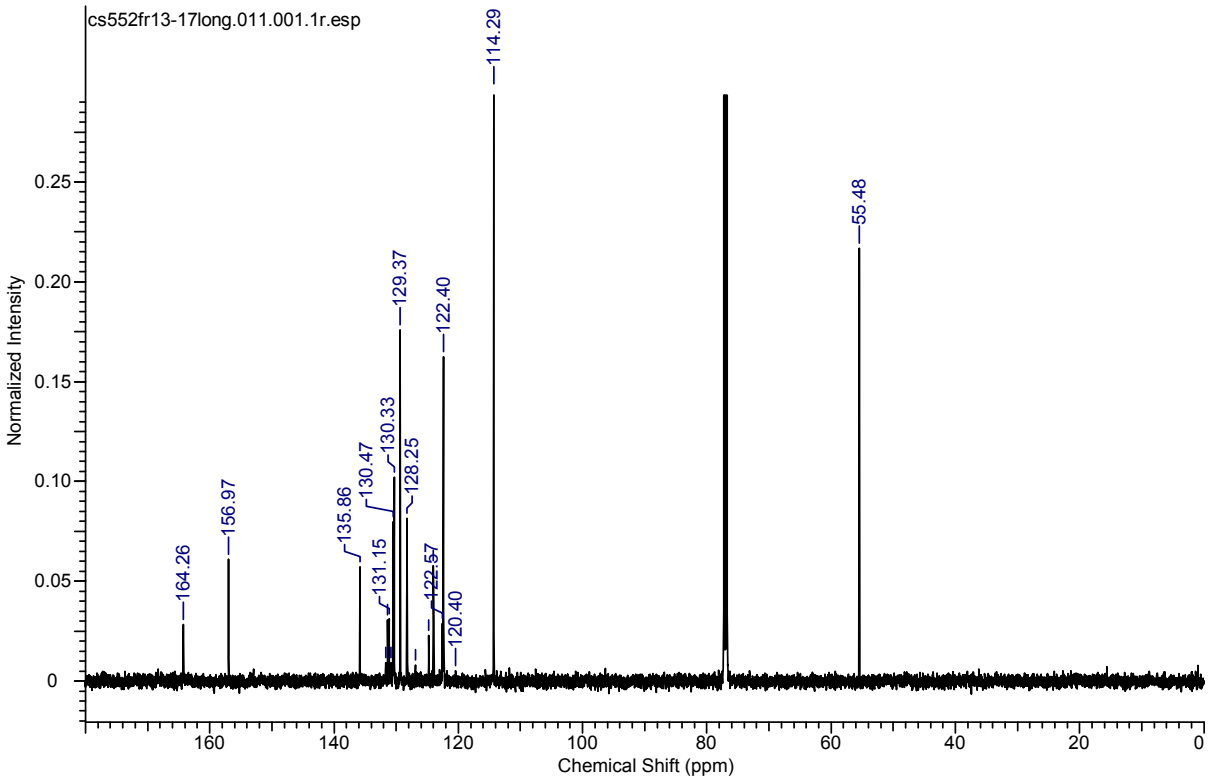


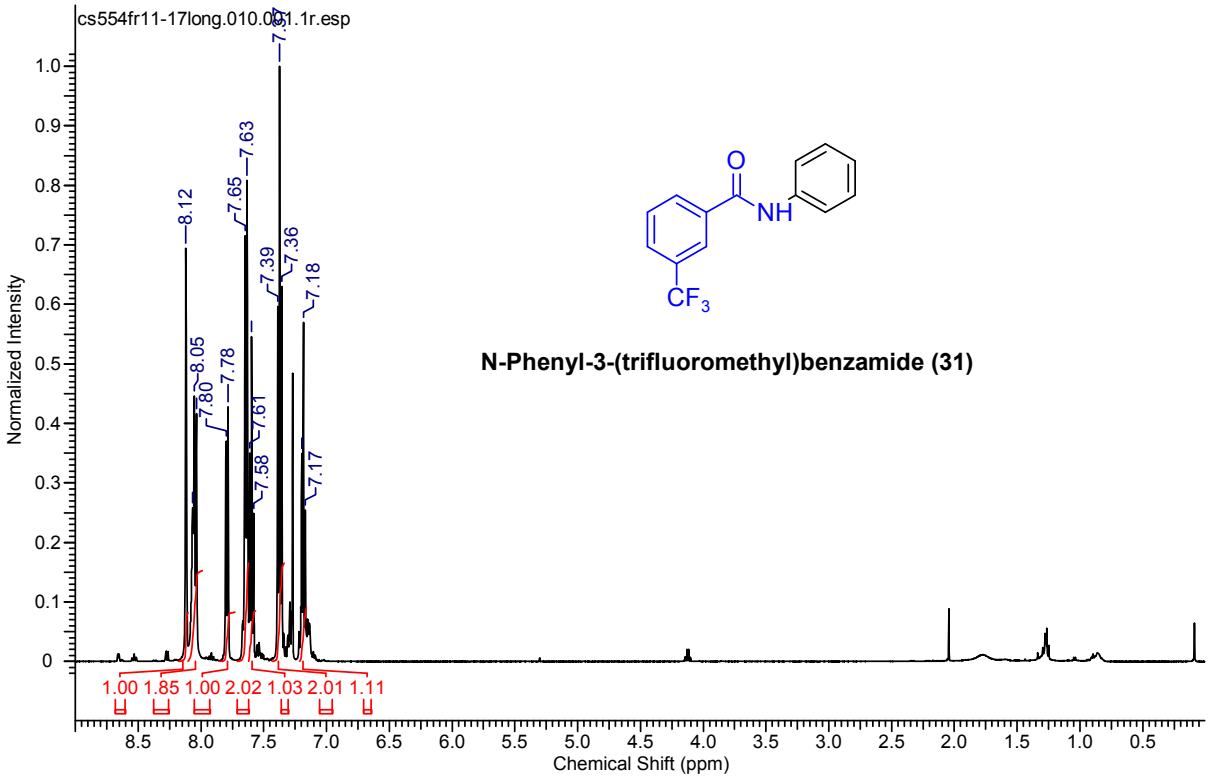

cs529fr17-42long.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
3.89
7.86
7.85
7.74
7.65
7.63
7.38
7.36
7.15
7.00
6.98
2.00 0.87 1.98 2.02 1.08 1.99
3.03
O
NH
MeO
4-Methoxy-N-phenylbenzamide (29)


cs529fr17-42long.012.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
165.15
162.69
138.31
129.09
128.91
127.50
124.38
120.27
114.15
55.48

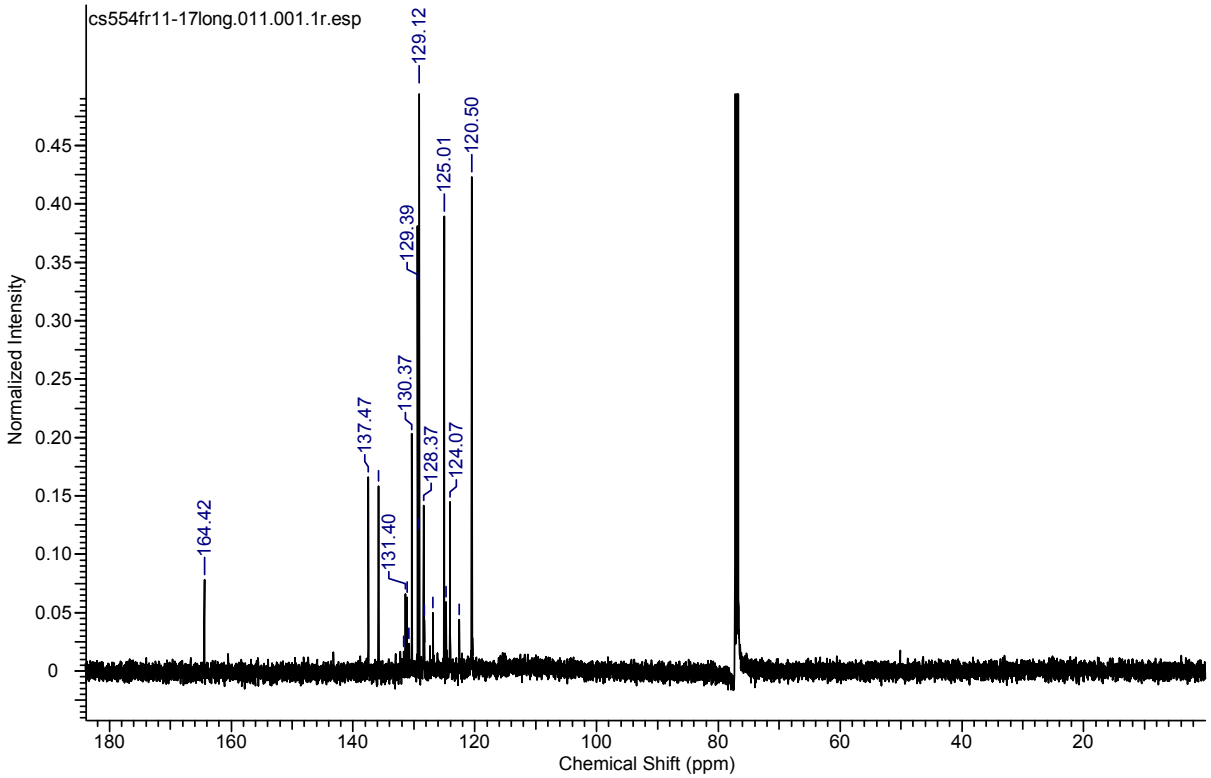


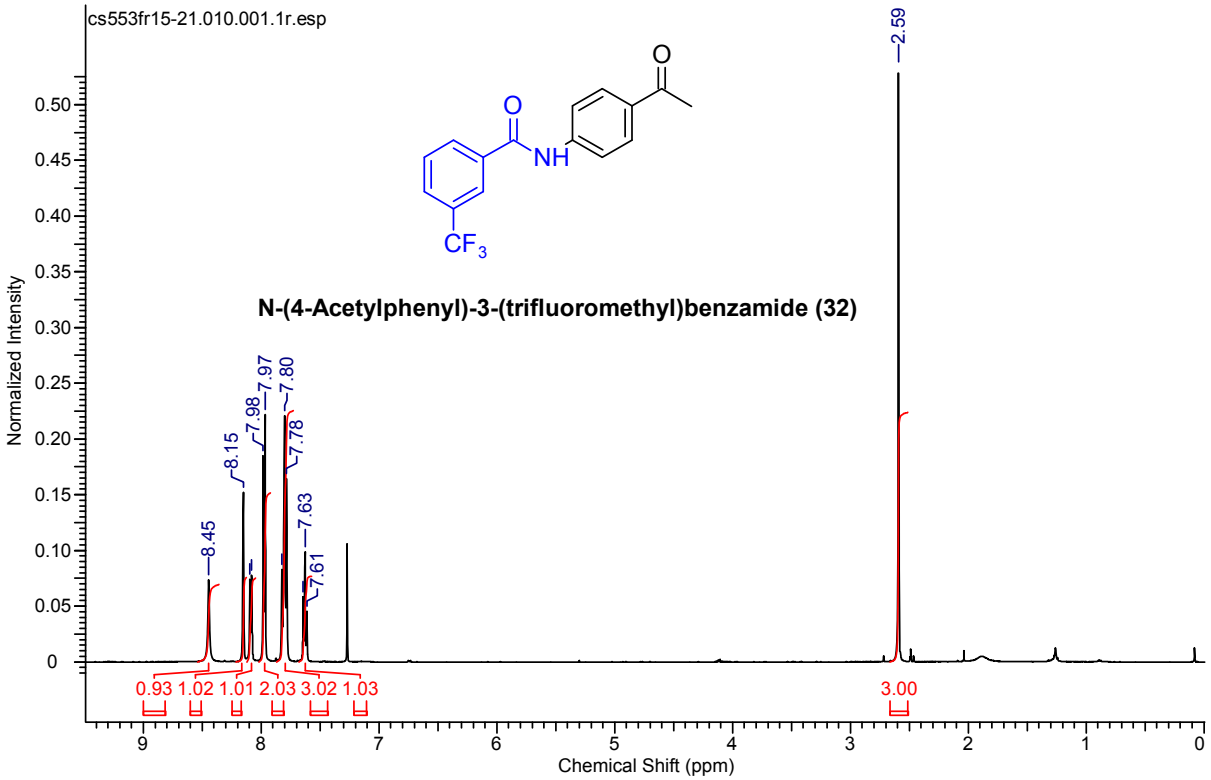
N-(4-Methoxyphenyl)-3-(trifluoromethyl) benzamide (30)

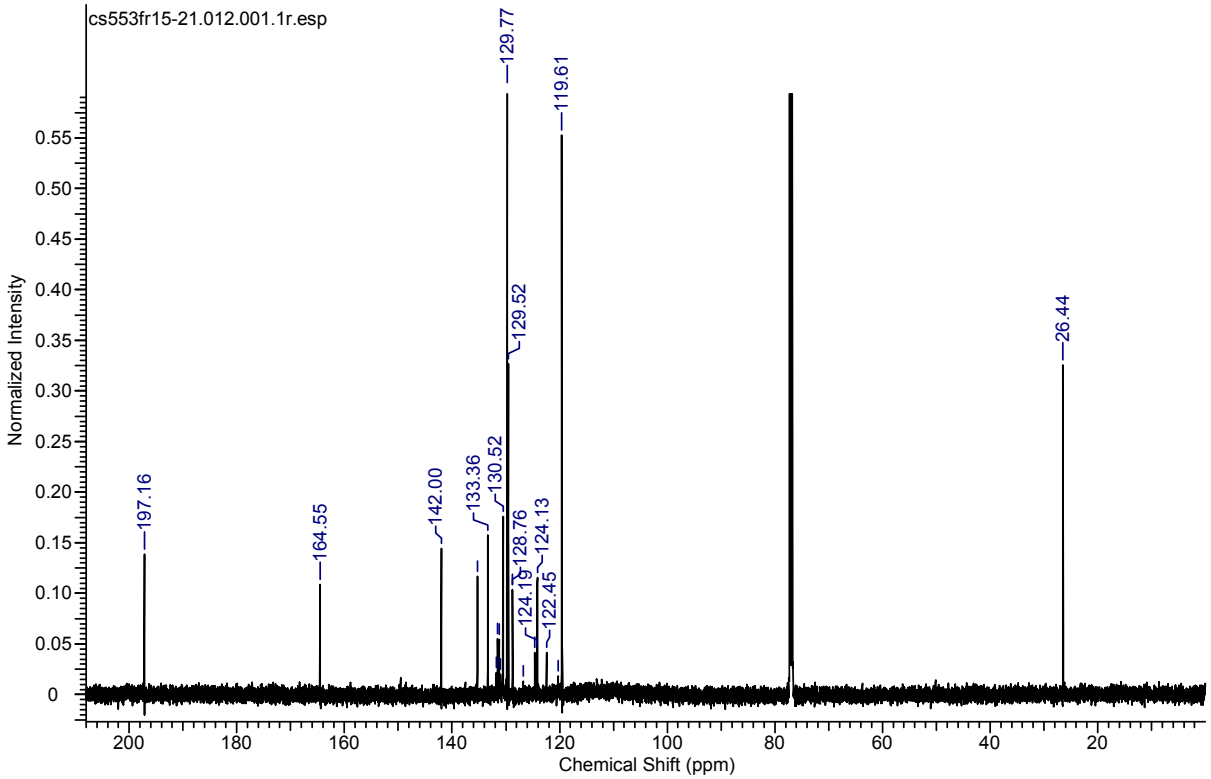


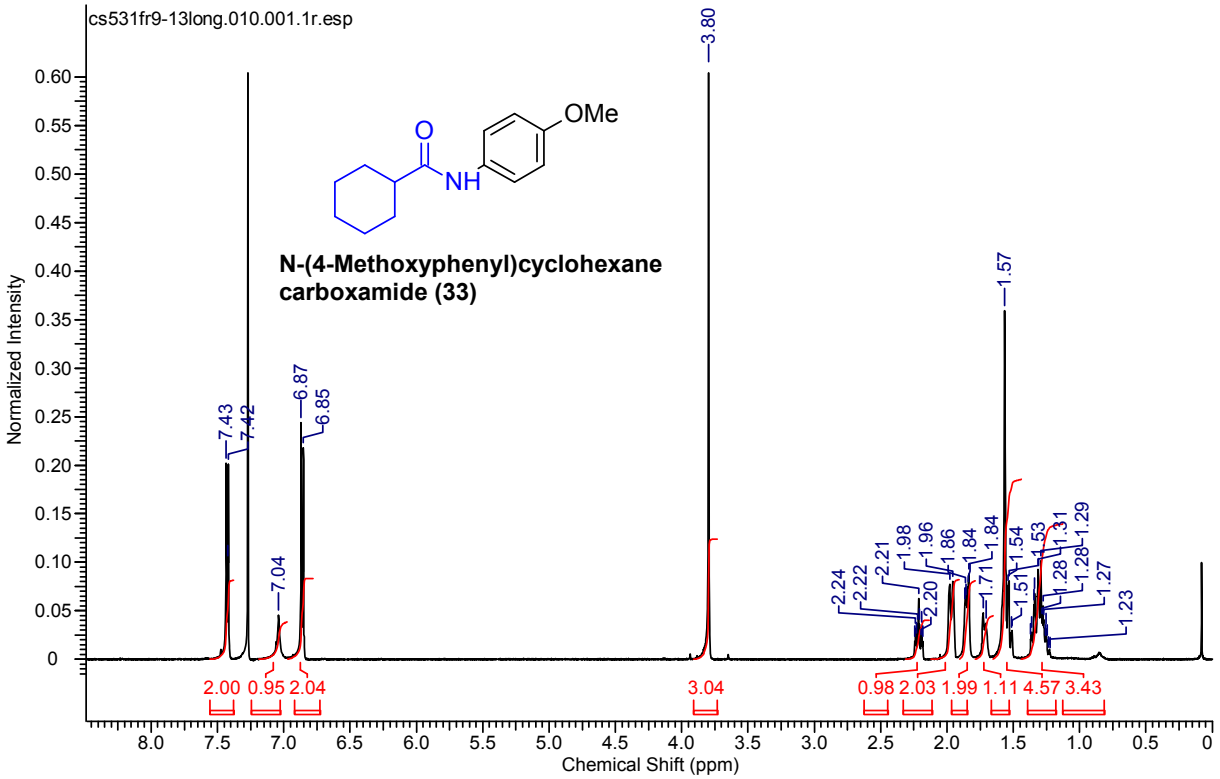


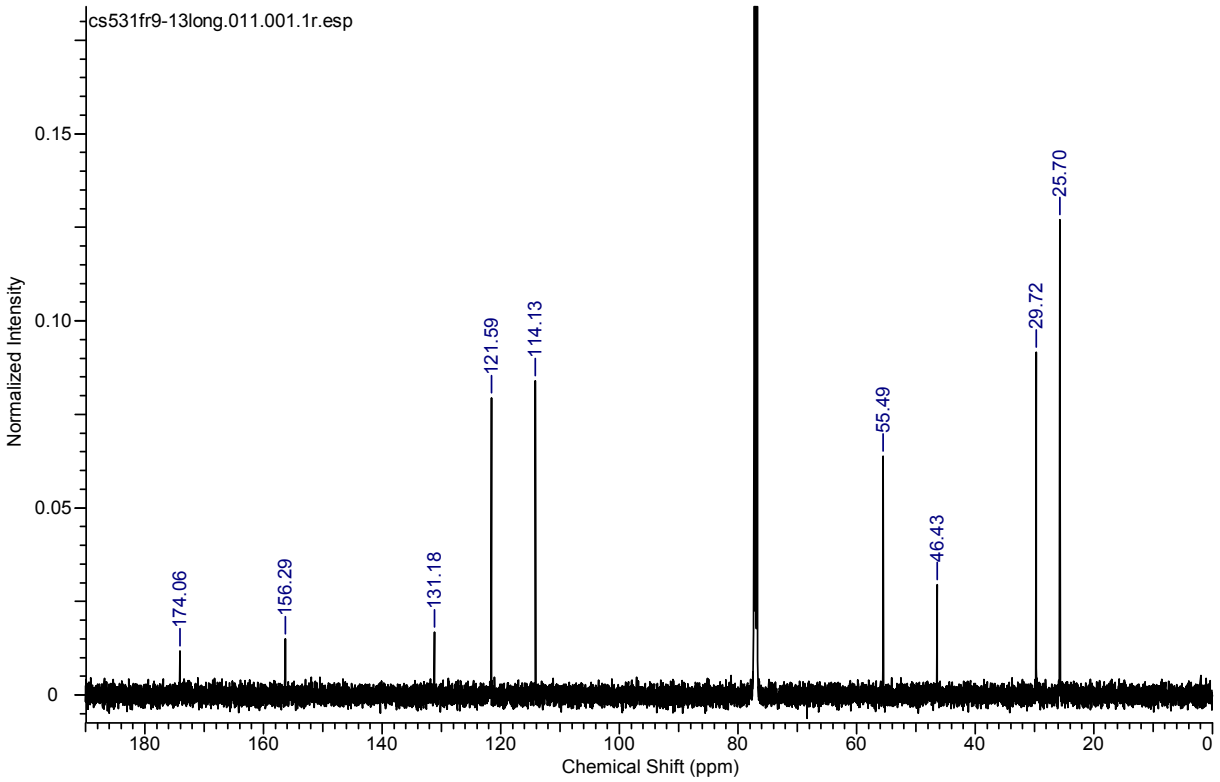
N-Phenyl-3-(trifluoromethyl)benzamide (31)

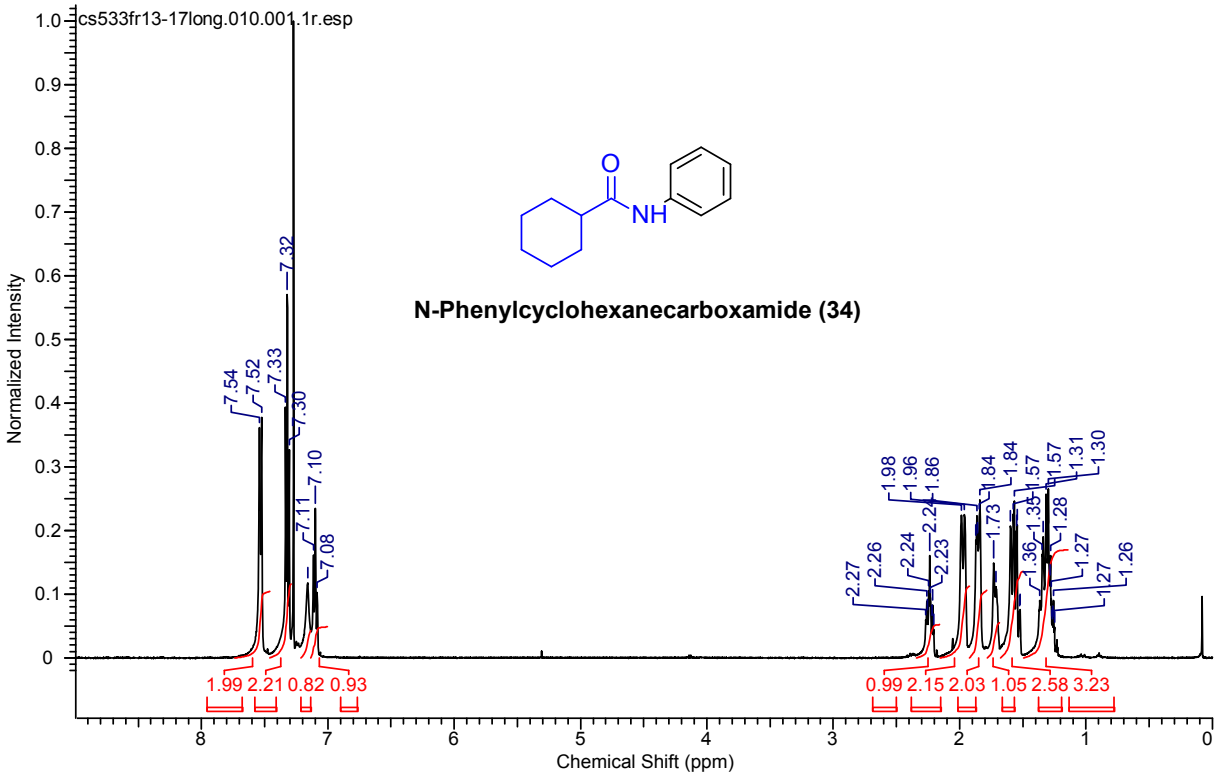



cs553fr15-21.010.001.1r.esp
O
NH
O
CF3
N-(4-Acetylphenyl)-3-(trifluoromethyl)benzamide (32)
Normalized Intensity
Chemical Shift (ppm)
2.59
8.45
8.15
7.98
7.97
7.80
7.78
7.63
7.61
0.93 1.02 1.01 2.03 3.02 1.03
3.00

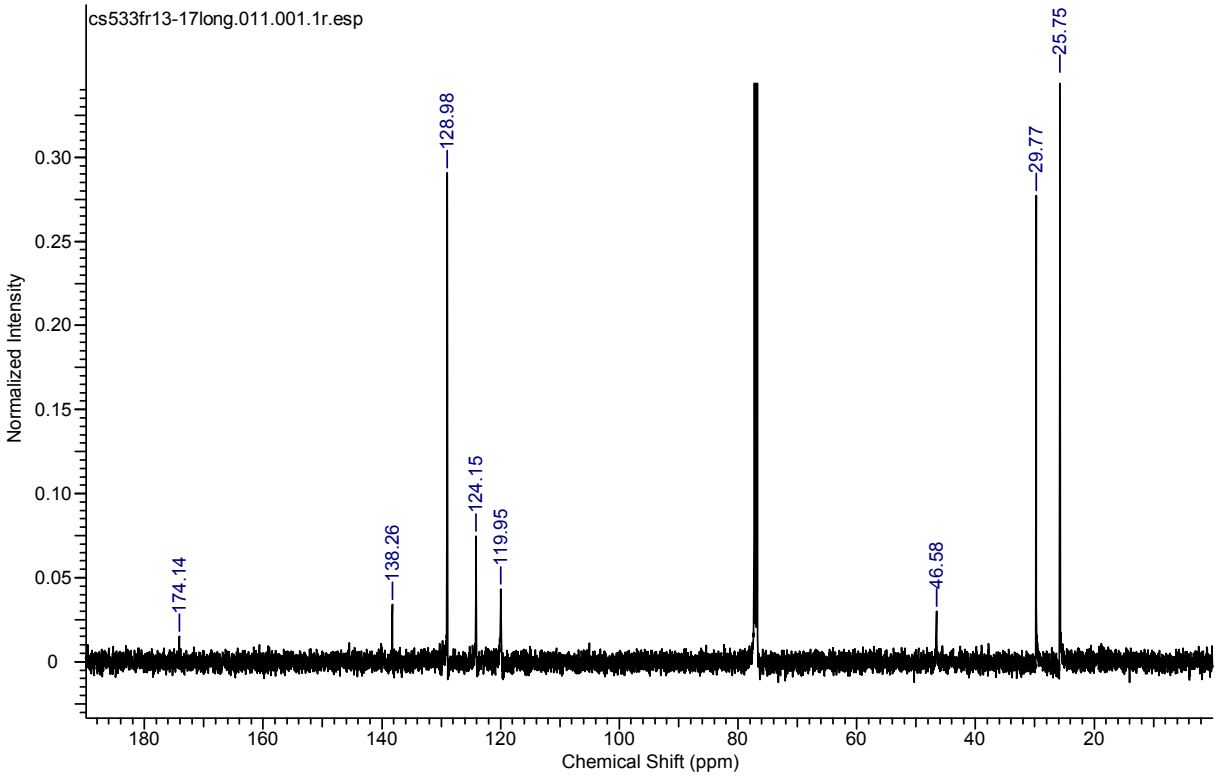

cs553fr15-21.012.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
197.16
164.55
142.00
133.36
130.52
129.77
129.52
128.76
124.19
124.13
122.45
119.61
26.44

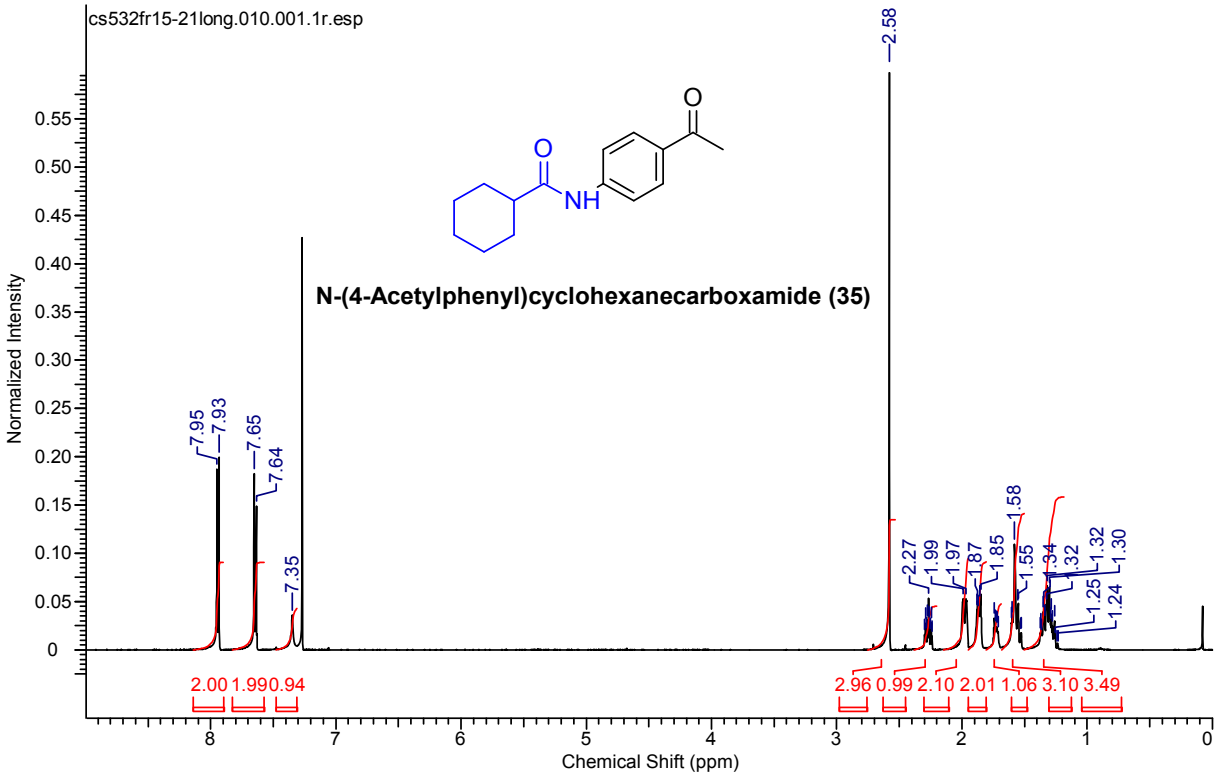

cs531fr9-13long.010.001.1r.esp
N-(4-Methoxyphenyl)cyclohexane carboxamide (33)
OMe
NH
O
Normalized Intensity
Chemical Shift (ppm)
3.80
1.57
7.43
7.42
6.87
6.85
7.04
2.24
2.22
2.21
1.98
1.96
2.20
1.86
1.84
1.84
1.71
1.54
1.53
1.51
1.31
1.29
1.28
1.28
1.27
1.23
2.00
0.95
2.04
3.04
0.98
2.03
1.99
1.11
4.57
3.43

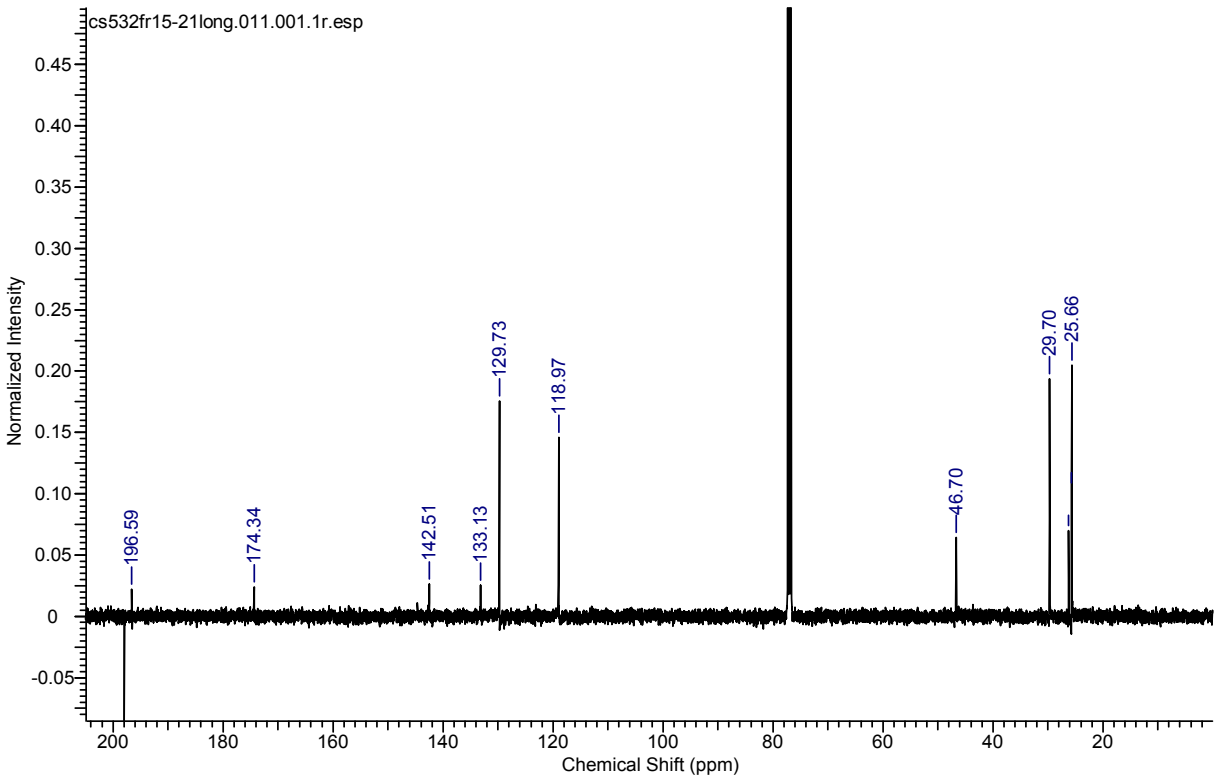

cs531fr9-13long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
174.06
156.29
131.18
121.59
114.13
55.49
46.43
29.72
25.70

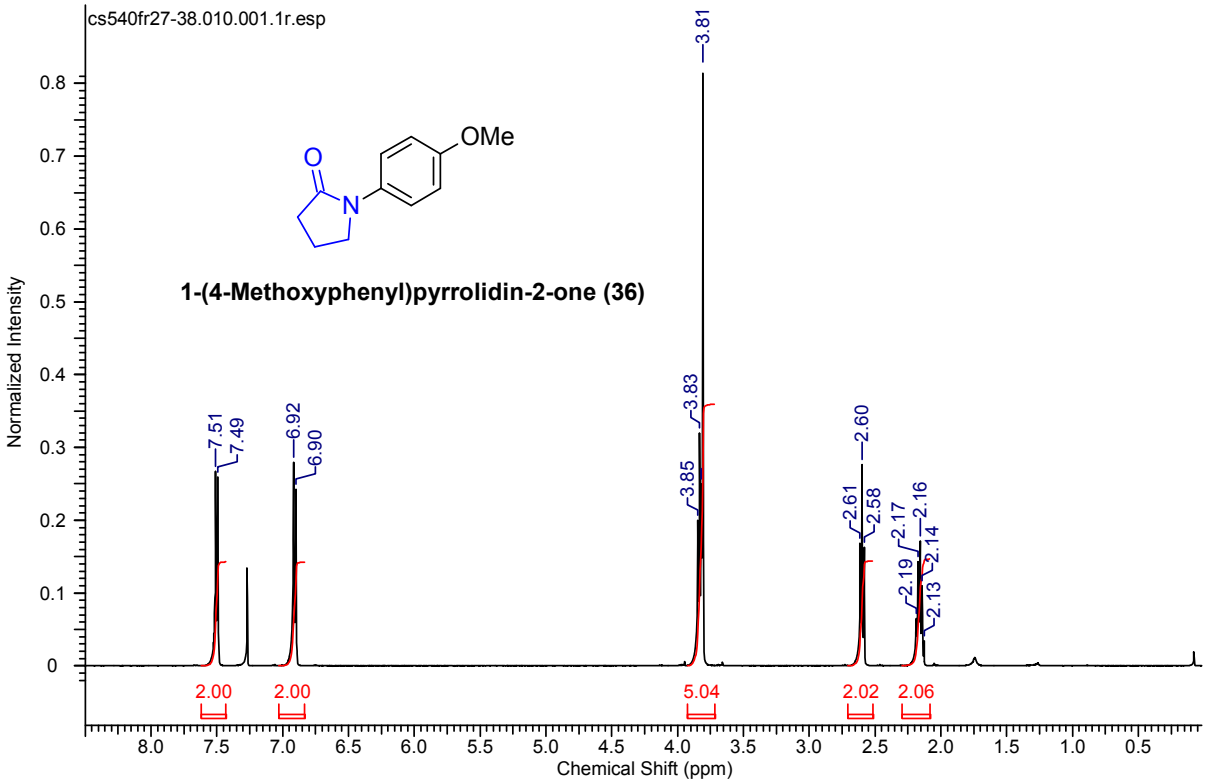


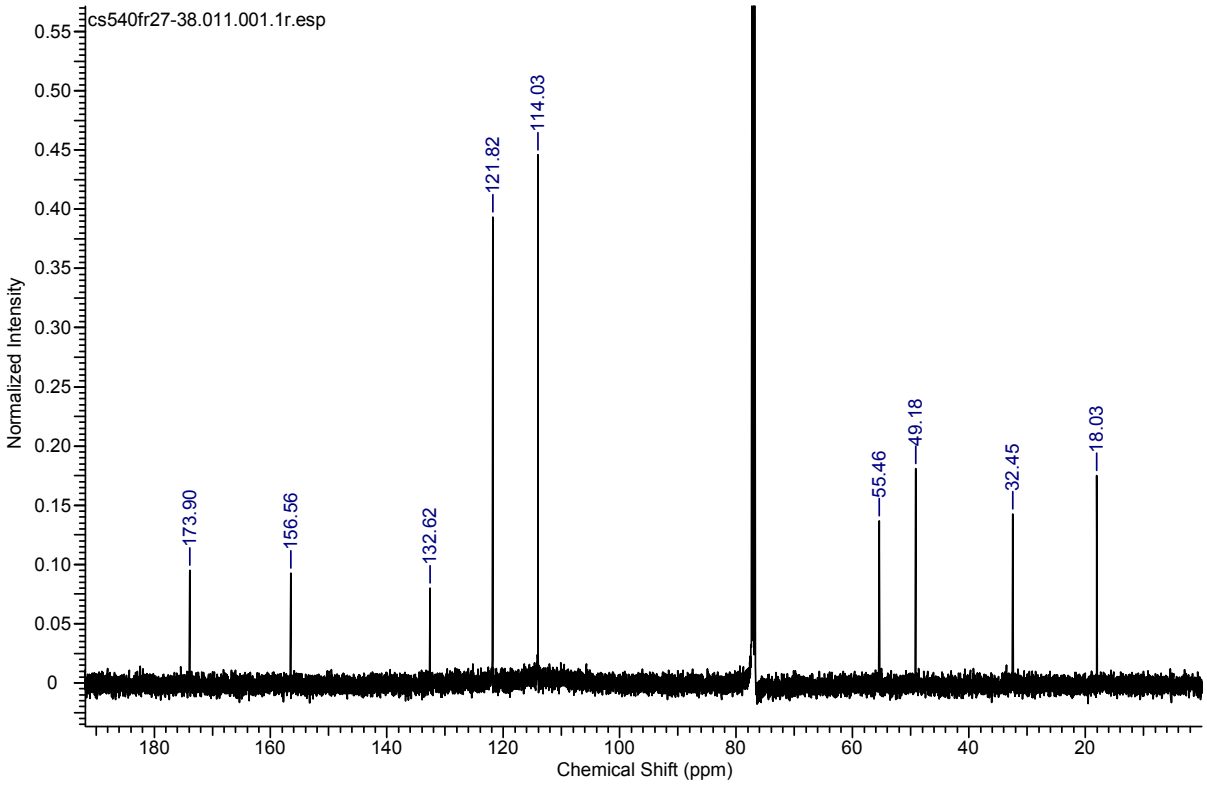
N-Phenylcyclohexanecarboxamide (34)

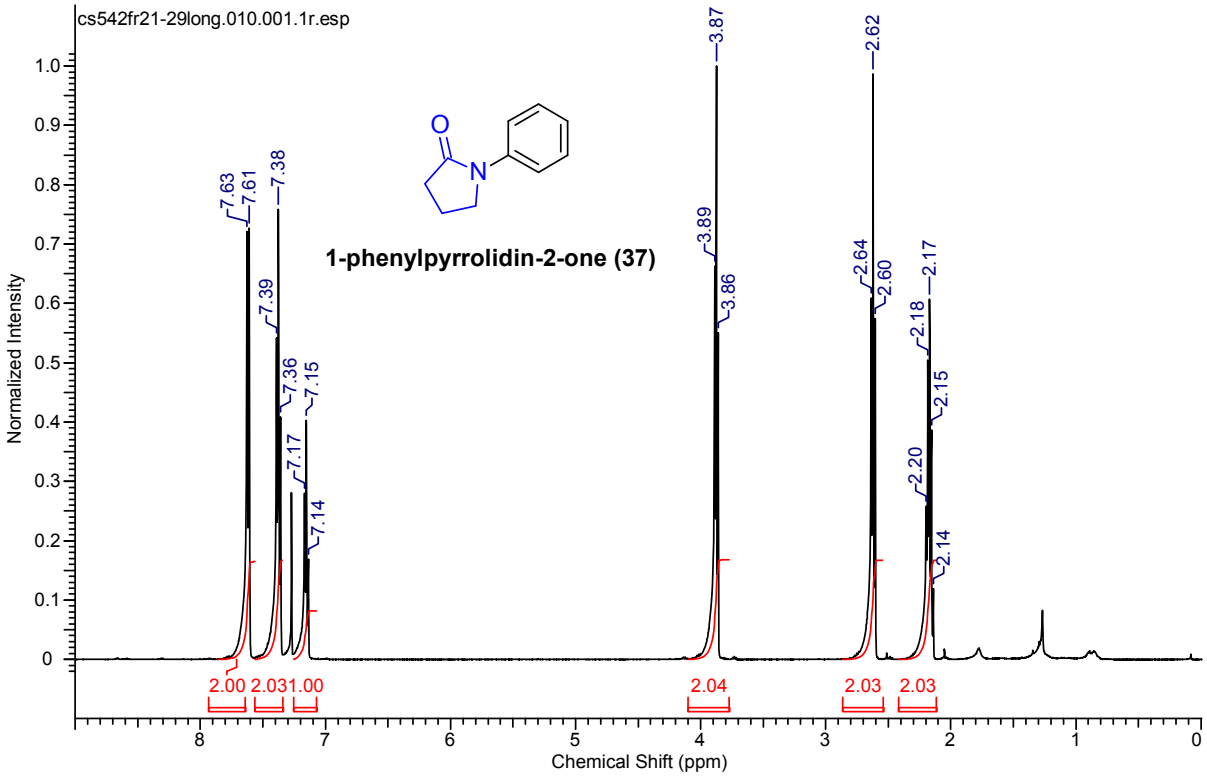


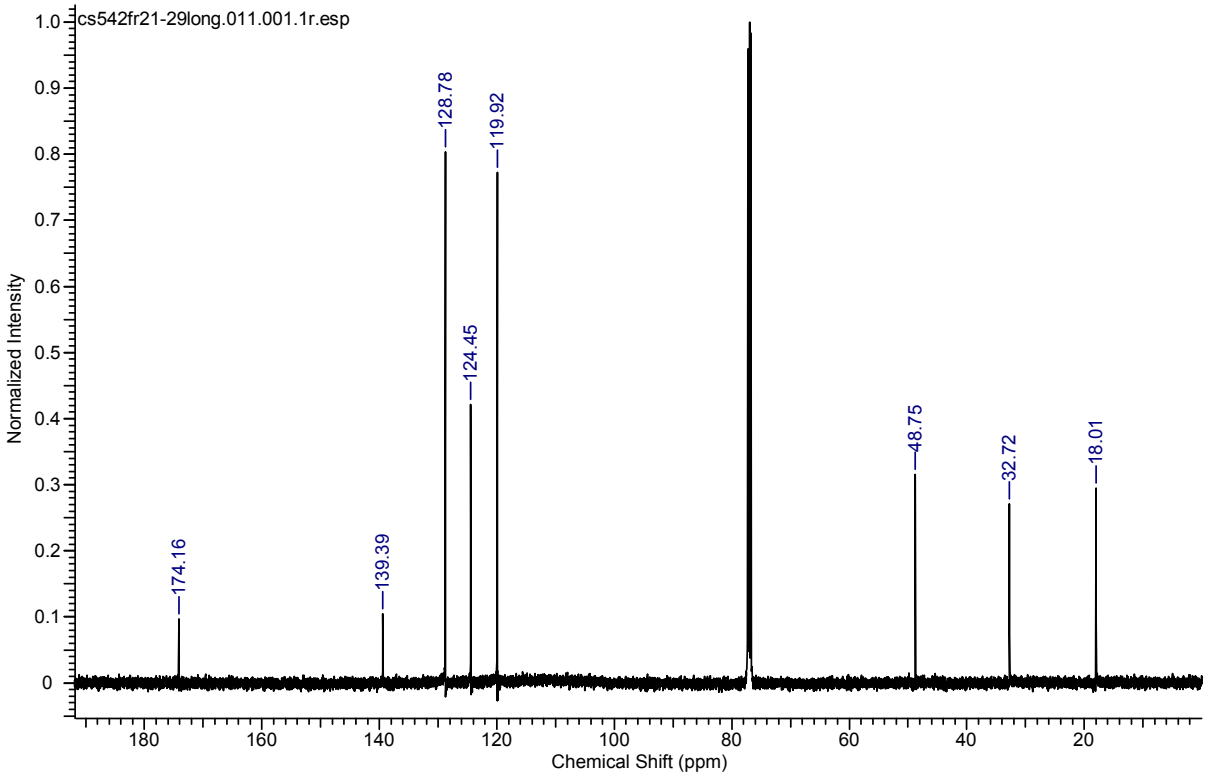

cs532fr15-21long.010.001.1r.esp
N-(4-Acetylphenyl)cyclohexanecarboxamide (35)
Normalized Intensity
Chemical Shift (ppm)
2.58
7.95
7.93
7.65
7.64
7.35
2.27
1.99
1.97
1.87
1.85
1.58
1.55
1.34
1.32
1.25
1.24
1.30
2.00 1.99 0.94
2.96 0.99 2.10 2.01 1.06 3.10 3.49

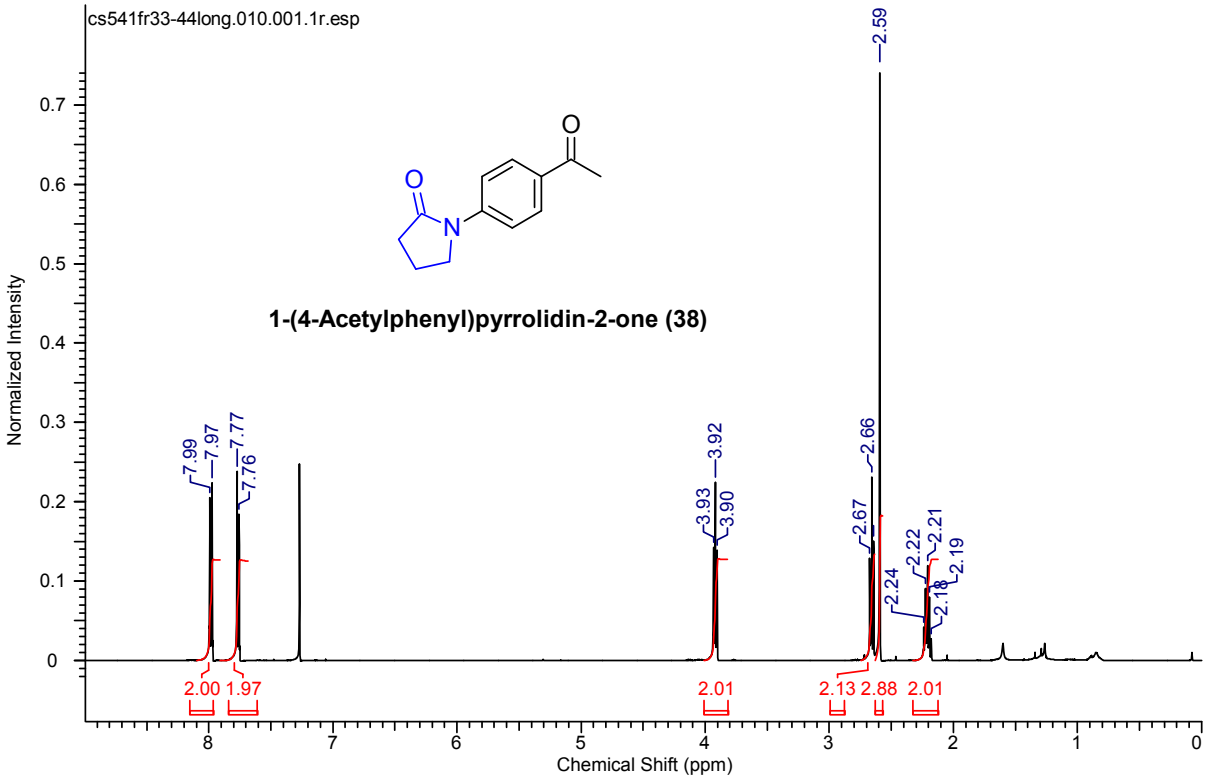

cs532fr15-21long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
196.59
174.34
142.51
133.13
129.73
118.97
46.70
29.70
25.66

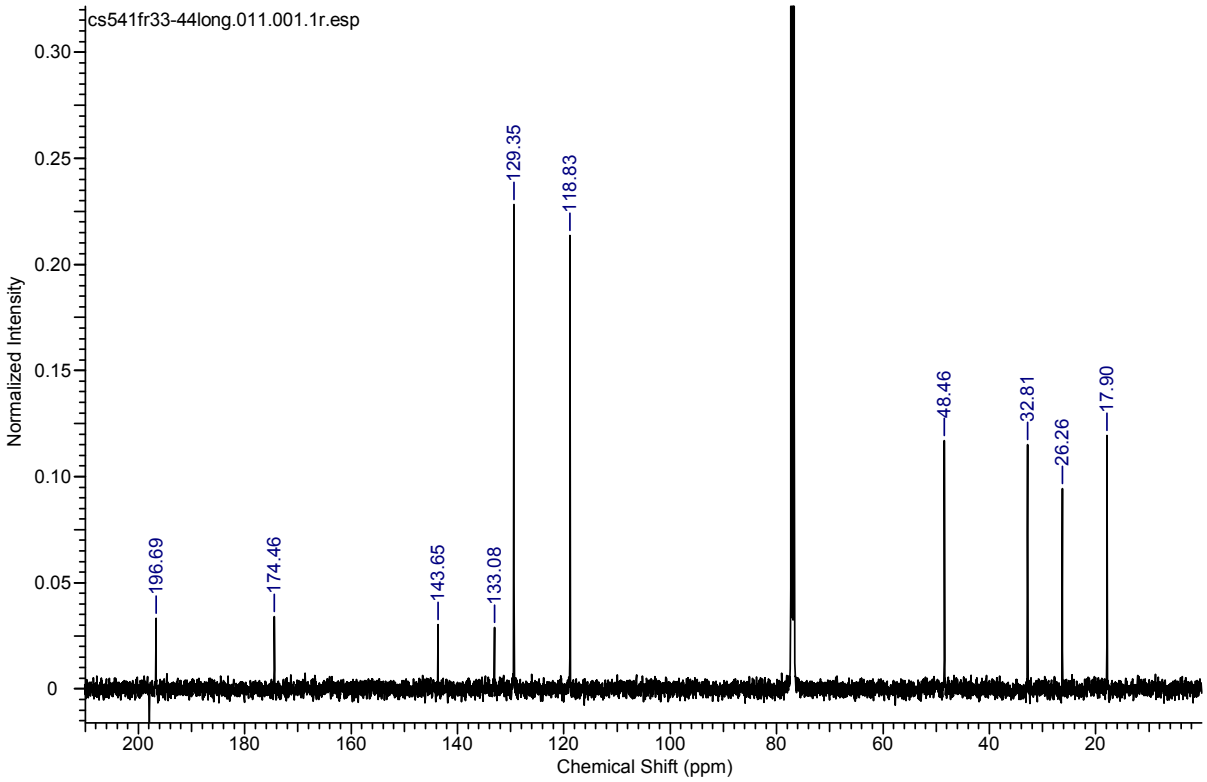

cs540fr27-38.010.001.1r.esp
OMe
O
N
1-(4-Methoxyphenyl)pyrrolidin-2-one (36)
Normalized Intensity
Chemical Shift (ppm)
3.81
7.51
7.49
6.92
6.90
3.83
3.85
2.60
2.61
2.58
2.17
2.16
2.19
2.14
2.13
2.00
2.00
5.04
2.02
2.06

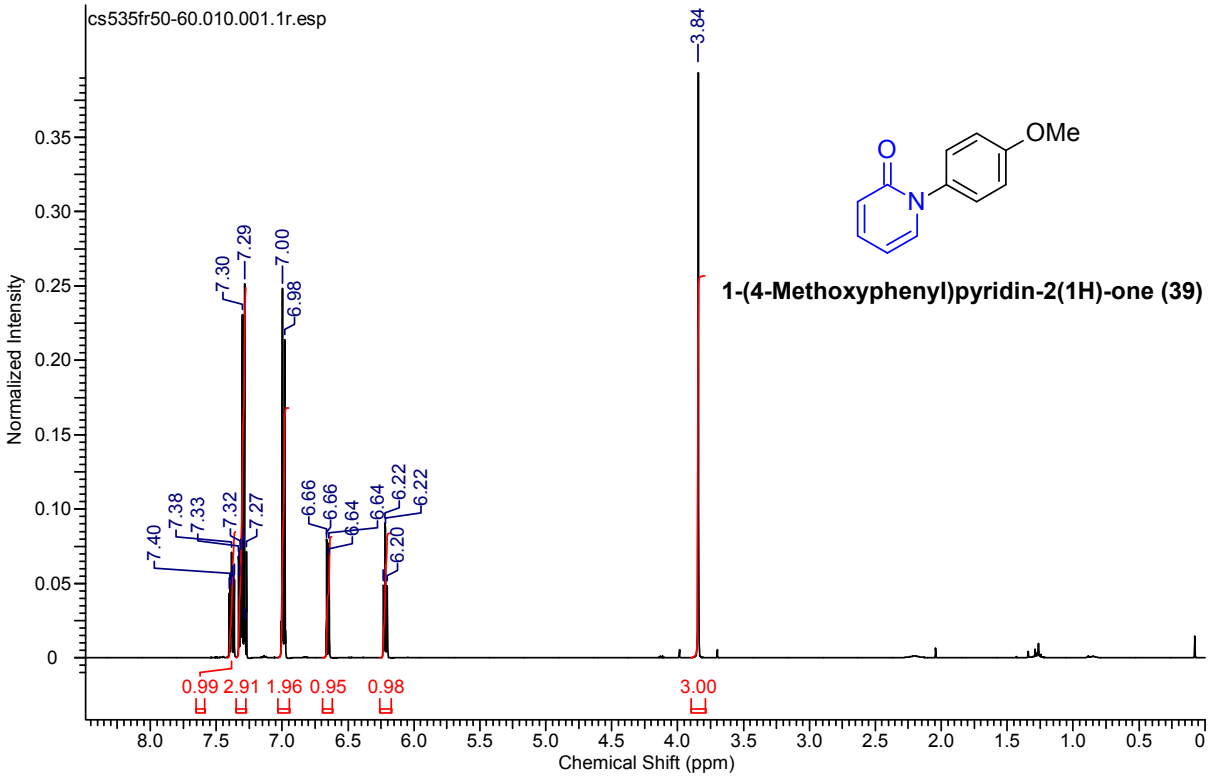

cs540fr27-38.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
173.90
156.56
132.62
121.82
114.03
55.46
49.18
32.45
18.03

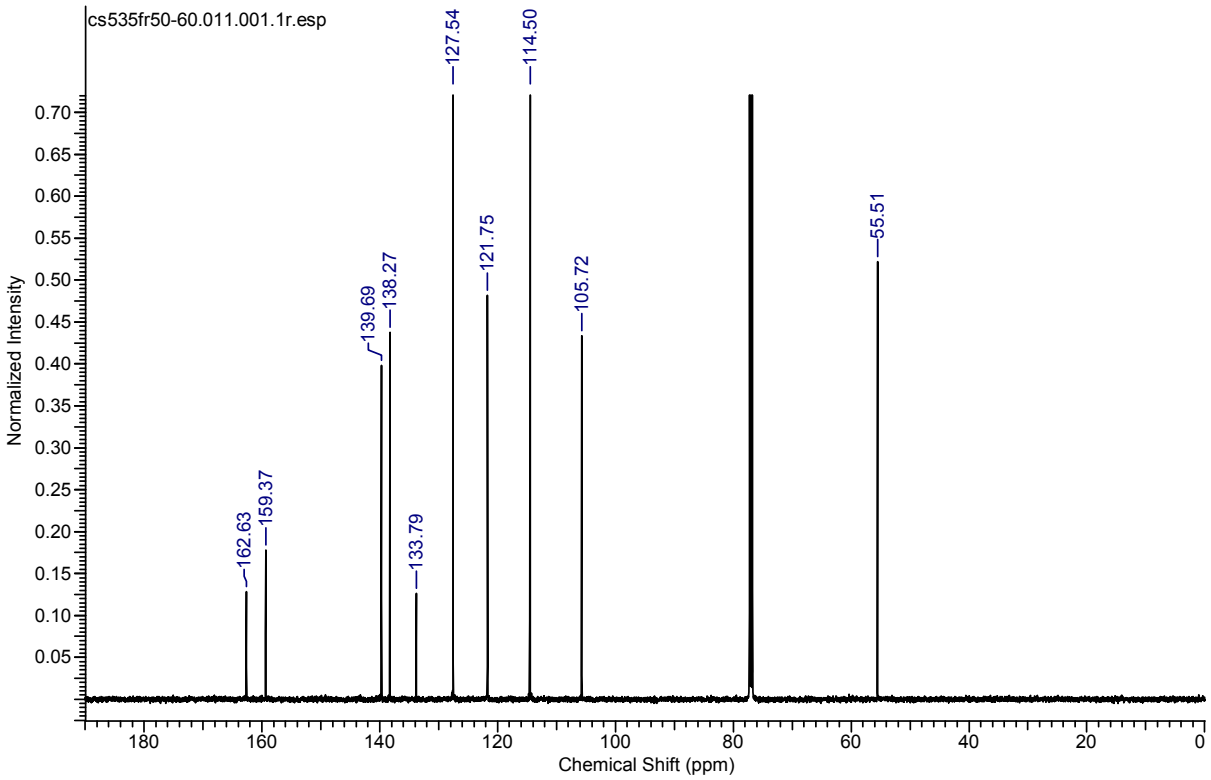

cs542fr21-29long.010.001.1r.esp
1-phenylpyrrolidin-2-one (37)
Normalized Intensity
Chemical Shift (ppm)
7.63
7.61
7.38
7.39
7.36
7.15
7.17
7.14
3.87
3.89
3.86
2.62
2.64
2.60
2.17
2.18
2.15
2.20
2.14
2.00
2.03
1.00
2.04
2.03
2.03

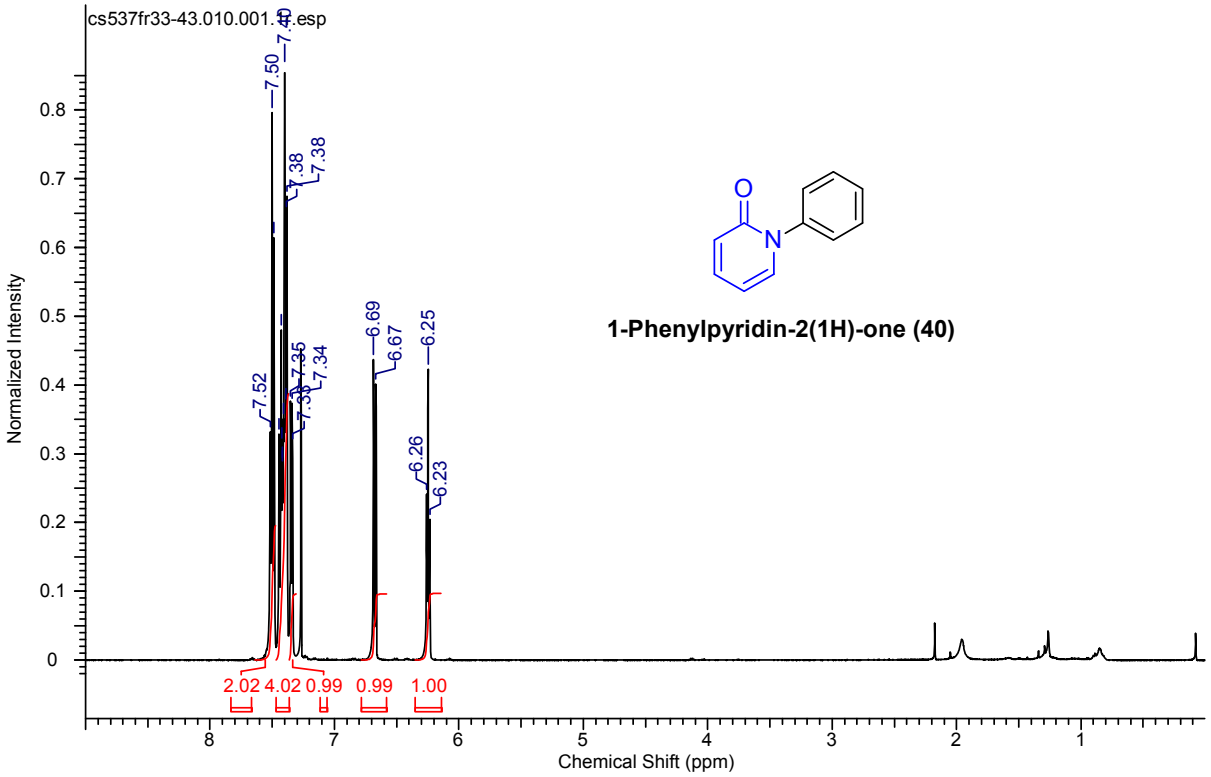

cs542fr21-29long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
174.16
139.39
128.78
124.45
119.92
48.75
32.72
18.01


cs541fr33-44long.010.001.1r.esp
1-(4-Acetylphenyl)pyrrolidin-2-one (38)
Normalized Intensity
Chemical Shift (ppm)
7.99
7.97
7.77
7.76
3.93
3.92
3.90
2.67
2.66
2.59
2.24
2.22
2.21
2.19
2.18
2.00
1.97
2.01
2.13
2.88
2.01

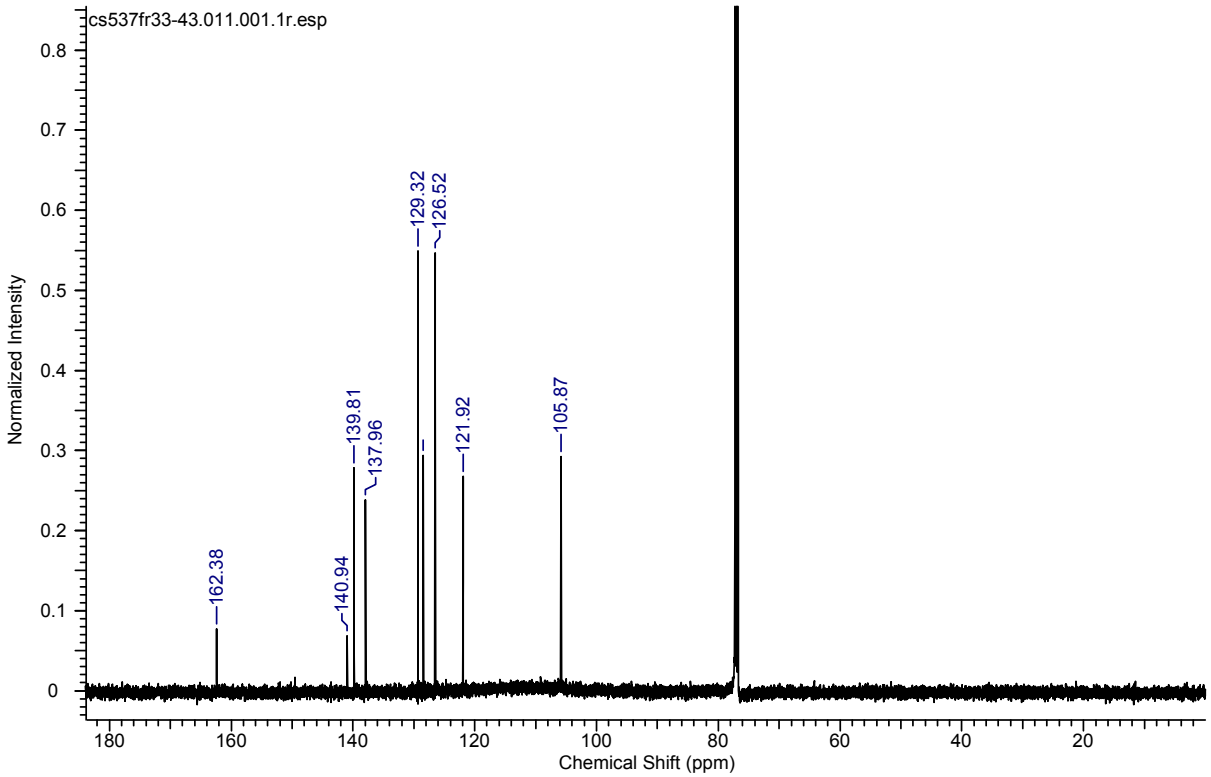

cs541fr33-44long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
196.69
174.46
143.65
133.08
129.35
118.83
48.46
32.81
26.26
17.90

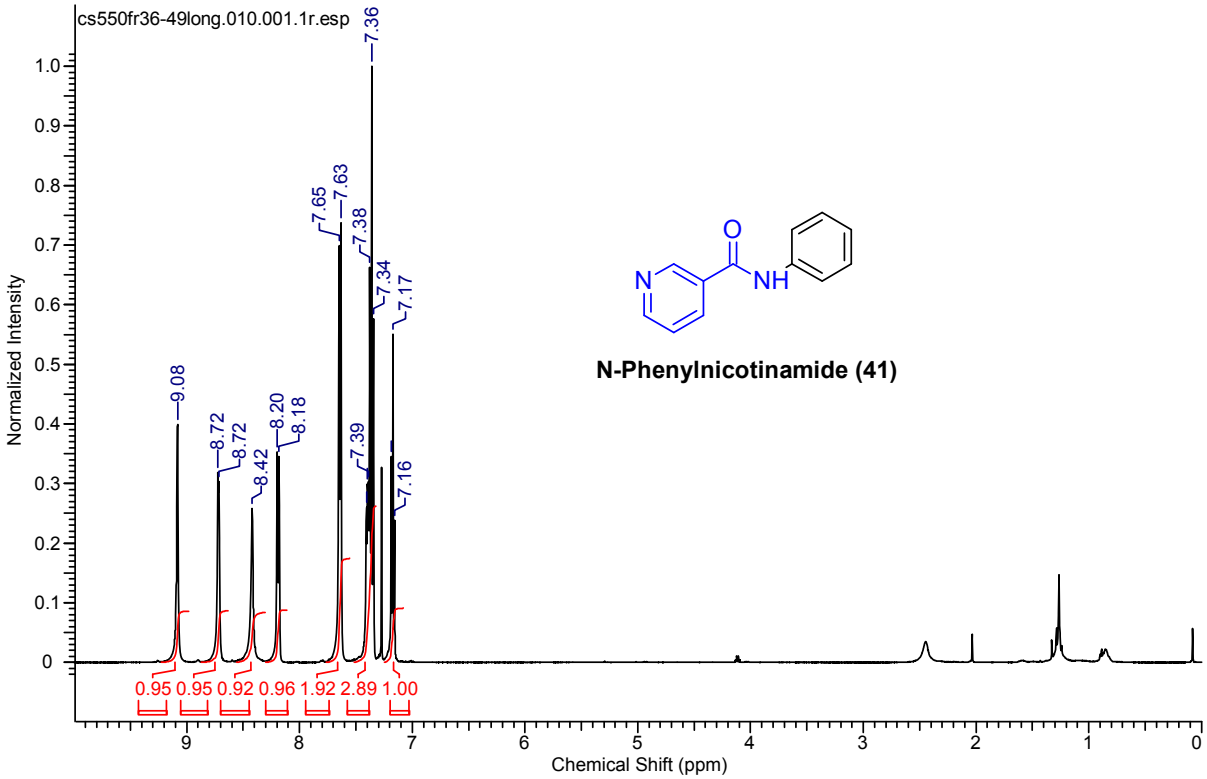

cs535fr50-60.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
3.84
7.40
7.38
7.33
7.32
7.30
7.29
7.27
7.00
6.98
6.66
6.66
6.64
6.64
6.22
6.22
6.20
0.99
2.91
1.96
0.95
0.98
3.00
OMe
O
N
1-(4-Methoxyphenyl)pyridin-2(1H)-one (39)


cs535fr50-60.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
162.63
159.37
139.69
138.27
133.79
127.54
121.75
114.50
105.72
55.51

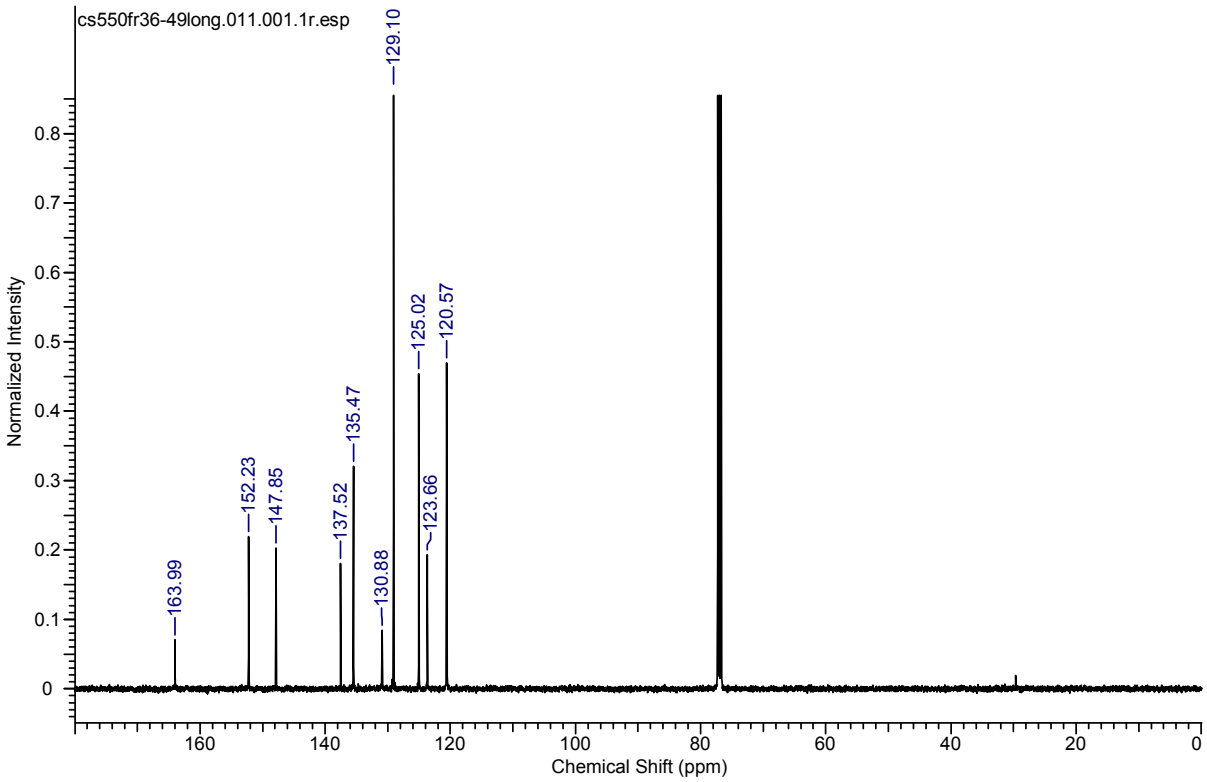


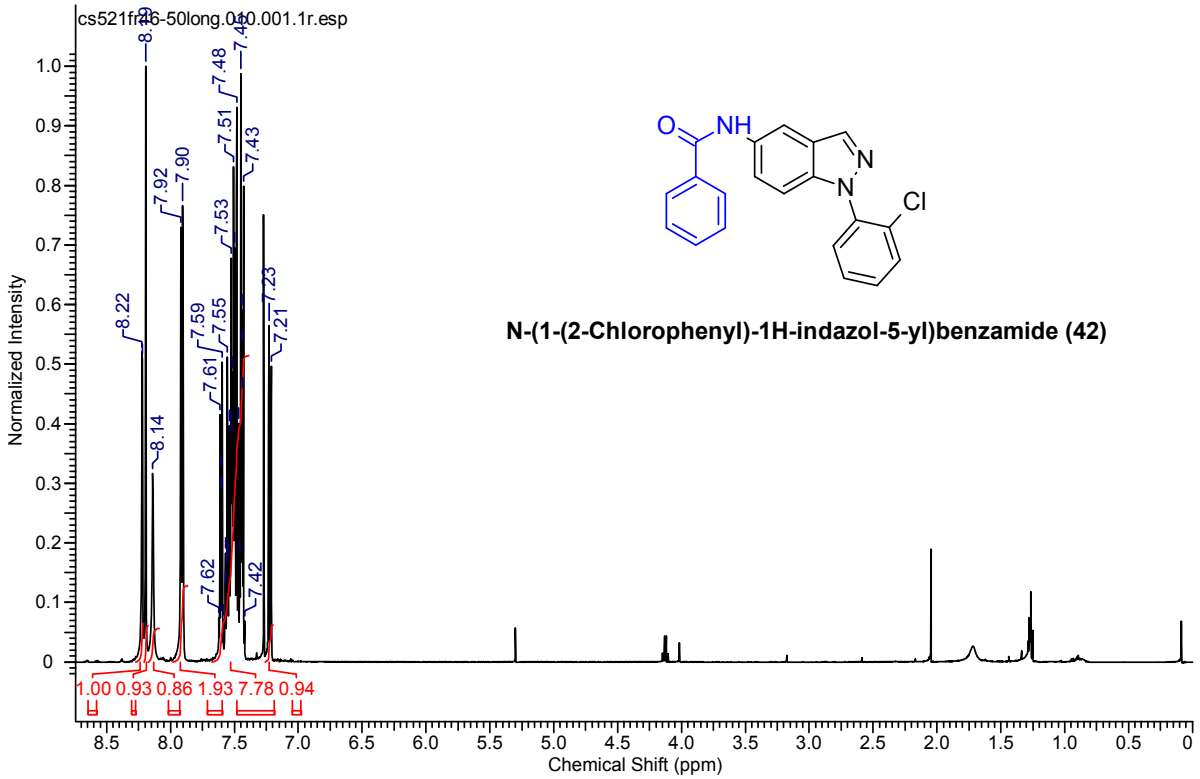
1-Phenylpyridin-2(1H)-one (40)



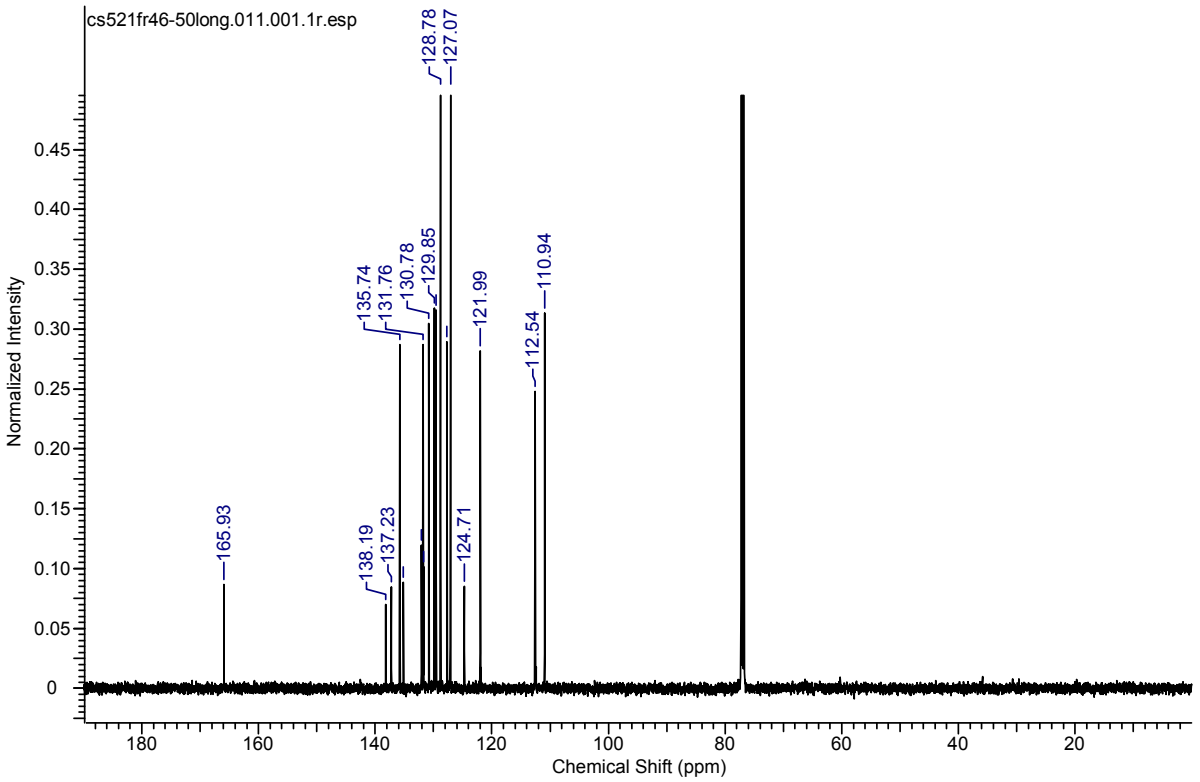


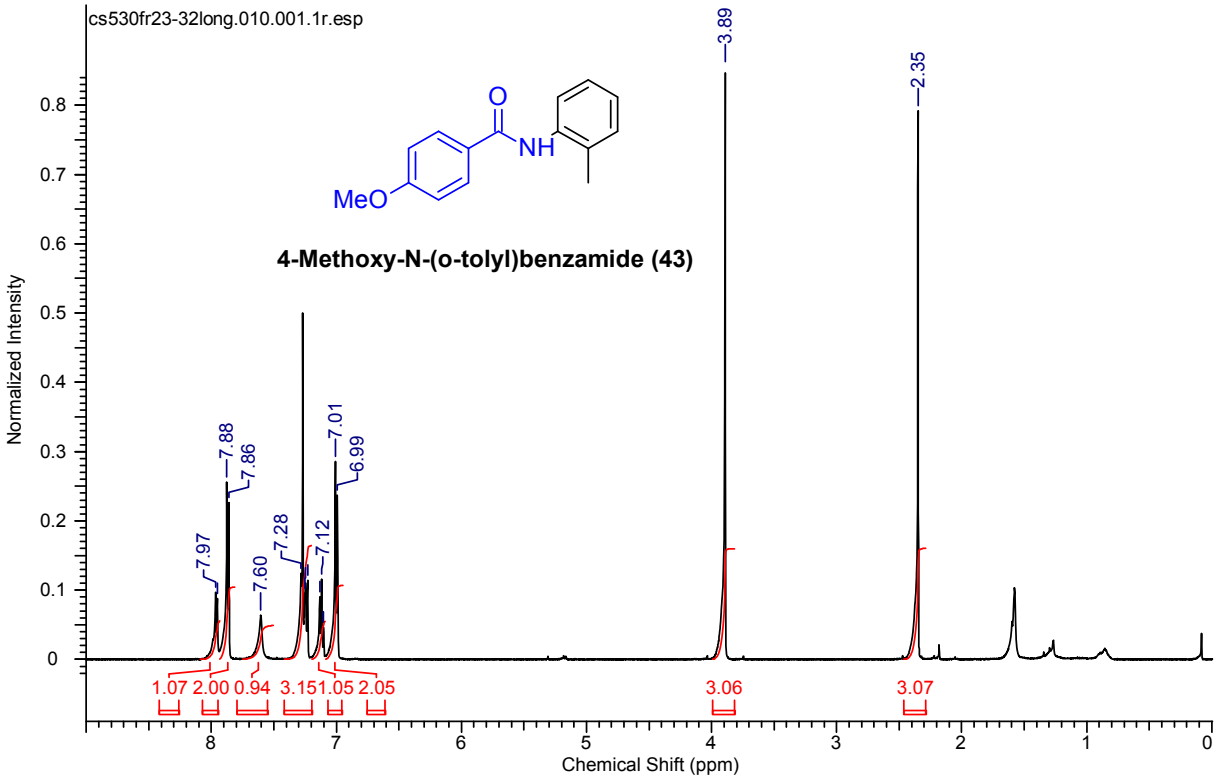
N-Phenylnicotinamide (41)

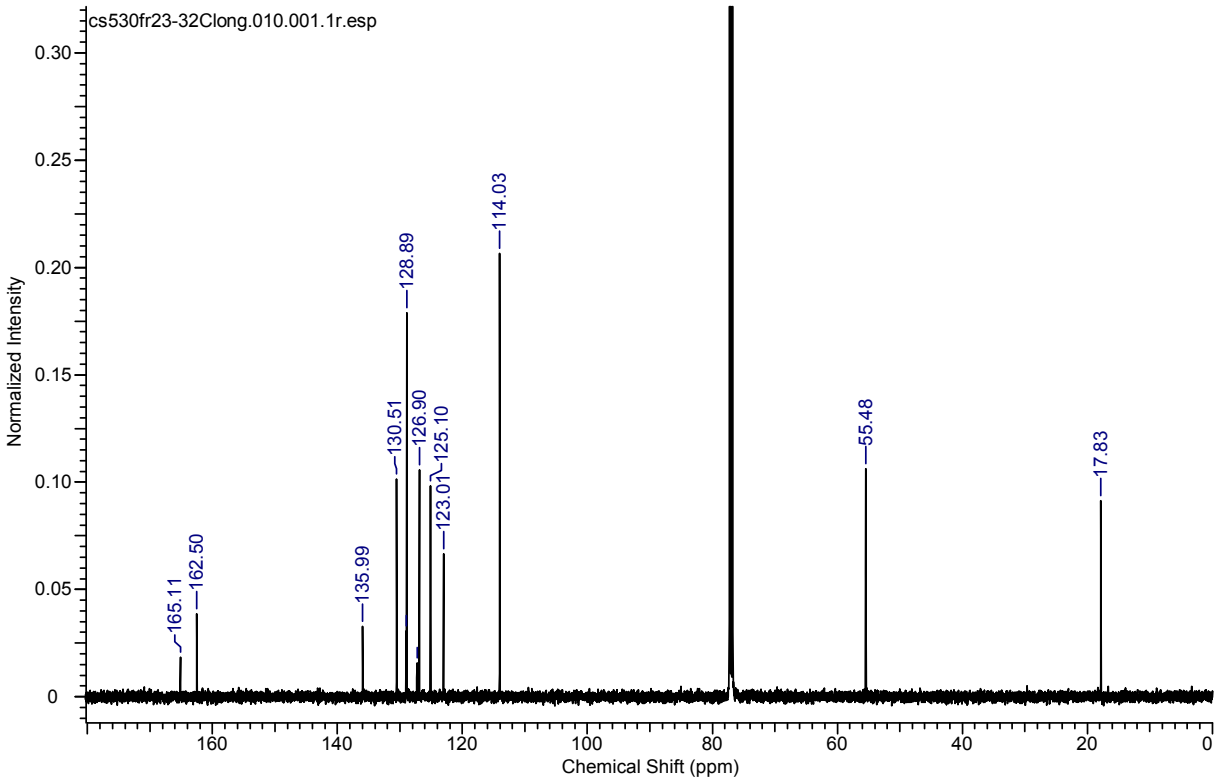


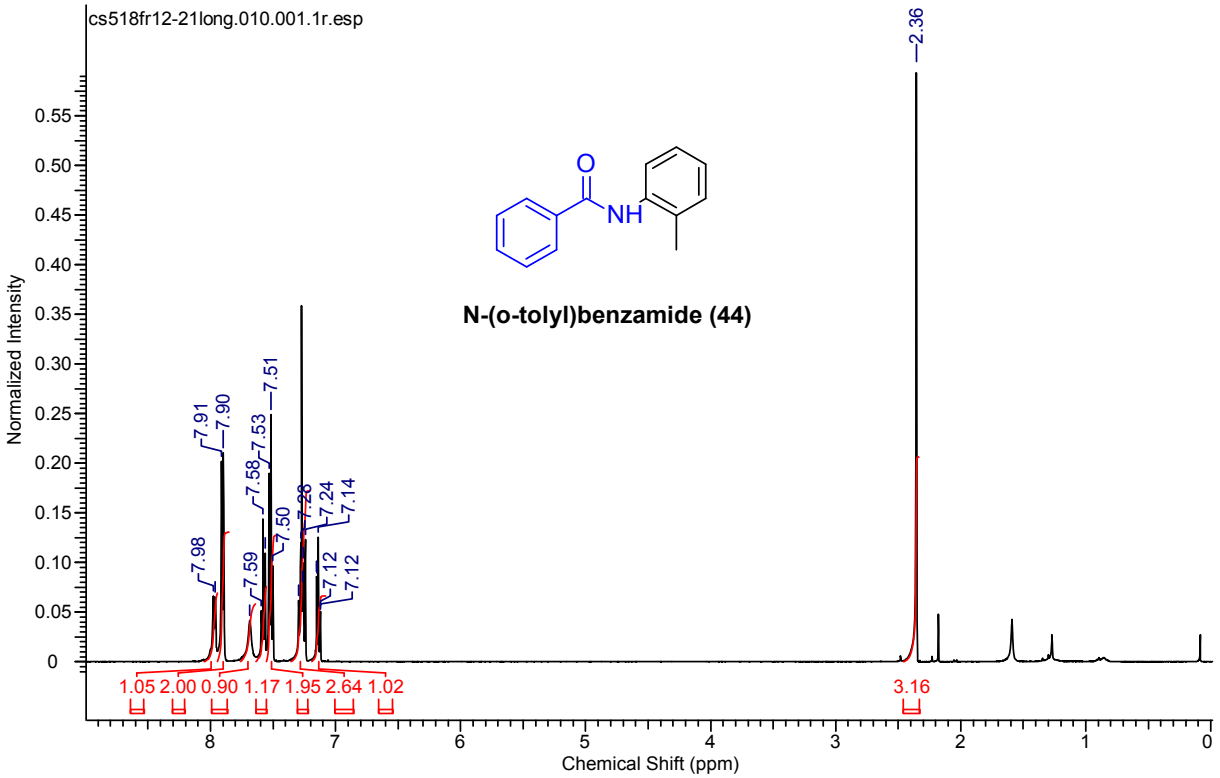


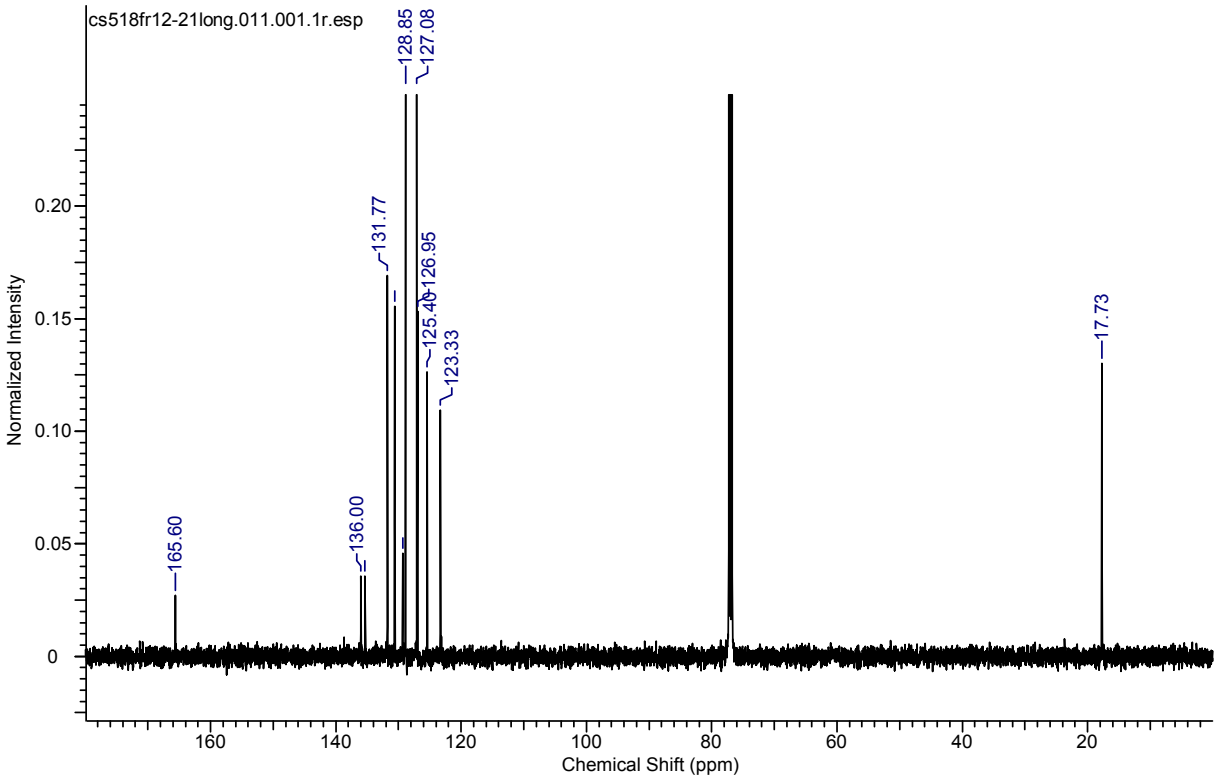
N-(1-(2-Chlorophenyl)-1H-indazol-5-yl)benzamide (42)

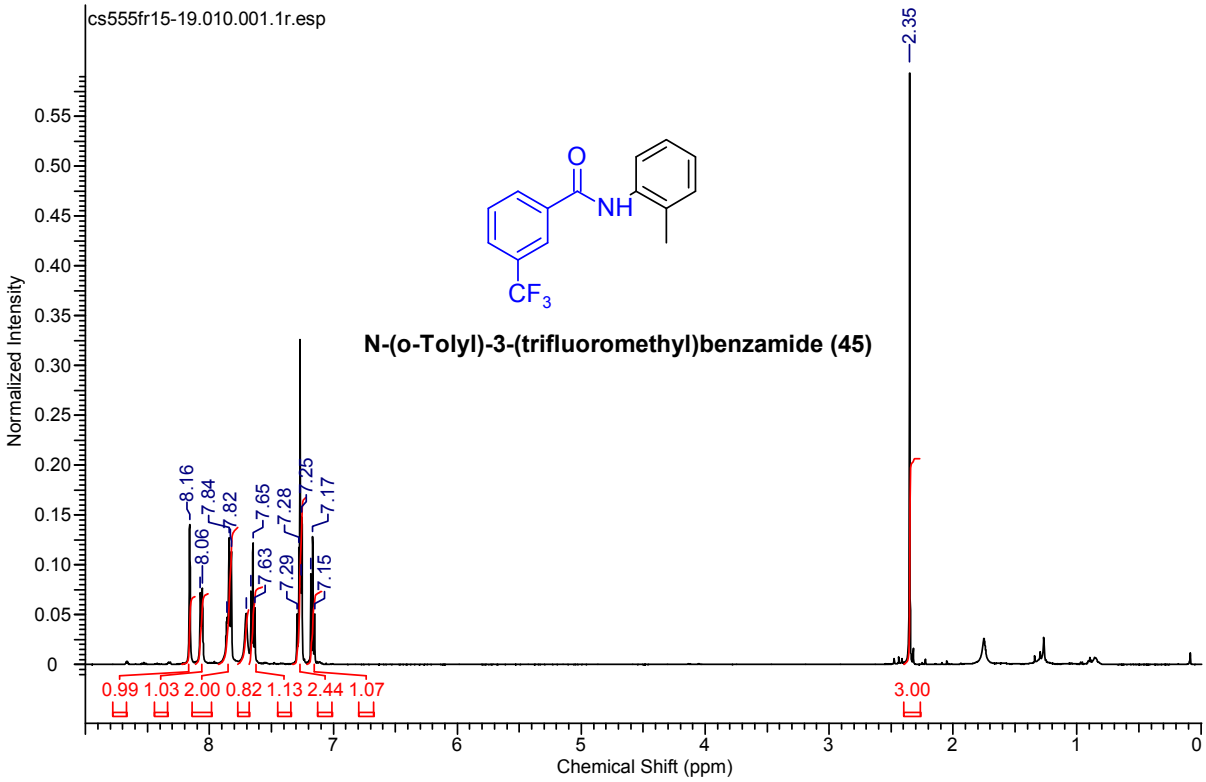


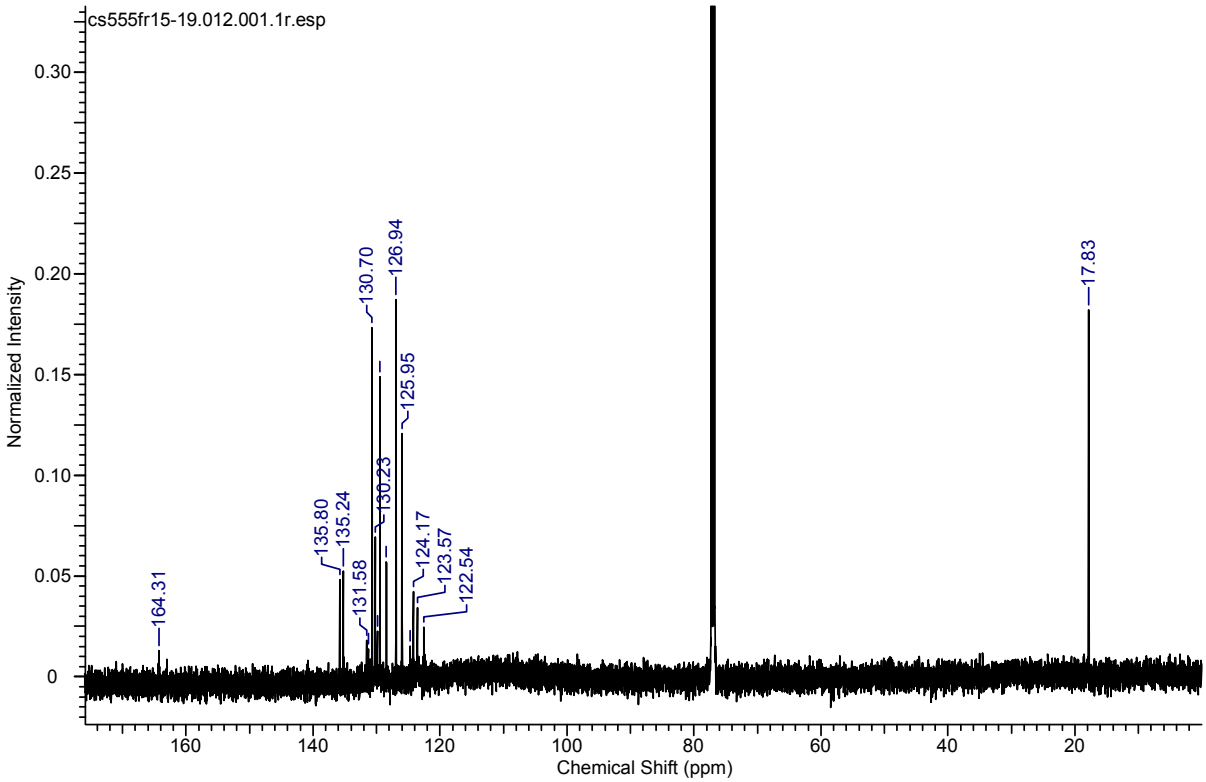

cs530fr23-32long.010.001.1r.esp
O
NH
MeO
4-Methoxy-N-(o-tolyl)benzamide (43)
3.89
2.35
7.88
7.86
7.97
7.60
7.28
7.12
7.01
6.99
1.07 2.00 0.94 3.15 1.05 2.05
3.06
3.07
Normalized Intensity
Chemical Shift (ppm)

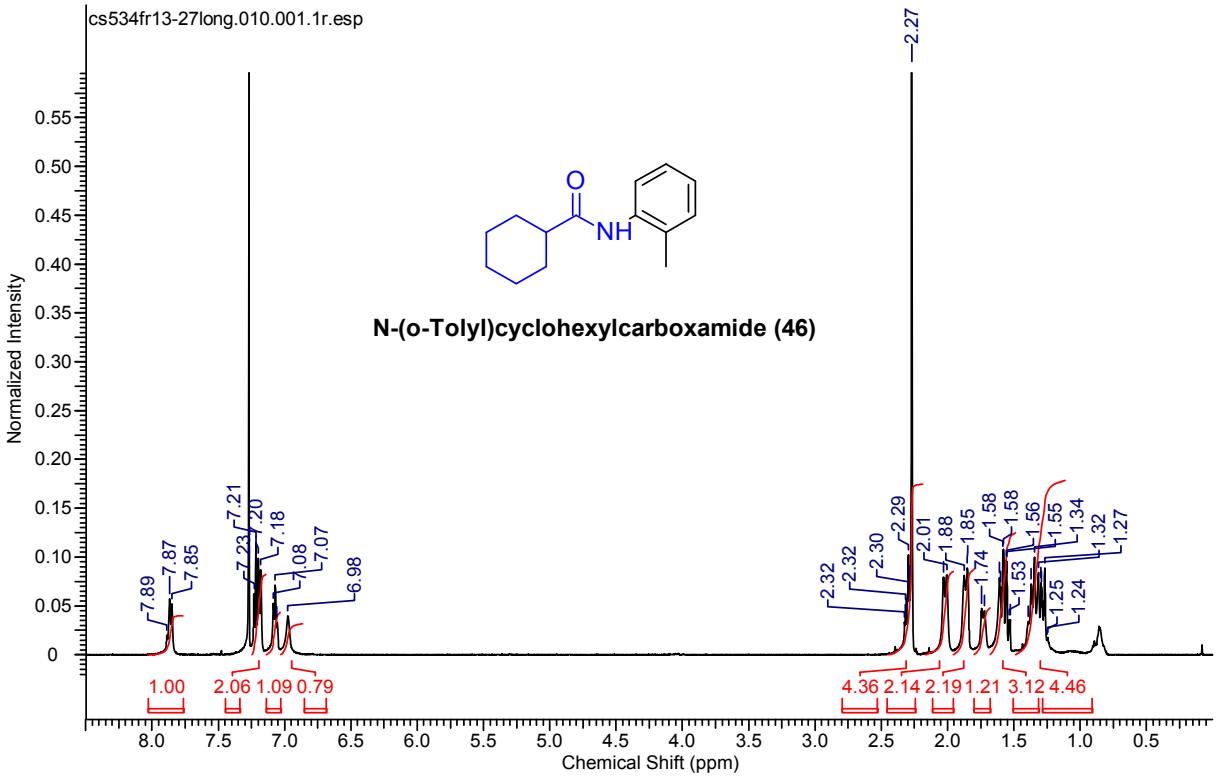

cs530fr23-32Clong.010.001.1r.esp
165.11
162.50
135.99
130.51
128.89
126.90
125.10
123.01
114.03
55.48
17.83
Normalized Intensity
Chemical Shift (ppm)

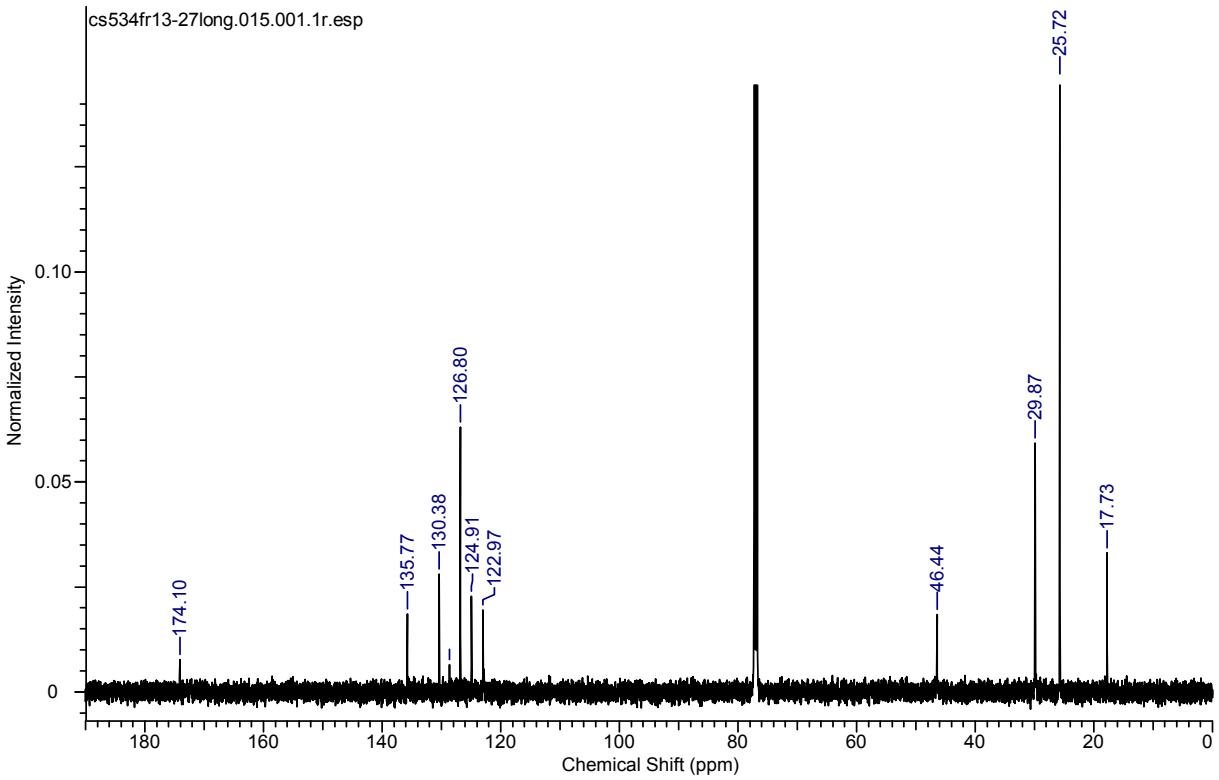

cs518fr12-21long.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
N-(o-tolyl)benzamide (44)
O
NH
2.36
7.91
7.90
7.53
7.51
7.58
7.50
7.28
7.24
7.14
7.98
7.59
7.12
7.12
1.05 2.00 0.90 1.17 1.95 2.64 1.02
3.16

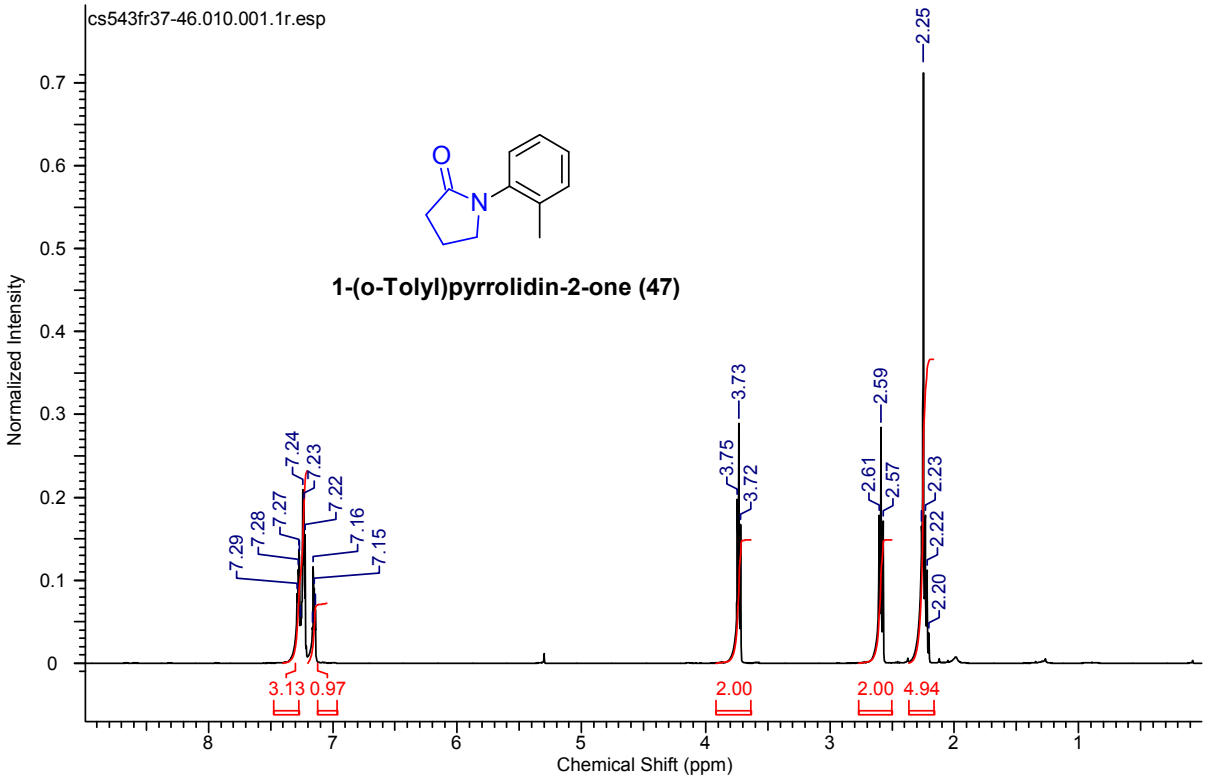

cs518fr12-21long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
128.85
127.08
131.77
126.95
125.40
123.33
17.73
165.60
136.00

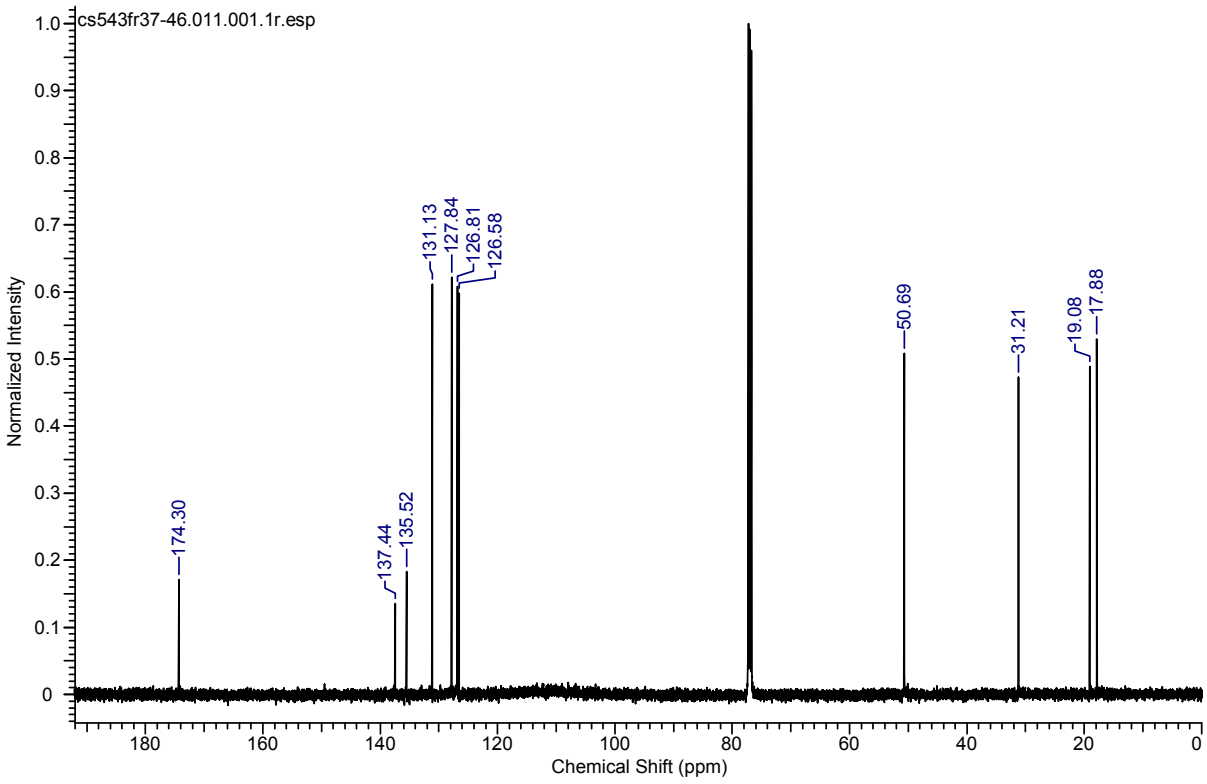

cs555fr15-19.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
8.16
8.06
7.84
7.82
7.65
7.63
7.29
7.28
7.25
7.17
7.15
2.35
0.99 1.03 2.00 0.82 1.13 2.44 1.07
3.00
O
NH
CF3
N-(o-Tolyl)-3-(trifluoromethyl)benzamide (45)

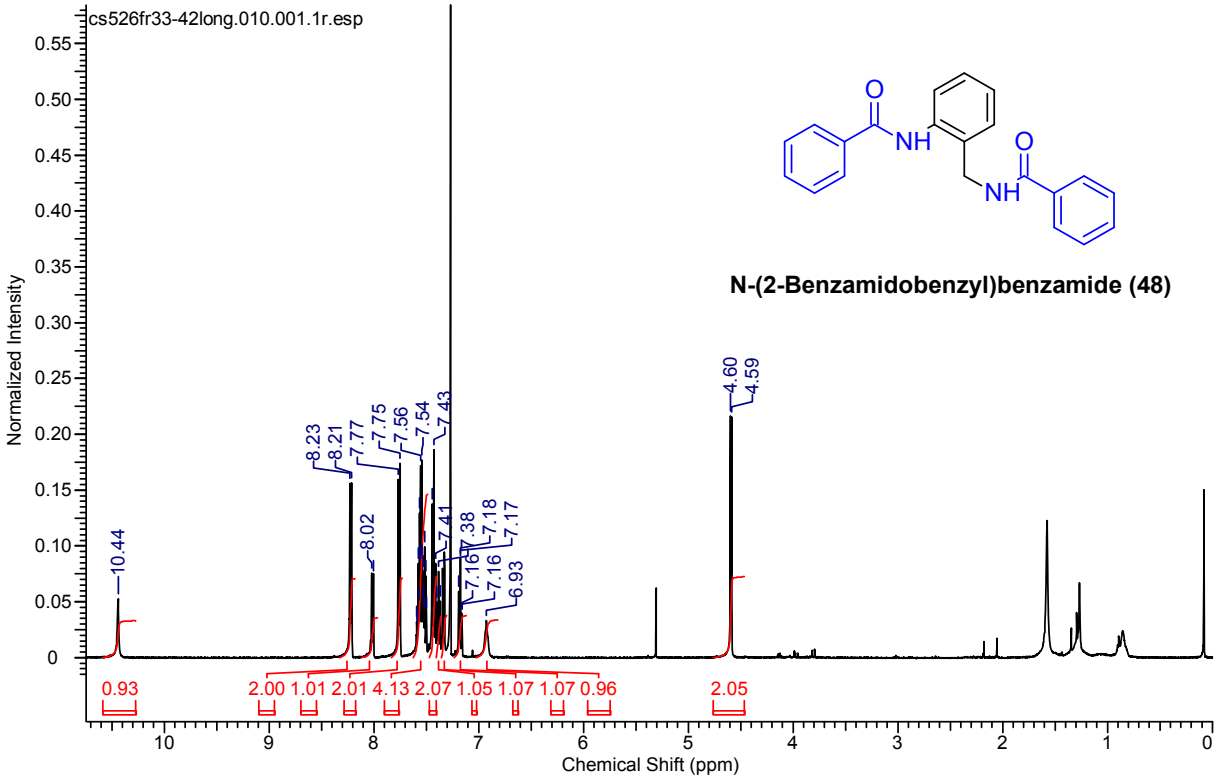

cs555fr15-19.012.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
164.31
135.80
135.24
131.58
130.70
130.23
126.94
125.95
124.17
123.57
122.54
17.83


cs534fr13-27long.010.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
N-(o-Tolyl)cyclohexylcarboxamide (46)
O
NH
2.27
7.89
7.87
7.85
7.21
7.20
7.18
7.08
7.07
6.98
2.32
2.32
2.30
2.29
2.01
1.88
1.85
1.74
1.58
1.58
1.56
1.55
1.34
1.32
1.27
1.53
1.25
1.24
1.00
2.06
1.09
0.79
4.36
2.14
2.19
1.21
3.12
4.46

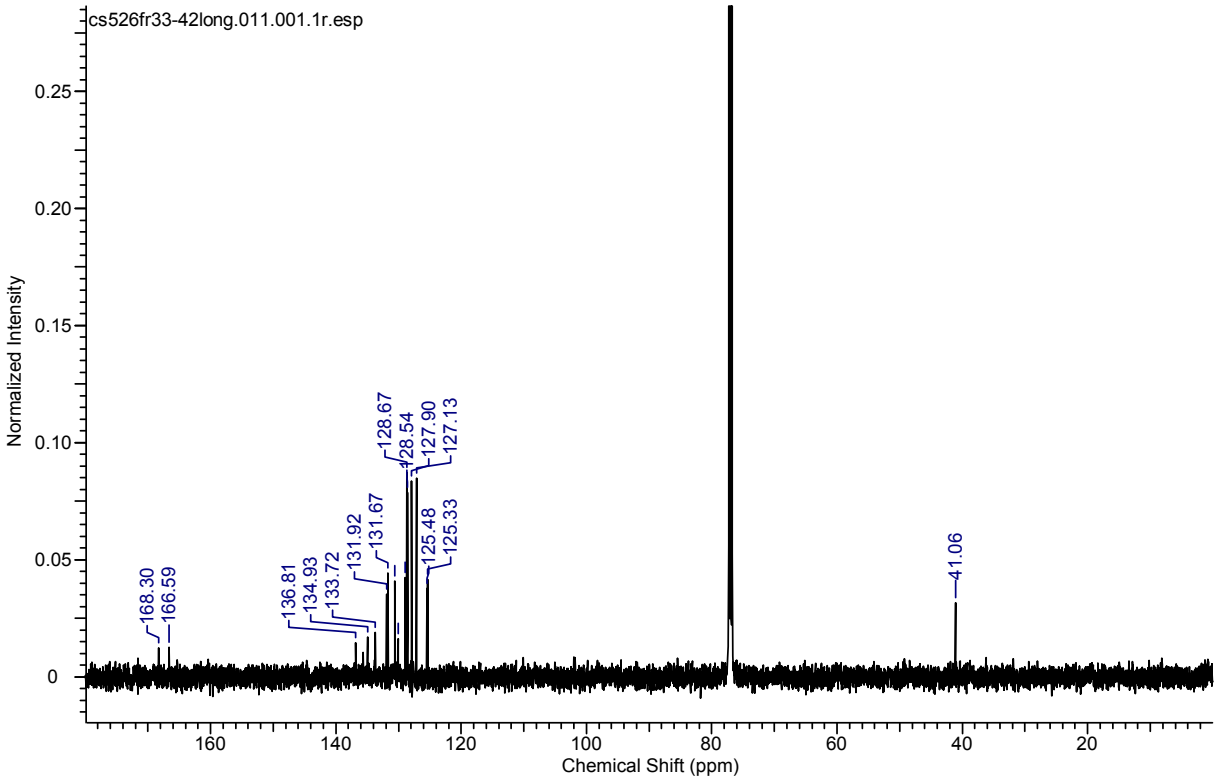

cs534fr13-27long.015.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
174.10
135.77
130.38
126.80
124.91
122.97
46.44
29.87
25.72
17.73

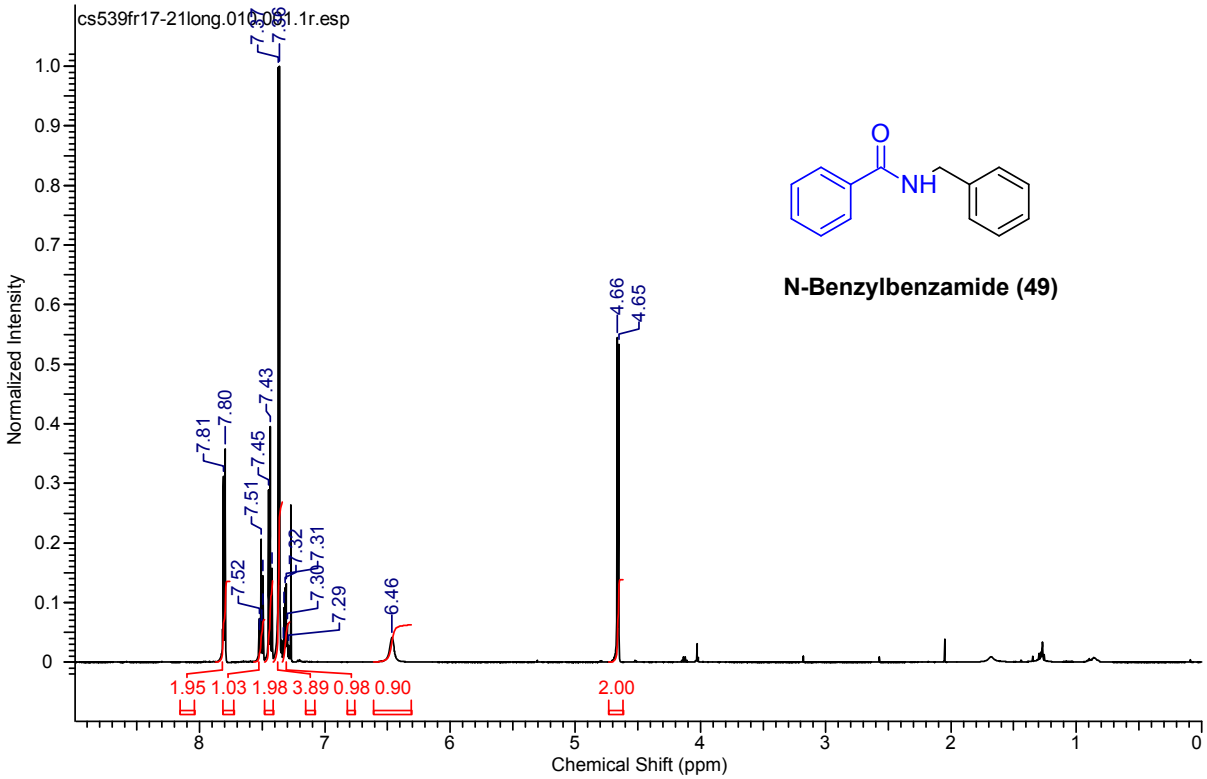

cs543fr37-46.010.001.1r.esp
1-(o-Tolyl)pyrrolidin-2-one (47)
Normalized Intensity
Chemical Shift (ppm)
7.29
7.28
7.27
7.24
7.23
7.22
7.16
7.15
3.75
3.73
3.72
2.61
2.59
2.57
2.25
2.23
2.22
2.20
3.13
0.97
2.00
2.00
4.94


cs543fr37-46.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
174.30
137.44
135.52
131.13
127.84
126.81
126.58
50.69
31.21
19.08
17.88

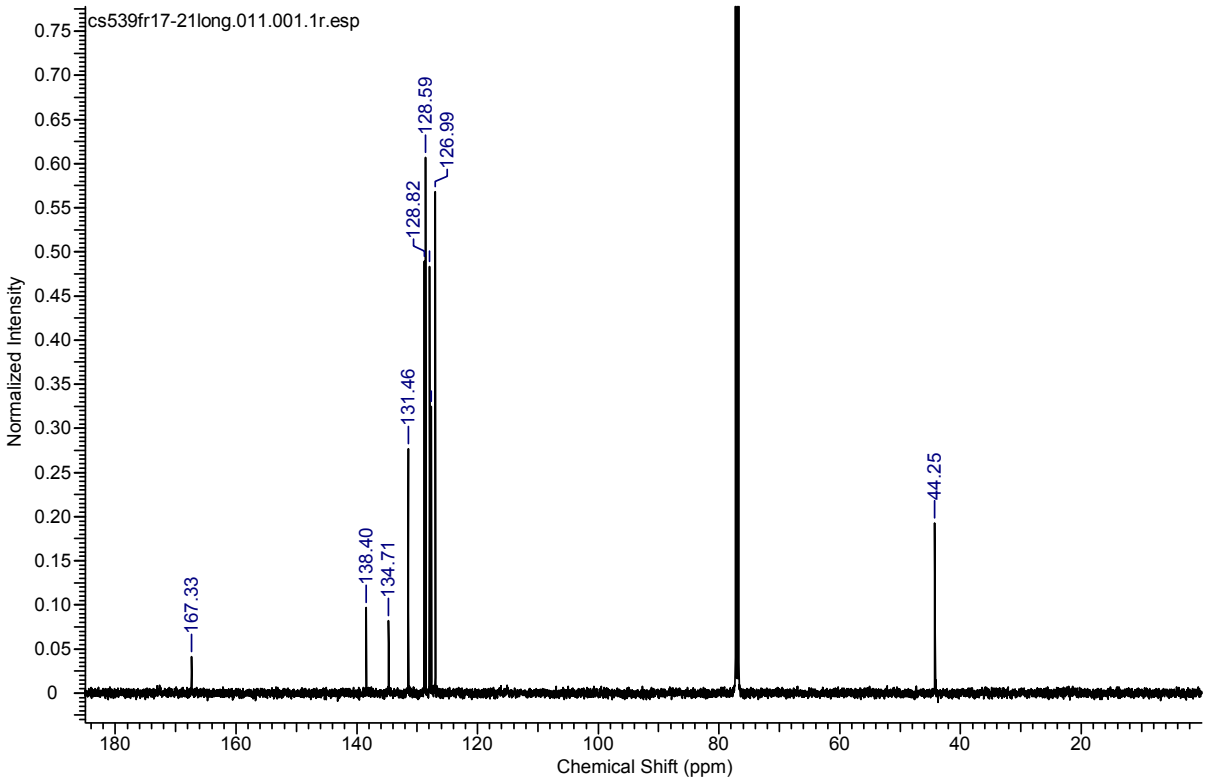


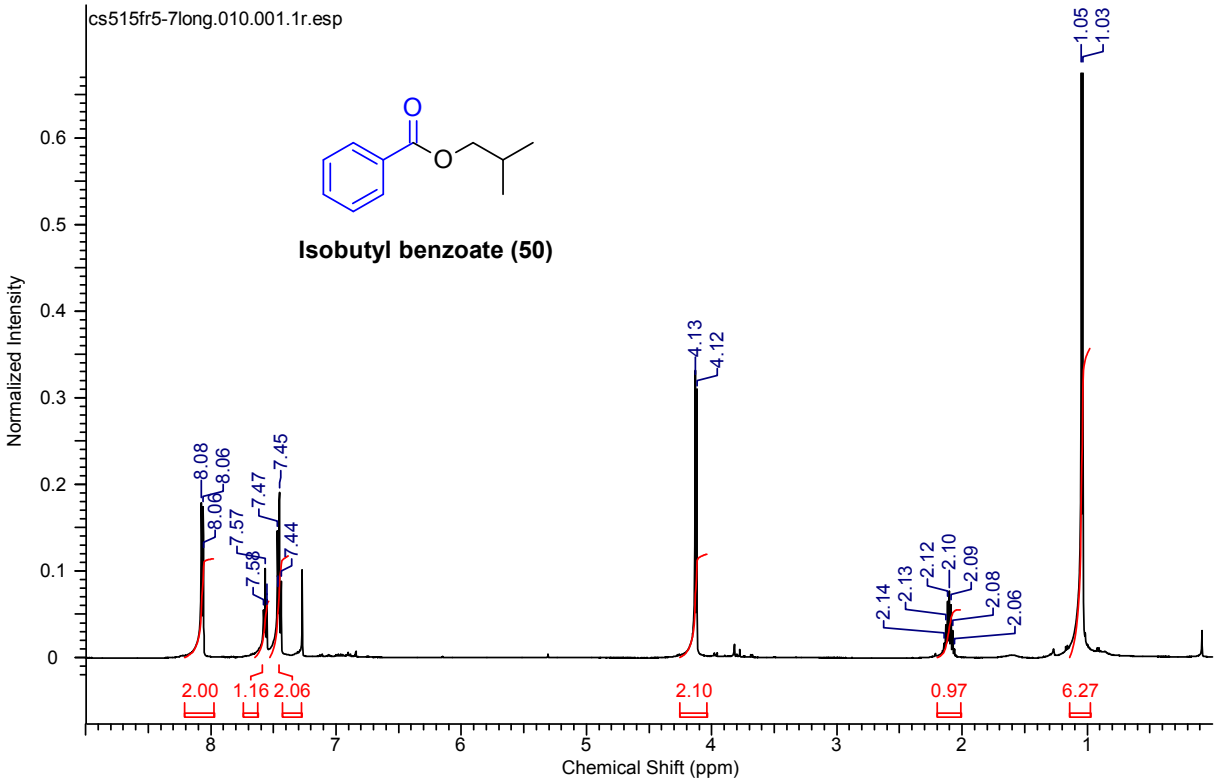
N-(2-Benzamidobenzyl)benzamide (48)

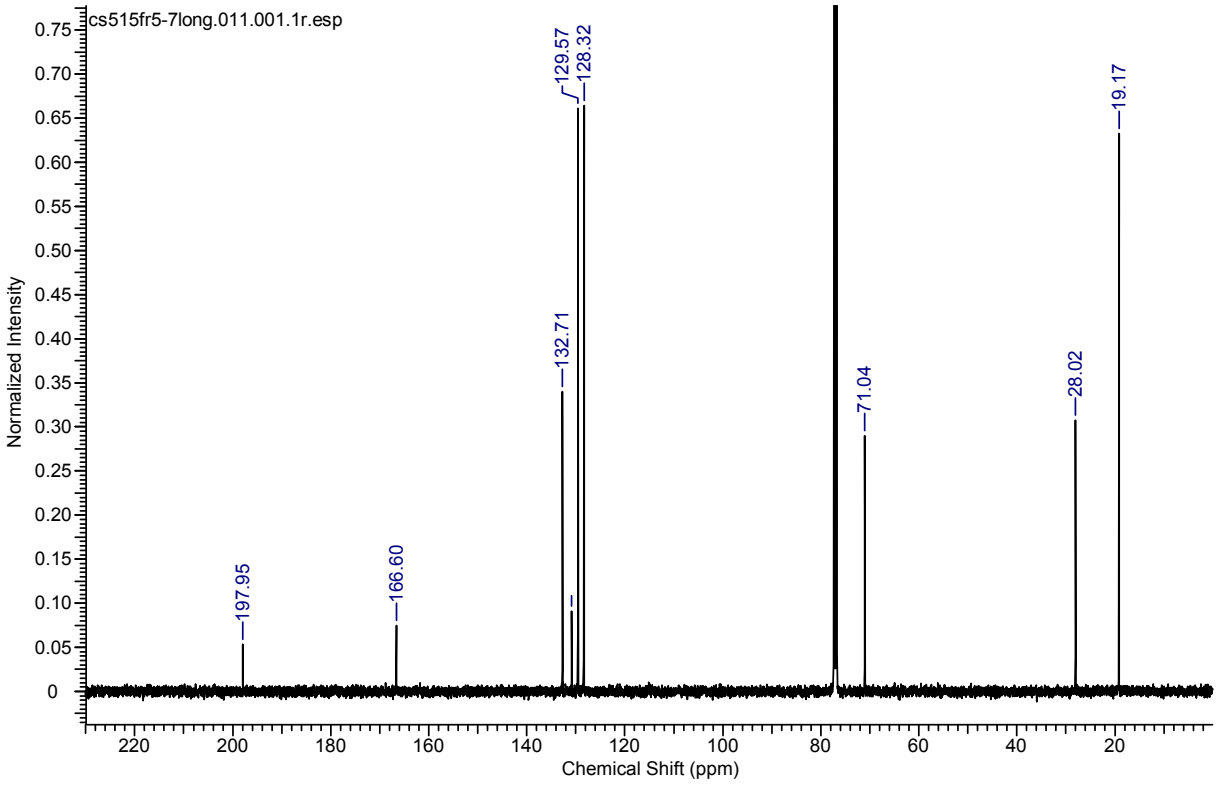


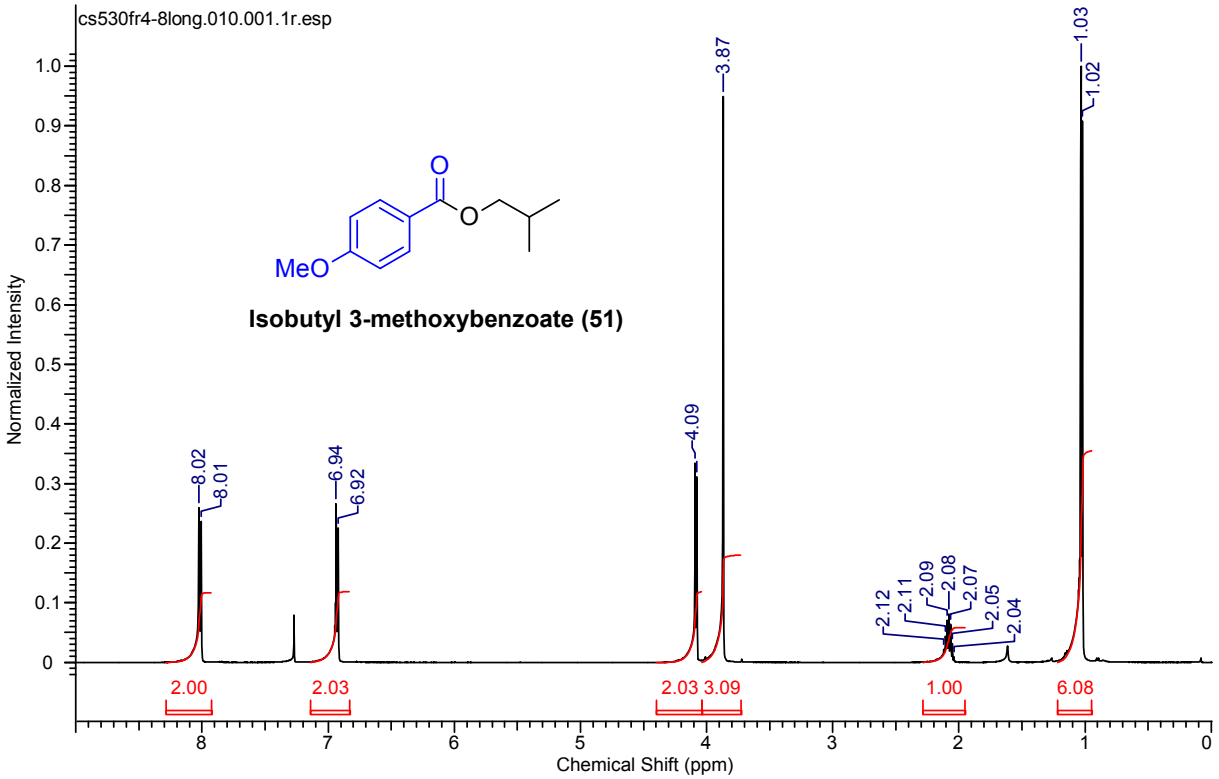


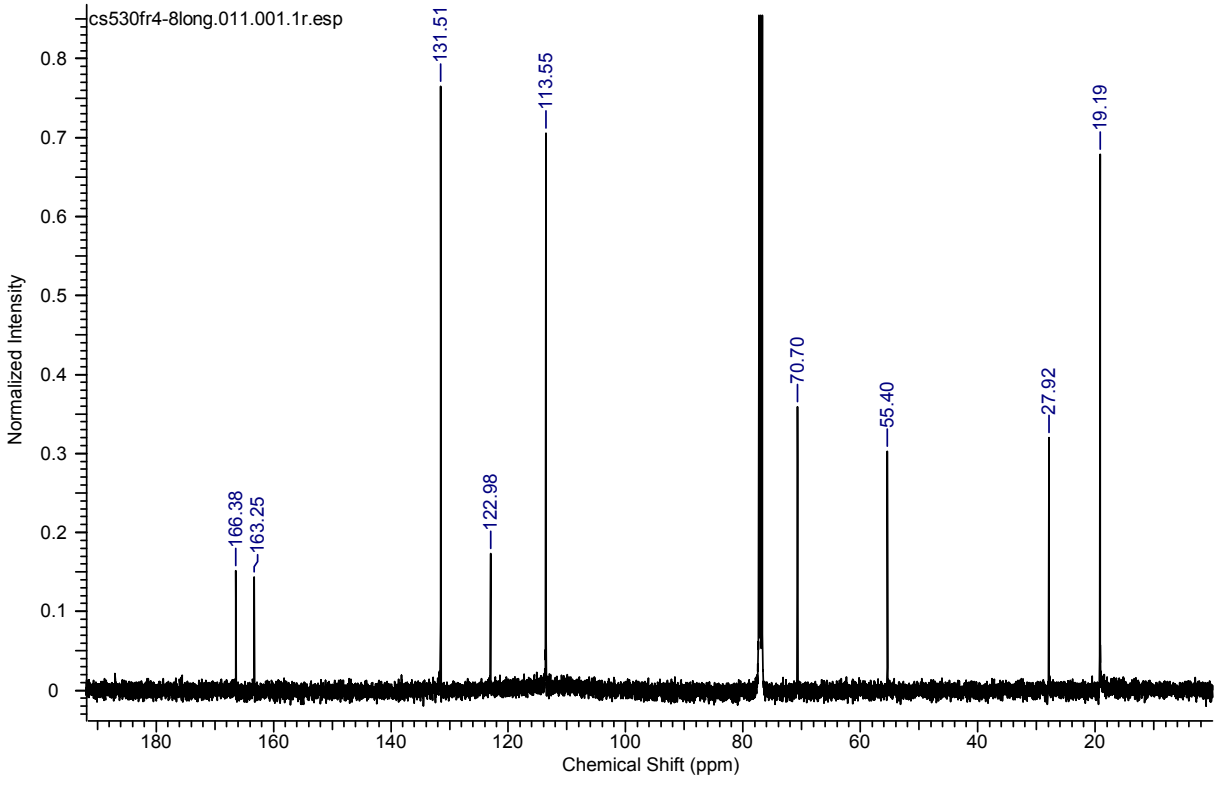
N-Benzylbenzamide (49)

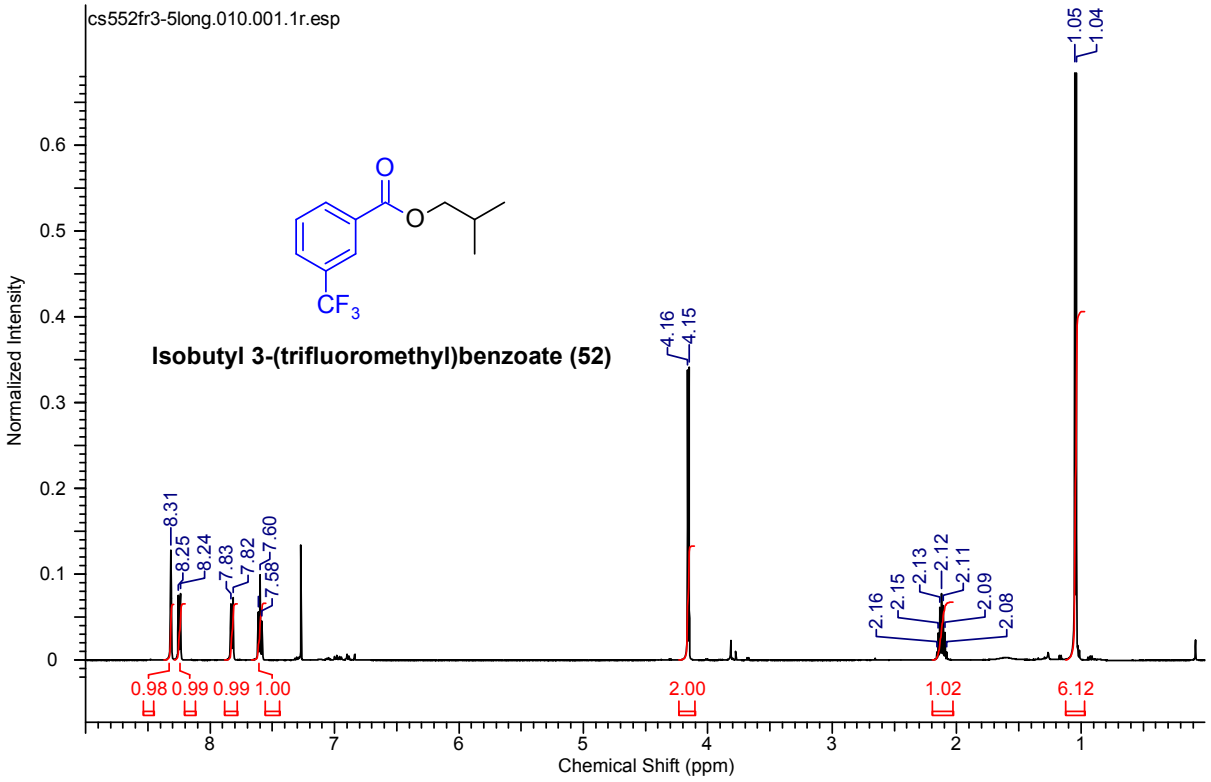


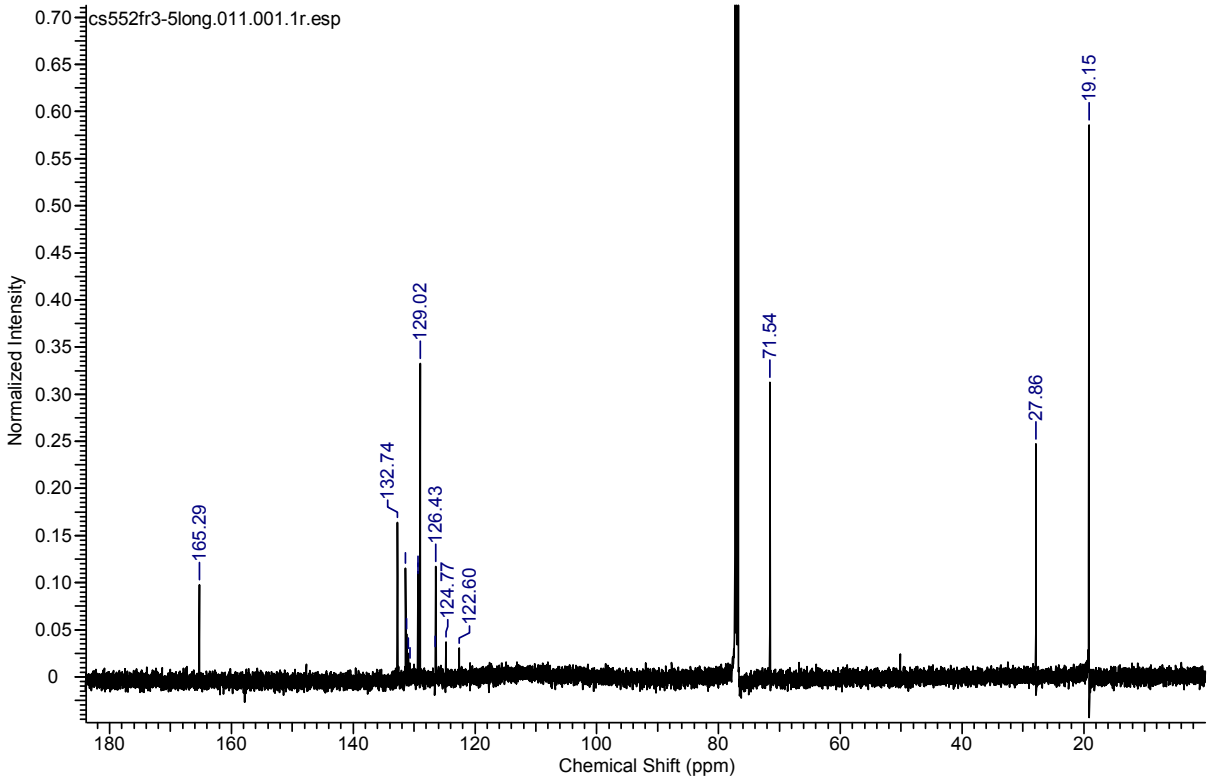

cs515fr5-7long.010.001.1r.esp
Isobutyl benzoate (50)
Normalized Intensity
Chemical Shift (ppm)
8.08
8.06
8.04
7.57
7.56
7.47
7.45
7.44
4.13
4.12
2.14
2.13
2.12
2.10
2.09
2.08
2.06
1.05
1.03
2.00
1.16
2.06
2.10
0.97
6.27

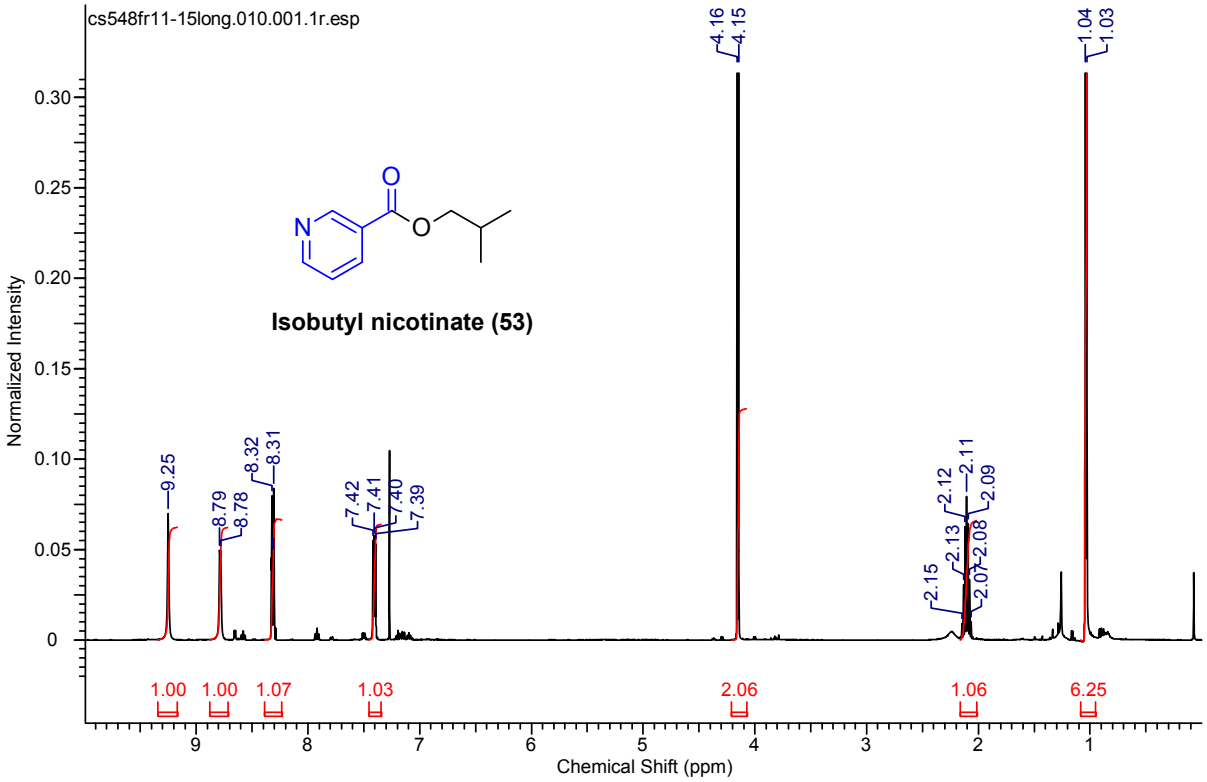

cs515fr5-7long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
197.95
166.60
132.71
129.57
128.32
71.04
28.02
19.17

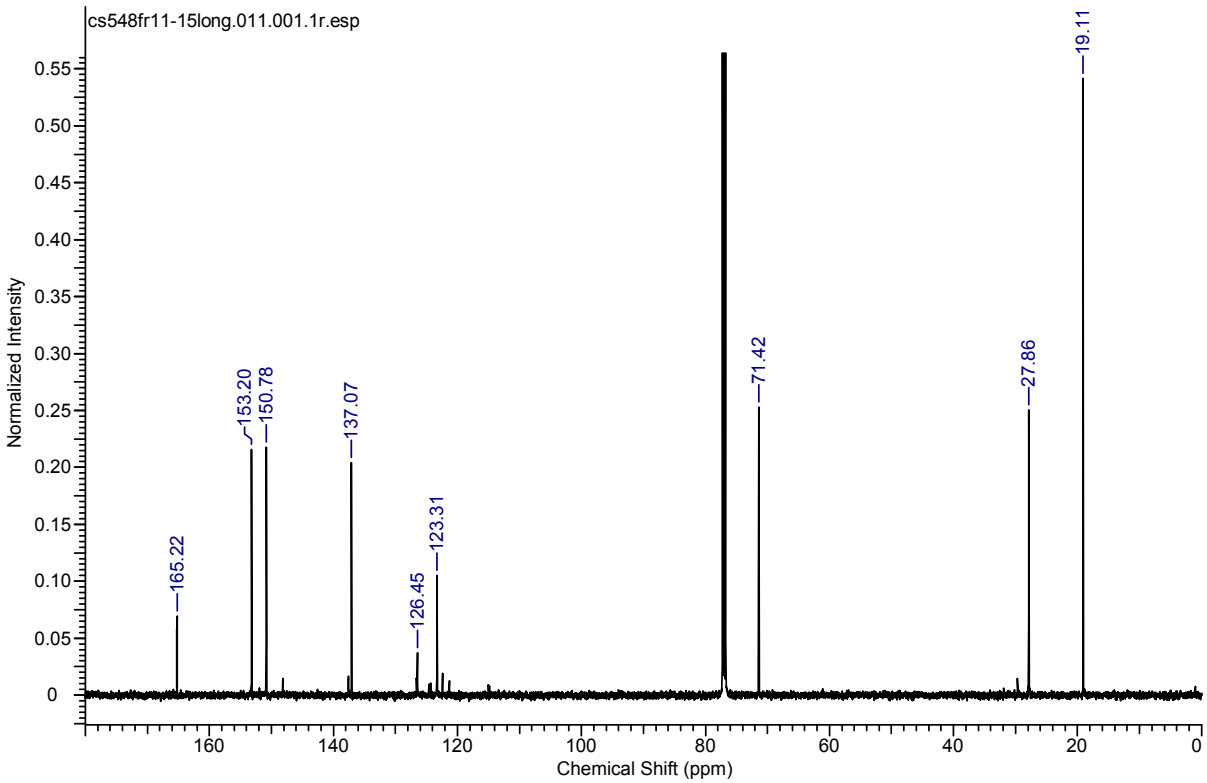

cs530fr4-8long.010.001.1r.esp
Isobutyl 3-methoxybenzoate (51)
MeO
O
O
Normalized Intensity
Chemical Shift (ppm)
8.02
8.01
6.94
6.92
4.09
3.87
2.12
2.11
2.09
2.08
2.07
2.05
2.04
1.03
1.02
2.00
2.03
2.03 3.09
1.00
6.08


cs530fr4-8long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
166.38
163.25
131.51
122.98
113.55
70.70
55.40
27.92
19.19


cs552fr3-5long.010.001.1r.esp
Isobutyl 3-(trifluoromethyl)benzoate (52)
Normalized Intensity
Chemical Shift (ppm)
8.31
8.25
8.24
7.83
7.82
7.60
7.58
4.16
4.15
2.16
2.15
2.13
2.12
2.11
2.09
2.08
1.05
1.04
0.98
0.99
0.99
1.00
2.00
1.02
6.12


cs552fr3-5long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
165.29
132.74
129.02
126.43
124.77
122.60
71.54
27.86
19.15


cs548fr11-15long.010.001.1r.esp
Isobutyl nicotinate (53)
Normalized Intensity
Chemical Shift (ppm)
9.25
8.79
8.78
8.32
8.31
7.42
7.41
7.40
7.39
4.16
4.15
2.15
2.13
2.12
2.11
2.09
2.08
2.07
1.04
1.03
1.00
1.00
1.07
1.03
2.06
1.06
6.25


cs548fr11-15long.011.001.1r.esp
Normalized Intensity
Chemical Shift (ppm)
165.22
153.20
150.78
137.07
126.45
123.31
71.42
27.86
19.11