Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

One Pot Tandem Dehydrogenative Cross-Coupling of Primary and Secondary Alcohols by Ruthenium Amido-Functionalized 1,2,4-Triazole Derived N-Heterocyclic Carbene Complexes

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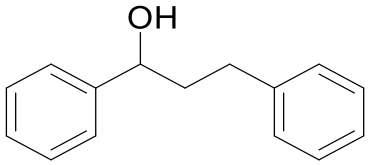
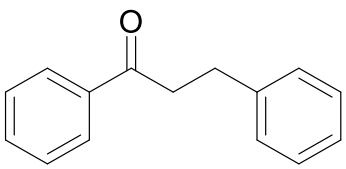
1,3-Diphenylpropan-1-ol (4)[1]



(**4**)

Colorless liquid [0.148 g, 70 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.37−7.36 (m, 4H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_6\underline{H}_5$), 7.31−7.26 (m, 3H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_6\underline{H}_5$), 7.21−7.17 (m, 3H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_6\underline{H}_5$), 4.71−4.68 (m, 1H, $C_6H_5C\underline{H}(OH)CH_2CH_2C_6H_5$), 2.69−2.63 (m, 2H, $C_6H_5CH(OH)C\underline{H}_2CH_2C_6H_5$), 2.19−1.99 (m, 2H, $C_6H_5CH(OH)CH_2C\underline{H}_2C_6H_5$), 1.61 (b, 1H, $C_6H_5CH(O\underline{H})CH_2CH_2C_6H_5$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 144.5 (*ipso*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_6H_5$), 141.8 ($C_6H_5CH(OH)CH_2CH_2$-*ipso*-$\underline{C}_6H_5$), 128.5 (*o*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_6H_5$), 128.4 ($C_6H_5CH(OH)CH_2CH_2$-*o*-$\underline{C}_6H_5$), 128.4 (*m*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_6H_5$), 128.2 (*p*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_6H_5$), 127.6 ($C_6H_5CH(OH)CH_2CH_2$-*m*-$\underline{C}_6H_5$), 125.8 ($C_6H_5CH(OH)CH_2CH_2$-*p*-$\underline{C}_6H_5$), 73.9 ($C_6H_5\underline{C}H(OH)CH_2CH_2C_6H_5$), 40.5 ($C_6H_5CH(OH)\underline{C}H_2CH_2C_6H_5$), 32.0 ($C_6H_5CH(OH)CH_2\underline{C}H_2C_6H_5$). GCMS (ESI): $[M]^+$ *m*/*z* = 212. Anal. Calcd. for $C_{15}H_{16}O$: C, 84.87; H, 7.60; Found: C, 85.72; H, 7.12 %.

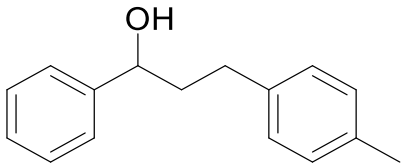
1,3-Diphenylpropan-1-one (4')[1]



(**4'**)

Colorless liquid [0.036 g, 17 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 500 MHz, 25 °C): δ ppm, 7.99 (d, 2H, $^{3}J_{HH}$ = 8 Hz, $C_6\underline{H}_5COCH_2CH_2C_6H_5$), 7.59 (t, 1H, $^{3}J_{HH}$ = 8 Hz, $C_6\underline{H}_5COCH_2CH_2C_6H_5$), 7.49 (t, 2H, $^{3}J_{HH}$ = 8 Hz, $C_6\underline{H}_5COCH_2CH_2C_6H_5$), 7.35–7.28 (m, 4H, $C_6H_5COCH_2CH_2C_6\underline{H}_5$), 7.24 (t, 1H, $^{3}J_{HH}$ = 7 Hz, $C_6H_5COCH_2CH_2C_6\underline{H}_5$), 3.34 (t, 2H, $^{3}J_{HH}$ = 8 Hz, $C_6H_5COC\underline{H}_2CH_2C_6H_5$), 3.11 (t, 2H, $^{3}J_{HH}$ = 8 Hz, $C_6H_5COCH_2C\underline{H}_2C_6H_5$). ^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz, 25 °C): δ ppm, 199.3 ($C_6H_5\underline{C}OCH_2CH_2C_6H_5$), 141.3 (*ipso*-$\underline{C}_6H_5COCH_2CH_2C_6H_5$), 136.9 ($C_6H_5COCH_2CH_2$-*ipso*-$\underline{C}_6H_5$), 133.0 (*p*-$\underline{C}_6H_5COCH_2CH_2C_6H_5$), 129.0 (*o*-$\underline{C}_6H_5COCH_2CH_2C_6H_5$), 128.6 (*m*-$\underline{C}_6H_5COCH_2CH_2C_6H_5$), 128.5 ($C_6H_5COCH_2CH_2$-*m*-$\underline{C}_6H_5$), 128.4 ($C_6H_5COCH_2CH_2$-*o*-$\underline{C}_6H_5$), 126.1 ($C_6H_5COCH_2CH_2$-*p*-$\underline{C}_6H_5$), 40.5 ($C_6H_5CO\underline{C}H_2CH_2C_6H_5$), 30.2 ($C_6H_5COCH_2\underline{C}H_2C_6H_5$). GCMS (ESI): $[M]^+$ *m*/*z* = 210. Anal. Calcd. for $C_{15}H_{14}O$: C, 85.68; H, 6.71; Found: C, 85.35; H, 6.24 %.

3-(4-Methyl-phenyl)-1-phenylpropan-1-ol (5)[1]

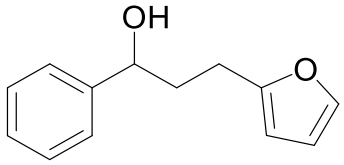


(**5**)

Colorless liquid [0.119 g, 53 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.44-7.43 (m, 4H, $C_6\underline{H}_5CH(OH)CH_2CH_2$-4-$CH_3$-$C_6H_4$), 7.38−7.35 (m, 1H, $C_6\underline{H}_5CH(OH)CH_2CH_2$-4-$CH_3$-$C_6H_4$), 7.21 (br, 4H, $C_6H_5CH(OH)CH_2CH_2$-4-CH_3-$C_6\underline{H}_4$), 4.76 (t, 1H, $^{3}J_{HH}$ = 6 Hz, $C_6H_5C\underline{H}(OH)CH_2CH_2$-4-$CH_3$-$C_6H_4$), 2.86−2.79 (m, 1H, $C_6H_5CH(OH)C\underline{H}_2CH_2$-4-$CH_3$-$C_6H_4$), 2.72−2.65 (m, 1H, $C_6H_5CH(OH)C\underline{H}_2CH_2$-4-$CH_3$-$C_6H_4$), 2.34 (s, 3H, $C_6H_5CH(OH)CH_2CH_2$-4-$C\underline{H}_3$-C_6H_4), 2.19-2.01 (m, 2H, $C_6H_5CH(OH)CH_2C\underline{H}_2$-4-$CH_3$-$C_6H_4$), 1.55 (d, 1H, $^{3}J_{HH}$ = 6 Hz, $C_6H_5CH(O\underline{H})CH_2CH_2$-4-$CH_3$-$C_6H_4$). ^{13}C{1H} NMR ($CDCl_3$, 100 MHz,

25 °C): δ ppm, 144.7 (*ipso*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-4-$CH_3$-$C_6H_4$), 140.1 ($C_6H_5CH(OH)CH_2CH_2$-4-$CH_3$-*ipso*-$\underline{C}_6H_4$), 136.0 ($C_6H_5CH(OH)CH_2CH_2$-4-$CH_3$-*p*-$\underline{C}_6H_4$), 130.2 ($C_6H_5CH(OH)CH_2CH_2$-4-$CH_3$-*m*-$\underline{C}_6H_4$), 128.8 (*m*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-4-$CH_3$-$C_6H_4$), 128.5 (*p*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-4-$CH_3$-$C_6H_4$), 127.6 ($C_6H_5CH(OH)CH_2CH_2$-4-$CH_3$-*o*-$\underline{C}_6H_4$), 126.0 (*o*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-4-$CH_3$-$C_6H_4$), 74.2 ($C_6H_5\underline{C}H(OH)CH_2CH_2$-4-$CH_3$-$C_6H_4$), 39.3 ($C_6H_5CH(OH)\underline{C}H_2CH_2$-4-$CH_3$-$C_6H_4$), 29.6 ($C_6H_5CH(OH)CH_2\underline{C}H_2$-4-$CH_3$-$C_6H_4$), 19.3 ($C_6H_5CH(OH)CH_2CH_2$-4-$\underline{C}H_3$-$C_6H_4$). GCMS (ESI): $[M]^+$ m/z = 226. Anal. Calcd. for $C_{16}H_{18}O$: C, 84.91; H, 8.02; Found: C, 84.70; H, 8.27 %.

3-(Furan-2-yl)-1-phenylpropan-1-ol (6)[1]

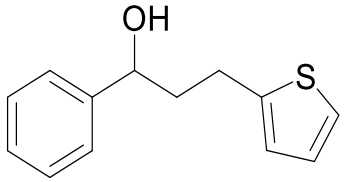


(**6**)

Colorless liquid [0.098 g, 49 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 500 MHz, 25 °C): δ ppm, 7.37−7.36 (m, 4H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_4H_3O$), 7.31−7.29 (m, 2H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_4\underline{H}_3O$), 6.29−6.28 (m, 1H, $C_6H_5CH(OH)CH_2CH_2C_4\underline{H}_3O$), 6.01−6.00 (m, 1H, $C_6H_5CH(OH)CH_2CH_2C_4\underline{H}_3O$), 4.73−4.70 (m, 1H, $C_6H_5C\underline{H}(OH)CH_2CH_2C_4H_3O$), 2.76−2.71 (m, 2H, $C_6H_5CH(OH)C\underline{H}_2CH_2C_4H_3O$), 2.16−2.02 (m, 2H, $C_6H_5CH(OH)CH_2C\underline{H}_2C_4H_3O$), 1.63 (br, 1H, $C_6H_5CH(O\underline{H})CH_2CH_2C_4H_3O$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 125 MHz, 25 °C): δ ppm, 155.5 ($C_6H_5CH(OH)CH_2CH_2$-*ipso*-$\underline{C}_4H_3O$), 144.3 (*ipso*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_4H_3O$), 140.9 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_4H_3O$), 128.5 (*m*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_4H_3O$), 127.7 (*p*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_4H_3O$), 125.8 (*o*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_4H_3O$), 110.1 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_4H_3O$), 105.0 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_4H_3O$), 73.7

($C_6H_5\underline{C}H(OH)CH_2CH_2C_4H_3O$), 37.1 ($C_6H_5CH(OH)\underline{C}H_2CH_2C_4H_3O$), 24.4 ($C_6H_5CH(OH)CH_2\underline{C}H_2C_4H_3O$). GCMS (ESI): $[M]^+$ *m*/*z* = 202. Anal. Calcd. for $C_{13}H_{14}O_2$: C, 77.20; H, 6.98; Found: C, 78.14; H, 5.89 %.

1-Phenyl-3-(thiophen-2-yl)-propan-1-ol (7)[1]

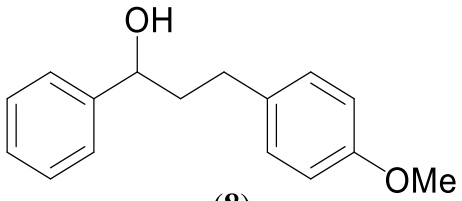


(**7**)

Colorless liquid [0.136 g, 64 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.39−7.38 (m, 4H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_4H_3S$), 7.34−7.32 (m, 1H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_4H_3S$), 7.15 (dd, 1H, $^3J_{HH}$ = 5 Hz, $^4J_{HH}$ = 1 Hz, $C_6H_5CH(OH)CH_2CH_2C_4\underline{H}_3S$), 6.95 (dd, 1H, $^3J_{HH}$ = 4 Hz, $^4J_{HH}$ = 2 Hz, $C_6H_5CH(OH)CH_2CH_2C_4\underline{H}_3S$), 6.84–6.83 (m, 1H, $C_6H_5CH(OH)CH_2CH_2C_4\underline{H}_3S$), 4.77−4.74 (m, 1H, $C_6H_5C\underline{H}(OH)CH_2CH_2C_4H_3S$), 2.99−2.94 (m, 2H, $C_6H_5CH(OH)C\underline{H}_2CH_2C_4H_3S$), 2.26−2.18 (m, 1H, $C_6H_5CH(OH)CH_2C\underline{H}_2C_4H_3S$), 2.26−2.07 (m, 1H, $C_6H_5CH(OH)CH_2C\underline{H}_2C_4H_3S$), 1.97 (br, 1H, $C_6H_5CH(O\underline{H})CH_2CH_2C_4H_3S$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 125 MHz, 25 °C): δ ppm, 144.6 (*ipso*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_4H_3S$), 144.3 ($C_6H_5CH(OH)CH_2CH_2$-*ipso*-$\underline{C}_4H_3S$), 128.5 (*m*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_4H_3S$), 127.7 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_4H_3S$), 126.5 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_4H_3S$), 125.9 (*o*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_4H_3S$), 124.8 (*p*-$C_6H_5CH(OH)CH_2CH_2C_4H_3S$), 123.2 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_4H_3S$), 73.5 ($C_6H_5\underline{C}H(OH)CH_2CH_2C_4H_3S$), 40.6 ($C_6H_5CH(OH)\underline{C}H_2CH_2C_4H_3S$), 26.2

($C_6H_5CH(OH)CH_2\underline{C}H_2C_4H_3S$). GCMS (ESI): $[M]^+$ m/z = 218. Anal. Calcd. for $C_{13}H_{14}OS$: C, 71.52; H, 6.46; S, 14.69; Found: C, 72.42; H, 6.18; S, 14.30 %.

3-(4-Methoxyphenyl)-1-phenylpropan-1-ol (8)[1]

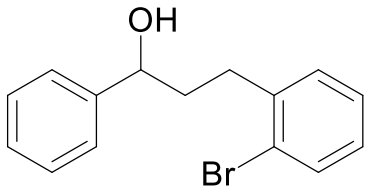


(**8**)

Colorless liquid [0.153 g, 66 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.38−7.37 (m, 4H, $C_6\underline{H}_5CH(OH)CH_2CH_2$-4-$OCH_3$-$C_6H_4$), 7.32−7.28 (m, 1H, $C_6\underline{H}_5CH(OH)CH_2CH_2$-4-$OCH_3$-$C_6H_4$), 7.13 (d, 2H, $^3J_{HH}$ = 9 Hz, $C_6H_5CH(OH)CH_2CH_2$-4-OCH_3-$C_6\underline{H}_4$), 6.85 (d, 2H, $^3J_{HH}$ = 8 Hz, $C_6H_5CH(OH)CH_2CH_2$-4-OCH_3-$C_6\underline{H}_4$), 4.71−4.68 (m, 1H, $C_6H_5C\underline{H}(OH)CH_2CH_2$-4-$OCH_3$-$C_6H_4$), 3.81 (s, 3H, $C_6H_5CH(OH)CH_2CH_2$-4-$OC\underline{H}_3$-C_6H_4), 2.75−2.60 (m, 2H, $C_6H_5CH(OH)C\underline{H}_2CH_2$-4-$OCH_3$-$C_6H_4$), 2.17−1.98 (m, 2H, $C_6H_5CH(OH)CH_2C\underline{H}_2$-4-$OCH_3$-$C_6H_4$), 1.94 (br, 1H, $C_6H_5CH(O\underline{H})CH_2CH_2$-4-$OCH_3$-$C_6H_4$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 157.8 ($C_6H_5CH(OH)CH_2CH_2$-4-OCH_3-*p*-$\underline{C}_6H_4$), 144.6 (*ipso*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-4-$OCH_3$-$C_6H_4$), 133.8 ($C_6H_5CH(OH)CH_2CH_2$-4-$OCH_3$-*ipso*-$\underline{C}_6H_4$), 129.5 ($C_6H_5CH(OH)CH_2CH_2$-4-$OCH_3$-*o*-$\underline{C}_6H_4$), 128.5 (*m*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-4-$OCH_3$-$C_6H_4$), 127.6 (*p*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-4-$OCH_3$-$C_6H_4$), 125.9 (*o*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-4-$OCH_3$-$C_6H_4$), 113.8 ($C_6H_5CH(OH)CH_2CH_2$-4-$OCH_3$-*o*-$\underline{C}_6H_4$), 73.8 ($C_6H_5\underline{C}H(OH)CH_2CH_2$-4-$OCH_3$-$C_6H_4$), 55.2 ($C_6H_5CH(OH)CH_2CH_2$-4-$O\underline{C}H_3$-$C_6H_4$), 40.7 ($C_6H_5CH(OH)\underline{C}H_2CH_2$-4-$OCH_3$-$C_6H_4$),

31.1 ($C_6H_5CH(OH)CH_2\underline{C}H_2$-4-$OCH_3$-$C_6H_4$). GCMS (ESI): $[M]^+$ m/z = 242. Anal. Calcd. for $C_{16}H_{18}O_2$: C, 79.31; H, 7.49; Found: C, 80.27; H, 7.05 %.

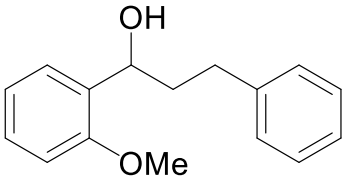
3-(2-Bromophenyl)-1-phenylpropan-1-ol (9)[1]



(**9**)

Colorless liquid [0.186 g, 64 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.54 (d, 1H, $^3J_{HH}$ = 8 Hz, $C_6H_5CH(OH)CH_2CH_2$-2-Br-$C_6\underline{H}_4$), 7.43−7.36 (m, 4H, $C_6\underline{H}_5CH(OH)CH_2CH_2$-2-Br-$C_6H_4$), 7.33−7.28 (m, 2H, $C_6\underline{H}_5CH(OH)CH_2CH_2$-2-Br-$C_6\underline{H}_4$), 7.25−7.23 (m, 1H, $C_6H_5CH(OH)CH_2CH_2$-2-Br-$C_6\underline{H}_4$), 7.09−7.05 (m, 1H, $C_6H_5CH(OH)CH_2CH_2$-2-Br-$C_6\underline{H}_4$), 4.78−4.74 (m, 1H, $C_6H_5C\underline{H}(OH)CH_2CH_2$-2-Br-$C_6H_4$), 2.96−2.76 (m, 2H, $C_6H_5CH(OH)C\underline{H}_2CH_2$-2-Br-$C_6H_4$), 2.13−2.02 (m, 2H, $C_6H_5CH(OH)CH_2C\underline{H}_2$-2-Br-$C_6H_4$), 1.96 (d, 1H, $^3J_{HH}$ = 4 Hz, $C_6H_5CH(O\underline{H})CH_2CH_2$-2-Br-$C_6H_4$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 144.3 (*ipso*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-2-Br-$C_6H_4$), 141.1 ($C_6H_5CH(OH)CH_2CH_2$-2-Br-*ipso*-$\underline{C}_6H_4$), 132.8 ($C_6H_5CH(OH)CH_2CH_2$-2-Br-*m*-$\underline{C}_6H_4$), 130.4 ($C_6H_5CH(OH)CH_2CH_2$-2-Br-*o*-$\underline{C}_6H_4$), 128.5 (*m*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-2-Br-$C_6H_4$), 127.6 ($C_6H_5CH(OH)CH_2CH_2$-2-Br-*p*-$\underline{C}_6H_4$), 127.4 (*o*-$\underline{C}_6H_5CH(OH)CH_2CH_2$-2-Br-$C_6H_4$), 125.9 ($C_6H_5CH(OH)CH_2CH_2$-2-Br-*m*-$\underline{C}_6H_4$), 124.4 ($C_6H_5CH(OH)CH_2CH_2$-2-Br-*o*-$\underline{C}_6H_4$), 73.9 ($C_6H_5\underline{C}H(OH)CH_2CH_2$-2-Br-$C_6H_4$), 38.9 ($C_6H_5CH(OH)\underline{C}H_2CH_2$-2-Br-$C_6H_4$), 32.5 ($C_6H_5CH(OH)CH_2\underline{C}H_2$-2-Br-$C_6H_4$). GCMS (ESI): $[M]^+$ m/z = 290. Anal. Calcd. for $C_{15}H_{15}BrO$: C, 61.87; H, 5.19; Found: C, 62.24; H, 4.61 %.

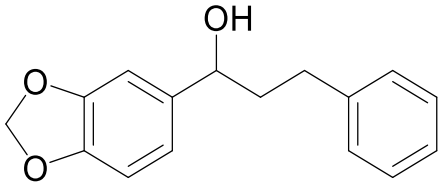
3-Phenyl-1-(*o*-methoxy)propan-1-ol (10)[1]



(**10**)

Colorless liquid [0.146 g, 60 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.39–7.19 (m, 7H, 4-OCH_3-$C_6\underline{H}_4CH(OH)CH_2CH_2C_6\underline{H}_5$), 7.02–6.98 (m, 1H, 4-$OCH_3$-$C_6\underline{H}_4CH(OH)CH_2CH_2C_6H_5$), 6.91 (d, 1H, $^{3}J_{HH}$ = 8 Hz, 4-OCH_3-$C_6\underline{H}_4CH(OH)CH_2CH_2C_6H_5$), 4.93 (br, 1H, 4-$OCH_3$-$C_6H_4C\underline{H}(OH)CH_2CH_2C_6H_5$), 3.87 (s, 3H, 4-$OC\underline{H}_3$-$C_6H_4CH(OH)CH_2CH_2C_6H_5$), 2.91−2.83 (m, 1H, 4-$OCH_3$-$C_6H_4CH(OH)C\underline{H}_2CH_2C_6H_5$), 2.75−2.70 (m, 1H, 4-$OCH_3$-$C_6H_4CH(OH)CH_2C\underline{H}_2C_6H_5$), 2.23−2.08 (m, 2H, 4-$OCH_3$-$C_6H_4CH(OH)CH_2C\underline{H}_2C_6H_5$), 1.55 (d, 1H, $^{3}J_{HH}$ = 6 Hz, 4-OCH_3-$C_6H_4CH(O\underline{H})CH_2CH_2C_6H_5$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 156.6 (4-OCH_3-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 142.2 (4-$OCH_3$-$C_6H_4CH(OH)CH_2CH_2$-*ipso*-$\underline{C}_6H_5$), 132.3 (4-$OCH_3C_6H_4CH(OH)CH_2CH_2$–*m*-$\underline{C}_6H_5$), 128.5 (4-$OCH_3$-$C_6H_4CH(OH)CH_2CH_2$–*o*-$\underline{C}_6H_5$), 128.3 (4-$OCH_3$-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 127.0 (4-$OCH_3$-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 126.1 (4-$OCH_3$-$C_6H_4CH(OH)CH_2CH_2$–*p*-$\underline{C}_6H_5$), 125.7 (4-$OCH_3$-*ipso*-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 120.8 (4-$OCH_3$-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 110.5 (4-$OCH_3$-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 70.6 (4-$OCH_3$-$C_6H_4\underline{C}H(OH)CH_2CH_2C_6H_5$), 55.2 (4-$O\underline{C}H_3$-$C_6H_4CH(OH)CH_2CH_2C_6H_5$), 38.7 (4-$OCH_3$-$C_6H_4CH(OH)\underline{C}H_2CH_2C_6H_5$), 32.3 (4-$OCH_3$-$C_6H_4CH(OH)CH_2\underline{C}H_2C_6H_5$). GCMS (ESI): $[M]^+$ *m*/*z* = 242. Anal. Calcd. for $C_{16}H_{18}O_2$: C, 79.31; H, 7.49; Found: C, 79.93; H, 6.38 %.

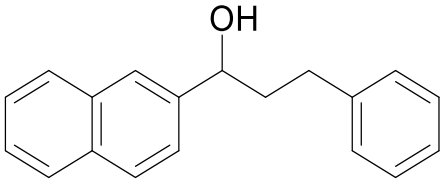
1-(benzo[1,3]dioxol-5-yl)-3-phenylpropan-1-ol (11)[1]



(**11**)

Colorless liquid [0.154 g, 60 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.32–7.28 (m, 1H, $OCH_2OC_6H_3CH(OH)CH_2CH_2C_6\underline{H}_5$), 7.22–7.20 (m, 2H, $OCH_2OC_6H_3CH(OH)CH_2CH_2C_6\underline{H}_5$), 6.92−6.89 (m, 2H, $OCH_2OC_6H_3CH(OH)CH_2CH_2C_6\underline{H}_5$), 6.85–6.78 (m, 3H, $OCH_2OC_6\underline{H}_3CH(OH)CH_2CH_2C_6H_5$), 5.97 (s, 2H, $OC\underline{H}_2OC_6H_3CH(OH)CH_2CH_2C_6H_5$), 4.87–4.82 (m, 1H, $OCH_2OC_6H_3C\underline{H}(OH)CH_2CH_2C_6H_5$), 2.77–2.62 (m, 2H, $OCH_2OC_6H_3CH(OH)C\underline{H}_2CH_2C_6H_5$), 2.19–1.96 (m, 2H, $OCH_2OC_6H_3CH(OH)CH_2C\underline{H}_2C_6H_5$), 2.19–1.85 (br, 1H, $OCH_2OC_6H_3CH(O\underline{H})CH_2CH_2C_6H_5$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 151.7 ($OCH_2O\underline{C}_6H_3CH(OH)CH_2CH_2C_6H_5$), 147.8 ($OCH_2O\underline{C}_6H_3CH(OH)CH_2CH_2C_6H_5$), 147.0 ($OCH_2O$-*ipso*-$\underline{C}_6H_3CH(OH)CH_2CH_2C_6H_5$), 141.7 ($OCH_2OC_6H_3CH(OH)CH_2CH_2$–*ipso*-$\underline{C}_6H_5$), 138.6 ($OCH_2O\underline{C}_6H_3CH(OH)CH_2CH_2C_6H_5$), 128.4 ($OCH_2OC_6H_3CH(OH)CH_2CH_2$–*m*-$\underline{C}_6H_5$), 125.8 ($OCH_2OC_6H_3CH(OH)CH_2CH_2$–*o*-$\underline{C}_6H_5$), 119.4 ($OCH_2OC_6H_3CH(OH)CH_2CH_2$–*p*-$\underline{C}_6H_5$), 108.1 ($OCH_2O\underline{C}_6H_3CH(OH)CH_2CH_2C_6H_5$), 106.4 ($OCH_2O\underline{C}_6H_3CH(OH)CH_2CH_2C_6H_5$), 101.0 ($O\underline{C}H_2OC_6H_3CH(OH)CH_2CH_2C_6H_5$), 73.7 ($OCH_2OC_6H_3\underline{C}H(OH)CH_2CH_2C_6H_5$), 40.4 ($OCH_2OC_6H_3CH(OH)\underline{C}H_2CH_2C_6H_5$), 32.0 ($OCH_2OC_6H_3CH(OH)CH_2\underline{C}H_2C_6H_5$). GCMS (ESI): $[M]^+$ *m*/*z* = 256. Anal. Calcd. for $C_{16}H_{16}O_3$: C, 74.98; H, 6.29; Found: C, 75.84; H, 5.38 %.

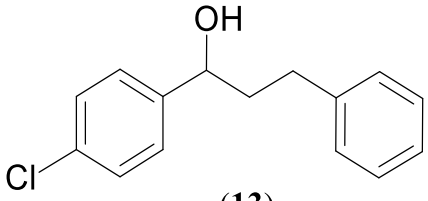
1-(Naphthyl)-3-phenylpropan-1-ol (12)[1]



(**12**)

Colorless liquid [0.185 g, 71 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.88–7.85 (m, 3H, $C_{10}\underline{H}_7CH(OH)CH_2CH_2C_6H_5$), 7.80 (br, 1H, $C_{10}\underline{H}_7CH(OH)CH_2CH_2C_6H_5$), 7.52–7.50 (m, 3H, $C_{10}\underline{H}_7CH(OH)CH_2CH_2C_6H_5$), 7.39–7.38 (m, 2H, $C_{10}H_7CH(OH)CH_2CH_2C_6\underline{H}_5$), 7.35–7.30 (m, 2H, $C_{10}H_7CH(OH)CH_2CH_2C_6\underline{H}_5$), 7.24–7.23 (m, 1H, $C_{10}H_7CH(OH)CH_2CH_2C_6\underline{H}_5$), 4.88−4.85 (m, 1H, $C_{10}H_7C\underline{H}(OH)CH_2CH_2C_6H_5$), 2.84−2.69 (m, 2H, $C_{10}H_7CH(OH)C\underline{H}_2CH_2C_6H_5$), 2.29−2.12 (m, 2H, $C_{10}H_7CH(OH)CH_2C\underline{H}_2C_6H_5$), 1.96 (br, 1H, $C_{10}H_7CH(O\underline{H})CH_2CH_2C_6H_5$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 141.8 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 140.8 ($C_{10}H_7CH(OH)CH_2CH_2$–*ipso*-$\underline{C}_6H_5$), 133.3 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 133.0 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 128.6 ($C_{10}H_7CH(OH)CH_2CH_2$–*m*-$\underline{C}_6H_5$), 128.5 ($C_{10}H_7CH(OH)CH_2CH_2$–*o*-$\underline{C}_6H_5$), 128.4 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 127.9 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 127.7 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 127.0 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 126.2 ($C_{10}H_7CH(OH)CH_2CH_2$–*p*-$\underline{C}_6H_5$), 125.9 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 124.7 ($\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 124.1 (*ipso*-$\underline{C}_{10}H_7CH(OH)CH_2CH_2C_6H_5$), 73.9 ($C_{10}H_7\underline{C}H(OH)CH_2CH_2C_6H_5$), 40.3 ($C_{10}H_7CH(OH)\underline{C}H_2CH_2C_6H_5$), 32.0 ($C_{10}H_7CH(OH)CH_2\underline{C}H_2C_6H_5$). GCMS (ESI): $[M]^+$ m/z = 262. Anal. Calcd. for $C_{19}H_{18}O$: C, 86.99; H, 6.92; Found: C, 87.33; H, 7.02 %.

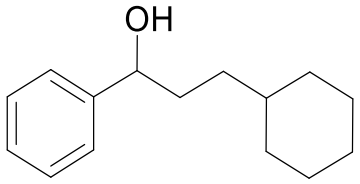
1-(4-Choloro phenyl)-3-phenylpropan-1-ol (13)[1]



(**13**)

Colorless liquid [0.139 g, 57 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.36–7.29 (m, 6H, 4-Cl-$C_6\underline{H}_4CH(OH)CH_2CH_2C_6\underline{H}_5$), 7.23–7.20 (m, 3H, 4-Cl-$C_6\underline{H}_4CH(OH)CH_2CH_2C_6\underline{H}_5$), 4.71–4.67 (m, 1H, 4-Cl-$C_6H_4C\underline{H}(OH)CH_2CH_2C_6H_5$), 2.79−2.65 (m, 2H, 4-Cl-$C_6H_4CH(OH)C\underline{H}_2CH_2C_6H_5$), 2.17−2.01 (m, 2H, 4-Cl-$C_6H_4CH(OH)CH_2C\underline{H}_2C_6H_5$), 2.00 (d, 1H, $^{3}J_{HH}$ = 4 Hz, 4-Cl-$C_6H_4CH(O\underline{H})CH_2CH_2C_6H_5$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 143.0 (4-Cl-*ipso*-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 141.5 (4-Cl-$C_6H_4CH(OH)CH_2CH_2$–*ipso*-$\underline{C}_6H_5$), 133.2 (4-Cl-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 128.6 (4-Cl-*m*-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 128.5 (4-Cl-$C_6H_4CH(OH)CH_2CH_2$–*m*-$\underline{C}_6H_5$), 128.4 (4-Cl-$C_6H_4CH(OH)CH_2CH_2$–*o*-$\underline{C}_6H_5$), 127.3 (4-Cl-*o*-$\underline{C}_6H_4CH(OH)CH_2CH_2C_6H_5$), 125.9 (4-Cl-$C_6H_4CH(OH)CH_2CH_2$–*p*-$\underline{C}_6H_5$), 73.1 (4-Cl-$C_6H_4\underline{C}H(OH)CH_2CH_2C_6H_5$), 40.5 (4-Cl-$C_6H_4CH(OH)\underline{C}H_2CH_2C_6H_5$), 31.9 (4-Cl-$C_6H_4CH(OH)CH_2\underline{C}H_2C_6H_5$). GCMS (ESI): $[M]^+$ *m*/*z* = 246. Anal. Calcd. for $C_{15}H_{15}ClO$: C, 73.02; H, 6.13; Found: C, 72.64; H, 5.39 %.

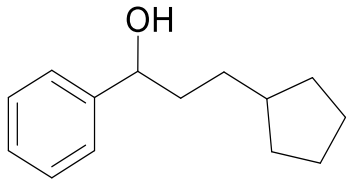
3-(Cyclohexyl)-1-phenylpropan-1-ol (14)[1]



(**14**)

Colorless liquid [0.149 g, 68 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 500 MHz, 25 °C): δ ppm, 7.37−7.36 (m, 4H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_6H_{11}$), 7.31−7.29 (m, 1H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_6H_{11}$), 4.67-4.64 (m, 1H, $C_6H_5C\underline{H}(OH)CH_2CH_2C_6H_{11}$), 1.87−1.65 (m, 8H, $C_6H_5CH(OH)C\underline{H}_2CH_2C_6H_{11}$ & $C_6H_5CH(OH)CH_2CH_2C_6\underline{H}_{11}$), 1.36 (sept, 1H, $C_6H_5CH(OH)CH_2CH_2C_6\underline{H}_{11}$), 1.27-1.13 (m, 4H, $C_6H_5CH(OH)CH_2CH_2C_6\underline{H}_{11}$), 0.93-0.85 (m, 1H, $C_6H_5CH(OH)CH_2C\underline{H}_2C_6H_{11}$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 125 MHz, 25 °C): δ ppm, 144.9 (*ipso*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_6H_{11}$), 128.4 (*m*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_6H_{11}$), 127.4 (*p*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_6H_{11}$), 125.9 (*o*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_6H_{11}$), 75.1 ($C_6H_5\underline{C}H(OH)CH_2CH_2C_6H_{11}$), 37.6 ($C_6H_5CH(OH)\underline{C}H_2CH_2C_6H_{11}$), 36.4 ($C_6H_5CH(OH)CH_2\underline{C}H_2C_6H_{11}$), 33.4 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_6H_{11}$), 33.4 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_6H_{11}$), 33.3 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_6H_{11}$), 36.6 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_6H_{11}$), 26.3 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_6H_{11}$). GCMS (ESI): $[M]^+$ *m*/*z* = 218. Anal. Calcd. for $C_{15}H_{22}O$: C, 82.52; H, 10.16; Found: C, 81.96; H, 9.70 %.

3-(Cyclopentyl)-1-phenylpropan-1-ol (15)[1]

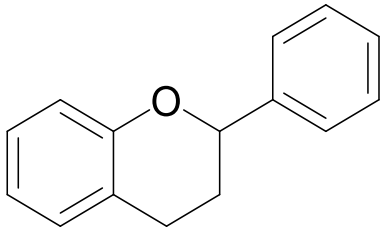


(**15**)

Colorless liquid [0.138 g, 67 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.37−7.36 (m, 4H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_5H_9$), 7.32−7.28 (m, 1H, $C_6\underline{H}_5CH(OH)CH_2CH_2C_5H_9$), 4.68-4.65 (m, 1H, $C_6H_5C\underline{H}(OH)CH_2CH_2C_5H_9$), 1.87−1.72 (m, 6H, $C_6H_5CH(OH)CH_2CH_2C_5\underline{H}_9$), 1.62−1.57 (m, 2H, $C_6H_5CH(OH)CH_2CH_2C_5\underline{H}_9$), 1.53−1.43 (m, 2H, $C_6H_5CH(OH)C\underline{H}_2CH_2C_5H_9$),

1.32-1.26 (m, 1H, $C_6H_5CH(OH)CH_2CH_2C_5\underline{H}_9$), 1.27-1.13 (m, 4H, $C_6H_5CH(OH)CH_2C\underline{H}_2C_5H_9$), 1.09-1.06 (m, 1H, $C_6H_5CH(OH)CH_2C\underline{H}_2C_5H_9$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 144.9 (*ipso*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_5H_9$), 128.4 (*m*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_5H_9$), 127.5 (*p*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_5H_9$), 125.9 (*o*-$\underline{C}_6H_5CH(OH)CH_2CH_2C_5H_9$), 74.9 ($C_6H_5\underline{C}H(OH)CH_2CH_2C_5H_9$), 40.1 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_5H_9$), 38.3 ($C_6H_5CH(OH)\underline{C}H_2CH_2C_5H_9$), 32.7 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_5H_9$), 32.6 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_5H_9$), 32.2 ($C_6H_5CH(OH)CH_2\underline{C}H_2C_5H_9$), 25.1 ($C_6H_5CH(OH)CH_2CH_2\underline{C}_5H_9$). GCMS (ESI): $[M]^+$ *m*/*z* = 186. Calcd. for $C_{14}H_{20}O$: C, 82.30; H, 9.87; Found: C, 81.67; H, 8.98 %.

Synthesis of 2-Phenylchroman (16)[2]

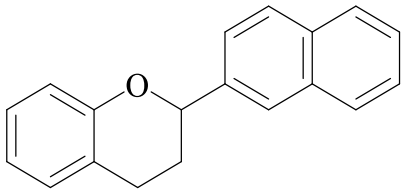


(**16**)

Colorless dense liquid [0.054 g, 26 % isolated yield (**1b**)]. ^1H NMR ($CDCl_3$, 500 MHz, 25 °C): δ ppm, 7.46 (d, 2H, $^3J_{HH}$ = 8 Hz, $C_6\underline{H}_4CH_2CH_2CH(O)C_6H_5$), 7.42 (t, 2H, $^3J_{HH}$ = 8 Hz, $C_6\underline{H}_4CH_2CH_2CH(O)C_6H_5$), 7.36–7.35 (m, 1H, $C_6H_4CH_2CH_2CH(O)C_6\underline{H}_5$), 7.17−7.11 (m, 2H, $C_6H_4CH_2CH_2CH(O)C_6\underline{H}_5$), 6.95–6.89 (m, 2H, $C_6H_4CH_2CH_2CH(O)C_6\underline{H}_5$), 5.10 (dd, 1H, $^3J_{HH}$ = 8 Hz, $^1J_{HH}$ = 2 Hz, $C_6H_4CH_2CH_2C\underline{H}(O)C_6H_5$), 3.06−2.99 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_6H_5$), 2.85−2.80 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_6H_5$), 2.27−2.22 (m, 1H, $C_6H_4CH_2C\underline{H}_2CH(O)C_6H_5$), 2.16–2.08 (m, 1H, $C_6H_4CH_2C\underline{H}_2CH(O)C_6H_5$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 125 MHz, 25 °C): δ ppm, 155.1 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_5$), 141.7 ($C_6H_4CH_2CH_2CH(O)$-*ipso*-$\underline{C}_6H_5$), 129.5 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_5$), 128.5 ($C_6H_4CH_2CH_2CH(O)$-*m*-$\underline{C}_6H_5$), 127.8 ($C_6H_4CH_2CH_2CH(O)$-*o*-

$\underline{C}_6H_5$), 127.3 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_5$), 126.0 ($C_6H_4CH_2CH_2CH(O)$-*p*-$\underline{C}_6H_5$), 121.8 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_5$), 120.3 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_5$), 116.9 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_5$), 77.7 ($C_6H_4CH_2CH_2\underline{C}H(O)C_6H_5$), 29.9 ($C_6H_4\underline{C}H_2CH_2CH(O)C_6H_5$), 25.1 ($C_6H_4CH_2\underline{C}H_2CH(O)C_6H_5$). GCMS (ESI): $[M]^+$ m/z = 210. Anal. Calcd. for $C_{15}H_{14}O$: C, 85.68; H, 6.71; Found: C, 84.82; H, 6.09 %.

2-(Naphthalen-2-yl)chroman (17)[2]

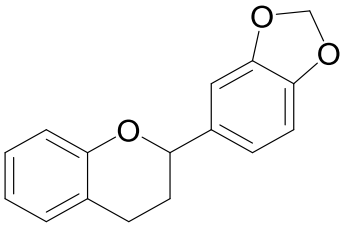


(**17**)

Yellow Solid [0.103 g, 40 % isolated yield (**1b**)]. ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.92−7.86 (m, 4H, $C_6H_4CH_2CH_2CH(O)C_{10}\underline{H}_7$), 7.58−7.48 (m, 3H, $C_6H_4CH_2CH_2CH(O)C_{10}\underline{H}_7$), 7.20−7.13 (m, 2H, $C_6\underline{H}_4CH_2CH_2CH(O)C_{10}H_7$), 7.00−6.98 (m, 1H, $C_6\underline{H}_4CH_2CH_2CH(O)C_{10}H_7$), 6.92 (td, 1H, $^3J_{HH}$ = 8 Hz, $^1J_{HH}$ = 2 Hz, $C_6\underline{H}_4CH_2CH_2CH(O)C_{10}H_7$), 5.26 (dd, 1H, $^3J_{HH}$ = 8 Hz, $^1J_{HH}$ = 2 Hz, $C_6H_4CH_2CH_2C\underline{H}(O)C_{10}H_7$), 3.11−3.03 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_{10}H_7$), 2.89−2.83 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_{10}H_7$), 2.35–2.16 (m, 1H, $C_6H_4CH_2C\underline{H}_2CH(O)C_{10}H_7$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 155.1 ($\underline{C}_6H_4CH_2CH_2CH(O)C_{10}H_7$), 139.1 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 133.3 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 133.0 ($\underline{C}_6H_4CH_2CH_2CH(O)C_{10}H_7$), 129.5 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 128.3 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 128.0 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 127.7 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 127.4 ($\underline{C}_6H_4CH_2CH_2CH(O)C_{10}H_7$), 126.1 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 125.9 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 124.8 ($C_6H_4CH_2CH_2CH(O)\underline{C}_{10}H_7$), 124.0 ($\underline{C}_6H_4CH_2CH_2CH(O)C_{10}H_7$), 121.8 ($C_6H_4CH_2CH_2CH(O)$-

ipso-$\underline{C}_{10}H_7$), 120.4 ($\underline{C}_6H_4CH_2CH_2CH(O)C_{10}H_7$), 116.9 ($\underline{C}_6H_4CH_2CH_2CH(O)C_{10}H_7$), 77.8 ($C_6H_4CH_2CH_2\underline{C}H(O)C_{10}H_7$), 29.9 ($C_6H_4\underline{C}H_2CH_2CH(O)C_{10}H_7$), 25.1 ($C_6H_4CH_2\underline{C}H_2CH(O)C_{10}H_7$). GCMS (ESI): $[M]^+$ *m*/*z* = 260. Anal. Calcd. for $C_{19}H_{16}O$: C, 87.66; H, 6.20; Found: C, 87.33; H, 7.02 %.

2-(Benzo[1,3]dioxol-5-yl)chroman (18)[2]

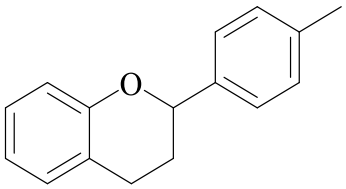


(**18**)

Colorless dense liquid [0.079 g, 32 % isolated yield (**1b**)]. ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.16−7.10 (m, 2H, $C_6\underline{H}_4CH_2CH_2CH(O)C_6\underline{H}_3OCH_2O$), 6.97−6.88 (m, 4H, $C_6\underline{H}_4CH_2CH_2CH(O)C_6\underline{H}_3OCH_2O$), 6.85−6.83 (m, 1H, $C_6\underline{H}_4CH_2CH_2CH(O)C_6H_3OCH_2O$), 5.99 (s, 2H, $C_6H_4CH_2CH_2CH(O)C_6H_3OC\underline{H}_2O$), 4.99 (dd, 1H, $^3J_{HH}$ = 8 Hz, $^1J_{HH}$ = 2 Hz, $C_6H_4CH_2CH_2C\underline{H}(O)C_6H_3OCH_2O$), 3.06−2.97 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_6H_3OCH_2O$), 2.86−2.80 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_6H_3OCH_2O$), 2.23–2.05 (m, 2H, $C_6H_4CH_2C\underline{H}_2CH(O)C_6H_3OCH_2O$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 155.1 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_3OCH_2O$), 147.8 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_3OCH_2O$), 147.2 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_3OCH_2O$), 135.7 ($C_6H_4CH_2CH_2CH(O)$-*ipso*-$\underline{C}_6H_3OCH_2O$), 129.5 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_3OCH_2O$), 127.3 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_3OCH_2O$), 121.7 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_3OCH_2O$), 120.3 ($\underline{C}_6H_4CH_2CH_2CH(O)\underline{C}_6H_3OCH_2O$), 119.5 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_3OCH_2O$), 116.9 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_3OCH_2O$), 108.2 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_3OCH_2O$), 106.7 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_3OCH_2O$), 101.1

($C_6H_4CH_2CH_2CH(O)C_6H_3O\underline{C}H_2O$), 77.6 ($C_6H_4CH_2CH_2\underline{C}H(O)C_6H_3OCH_2O$), 29.9 ($C_6H_4\underline{C}H_2CH_2CH(O)C_6H_3OCH_2O$), 25.1 ($C_6H_4CH_2\underline{C}H_2CH(O)C_6H_3OCH_2O$). GCMS (ESI): $[M]^+$ m/z = 254. Anal. Calcd. for $C_{16}H_{14}O_3$: C, 75.58; H, 5.55; Found: C, 76.00; H, 4.89 %.

2-(4-Tolyl)chroman (19)[2]

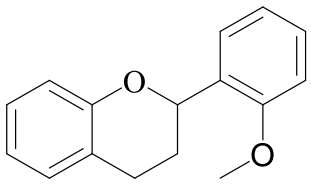


(**19**)

Colorless solid [0.067 g, 30 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.34 (d, 2H, $^3J_{HH}$ = 8 Hz, $C_6\underline{H}_4CH_2CH_2CH(O)C_6H_4CH_3$), 7.21 (d, 2H, $^3J_{HH}$ = 8 Hz, $C_6\underline{H}_4CH_2CH_2CH(O)C_6H_4CH_3$), 7.15−7.09 (m, 2H, $C_6H_4CH_2CH_2CH(O)C_6\underline{H}_4CH_3$), 6.93–6.89 (m, 2H, $C_6H_4CH_2CH_2CH(O)C_6\underline{H}_4CH_3$), 5.07–5.04 (m, 1H, $C_6H_4CH_2CH_2C\underline{H}(O)C_6H_4CH_3$), 3.05−2.97 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_6H_4CH_3$), 2.85−2.79 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_6H_4CH_3$), 2.38 (s, 3H, $C_6H_4CH_2CH_2CH(O)C_6H_4C\underline{H}_3$), 2.24–2.06 (m, 2H, $C_6H_4CH_2C\underline{H}_2CH(O)C_6H_4CH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 155.2 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4CH_3$), 138.7 ($C_6H_4CH_2CH_2CH(O)$-*ipso*-$\underline{C}_6H_4CH_3$), 137.5 ($C_6H_4CH_2CH_2CH(O)$-*p*-$\underline{C}_6H_4CH_3$), 129.5 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4CH_3$), 129.1 ($C_6H_4CH_2CH_2CH(O)$-*m*-$\underline{C}_6H_4CH_3$), 127.3 ($C_6H_4CH_2CH_2CH(O)$-*o*-$\underline{C}_6H_4CH_3$), 125.9 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4CH_3$), 121.8 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4CH_3$), 120.2 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4CH_3$), 116.9 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4CH_3$), 77.6 ($C_6H_4CH_2CH_2\underline{C}H(O)C_6H_4CH_3$), 29.8 ($C_6H_4\underline{C}H_2CH_2CH(O)C_6H_4CH_3$), 25.1 ($C_6H_4CH_2\underline{C}H_2CH(O)C_6H_4CH_3$), 21.1

($C_6H_4CH_2CH_2CH(O)C_6H_4\underline{C}H_3$). GCMS (ESI): $[M]^+$ m/z = 224. Anal. Calcd. for $C_{16}H_{16}O$: C, 85.68; H, 7.19; Found: C, 84.86; H, 8.16 %.

2-(2-Methoxyphenyl)chroman (20)[2]



(**20**)

Colorless solid [0.088 g, 37 % isolated yield (**1b**)] ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C): δ ppm, 7.52 (dd, 1H, $^3J_{HH}$ = 8 Hz, $^1J_{HH}$ = 2 Hz, $C_6H_4CH_2CH_2CH(O)C_6\underline{H}_4OCH_3$), 7.33–7.29 (m, 1H, $C_6H_4CH_2CH_2CH(O)C_6\underline{H}_4OCH_3$), 7.16–7.10 (m, 2H, $C_6\underline{H}_4CH_2CH_2CH(O)C_6\underline{H}_4OCH_3$), 7.02 (t, 1H, $^3J_{HH}$ = 8 Hz, $C_6H_4CH_2CH_2CH(O)C_6\underline{H}_4OCH_3$), 6.95-6.87 (m, 3H, $C_6\underline{H}_4CH_2CH_2CH(O)C_6H_4OCH_3$), 5.47 (dd, 1H, $^3J_{HH}$ = 8 Hz, $^1J_{HH}$ = 2 Hz, $C_6H_4CH_2CH_2C\underline{H}(O)C_6H_4OCH_3$), 3.87 (s, 3H, $C_6H_4CH_2CH_2CH(O)C_6H_4OC\underline{H}_3$), 3.06−2.98 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_6H_4OCH_3$), 2.81−2.75 (m, 1H, $C_6H_4C\underline{H}_2CH_2CH(O)C_6H_4OCH_3$), 2.30-2.24 (m, 1H, $C_6H_4CH_2C\underline{H}_2CH(O)C_6H_4OCH_3$), 2.03–1.93 (m, 1H, $C_6H_4CH_2C\underline{H}_2CH(O)C_6H_4OCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz, 25 °C): δ ppm, 155.9 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_4OCH_3$), 155.5 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4OCH_3$), 130.2 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4OCH_3$), 129.5 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_4OCH_3$), 128.4 ($C_6H_4CH_2CH_2CH(O)$-*p*-$\underline{C}_6H_4OCH_3$), 127.2 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4OCH_3$), 126.4 ($C_6H_4CH_2CH_2CH(O)$-*ipso*-$\underline{C}_6H_4OCH_3$), 122.2 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4OCH_3$), 120.7 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_4OCH_3$), 120.0 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4OCH_3$), 116.8 ($\underline{C}_6H_4CH_2CH_2CH(O)C_6H_4OCH_3$), 110.3 ($C_6H_4CH_2CH_2CH(O)\underline{C}_6H_4OCH_3$), 72.3

($C_6H_4CH_2CH_2\underline{C}H(O)C_6H_4OCH_3$), 55.4 ($C_6H_4CH_2CH_2CH(O)C_6H_4O\underline{C}H_3$), 28.5 ($C_6H_4\underline{C}H_2CH_2CH(O)C_6H_4OCH_3$), 25.2 ($C_6H_4CH_2\underline{C}H_2CH(O)C_6H_4OCH_3$). GCMS (ESI): $[M]^+$ m/z = 240. Anal. Calcd. for $C_{16}H_{14}O_2$: C, 79.97; H, 6.71; Found: C, 79.77; H, 7.15 %.

PG-AK-4-201-A-1H

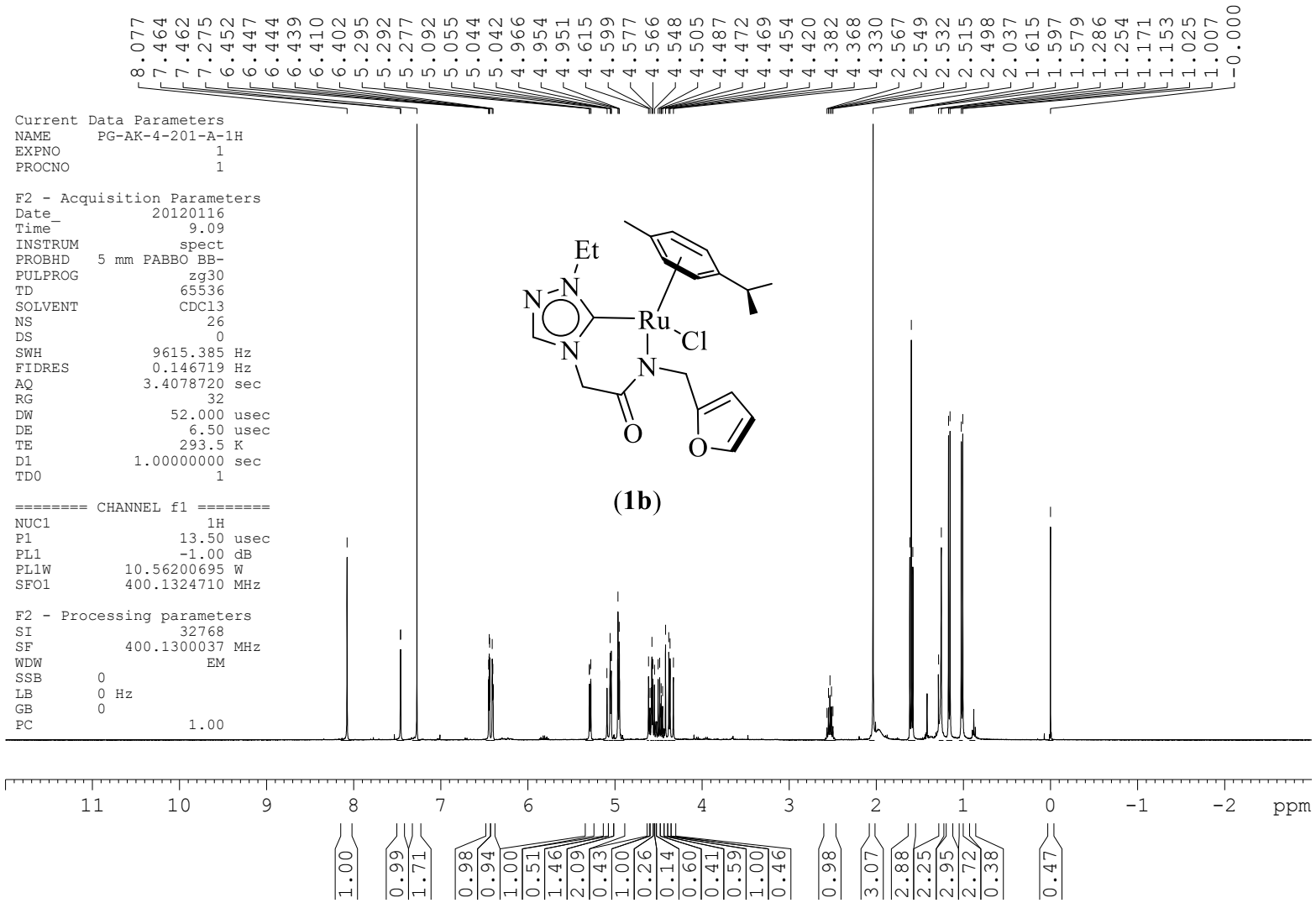


Figure S1. ^{1}H NMR spectrum of **1b** in $CDCl_3$.

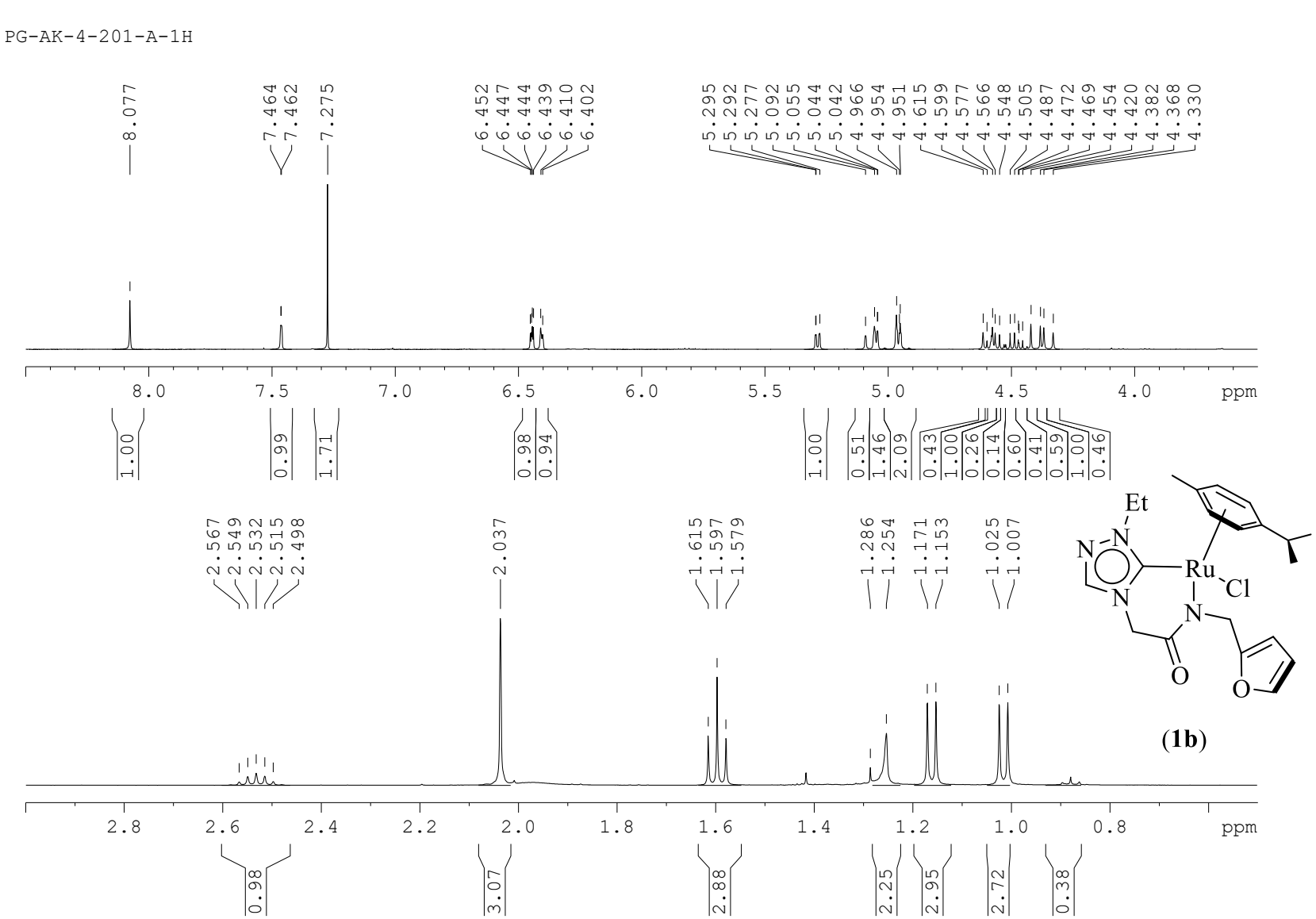


Figure S2. Expanded ^{1}H NMR spectrum of **1b** in $CDCl_3$.

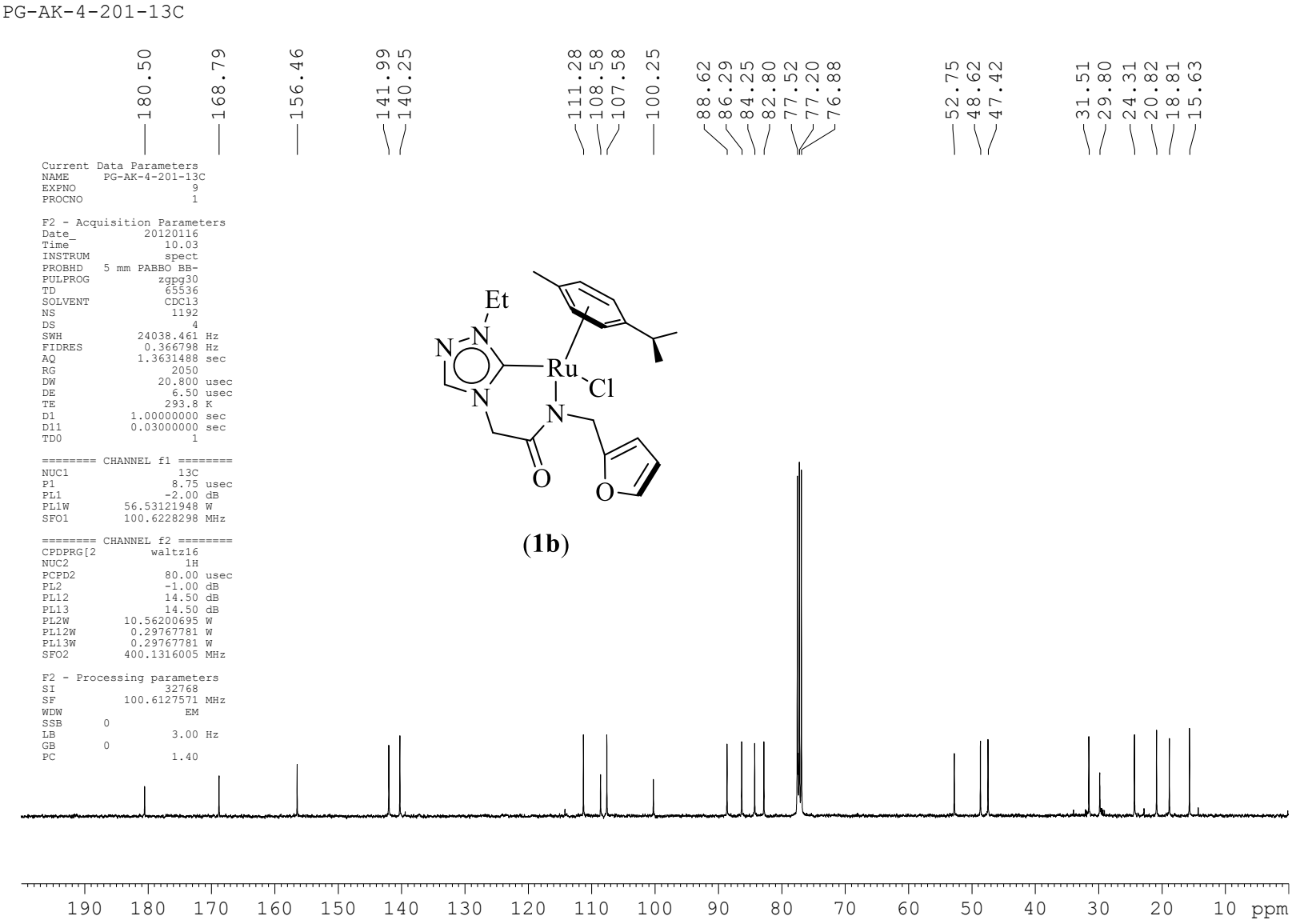


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of **1b** in $CDCl_3$.

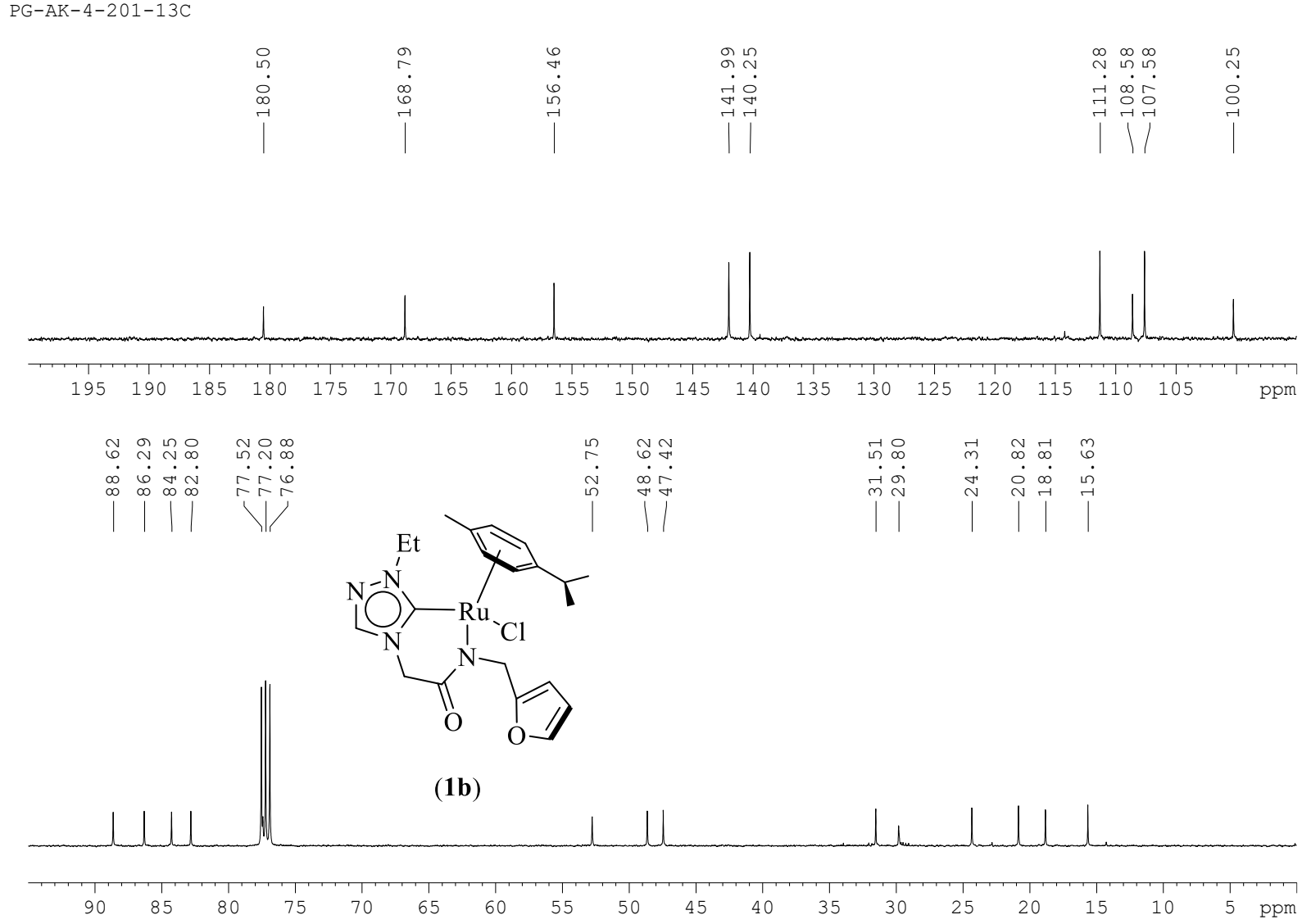
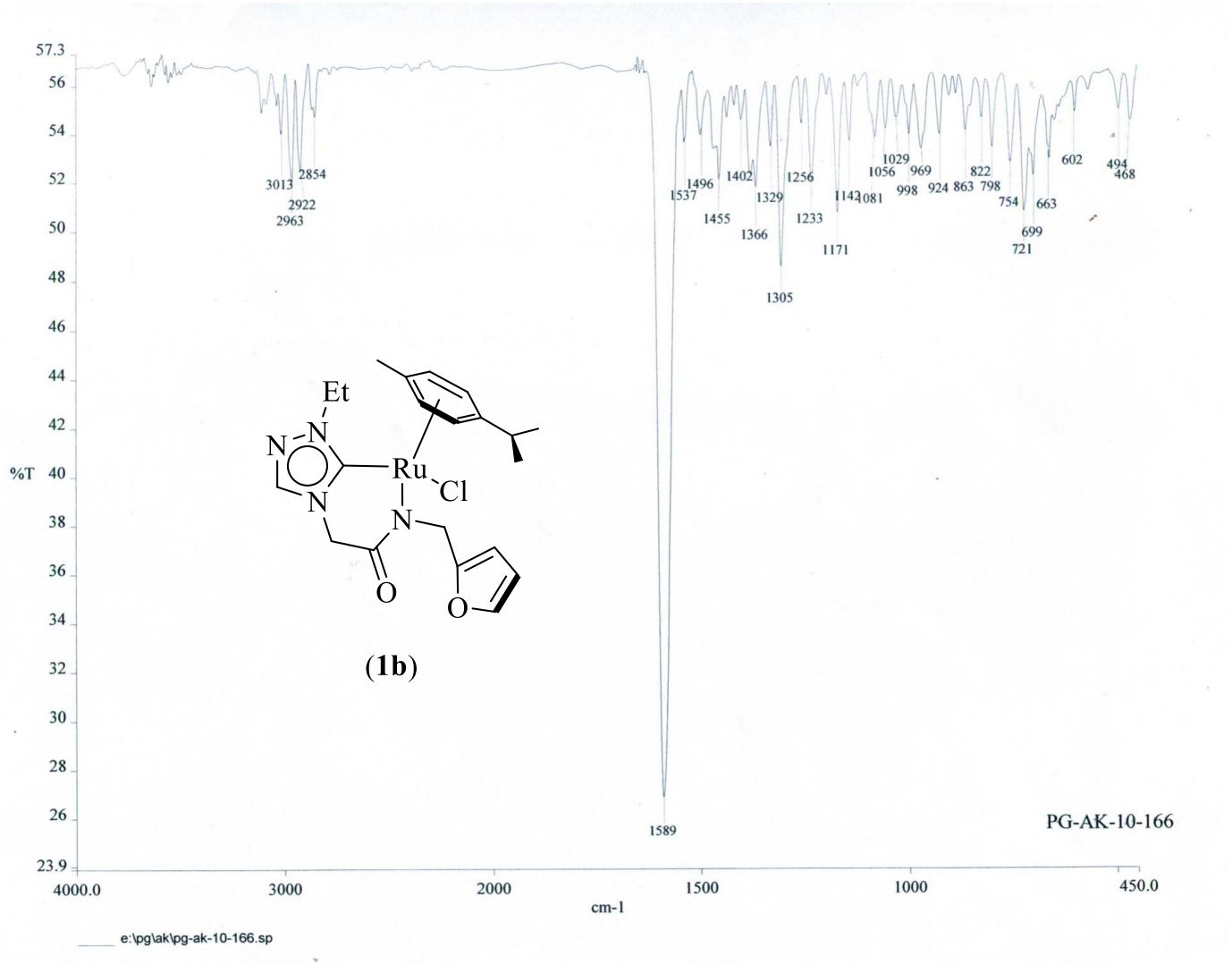
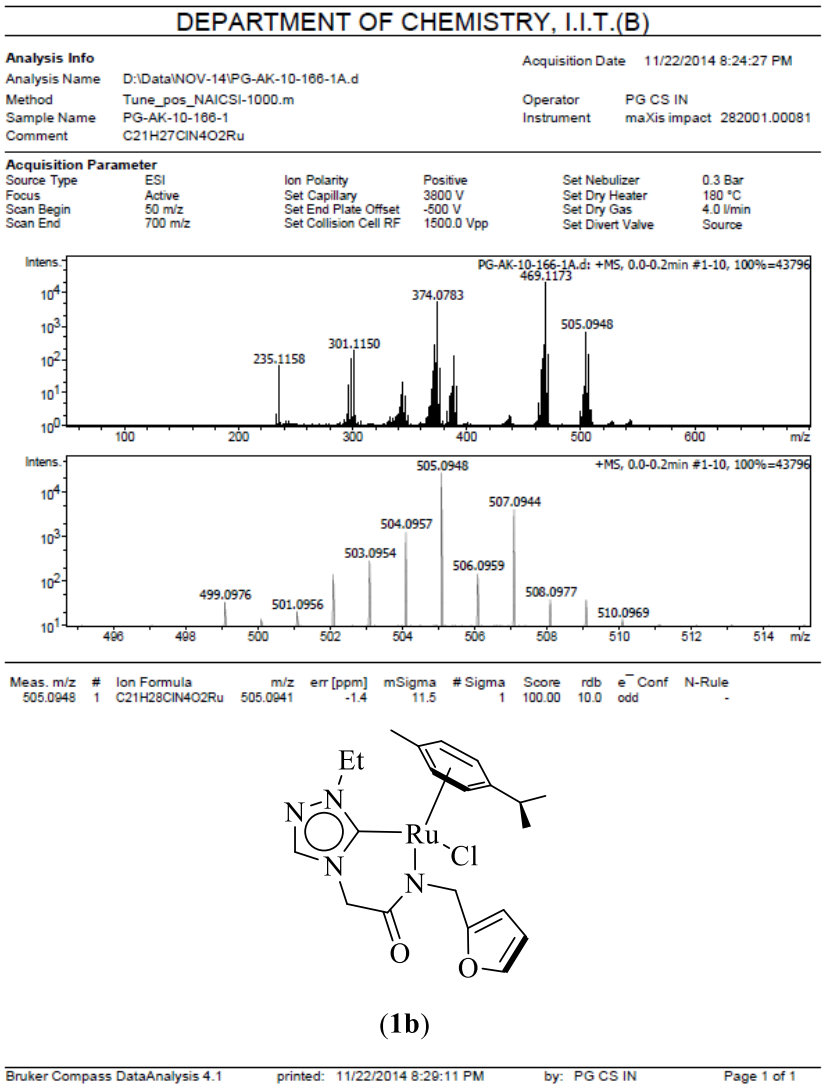


Figure S4. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of **1b** in $CDCl_3$



(**1b**)

Figure S5. Infrared spectrum of **1b** in KBr



(**1b**)

Figure S6. High Resolution Mass Spectrometry (HRMS) data of **1b**.

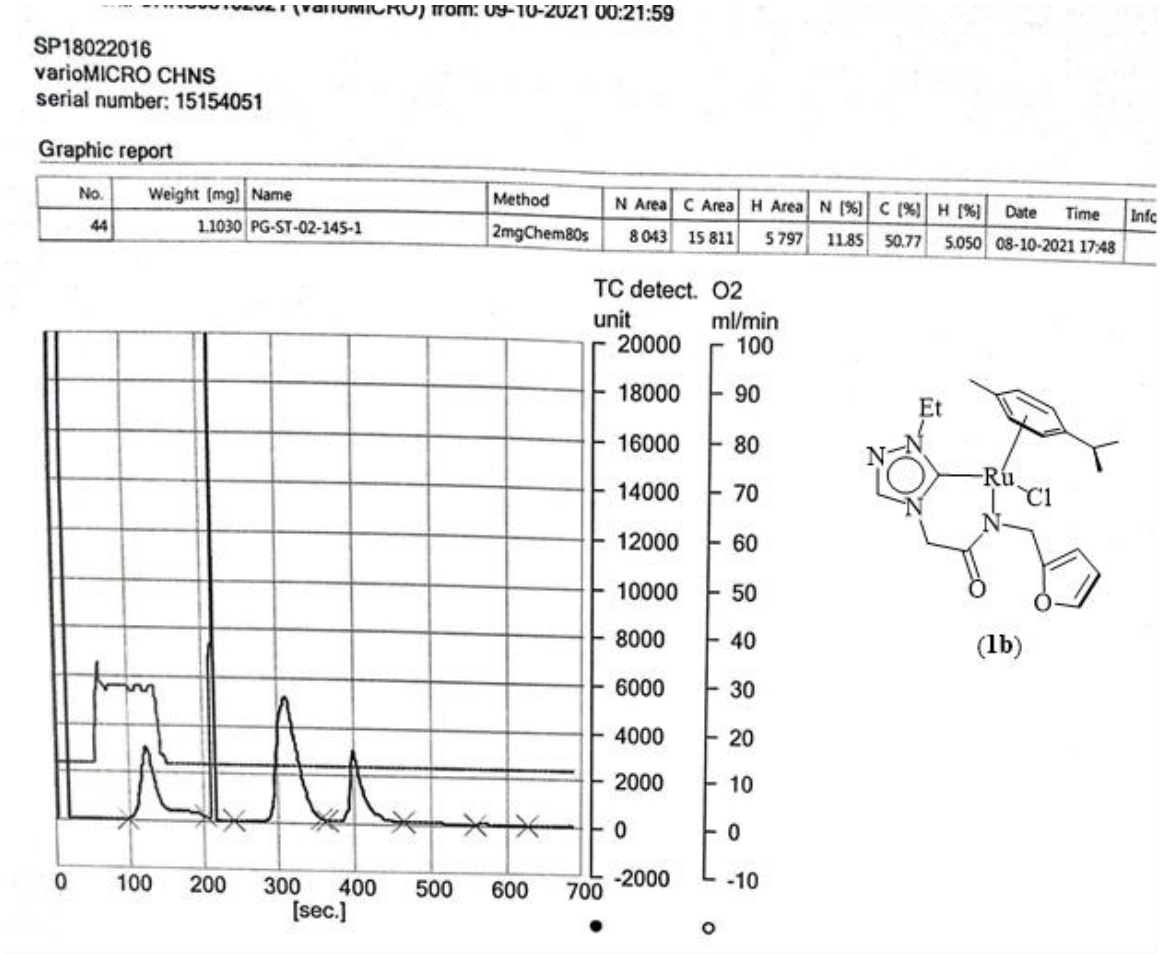


Figure S7. Elemental analysis data of **1b**.

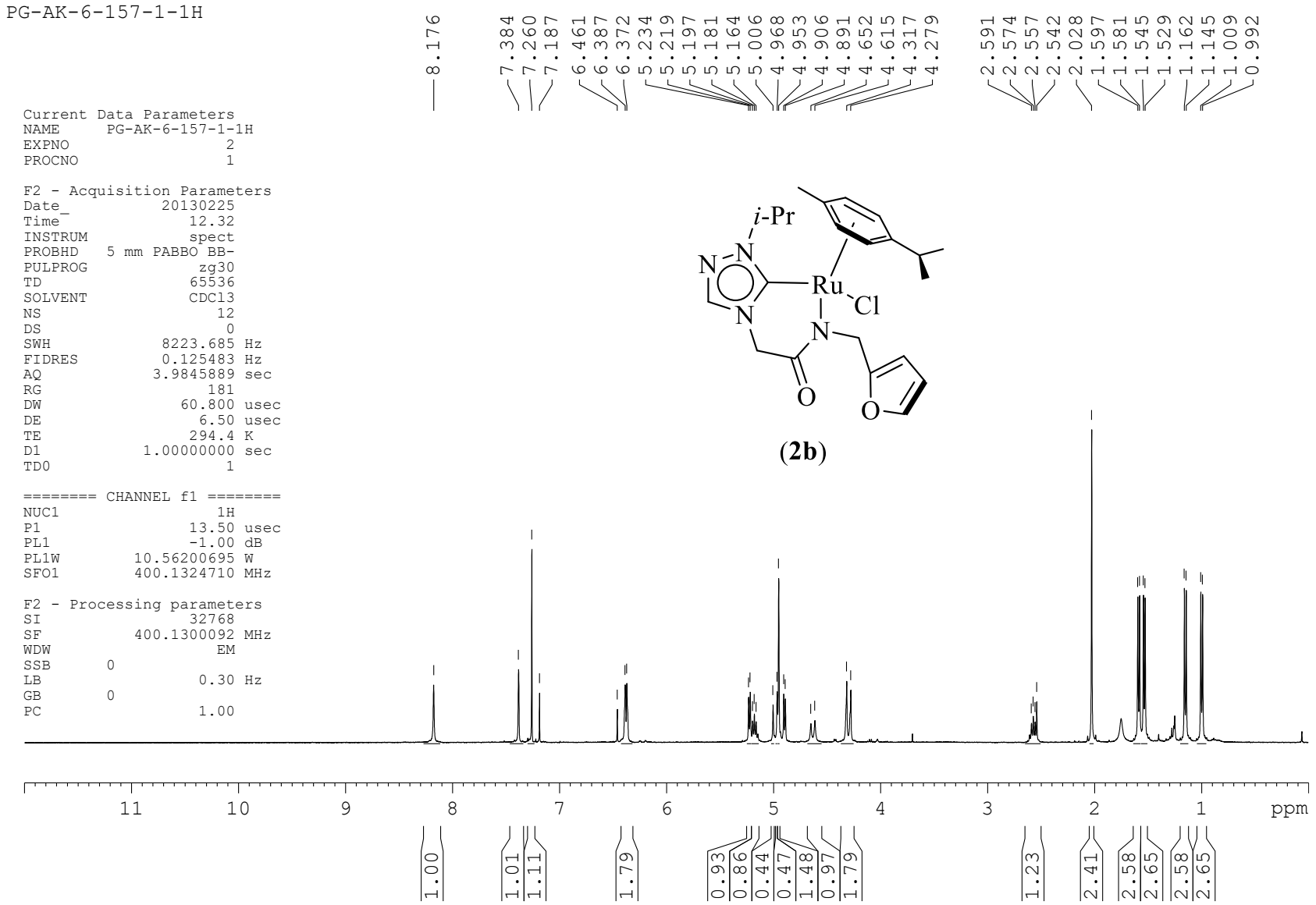


Figure S8. ^{1}H NMR spectrum of **2b** in $CDCl_3$.

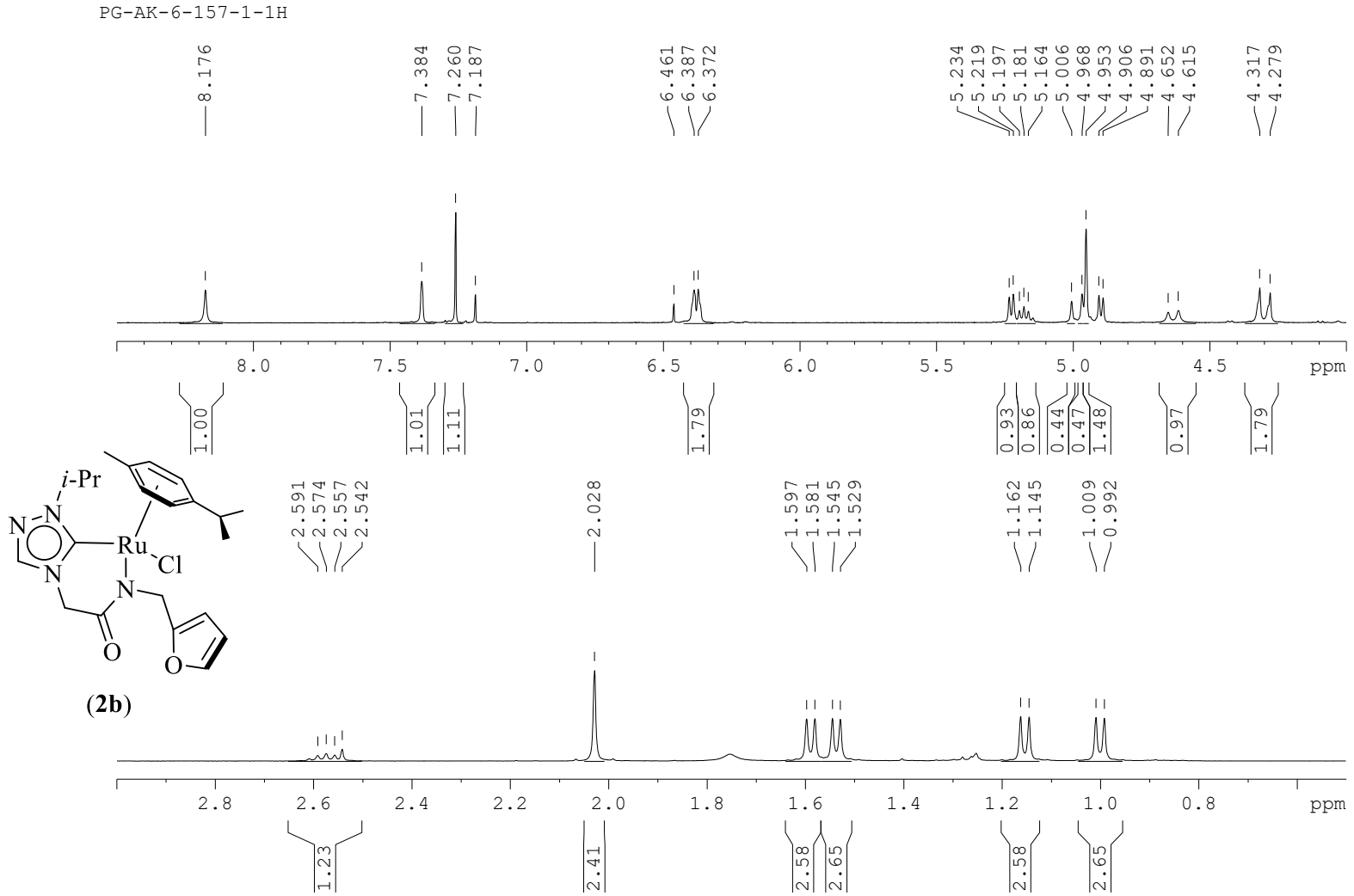


Figure S9. Expanded ^{1}H NMR spectrum of **2b** in $CDCl_3$.

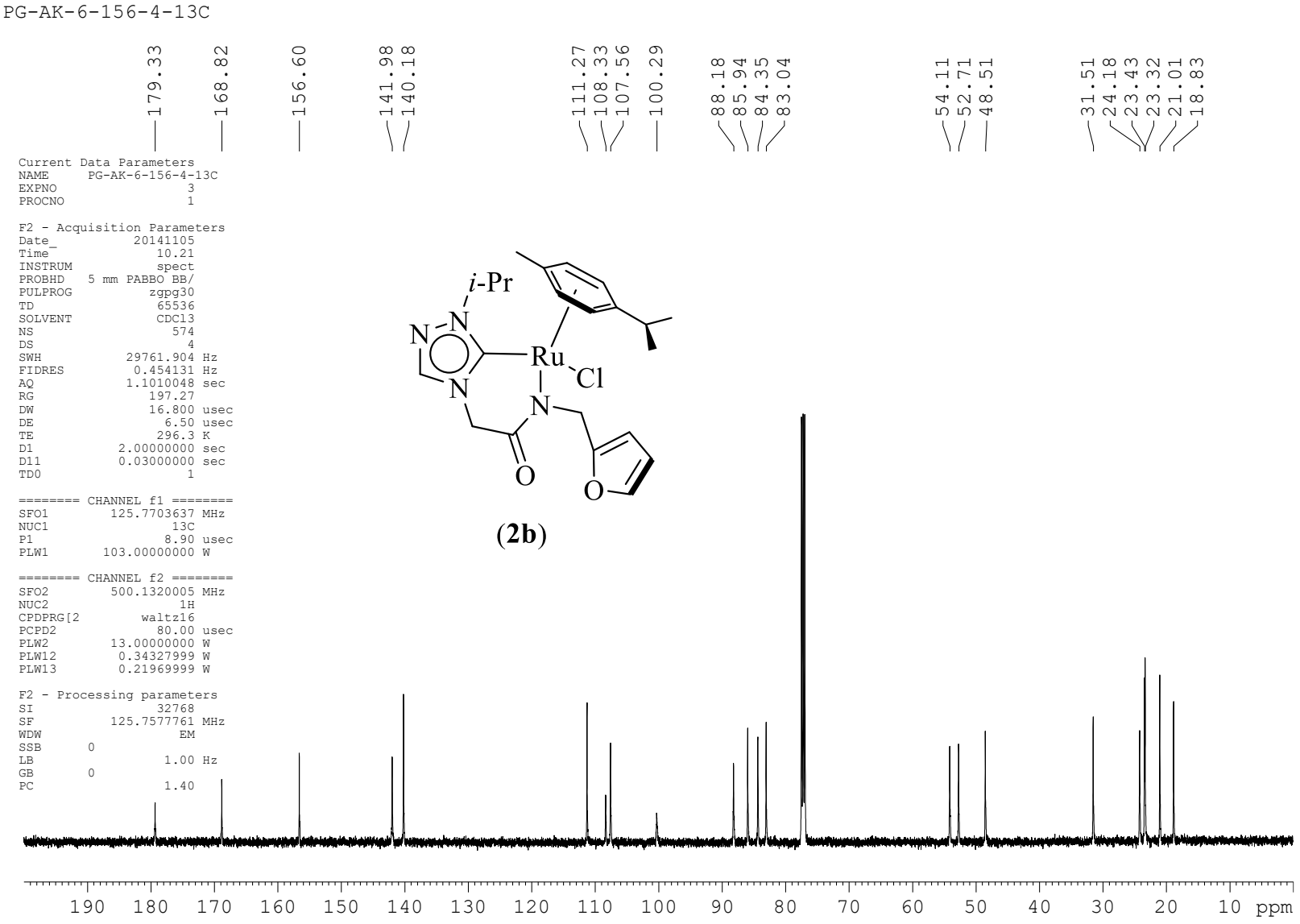


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **2b** in $CDCl_3$.

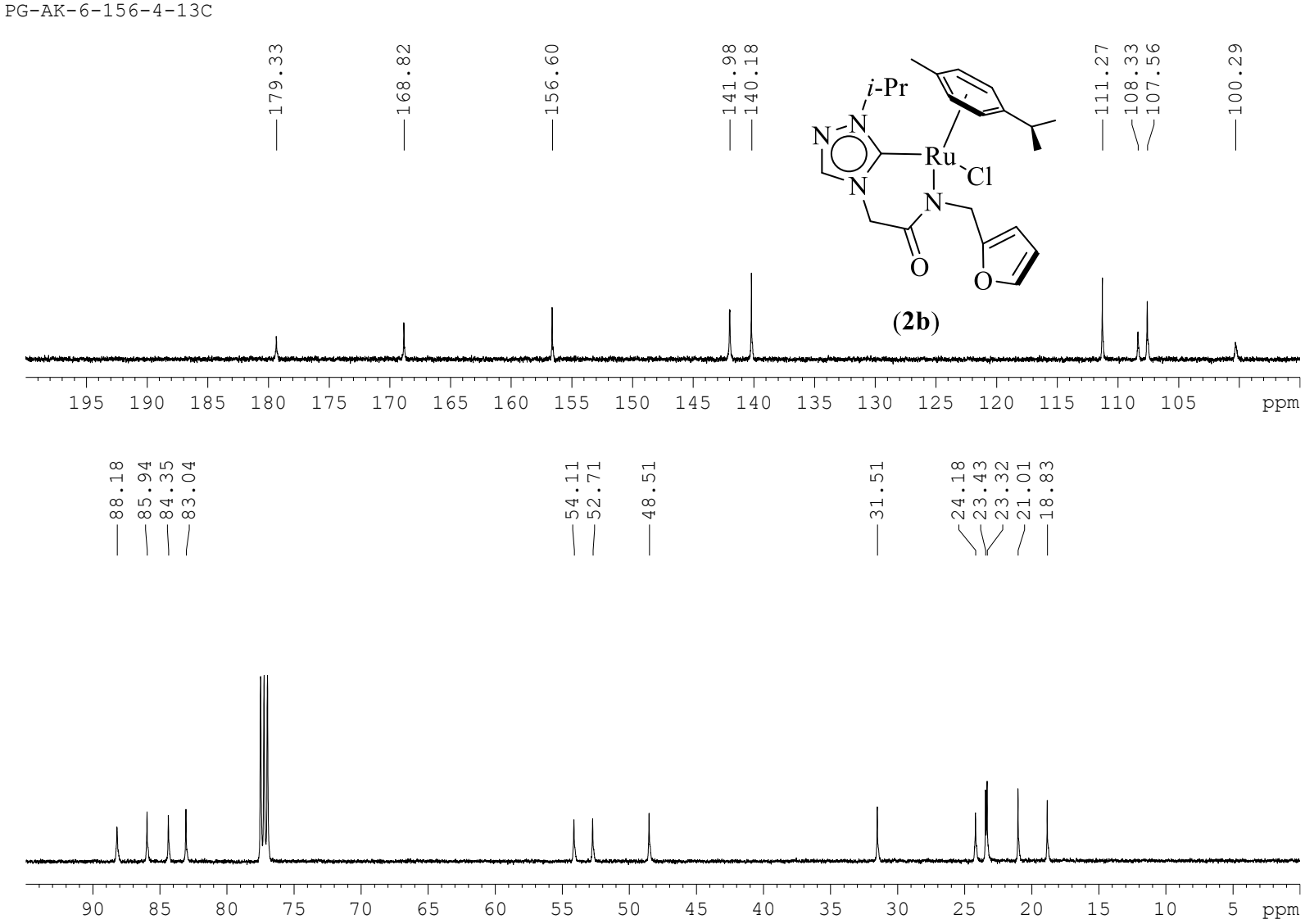
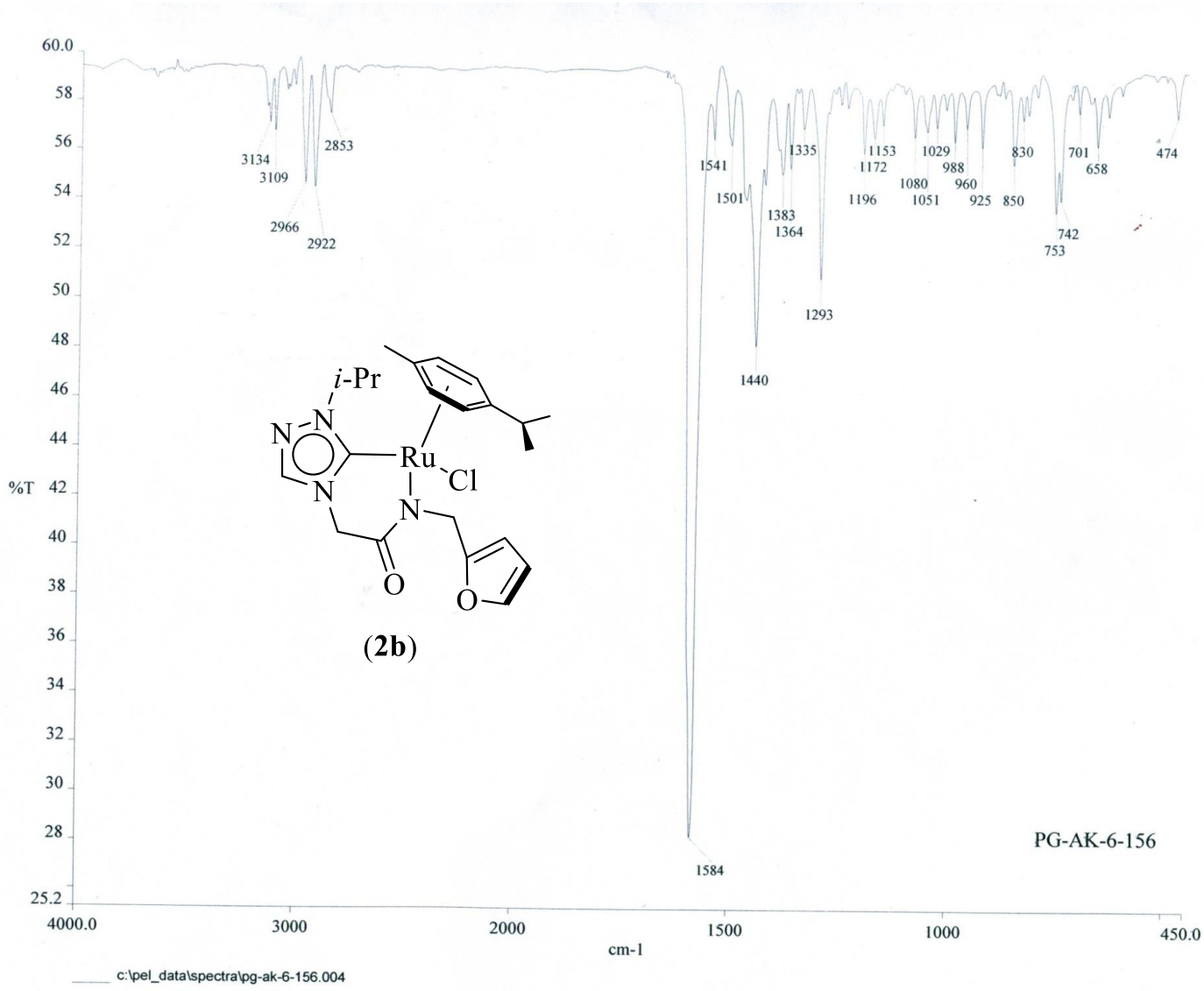
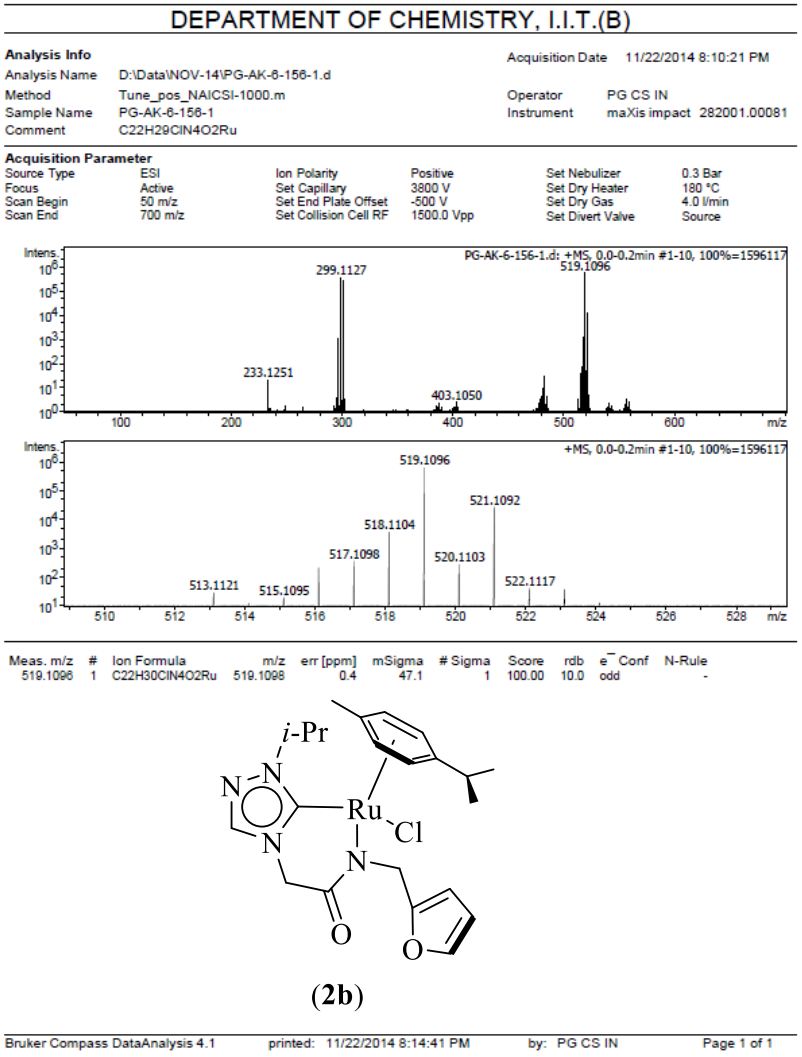


Figure S11. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of **2b** in $CDCl_3$.



(**2b**)

Figure S12. Infrared spectrum of **2b** in KBr



(**2b**)

Figure S13. High Resolution Mass Spectrometry (HRMS) data of **2b**.

Eager 300 Report

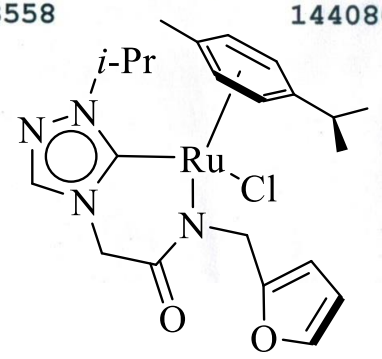
Page: 1 Sample: PG-AK-6-Ru-180 (PG-AK-6-Ru-180)

Method Name : SP-130513
Method File : D:\CHNS2012\SP-130513.mth
Chromatogram : PG-AK-6-Ru-180
Operator ID : MNRAO
Company Name : C.E. Instruments
Analysed : 05/13/2013 16:39
Printed : 5/13/2013 18:54
Sample ID : PG-AK-6-Ru-180 (# 16)
Instrument N. : Instrument #1
Analysis Type : UnkNown (Area)
Sample weight : .735

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	11.2174	43	166571	FU	6.007363	.101682E+07
Carbon	50.6220	66	1000650	FU	1.000000	.268086E+07
Hydrogen	5.5164	178	273582	RS	3.657588	.630570E+07
Totals	67.3558		1440803			



(**2b**)

Figure S14. Elemental analysis data of **2b**.

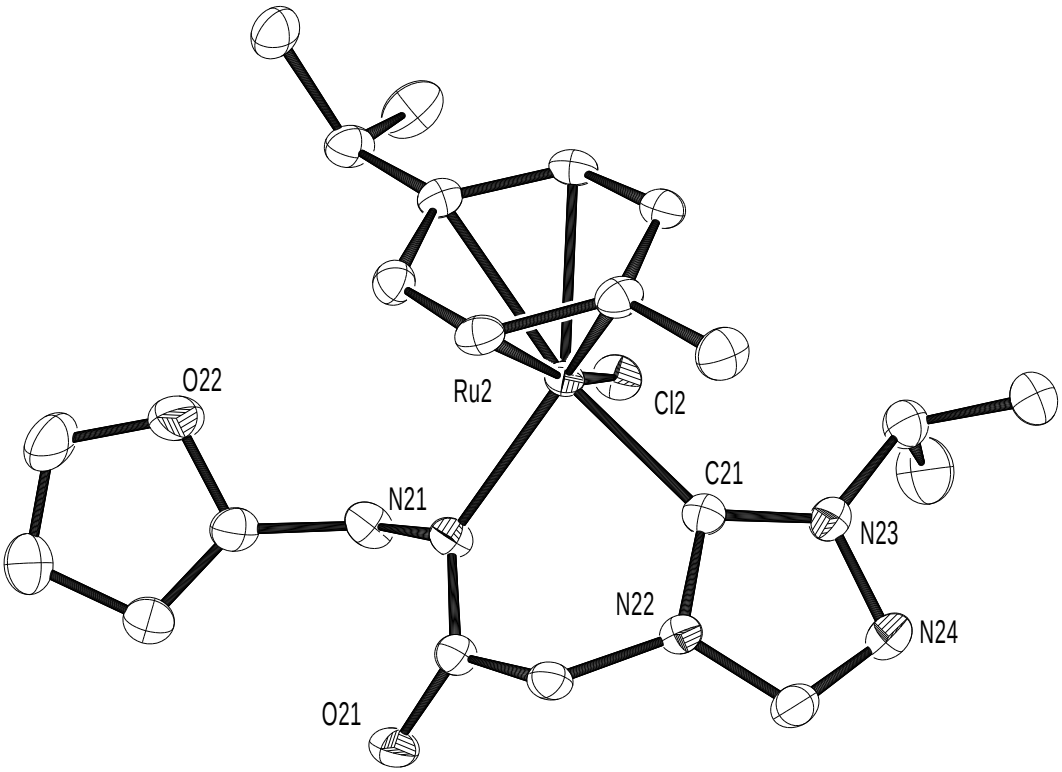


Figure S15. ORTEP diagram of **2b** with thermal ellipsoids are shown at the 50 % probability level. Selected bond lengths (Å) and angles (°): Ru2−C21 2.0384(19), Ru2−N21 2.1230(16), Ru2−Cl2 2.4319(5), C21−Ru2−N21 83.29(7), N21−Ru2−Cl2 86.37(4).

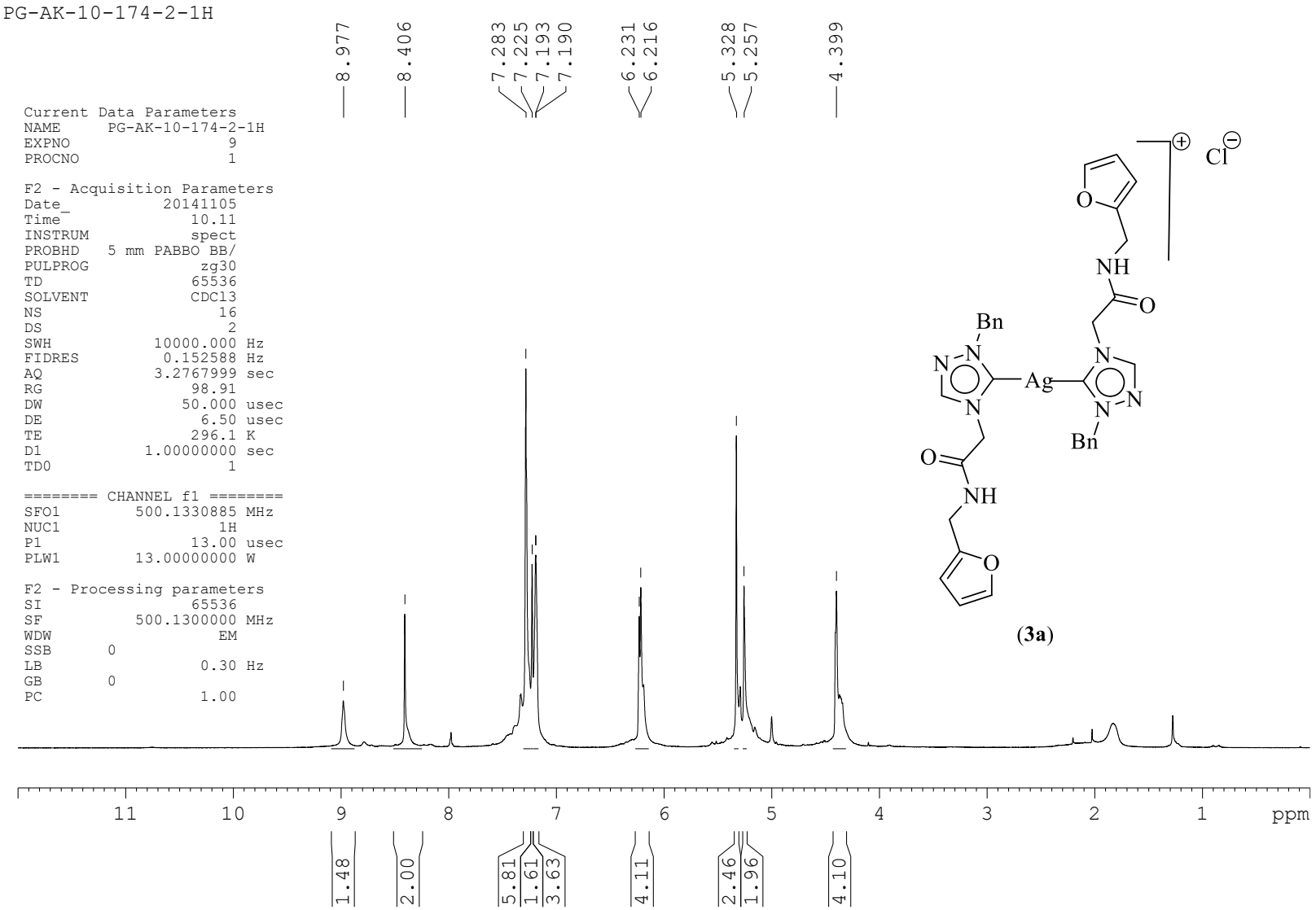


Figure S16. ^{1}H NMR spectrum of **3a** in $CDCl_3$.

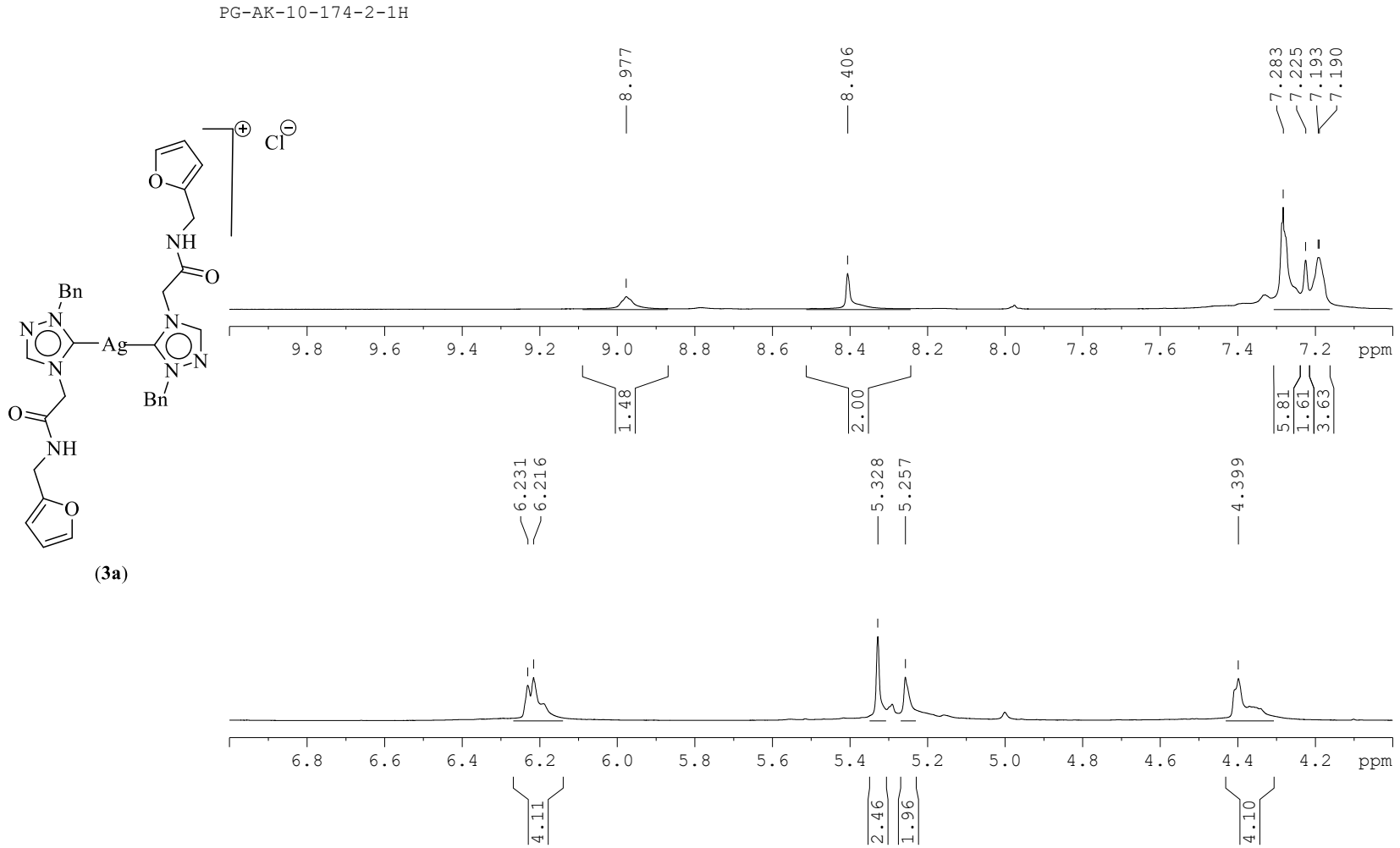


Figure S17. Expanded ^{1}H NMR spectrum of **3a** in $CDCl_3$

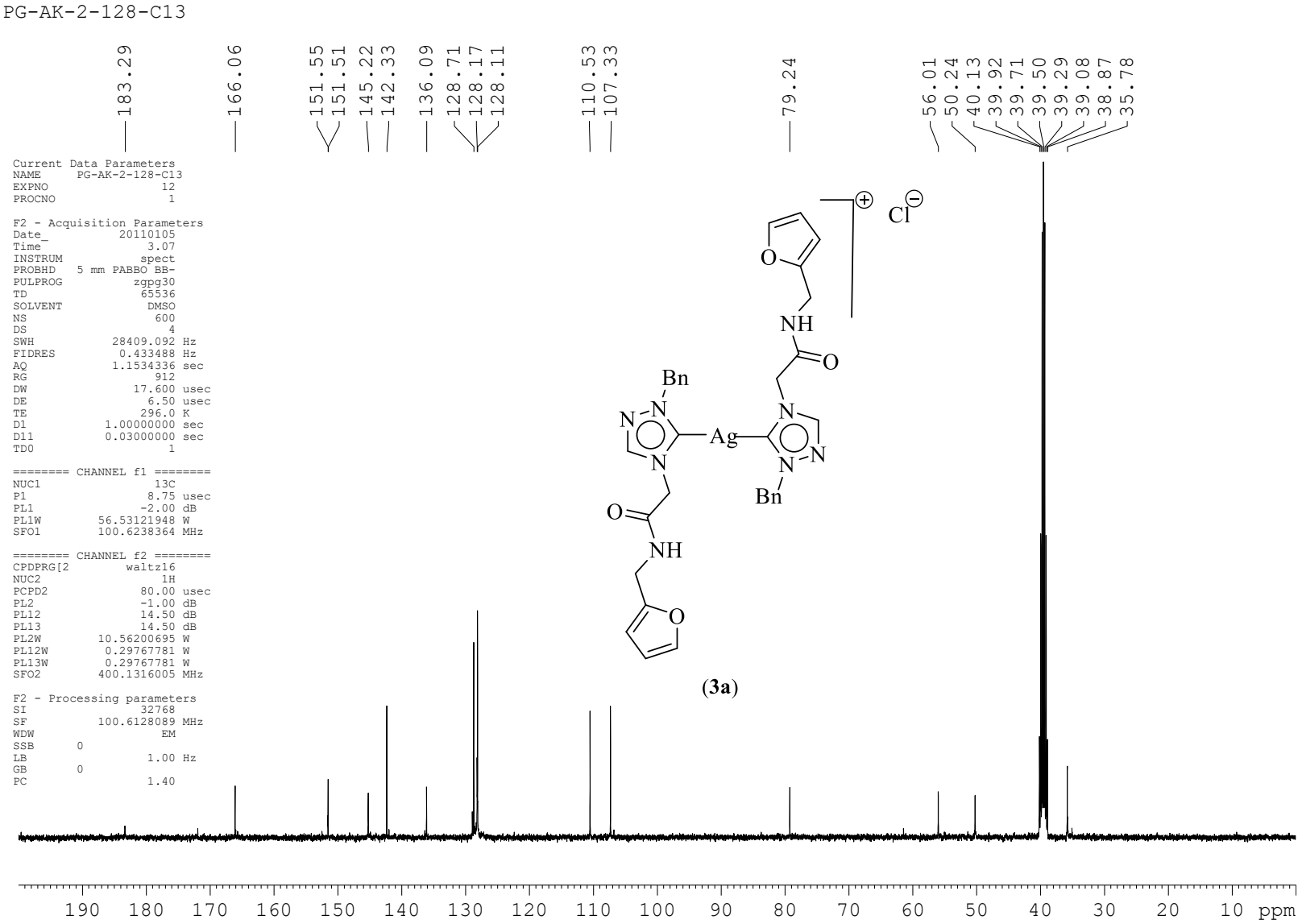


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **3a** in DMSO-d_6.

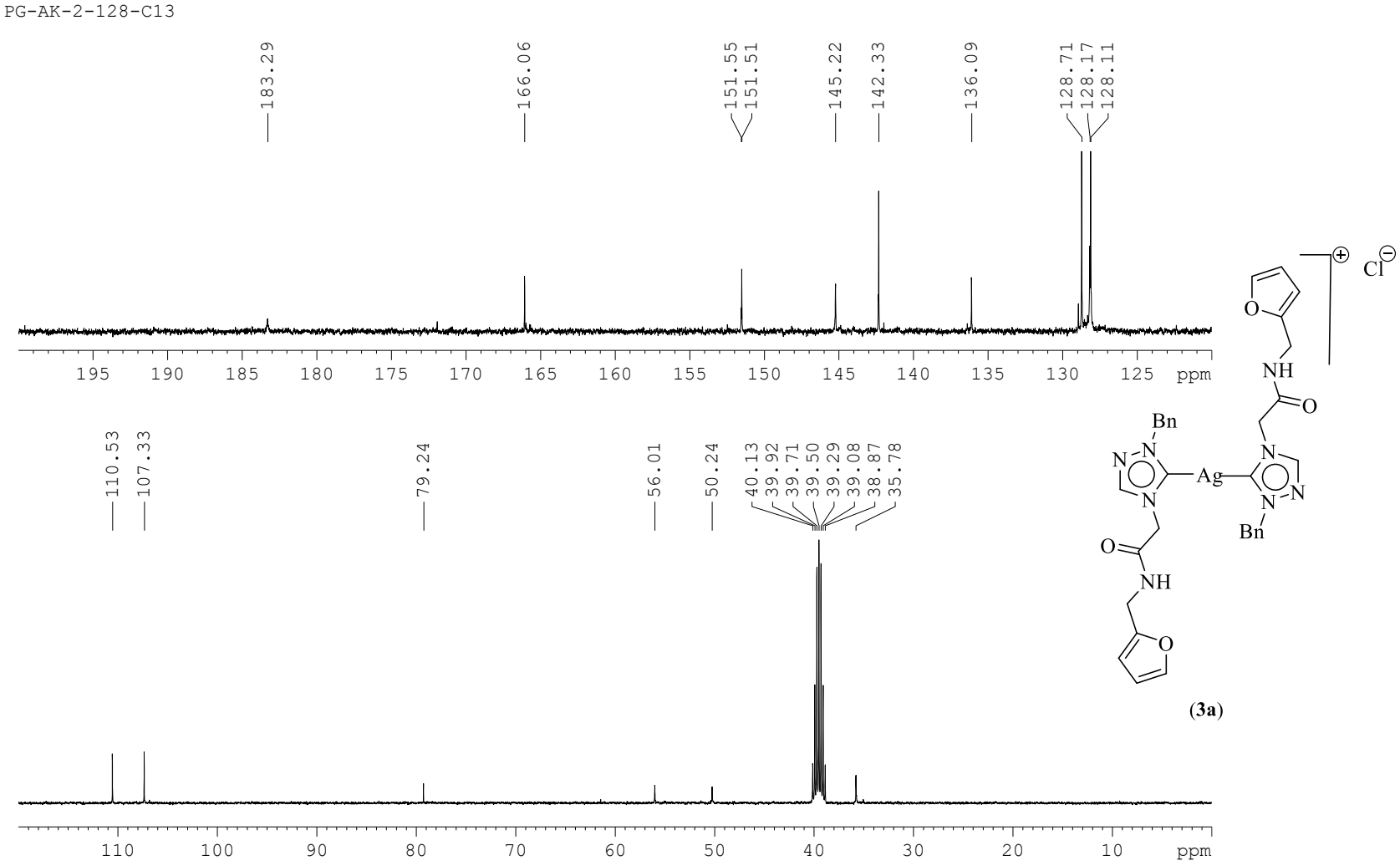


Figure S19. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of **3a** in DMSO-d_6.

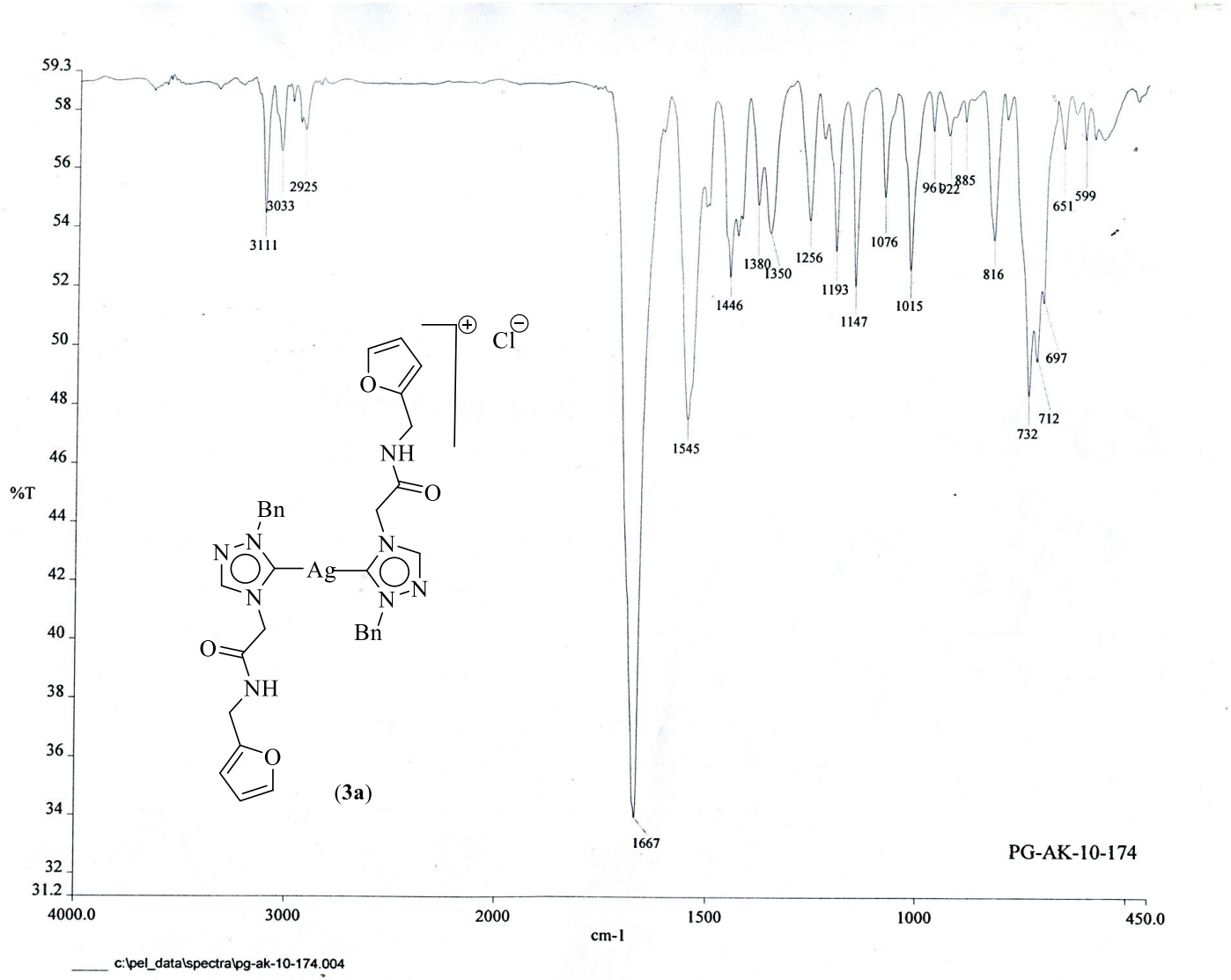


Figure S20. Infrared spectrum of **3a** in KBr.

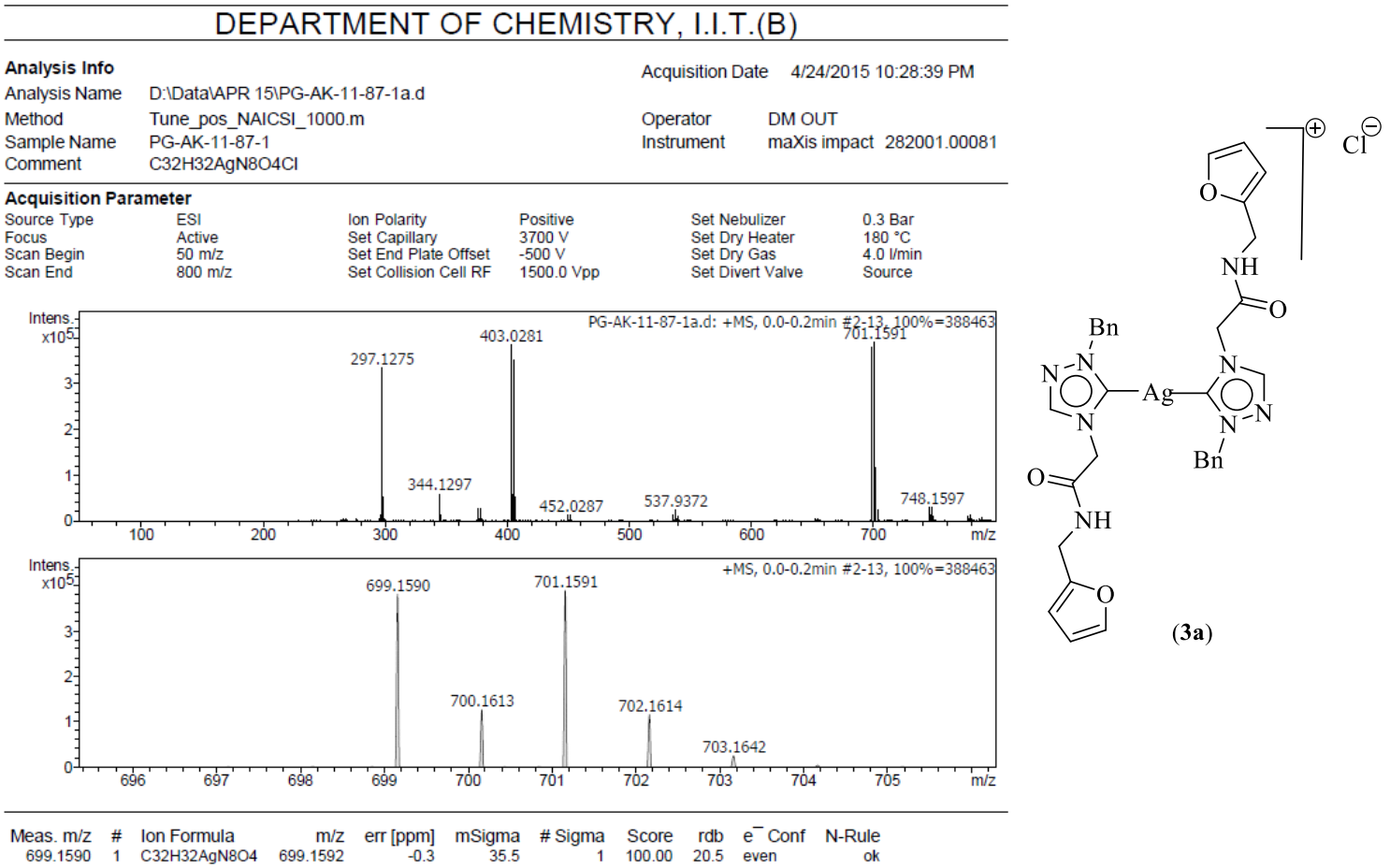
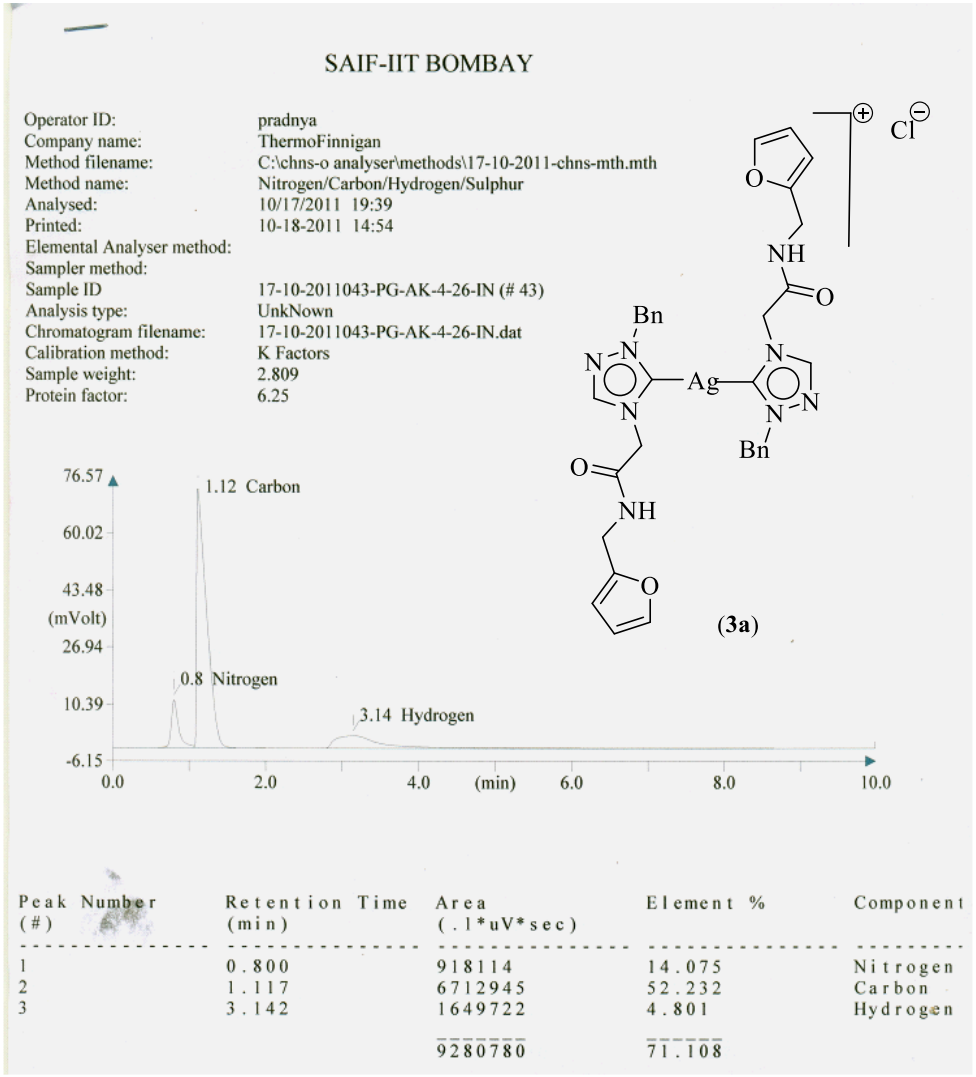


Figure S21. High Resolution Mass Spectrometry (HRMS) data of **3a**.



Peak Number (#)	Retention Time (min)	Area (.1*uV*sec)	Element %	Component
1	0.800	918114	14.075	Nitrogen
2	1.117	6712945	52.232	Carbon
3	3.142	1649722	4.801	Hydrogen
		9280780	71.108	

Figure S22. Elemental analysis data of **3a**.

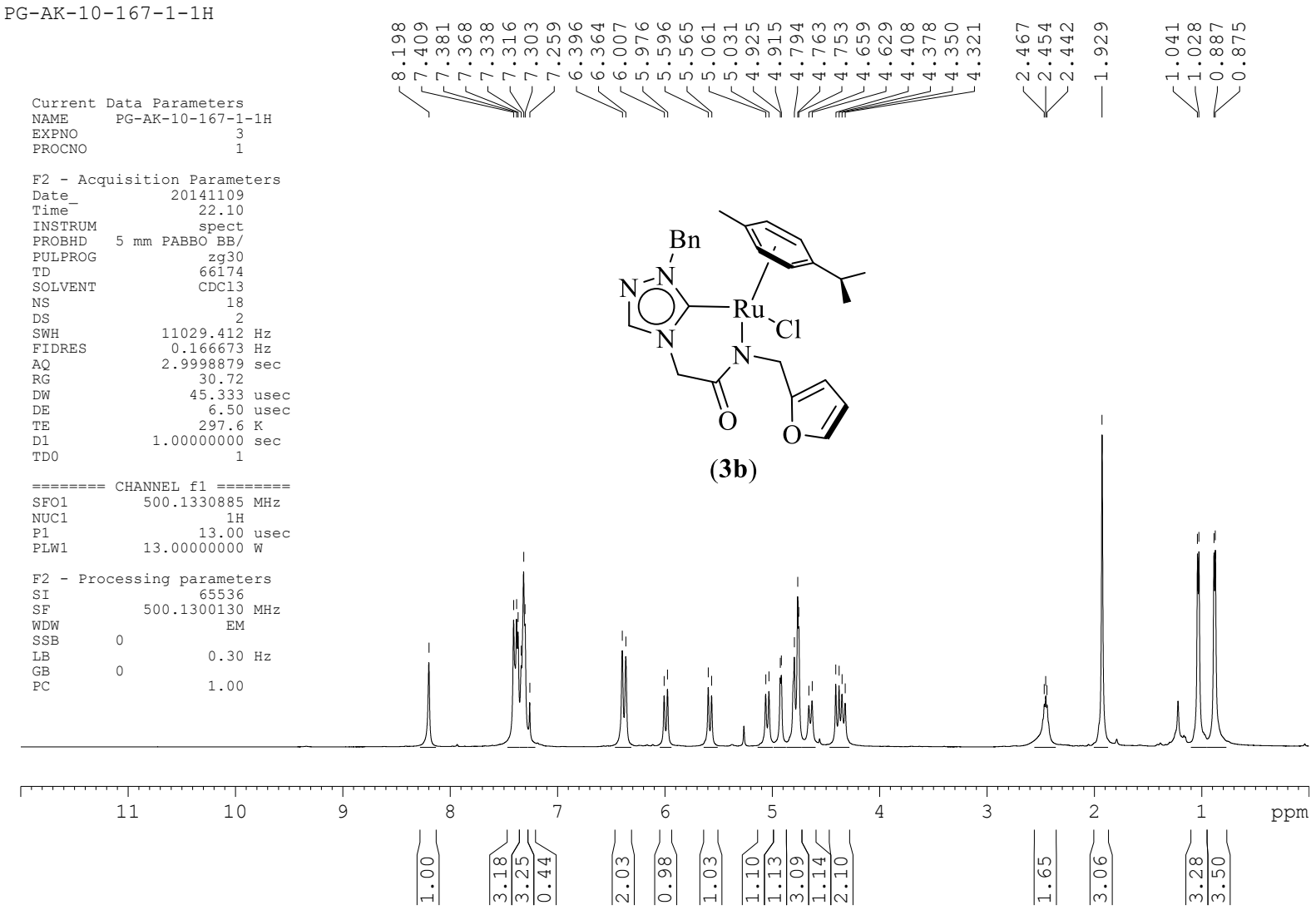


Figure S23. ^{1}H NMR spectrum of **3b** in $CDCl_3$.

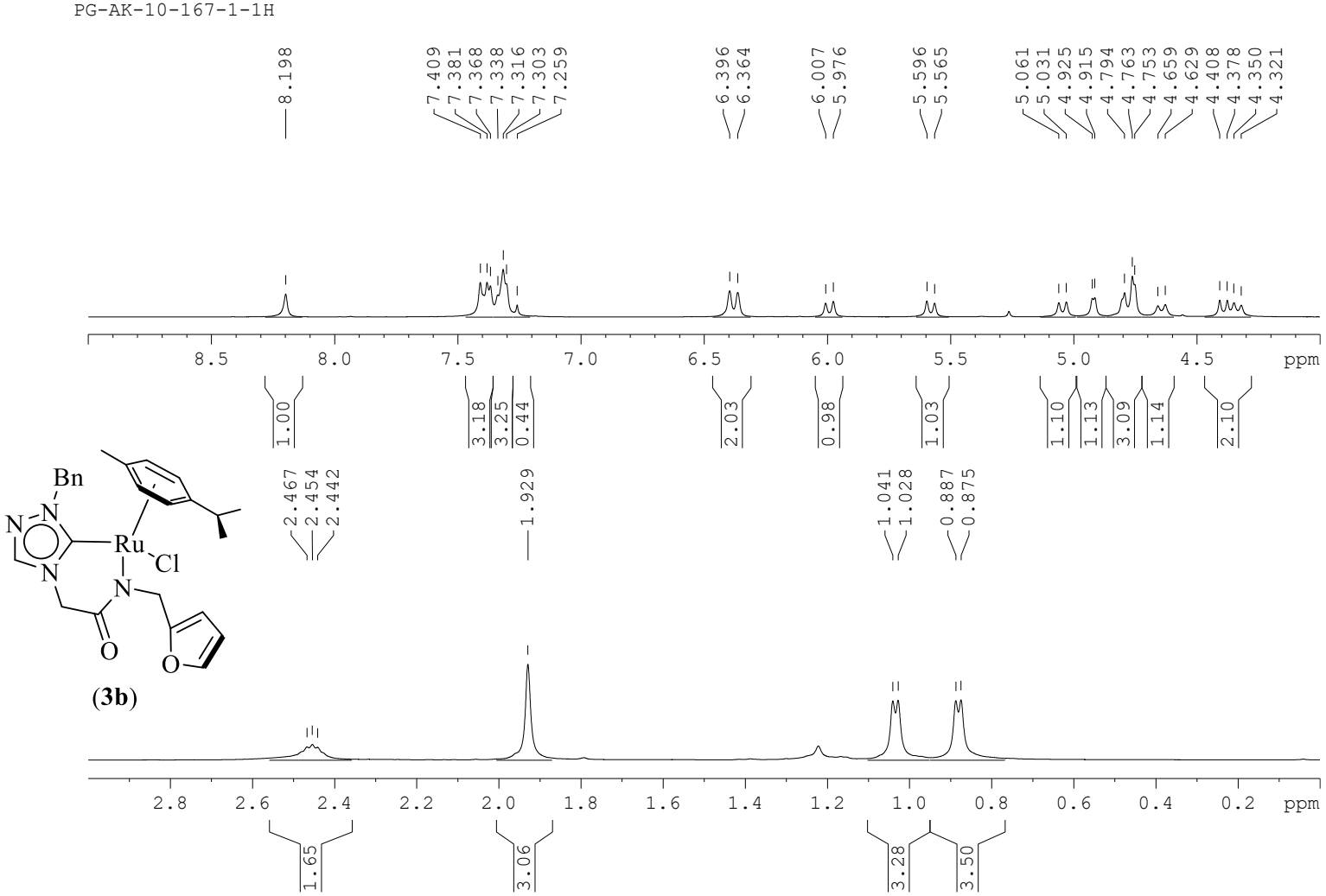


Figure S24. Expanded ^{1}H NMR spectrum of **3b** in $CDCl_3$.

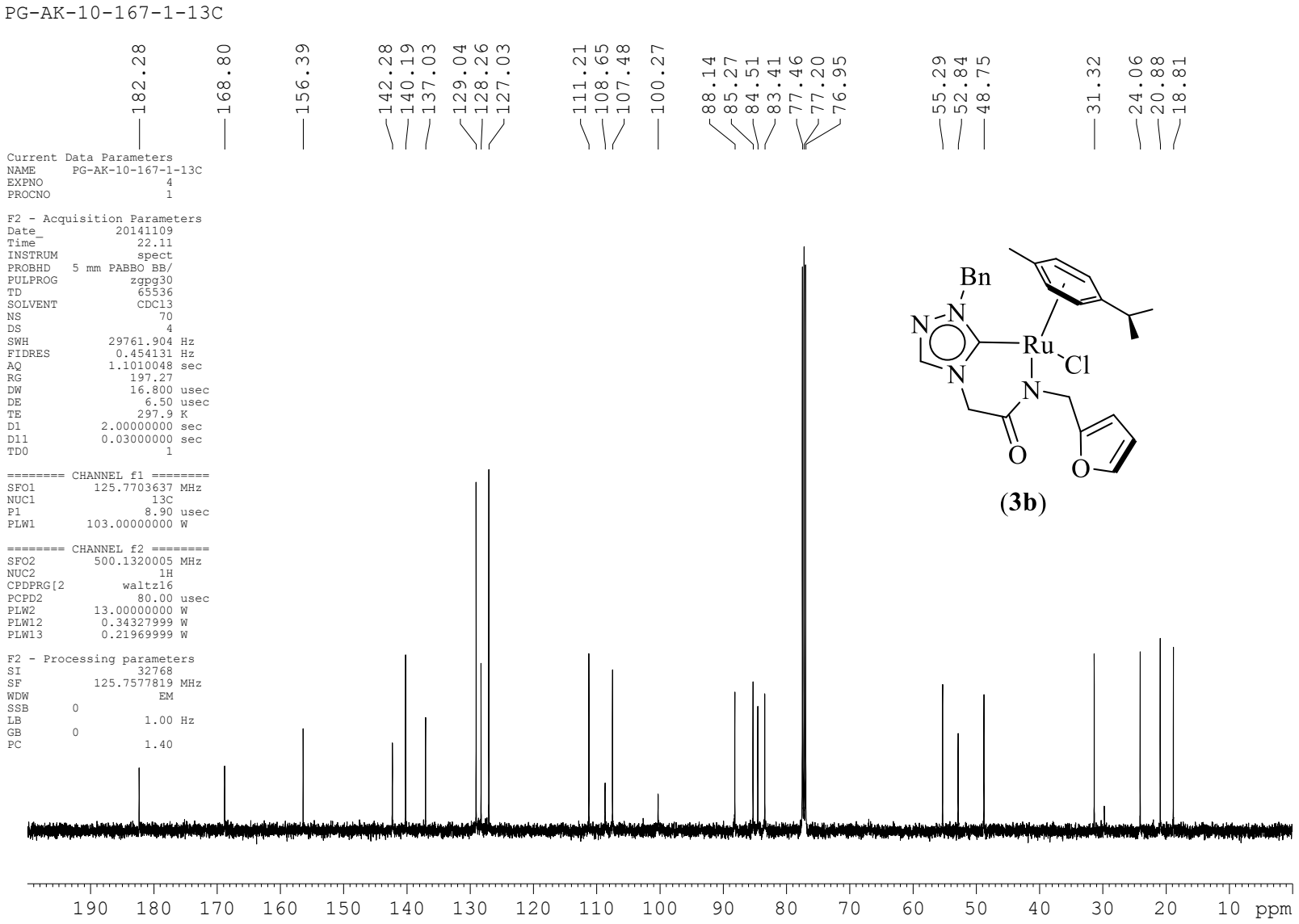


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of **3b** in $CDCl_3$.

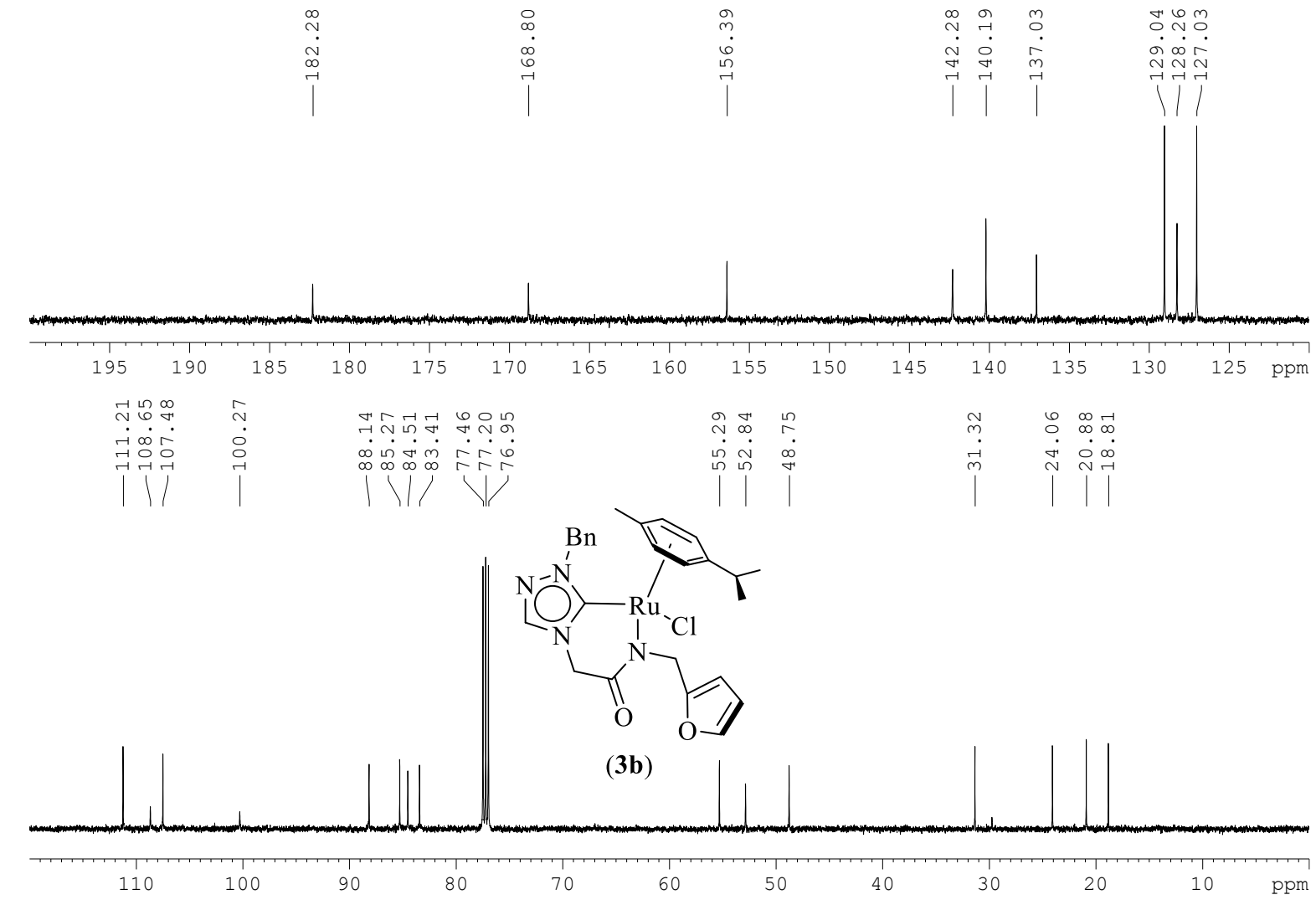


Figure S26. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of **3b** in $CDCl_3$.

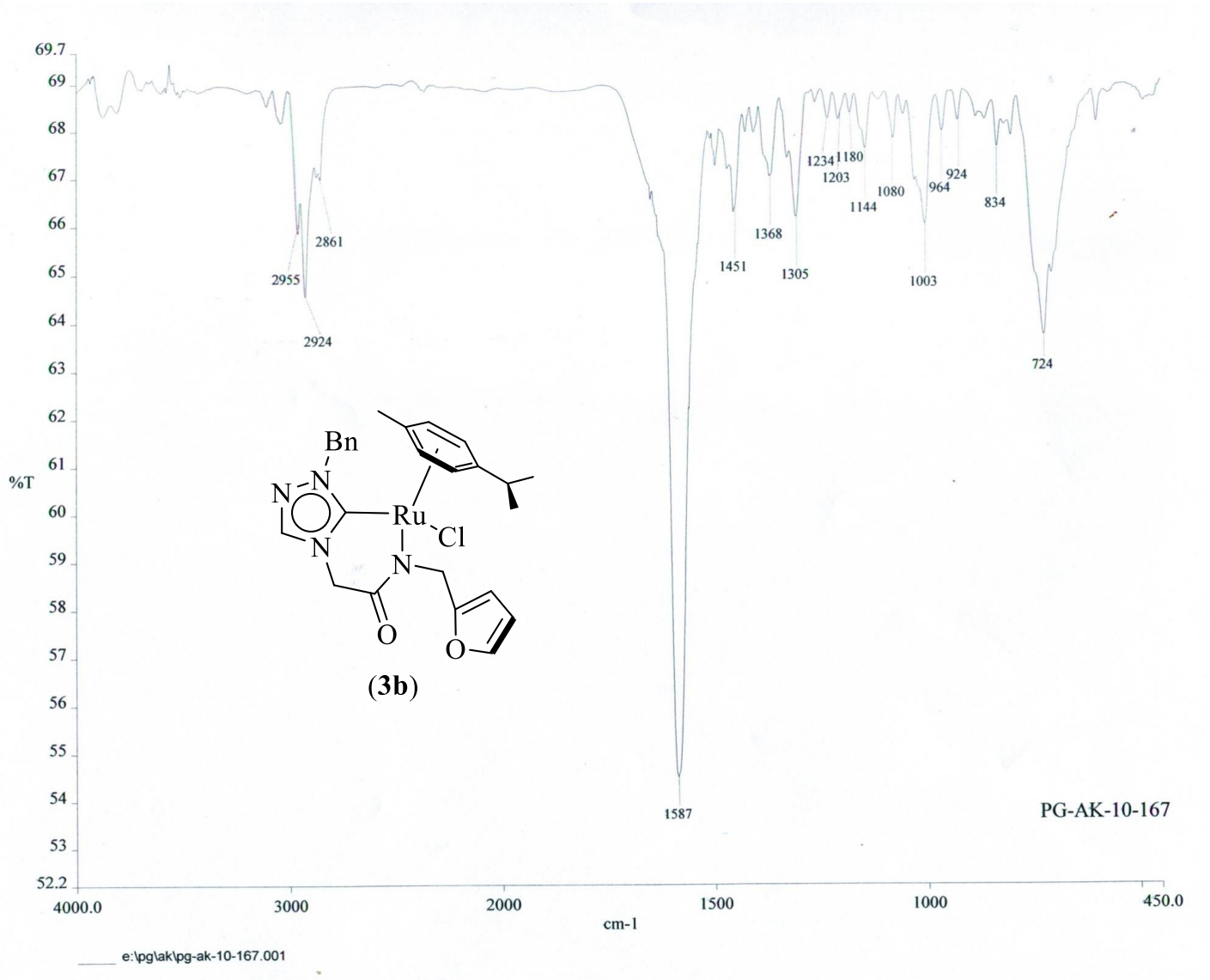


Figure S27. Infrared spectrum of **3b** in KBr.

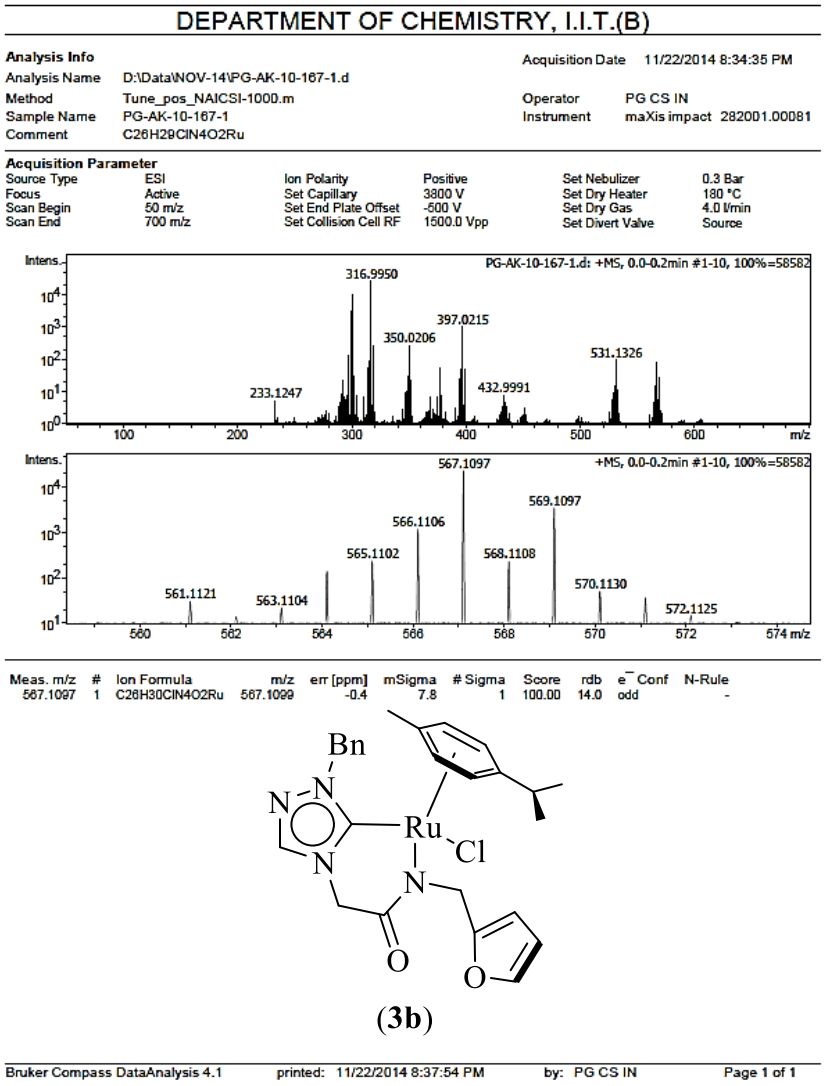


Figure S28. High Resolution Mass Spectrometry (HRMS) data of **3b**.

Eager 300 Report

Page: 1 Sample: AK-2-125-3 (AK-2-125-3)

Method Name : SP060111
Method File : D:\CHNS2011\SP060111.mth
Chromatogram : AK-2-125-3
Operator ID : sks
Company Name : C.E. Instruments
Analysed : 01/05/2011 16:22
Printed : 1/5/2011 18:51
Sample ID : AK-2-125-3 (# 23)
Instrument N. : Instrument #1
Analysis Type : UnkNown (Area)
Sample weight : .699

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

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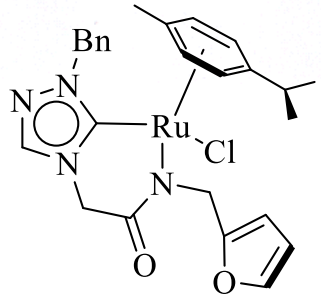
Carbon	54.3813	66	927536	FU	1.000000	.244008E+07
Hydrogen	5.5634	172	224030	RS	4.140230	.545526E+07
Totals	70.4505		1257951			



(**3b**)

Figure S29. Elemental analysis data of **3b**.

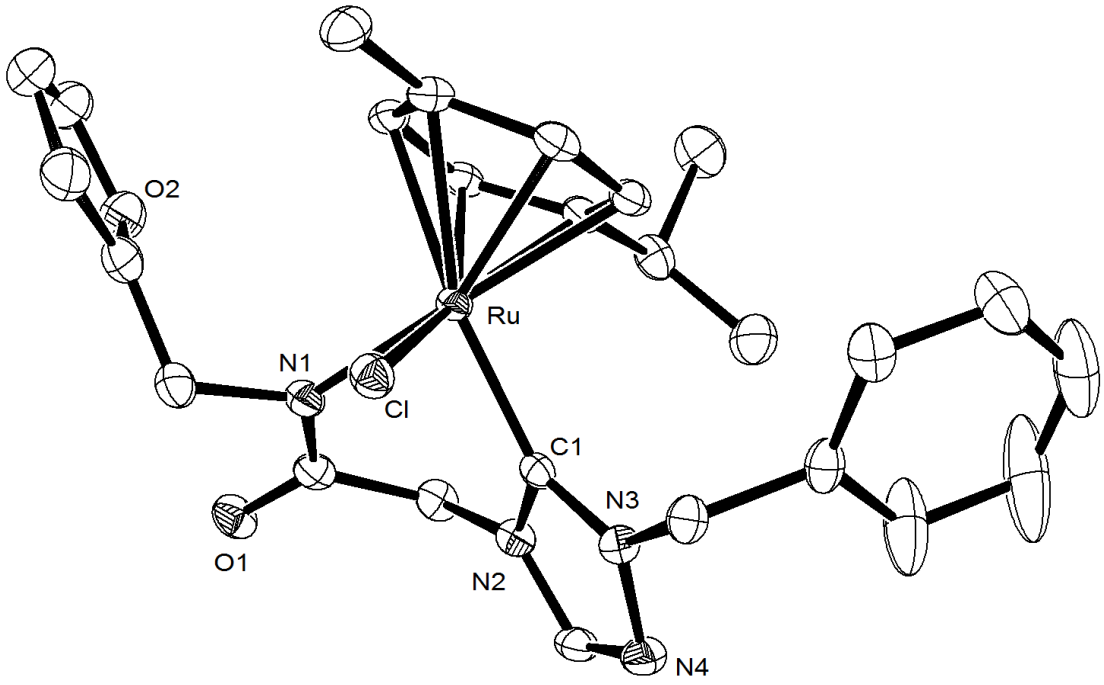


Figure S30. ORTEP diagram of **3b** with thermal ellipsoids are shown at the 50 % probability level. Selected bond lengths (Å) and angles (°): Ru1−C1 2.016(3), Ru−N1 2.131(2), Ru1−Cl 2.4347(7), C1−Ru−N1 82.74(10), N1−Ru−Cl1 87.71(7).

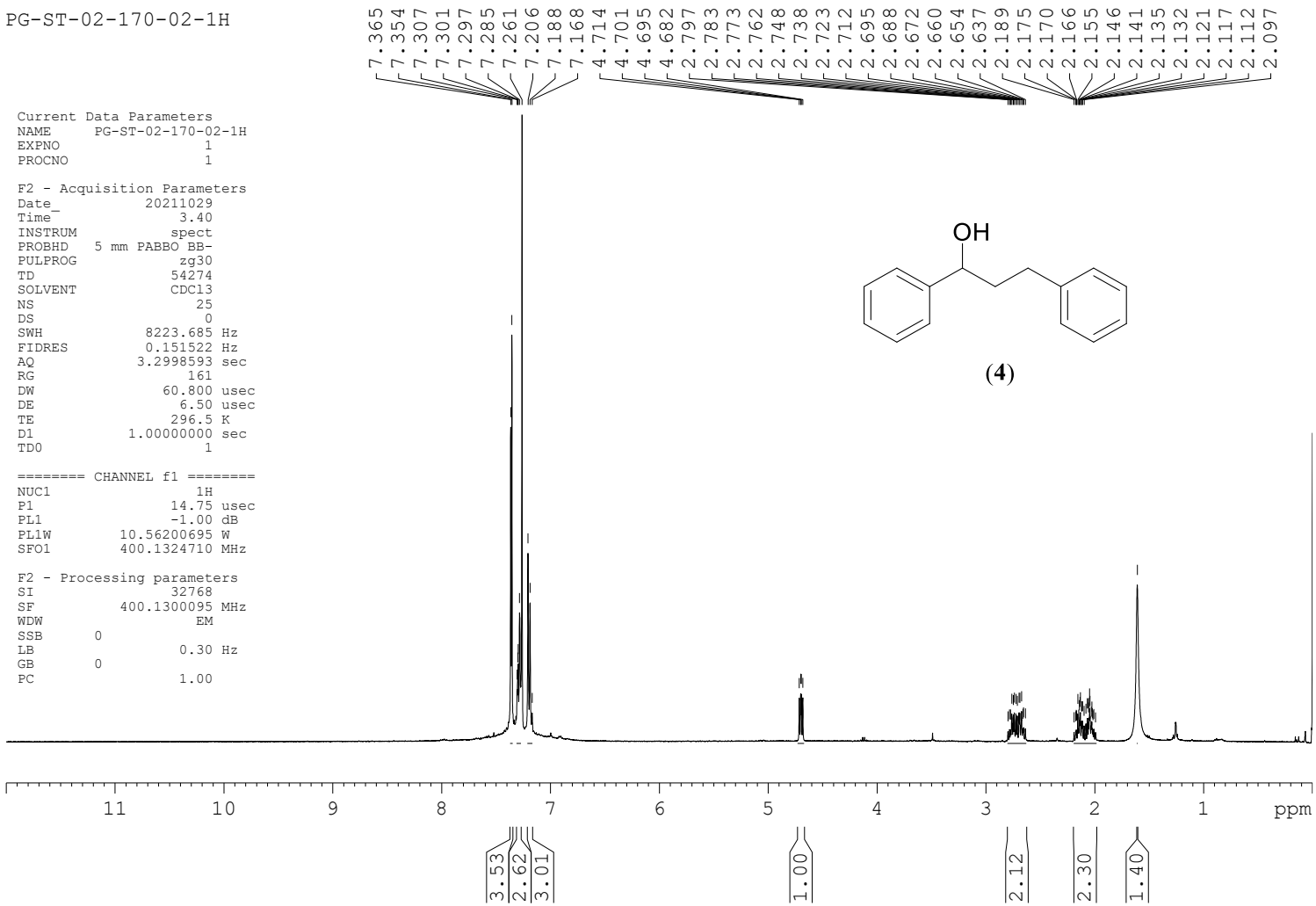


Figure S31. ^{1}H NMR spectrum of (**4**) in $CDCl_3$.

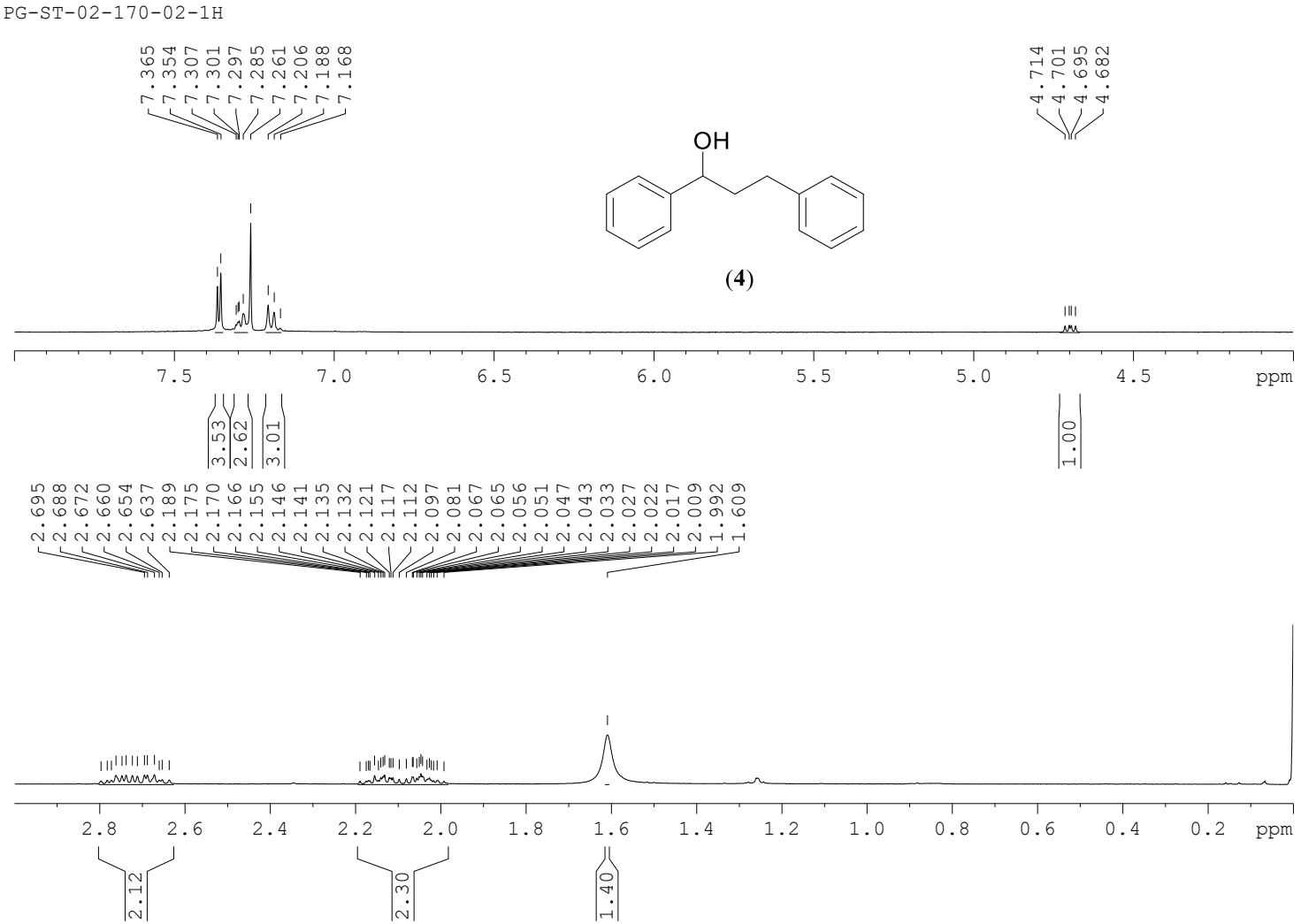


Figure S32. Expanded ^{1}H NMR spectrum of (**4**) in $CDCl_3$.

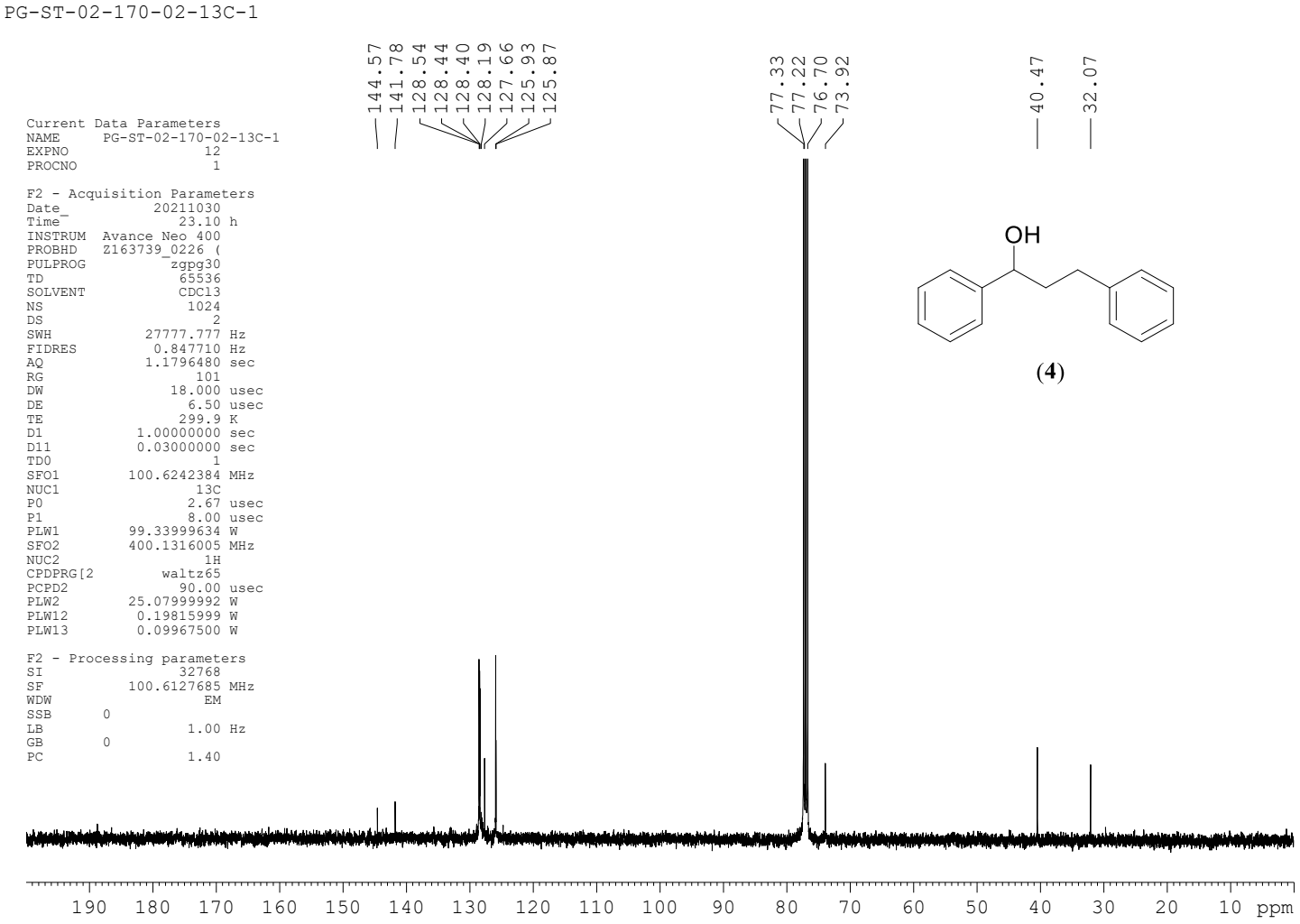


Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum of (**4**) in $CDCl_3$.

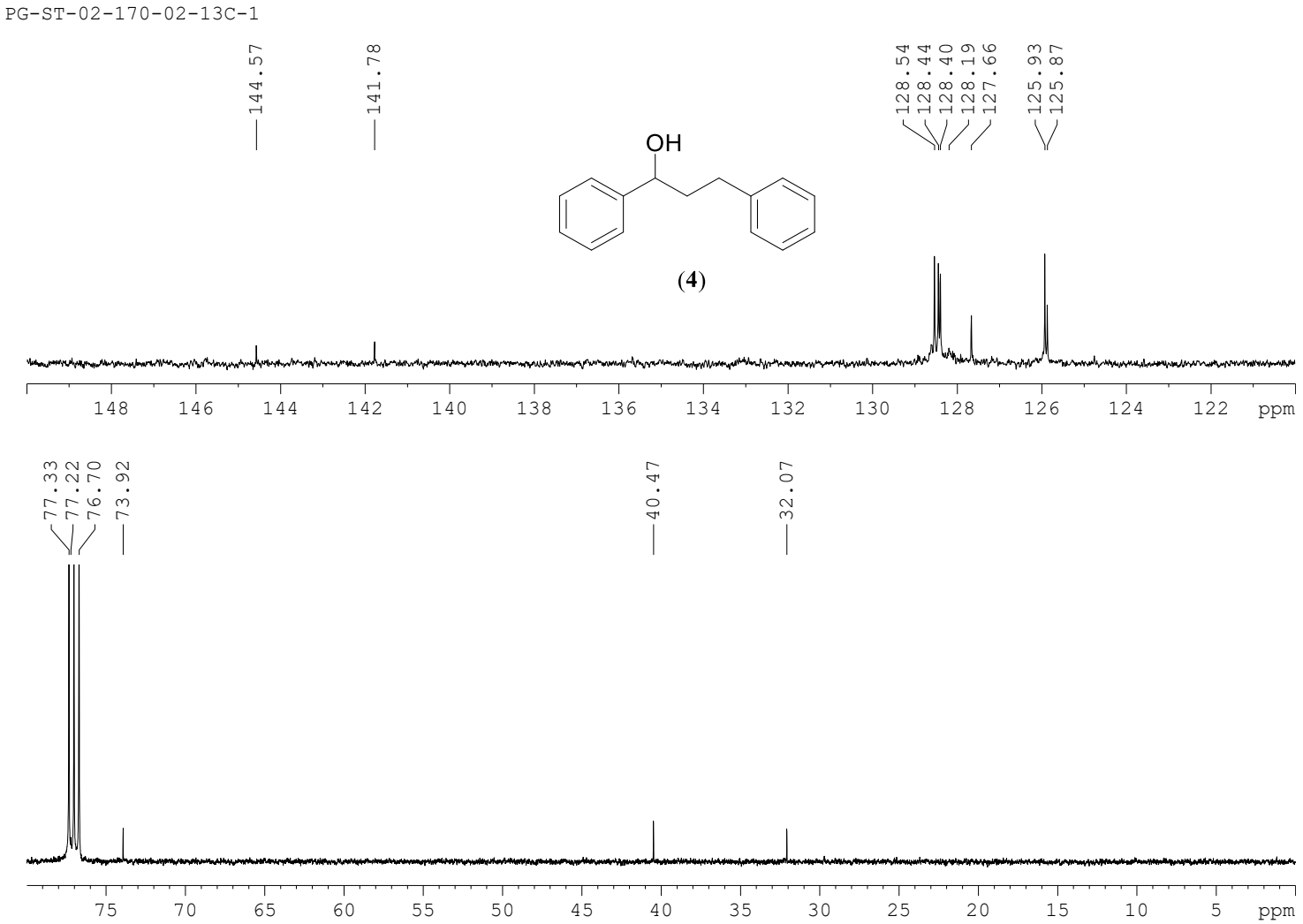


Figure S34. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**4**) in $CDCl_3$.

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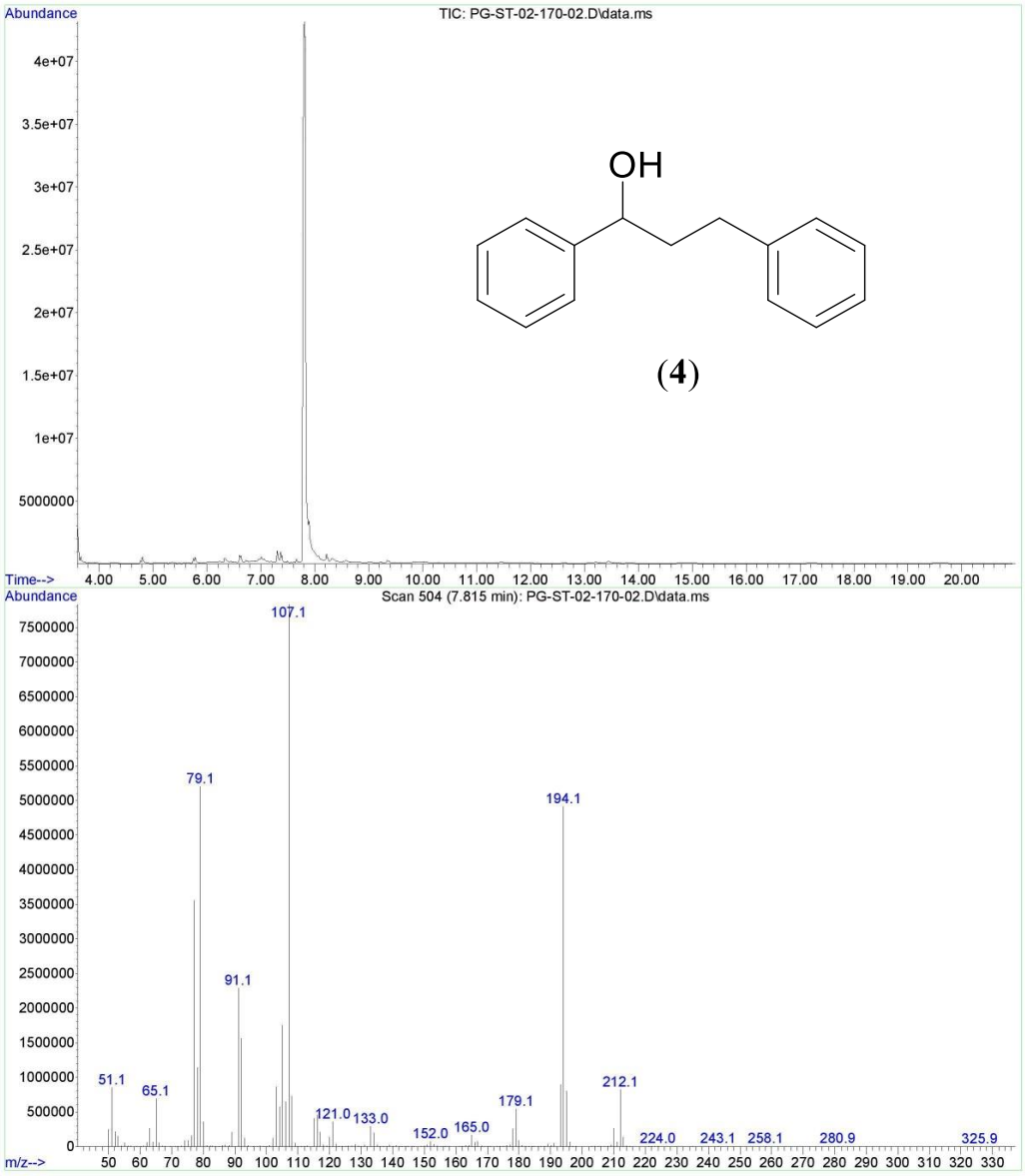

Figure S35. GCMS trace in EtOAc of (**4**) showing the M^+ peak at *m/z* 212.

SP18022016
varioMICRO CHNS
serial number: 15154051

Graphic report

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date Time	Info
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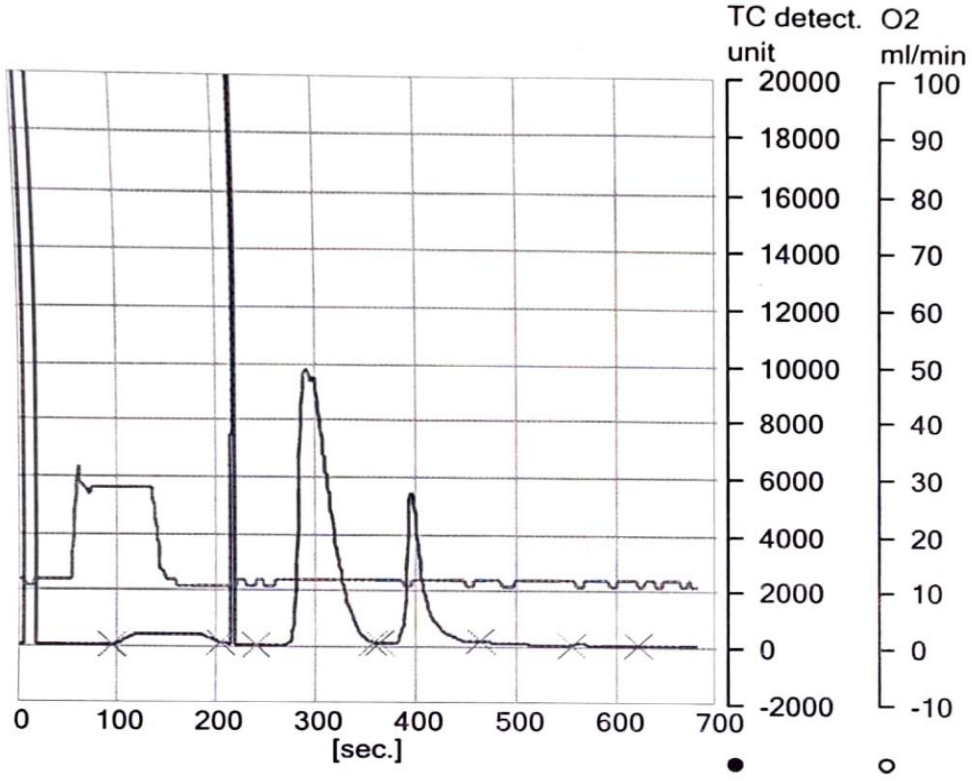

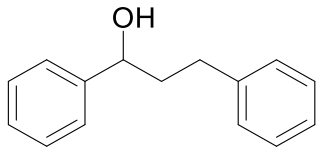

(**4**)

Figure S36. Elemental analysis data of (**4**).

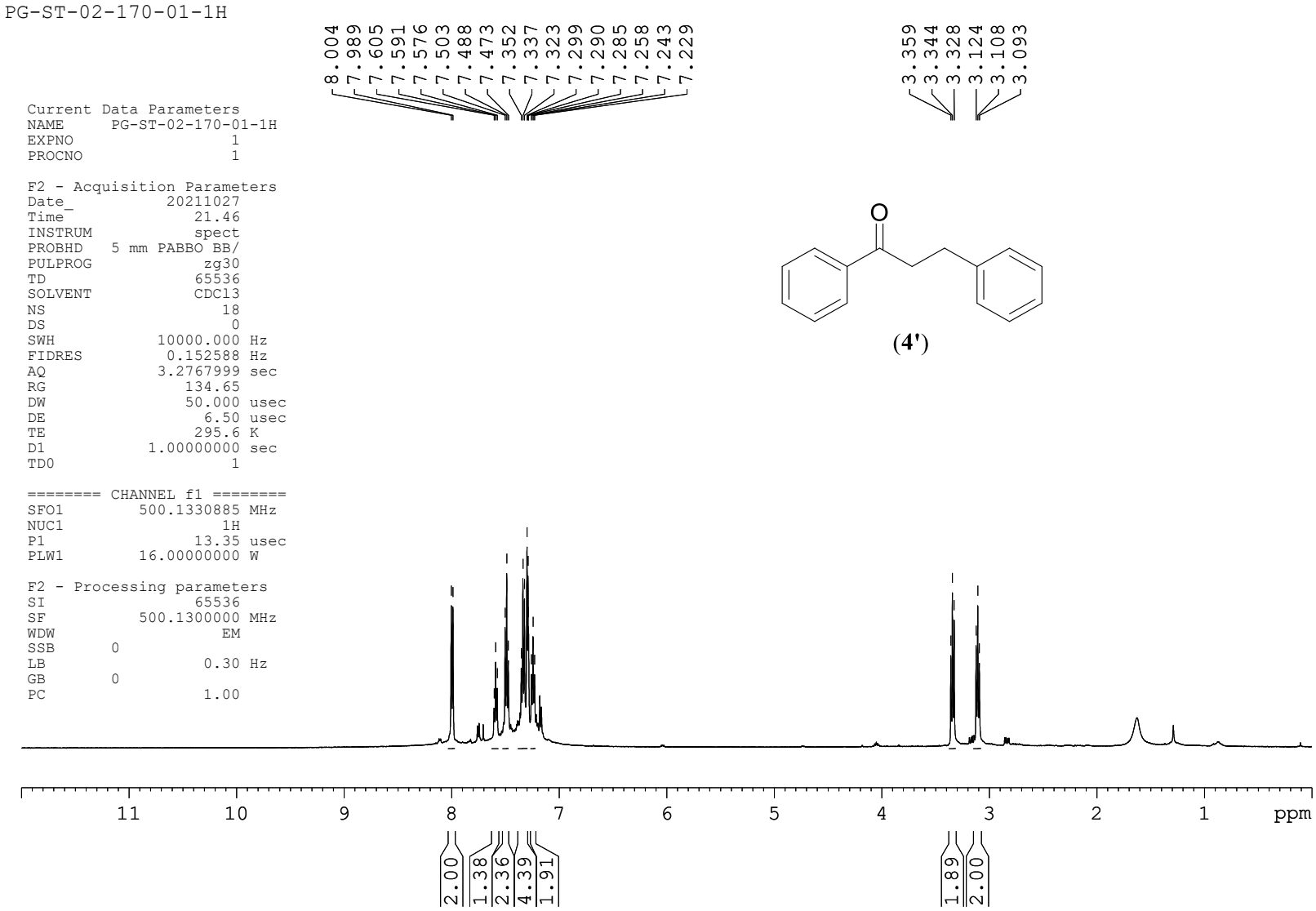

Figure S37. ^{1}H NMR spectrum of (**4'**) in $CDCl_3$.

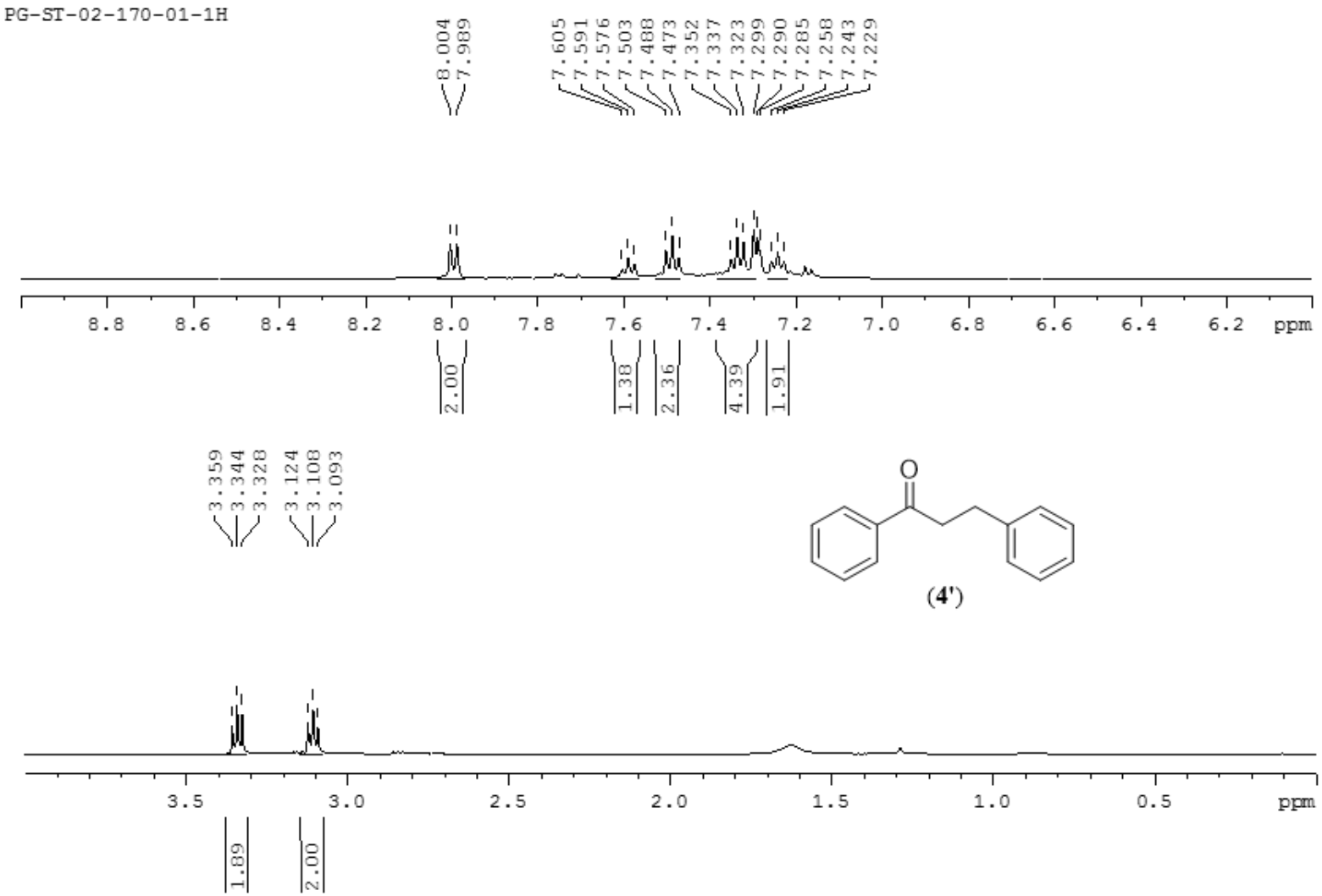

Figure S38. Expanded ^{1}H NMR spectrum of (**4'**) in $CDCl_3$.

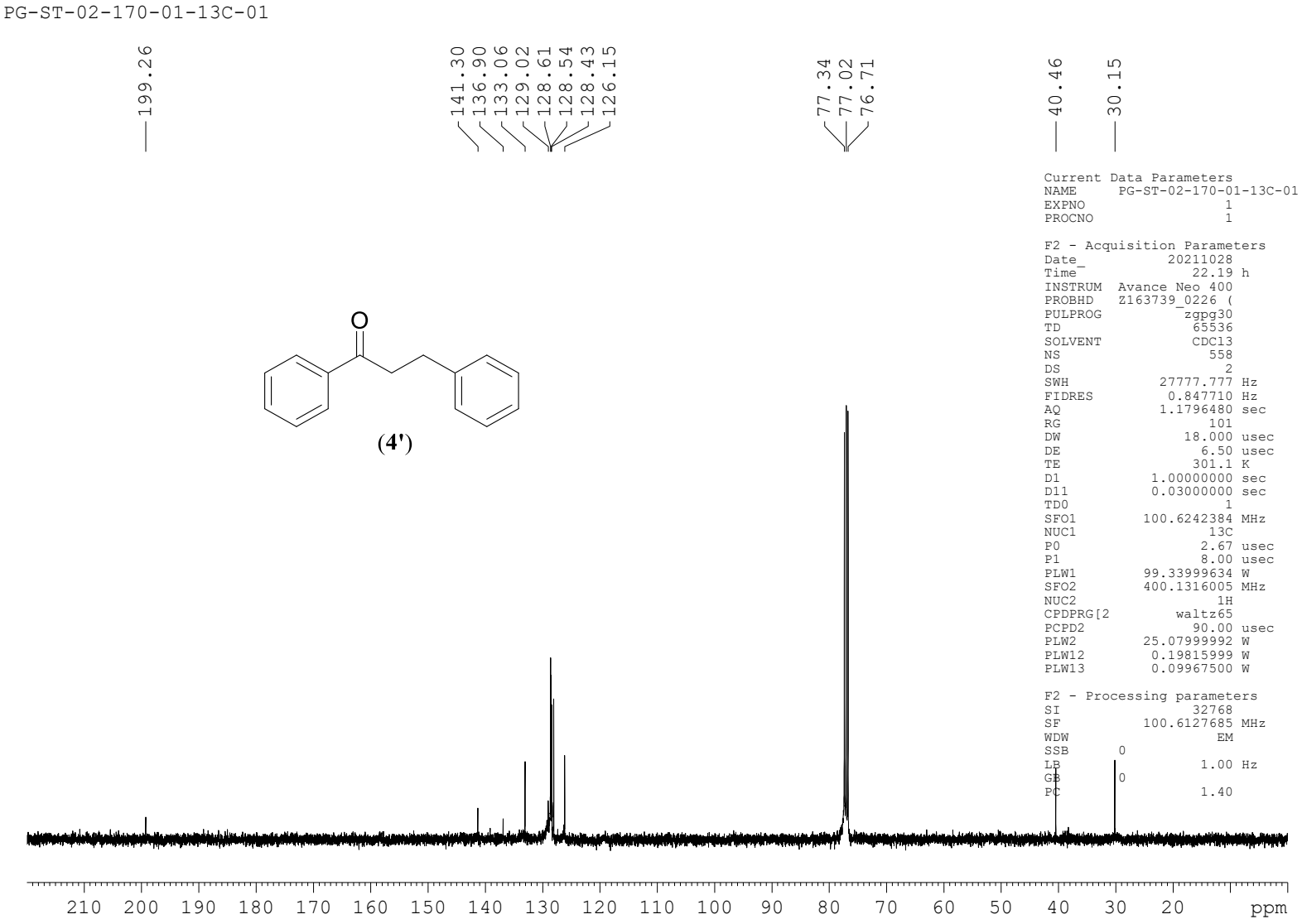

Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum of (**4'**) in $CDCl_3$.

Figure S40. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**4'**) in $CDCl_3$.

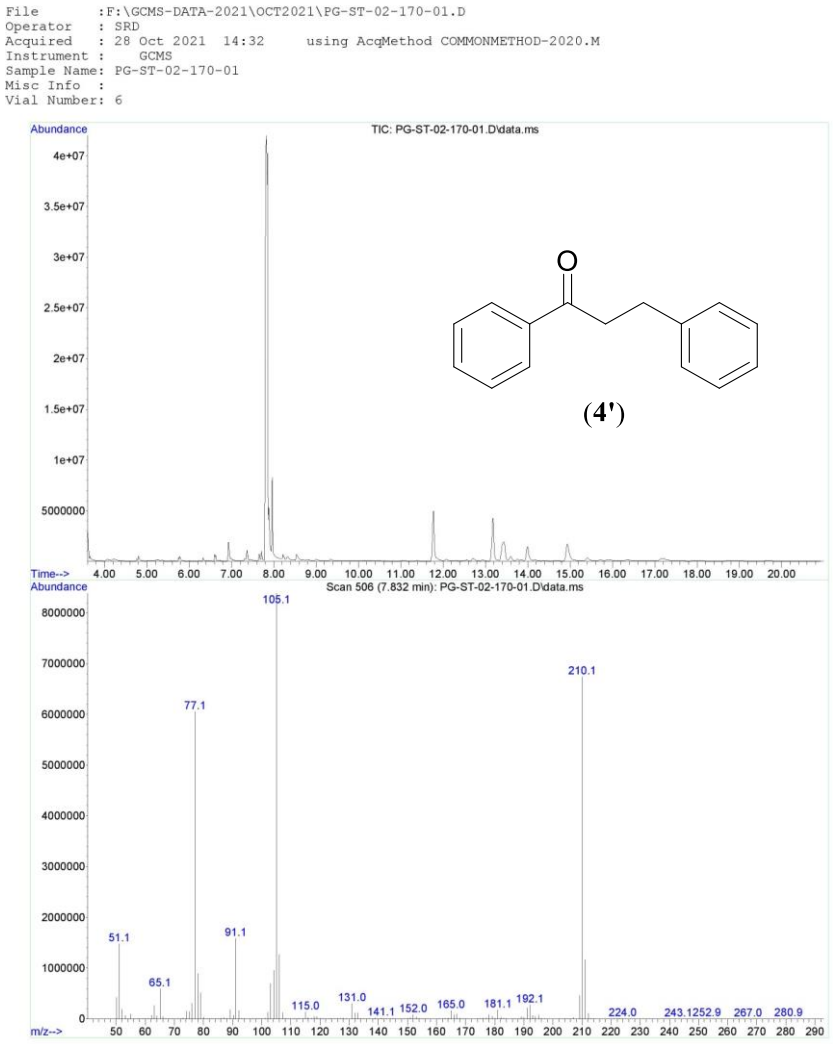

Figure S41. GCMS trace in EtOAc of (**4'**) showing the M^+ peak at *m/z* 210.

Document: CHNS11112021 (varioMICRO) from: 12-11-2021 10:04:06

SP18022016
varioMICRO CHNS
serial number: 15154051

Graphic report

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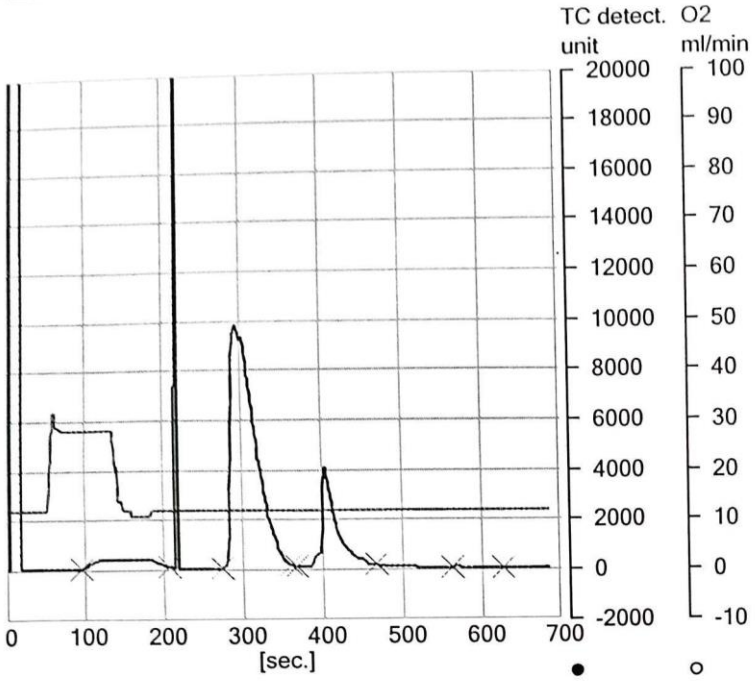

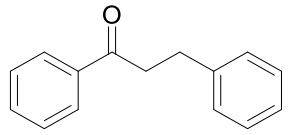

(4')

Figure S42. Elemental analysis data of (**4'**).

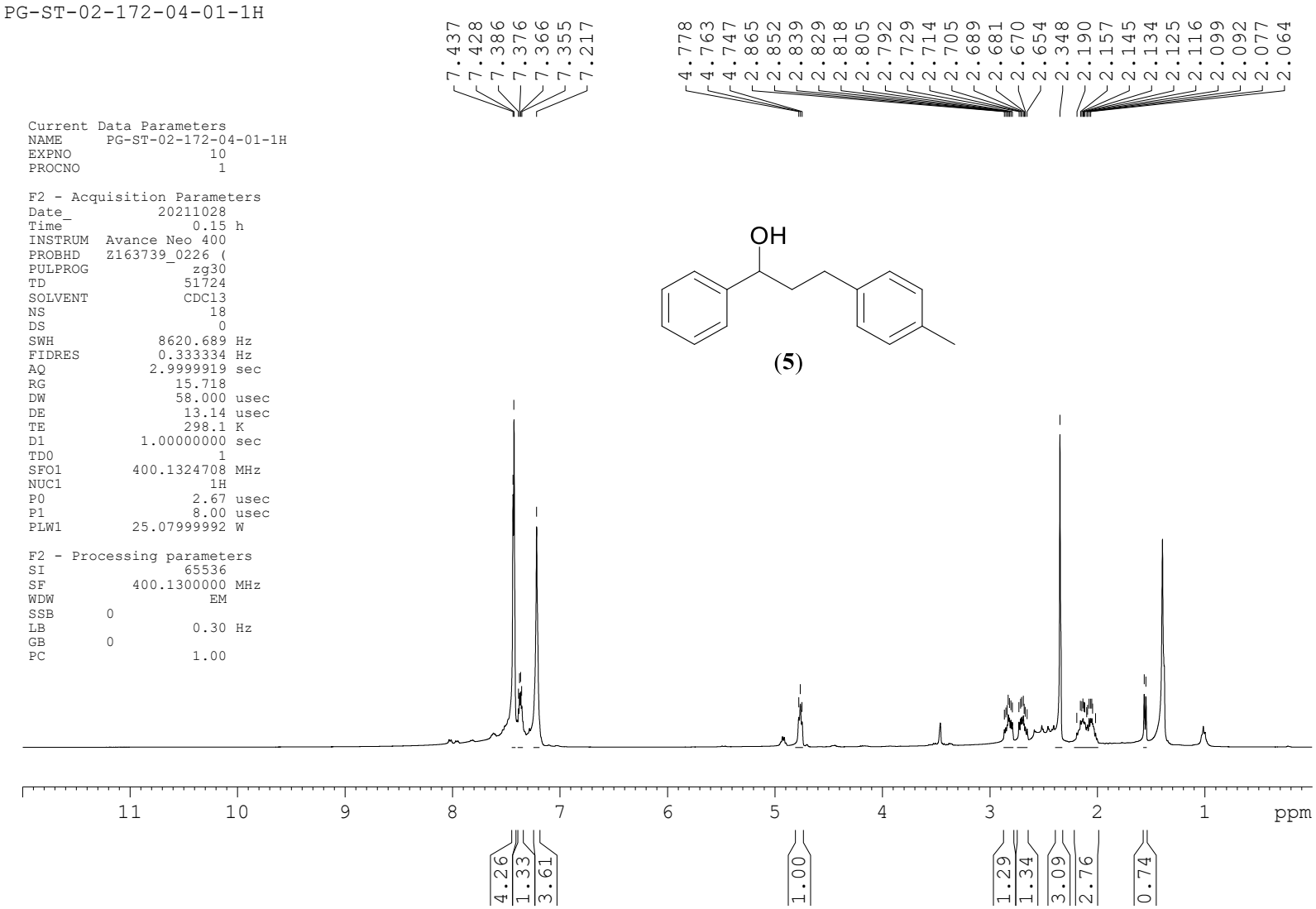

Figure S43. ^{1}H NMR spectrum of (**5**) in $CDCl_3$.

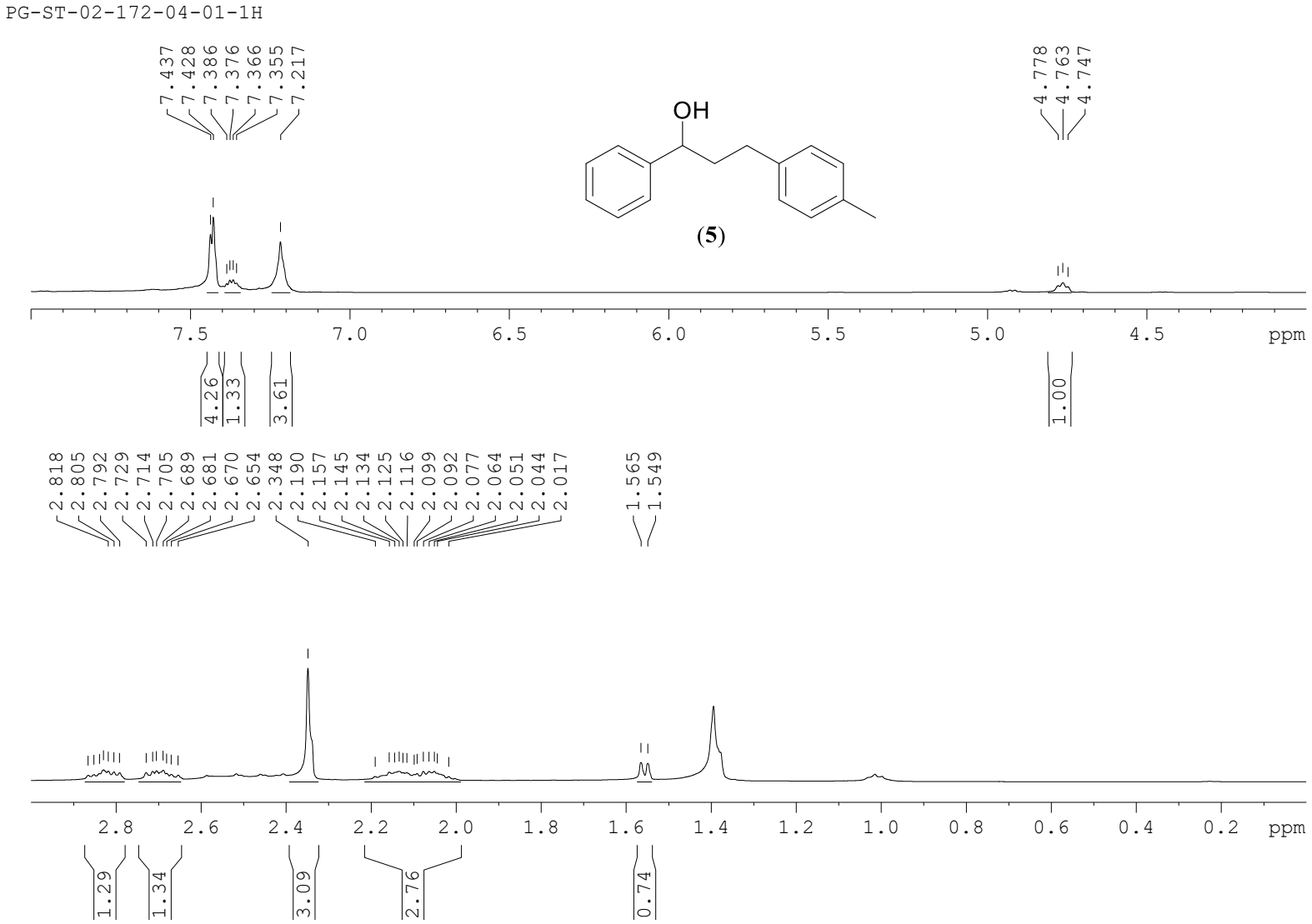

Figure S44. Expanded ^{1}H NMR spectrum of (**5**) in $CDCl_3$.

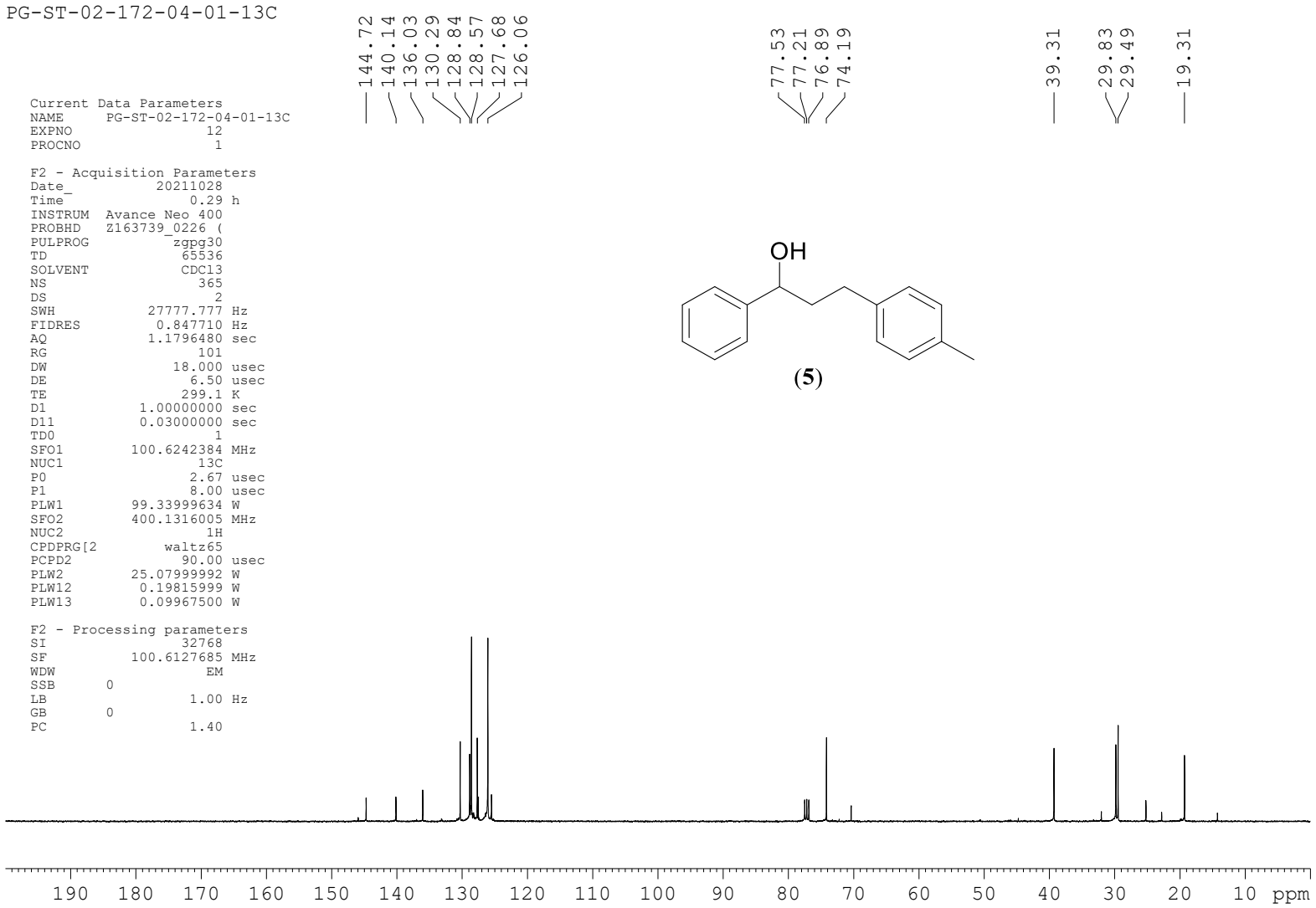

Figure S45. $^{13}C\{^{1}H\}$ NMR spectrum of (**5**) in $CDCl_3$.

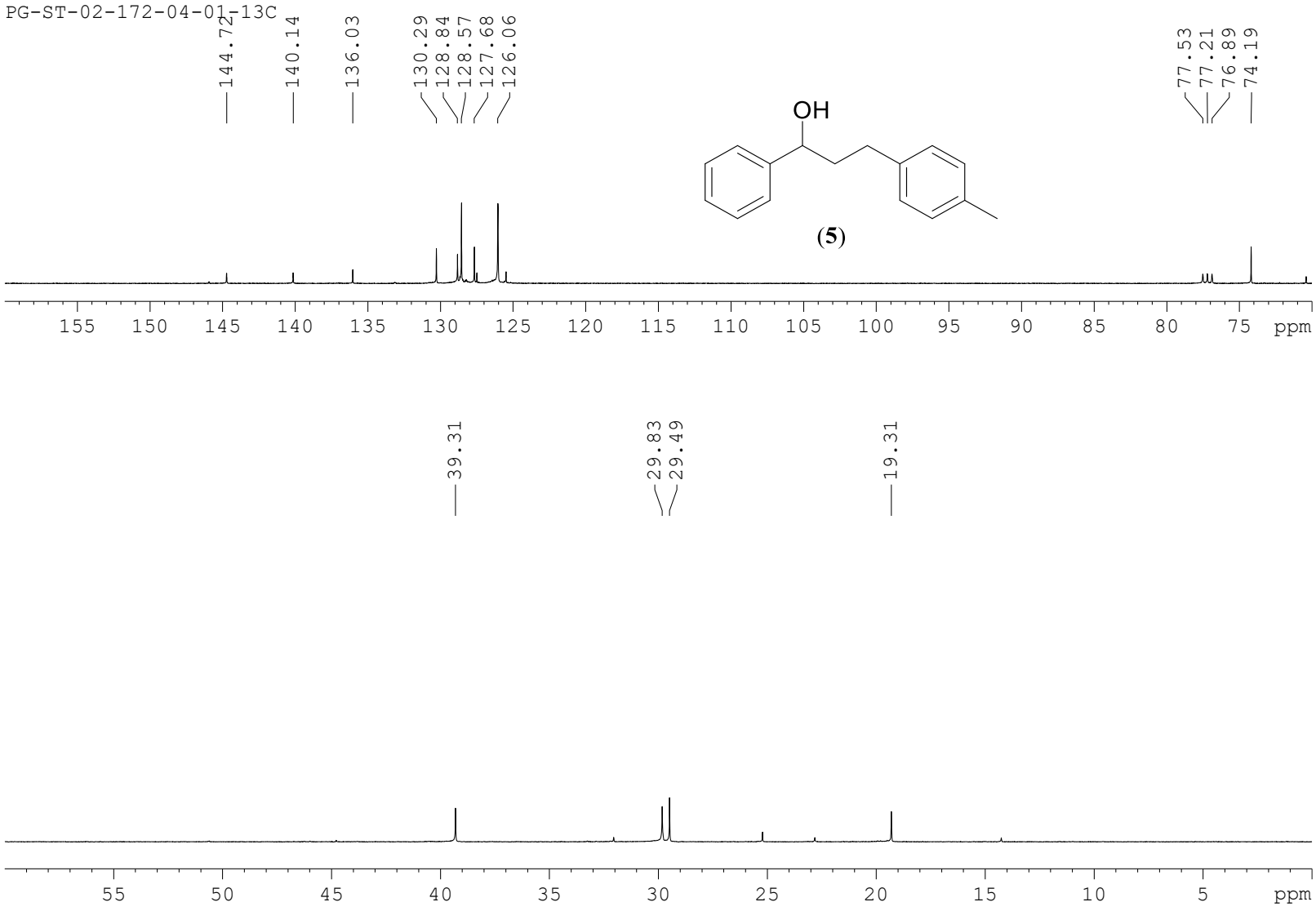

Figure S46. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**5**) in $CDCl_3$.

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Vial Number: 4
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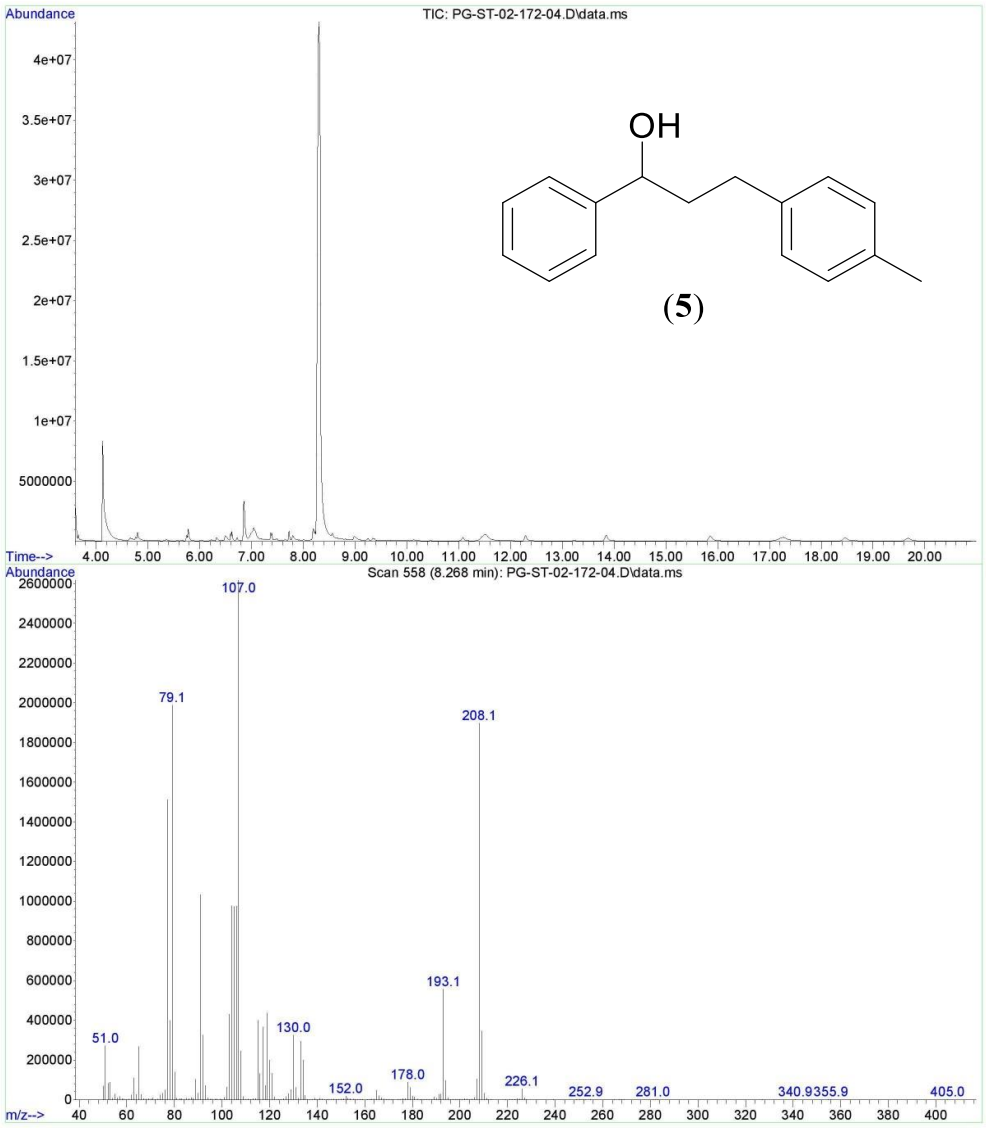

Figure S47. GCMS trace in EtOAc of (**5**) showing the M^+ peak at *m/z* 226.

Document: CHNS21012022 (varioMICRO) from: --.--.-- (modified)

SP18022016
varioMICRO CHNS
serial number: 15154051

Graphic report

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date Time	Info
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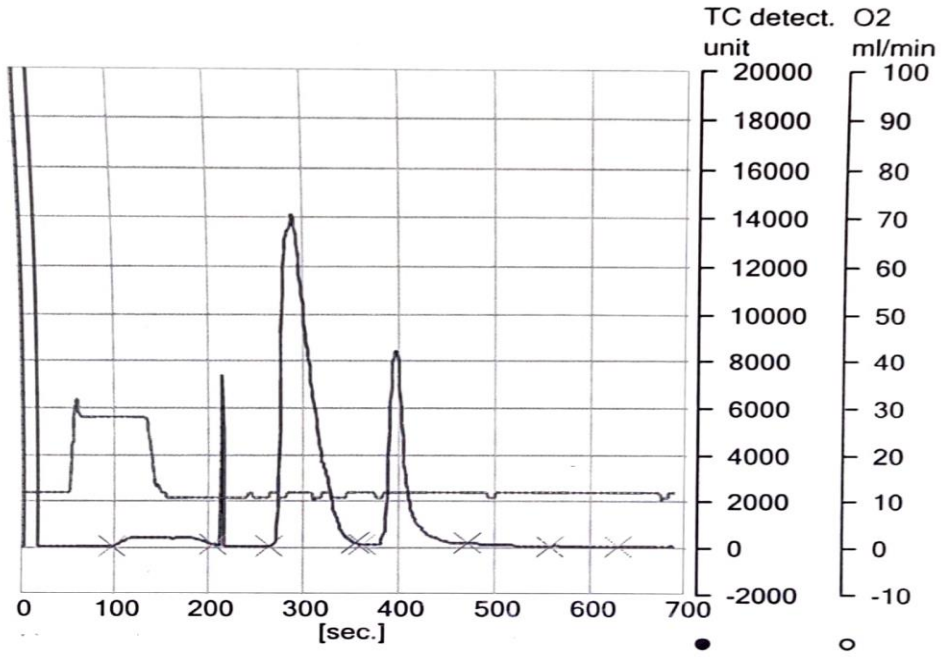

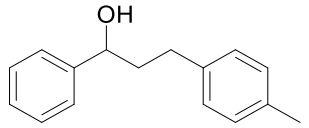

(**5**)

Figure S48. Elemental analysis data of (**5**).

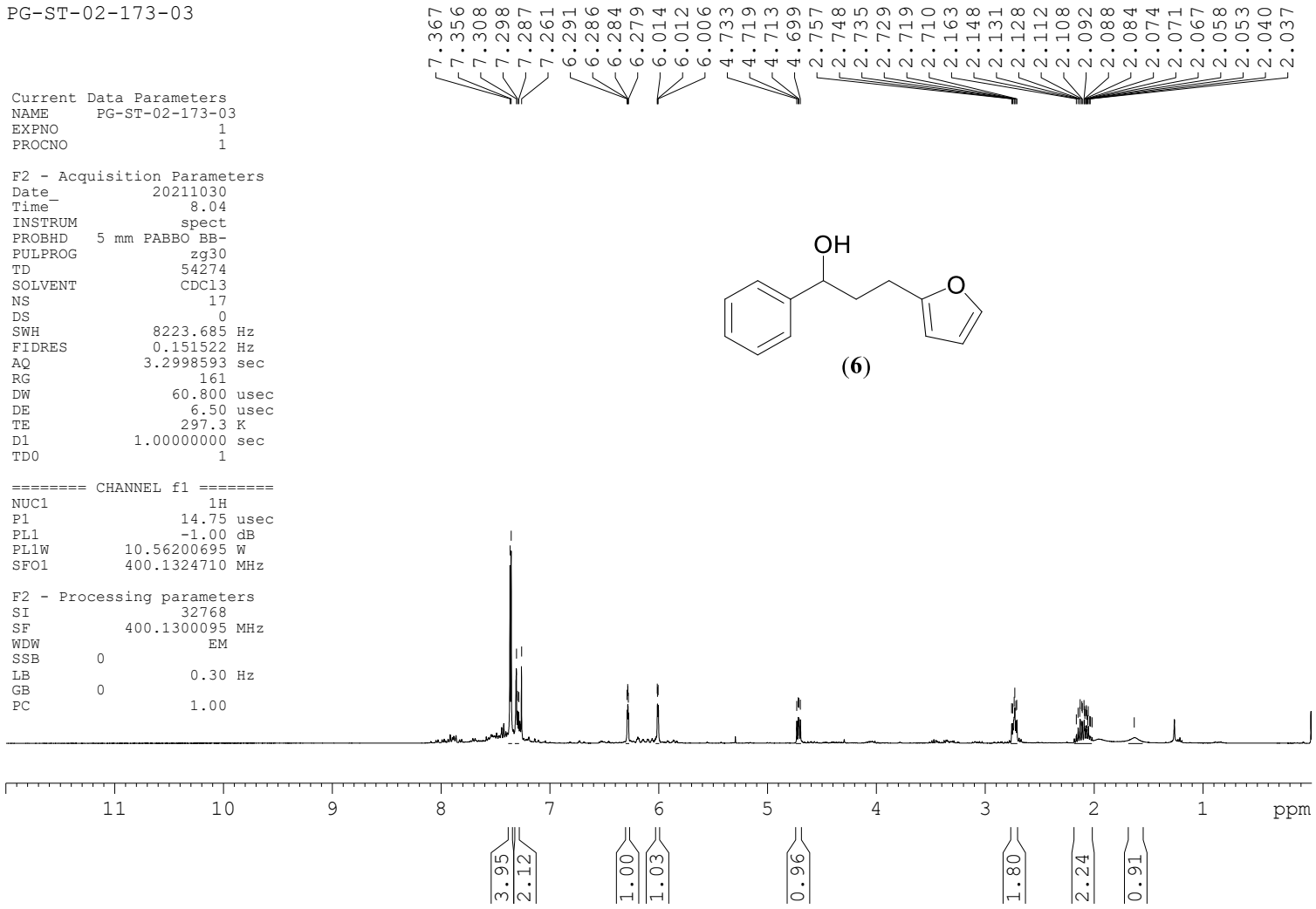

Figure S49. ^{1}H NMR spectrum of (**6**) in $CDCl_3$.

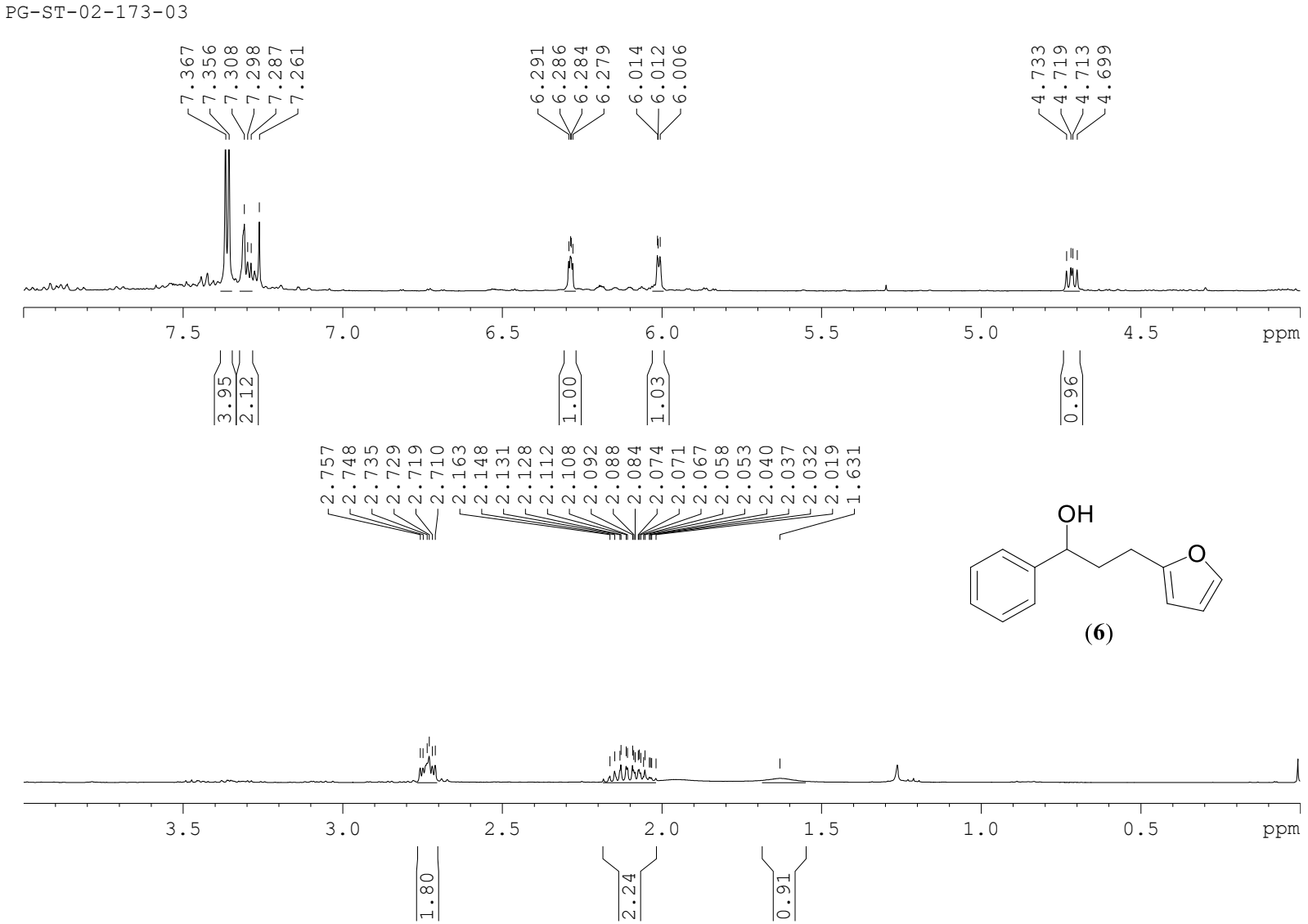

Figure S50. Expanded ^{1}H NMR spectrum of (**6**) in $CDCl_3$.

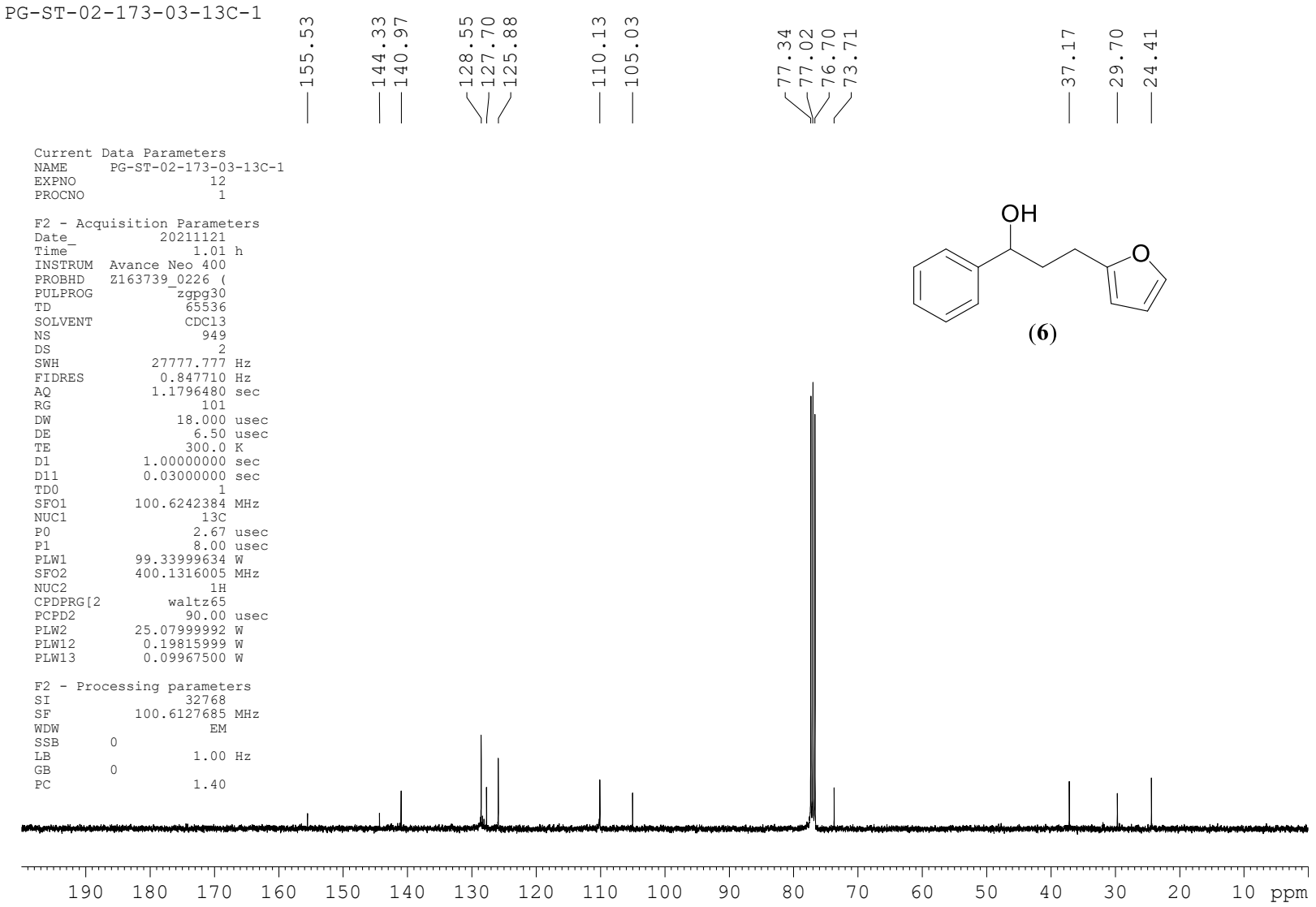

Figure S51. $^{13}C\{^{1}H\}$ NMR spectrum of (**6**) in $CDCl_3$.

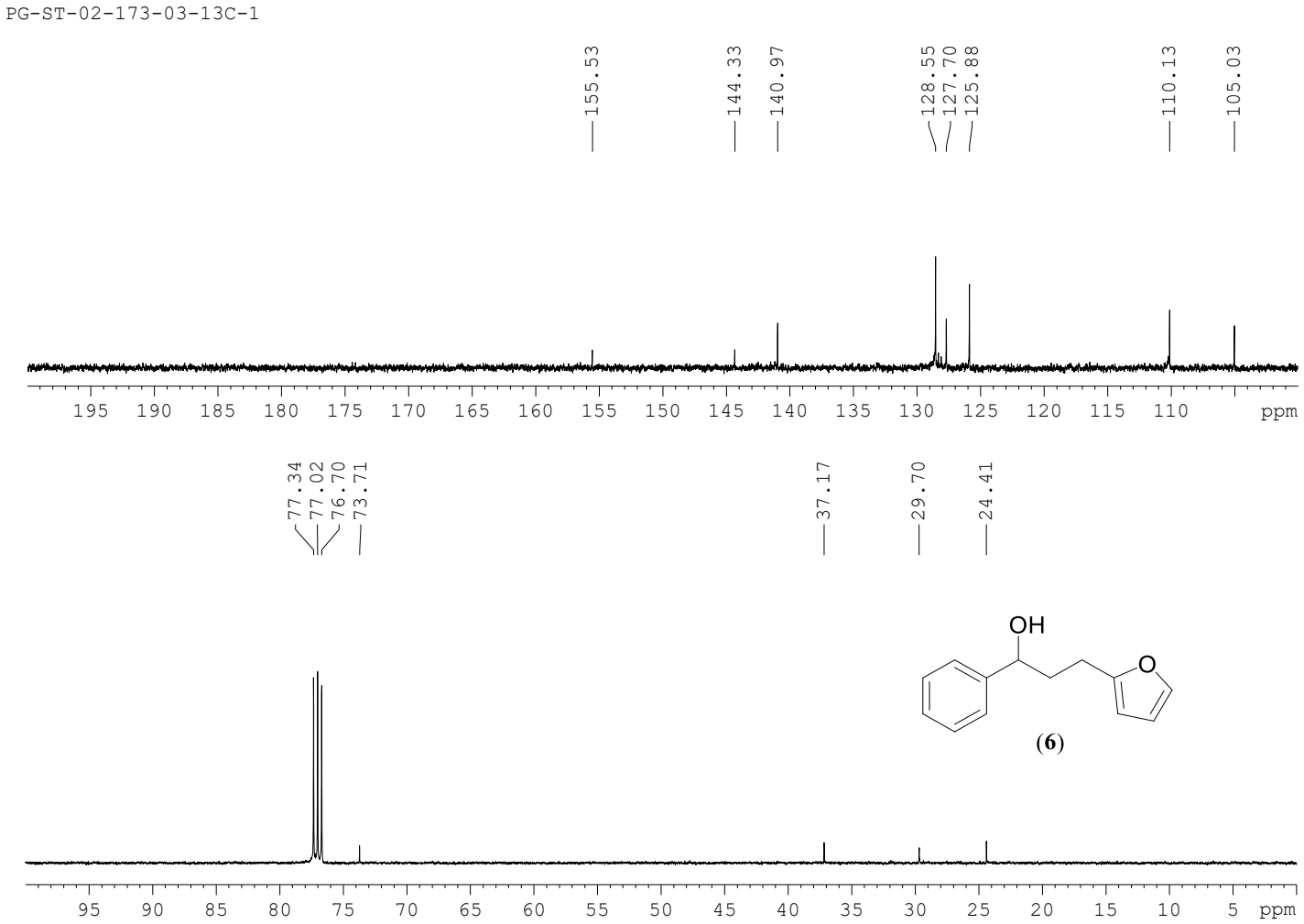

Figure S52. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**6**) in $CDCl_3$.

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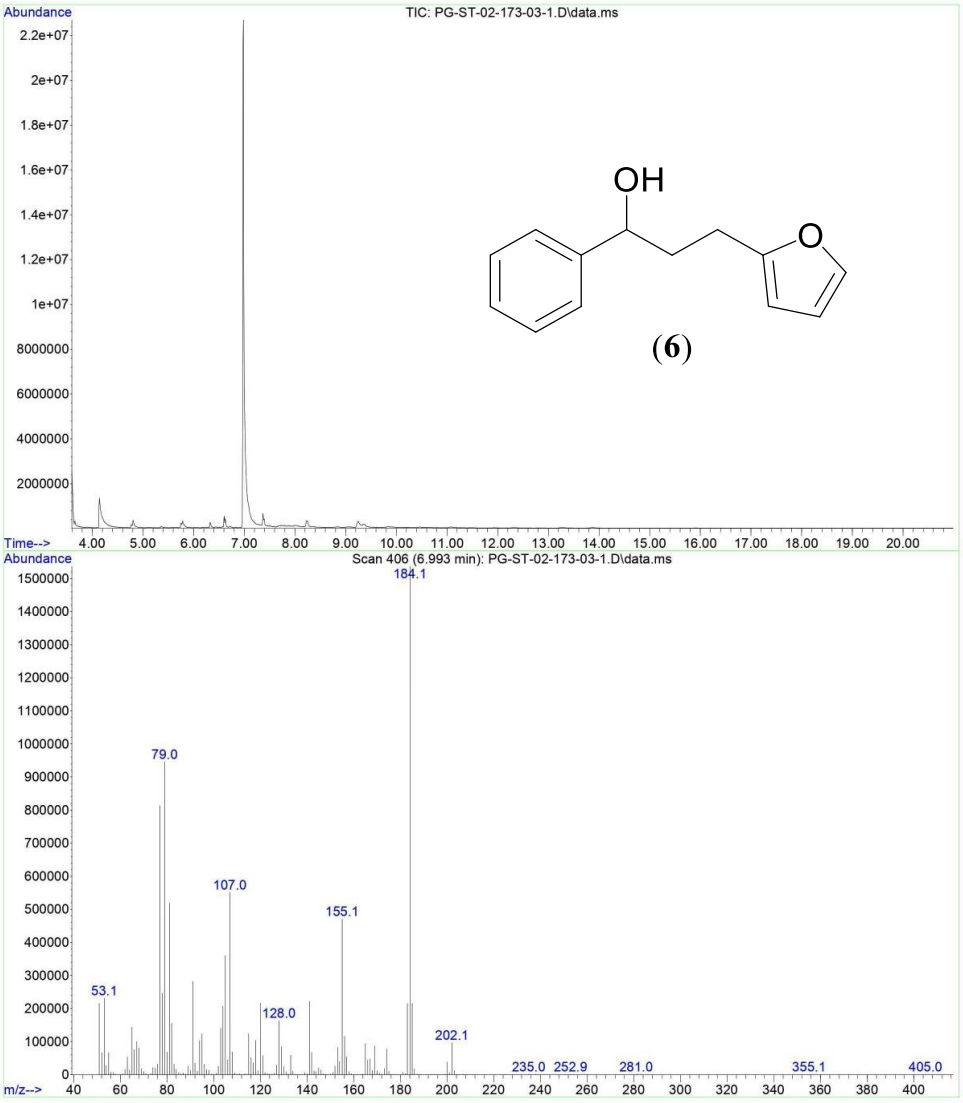

Figure S53. GCMS trace in EtOAc of (**6**) showing the M^+ peak at *m/z* 202.

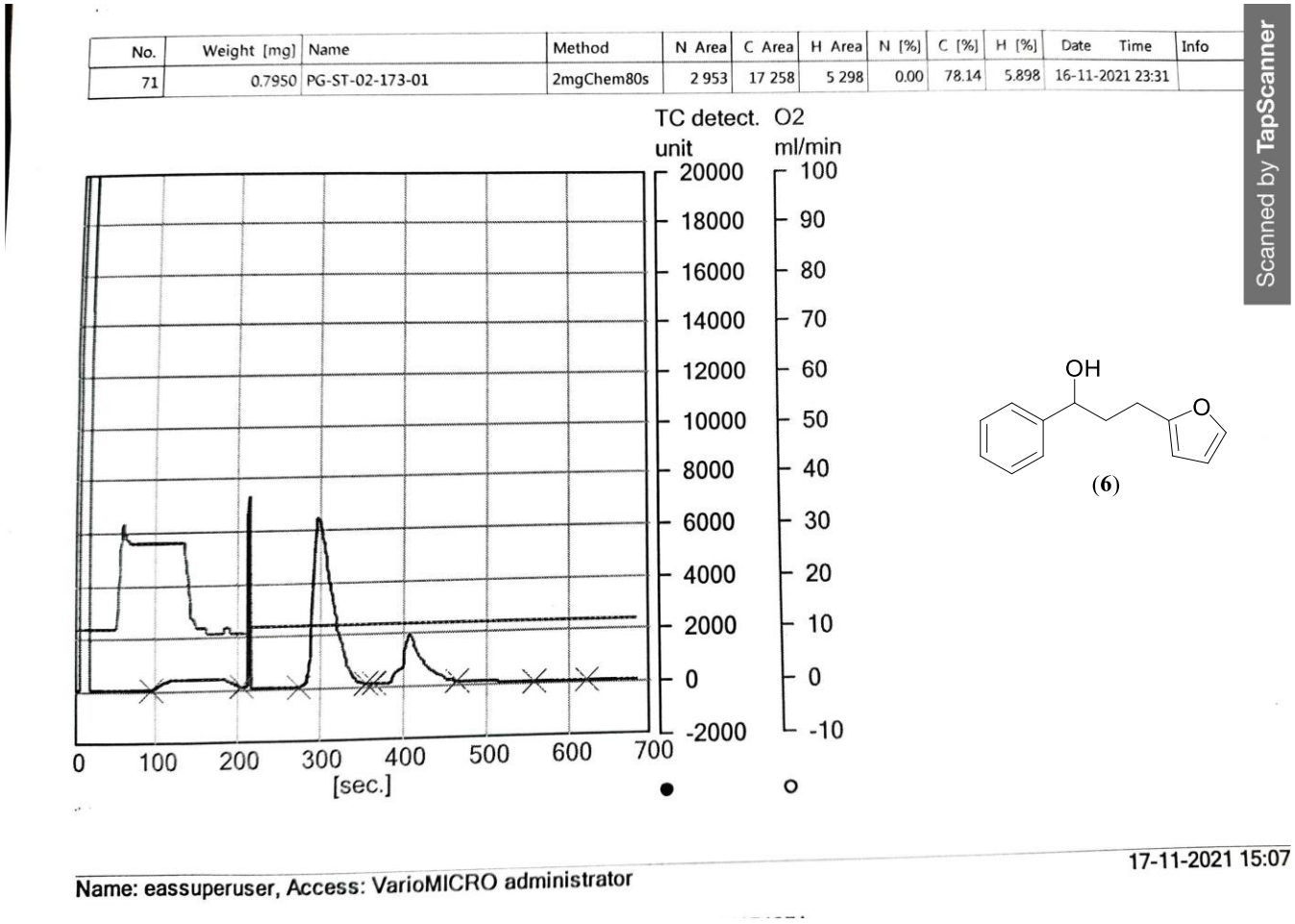

Figure S54. Elemental analysis data of (**6**).

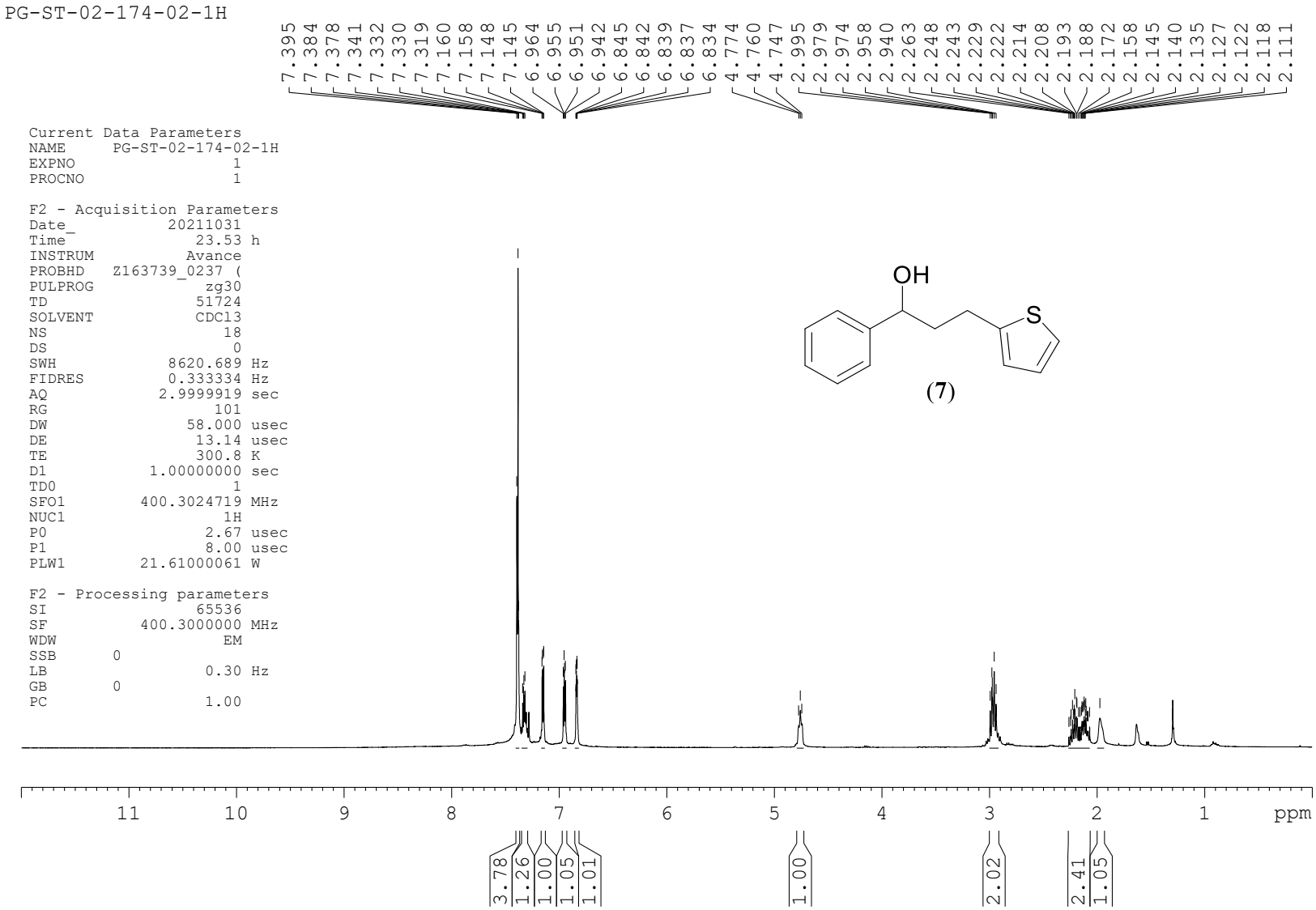

Figure S55. ^{1}H NMR spectrum of (**7**) in $CDCl_3$.

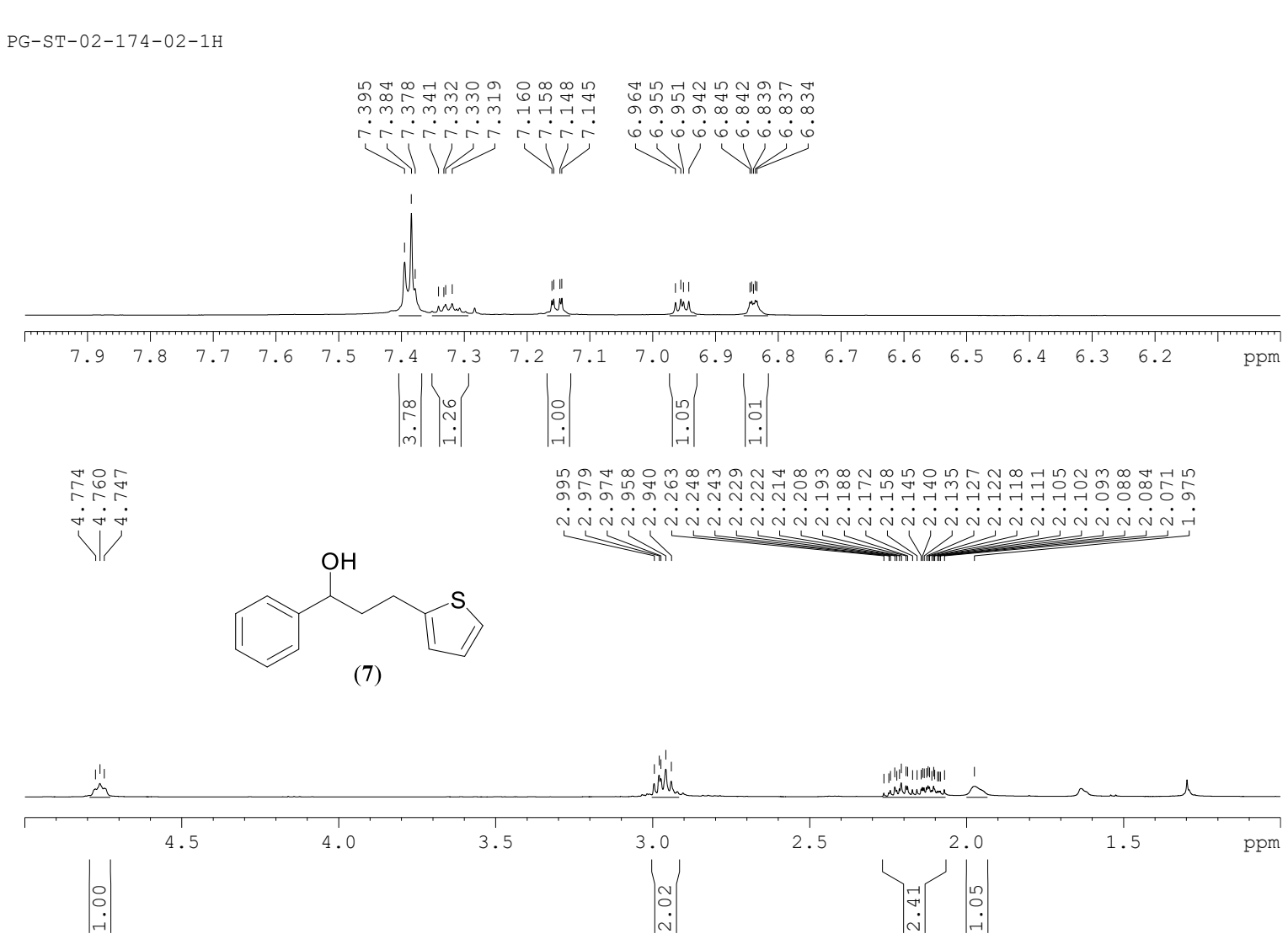

Figure S56. Expanded ^{1}H NMR spectrum of (**7**) in $CDCl_3$.

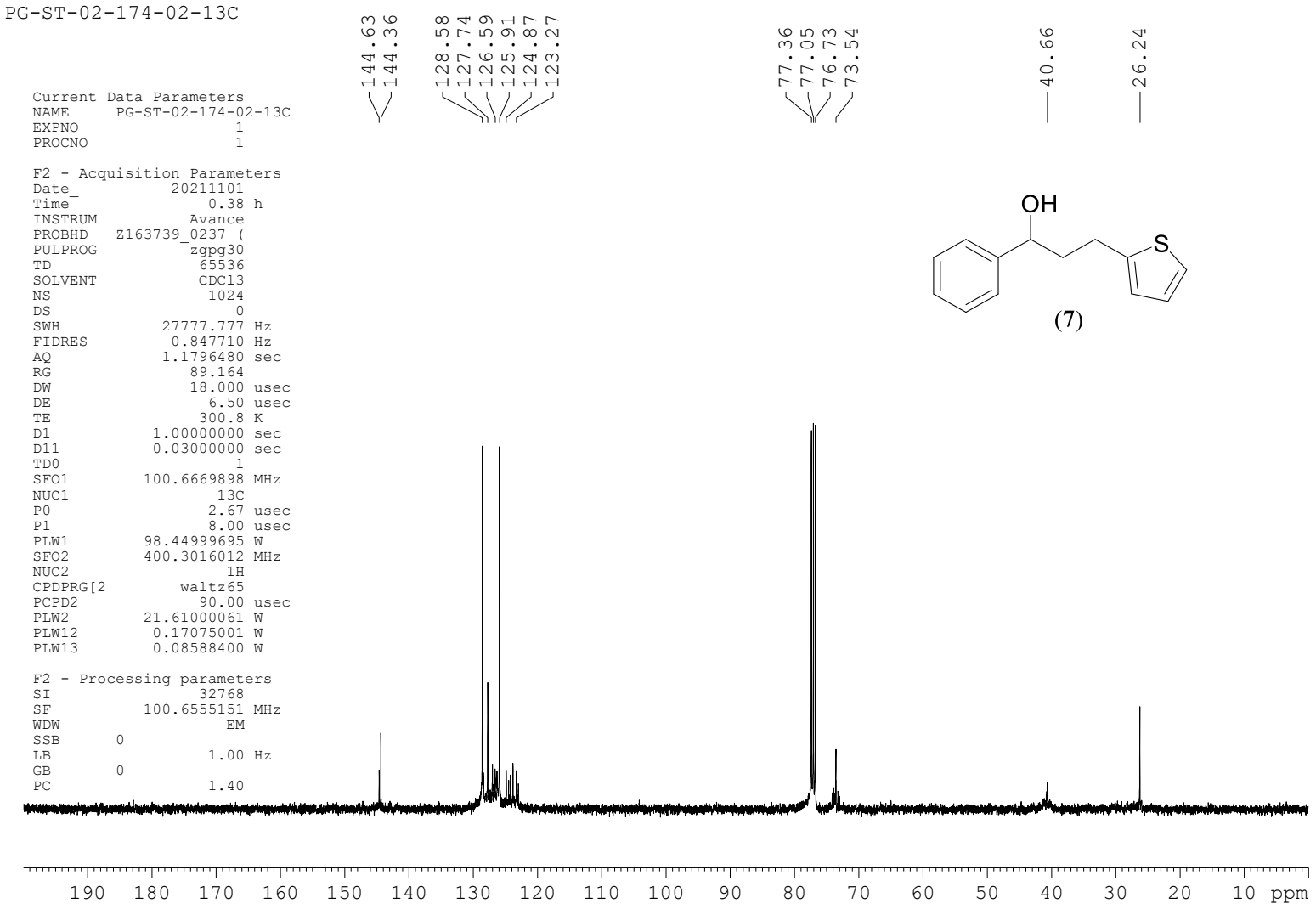

Figure S57. $^{13}C\{^{1}H\}$ NMR spectrum of (**7**) in $CDCl_3$.

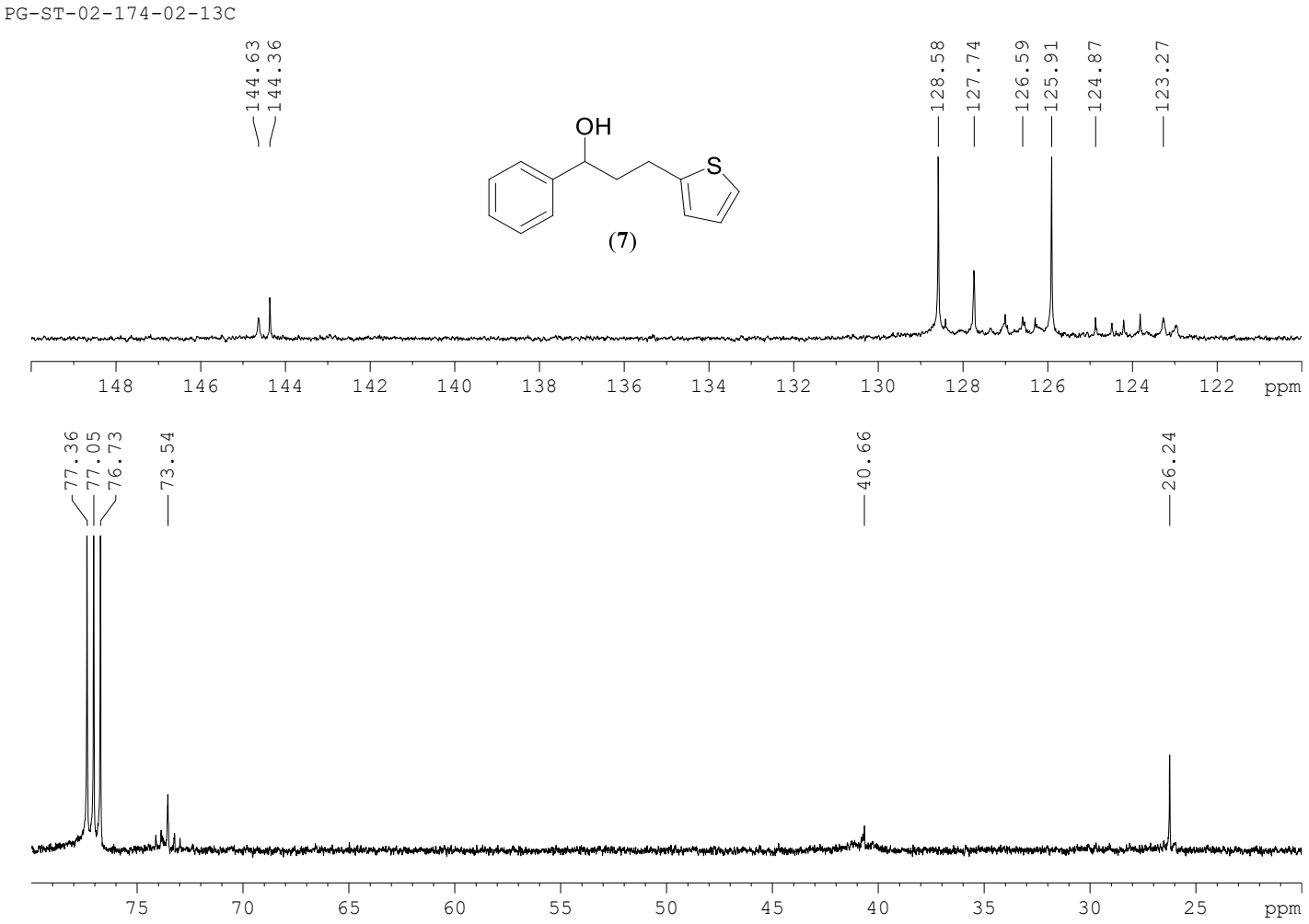

Figure S58. $^{13}C\{^{1}H\}$ NMR spectrum of (**7**) in $CDCl_3$.

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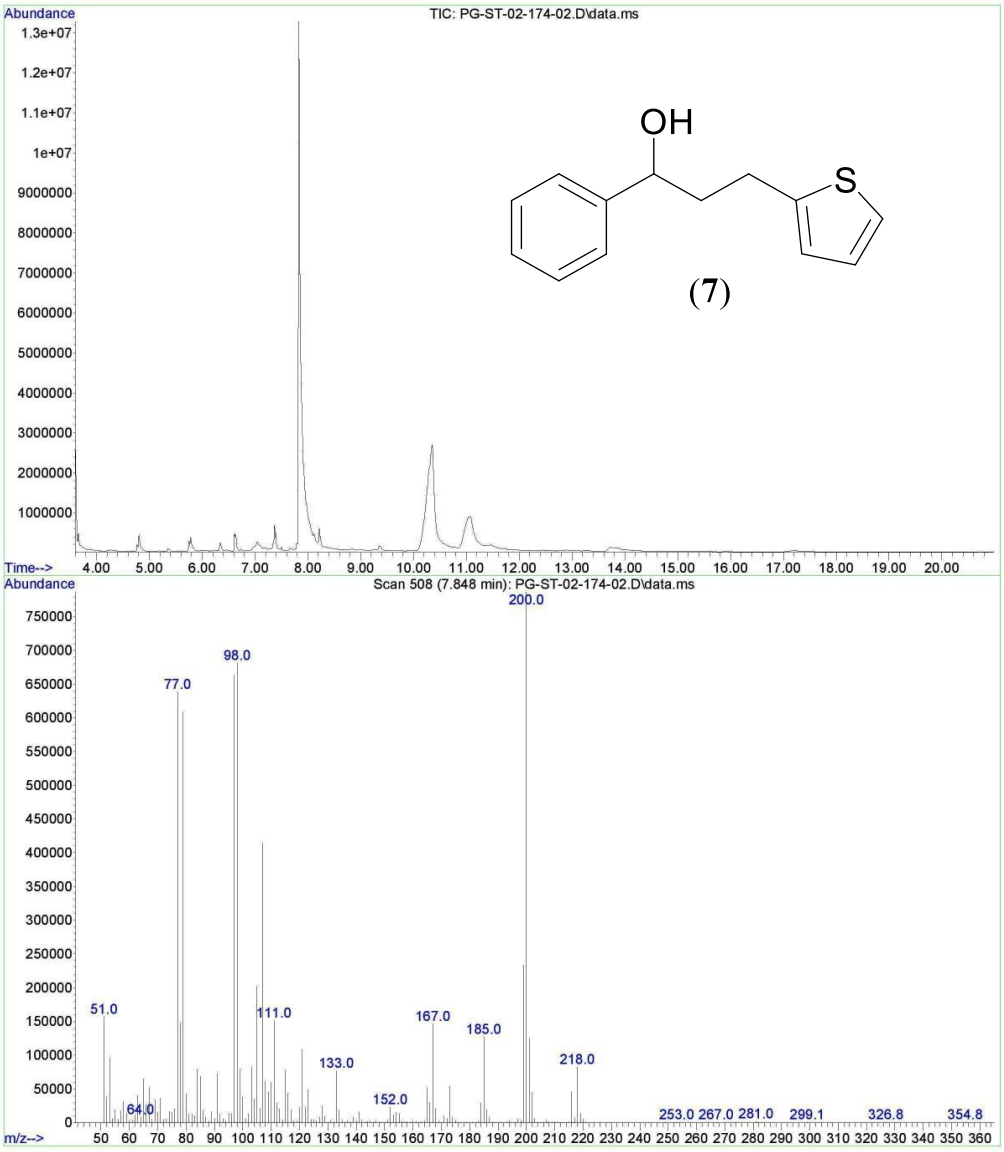

Figure S59. GCMS trace in EtOAc of (**7**) showing the M^+ peak at *m/z* 218.

Document: CHNS21012022 (varioMICRO) from: --.--.-- (modified)

SP18022016
varioMICRO CHNS
serial number: 15154051

Graphic report

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	S Area	N [%]	C [%]	H [%]	S [%]	Date	Time	Info
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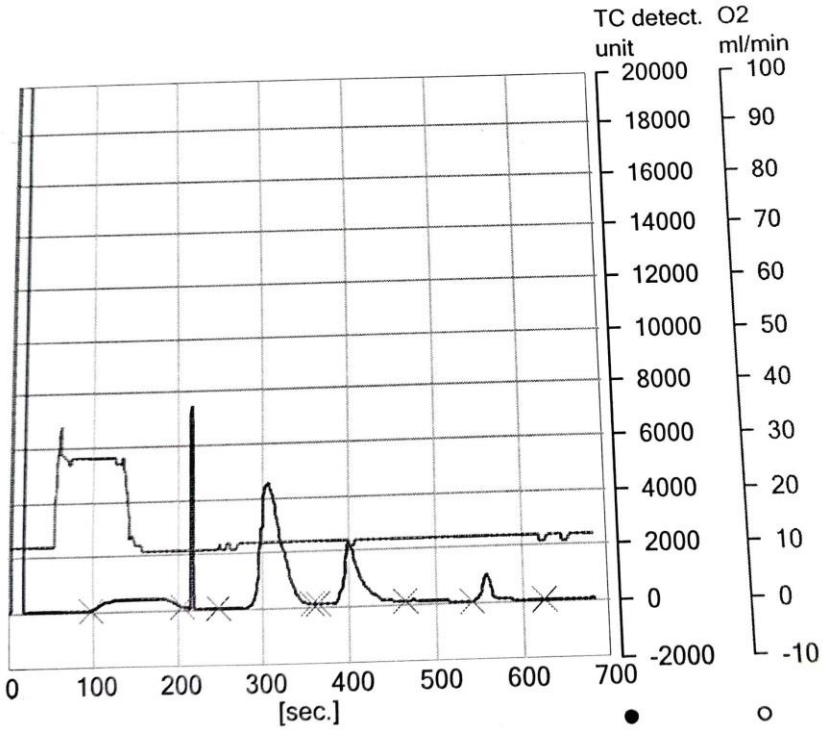

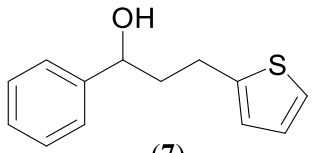

(**7**)

Figure S60. Elemental analysis data of (**7**).

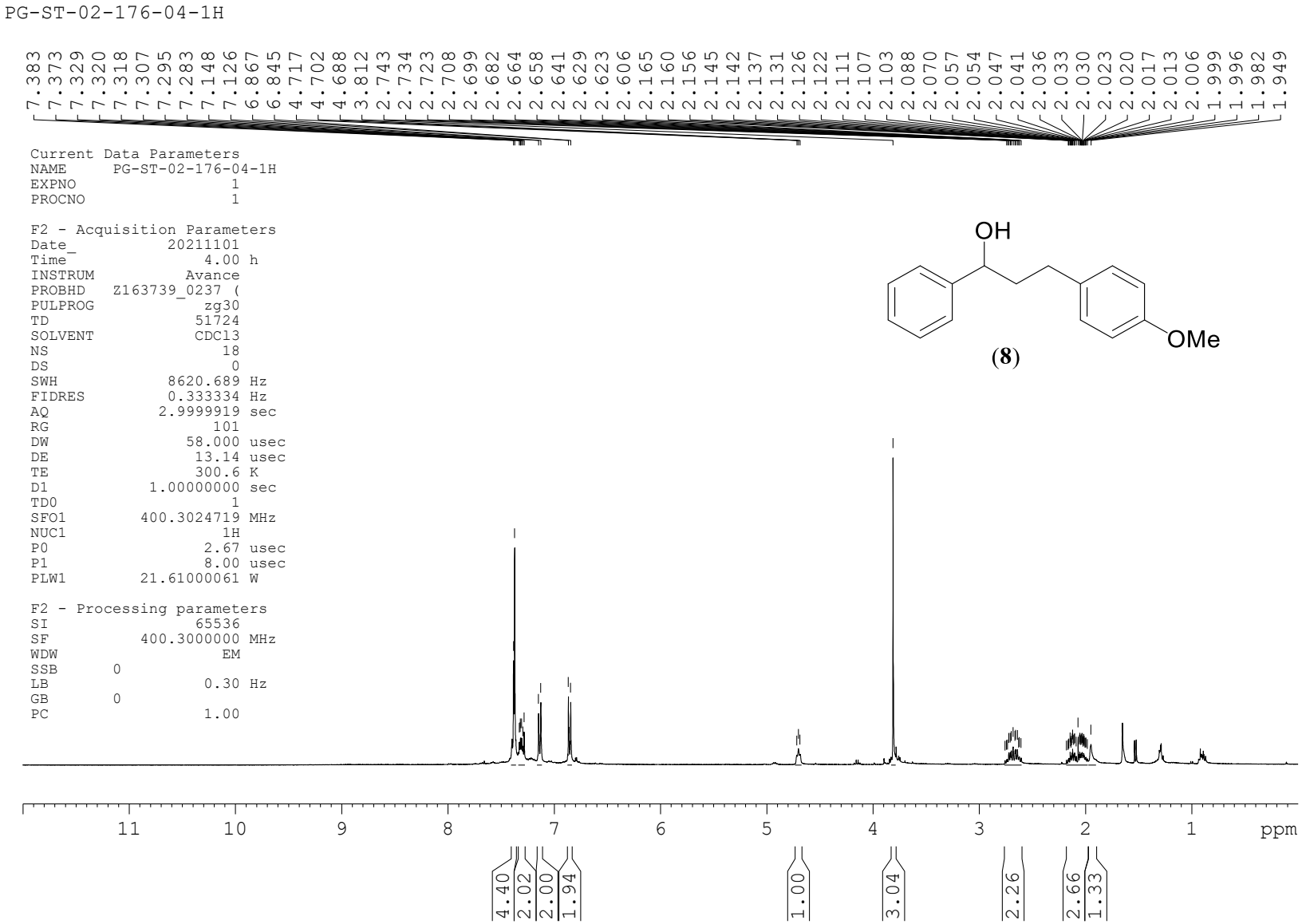

Figure S61. ^{1}H NMR spectrum of (**8**) in $CDCl_3$.

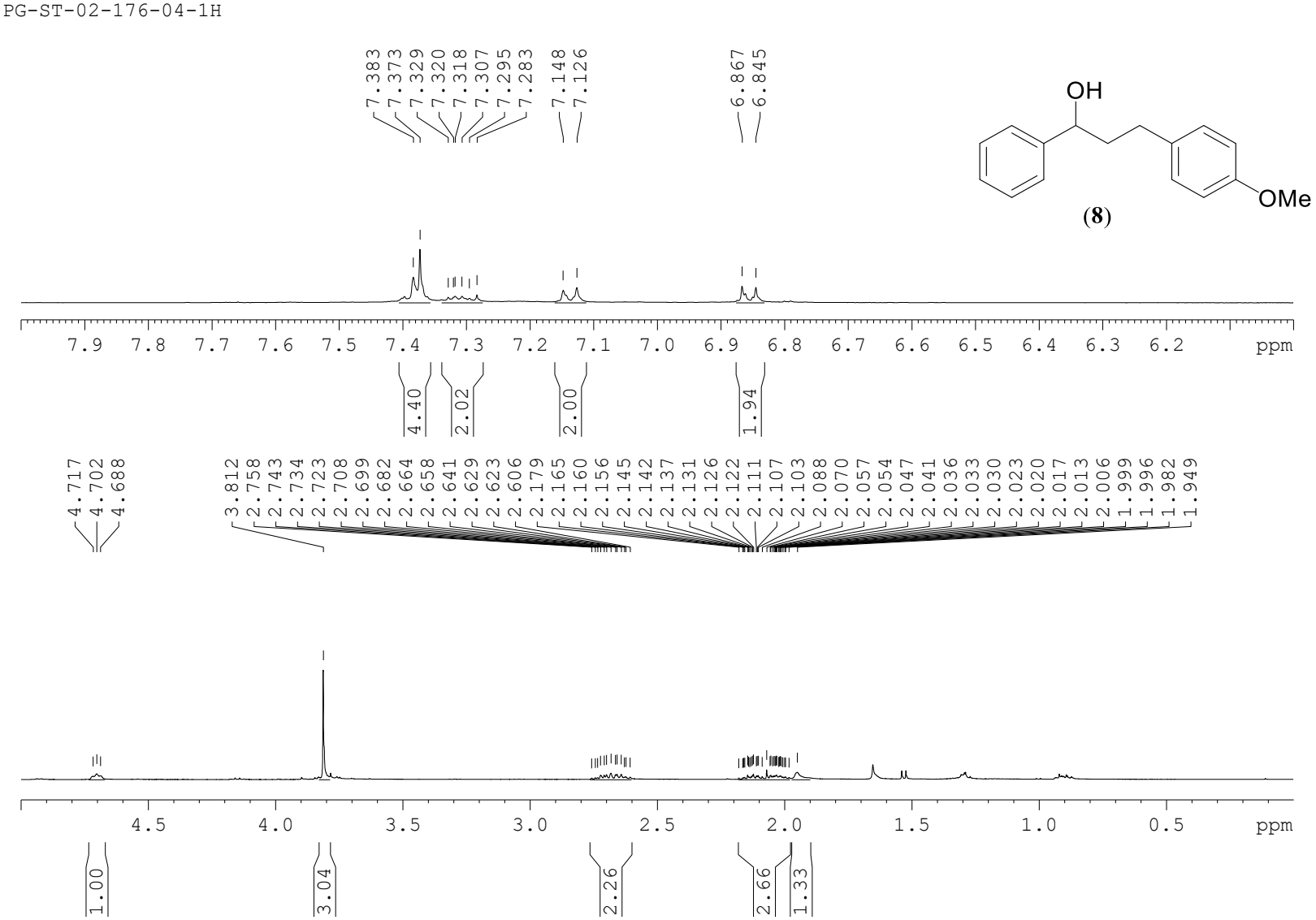

Figure S62. Expanded ^{1}H NMR spectrum of (**8**) in $CDCl_3$.

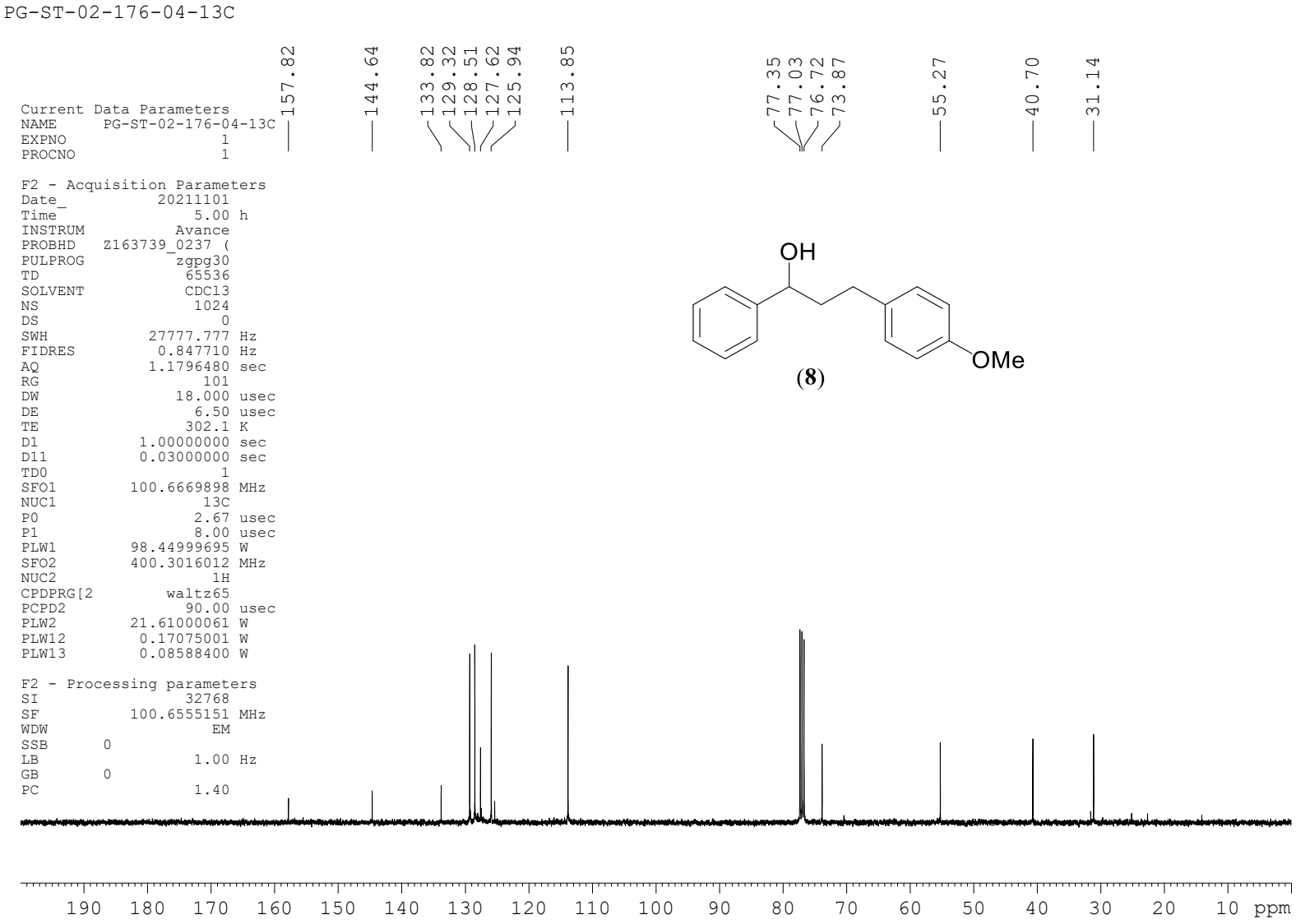

Figure S63. $^{13}C\{^{1}H\}$ NMR spectrum of (**8**) in $CDCl_3$.

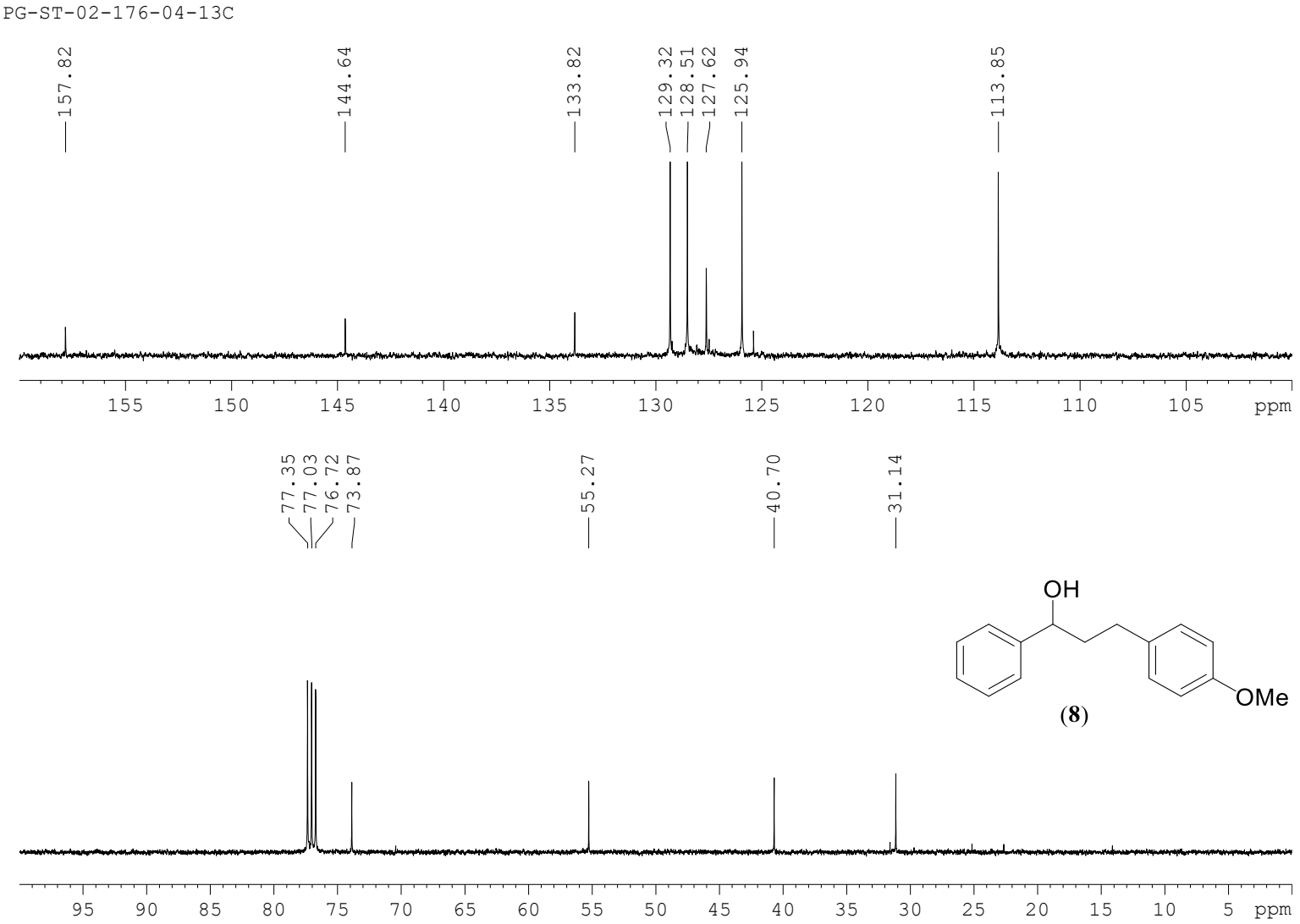

Figure S64. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**8**) in $CDCl_3$

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Acquired   :  1 Nov 2021  18:43     using AcqMethod COMMONMETHOD-2020.M
Instrument :    GCMS
Sample Name: PG-ST-02-176-04
Misc Info  :
Vial Number: 7
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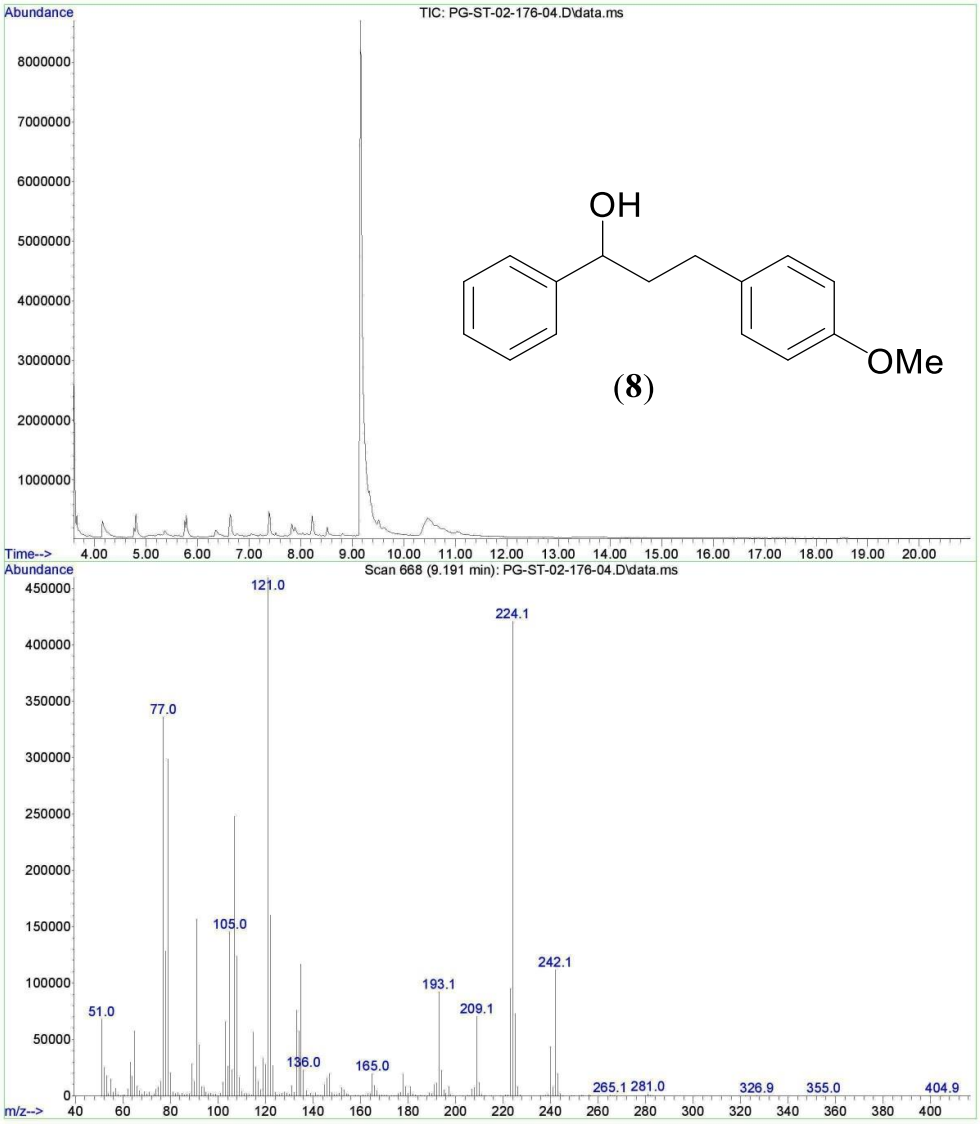

Figure S65. GCMS trace in EtOAc of (**8**) showing the M^+ peak at *m/z* 242.

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date Time	Info
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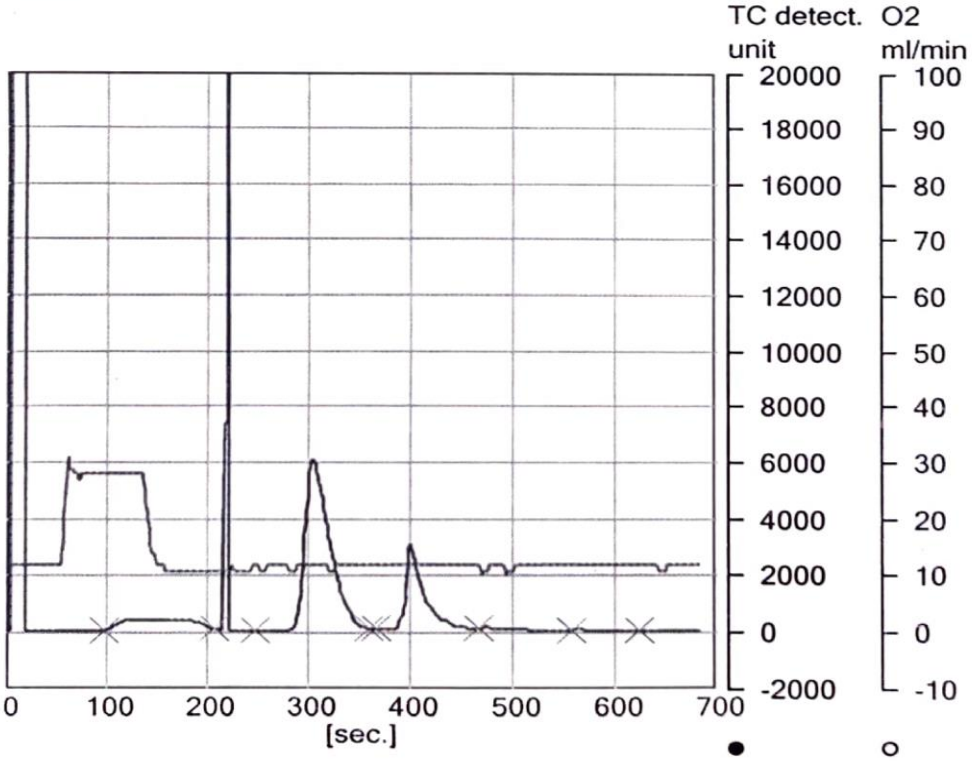

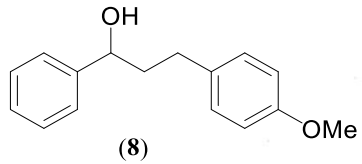

(**8**)

Figure S66. Elemental analysis data of (**8**).

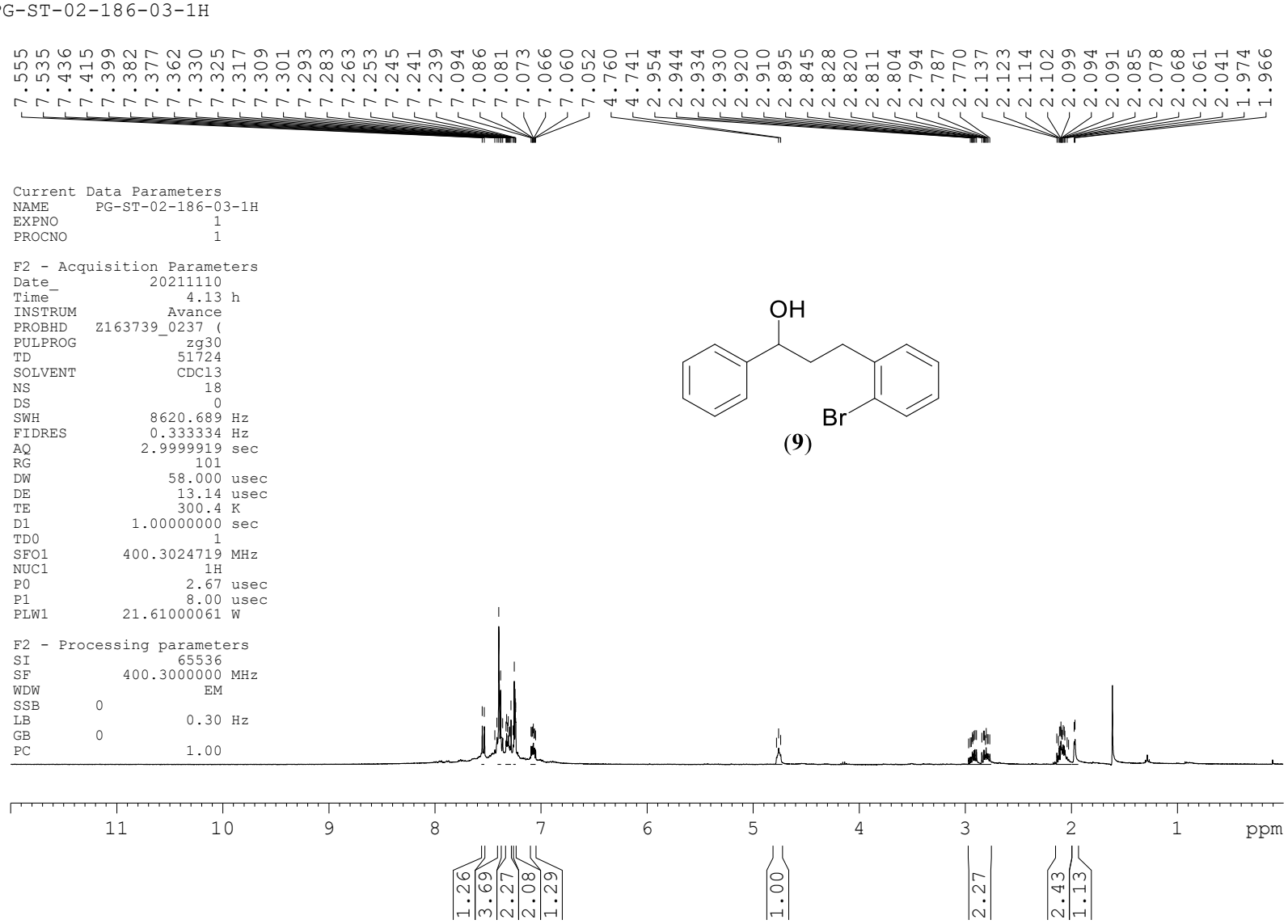

Figure S67. ^{1}H NMR spectrum of (**9**) in $CDCl_3$.

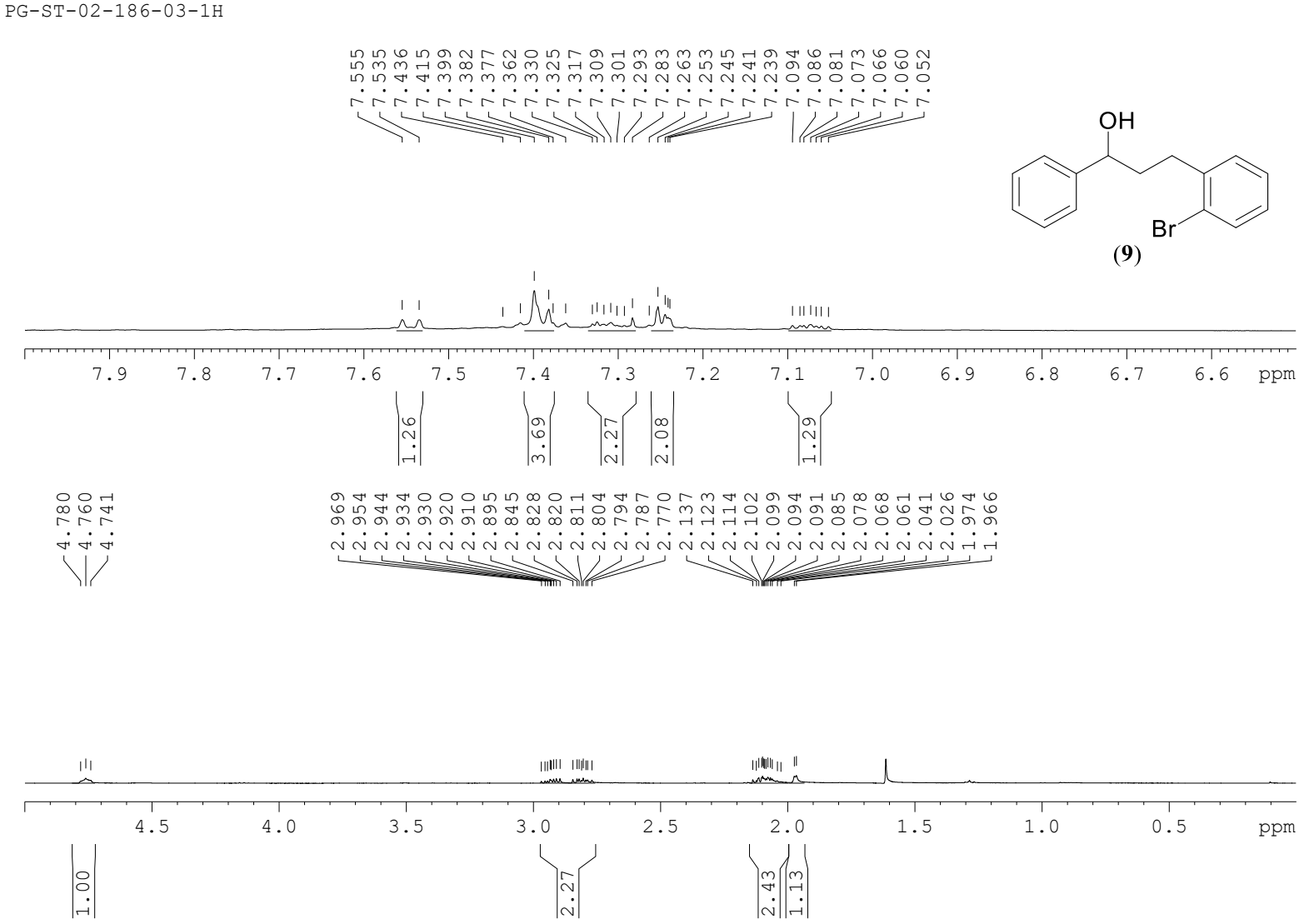

Figure S68. Expanded ^{1}H NMR spectrum of (**9**) in $CDCl_3$.

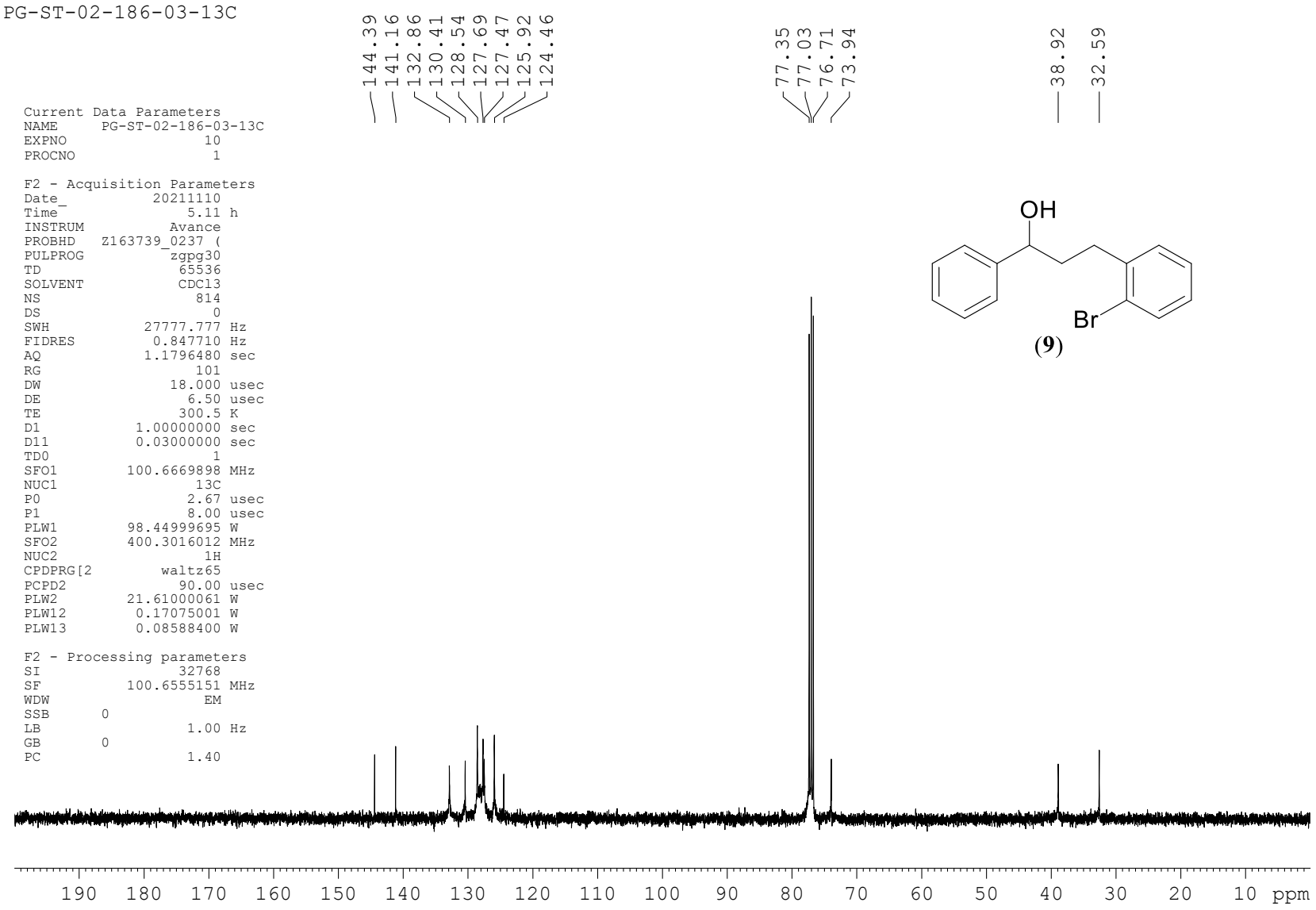

Figure S69. $^{13}C\{^{1}H\}$ NMR spectrum of (**9**) in $CDCl_3$.

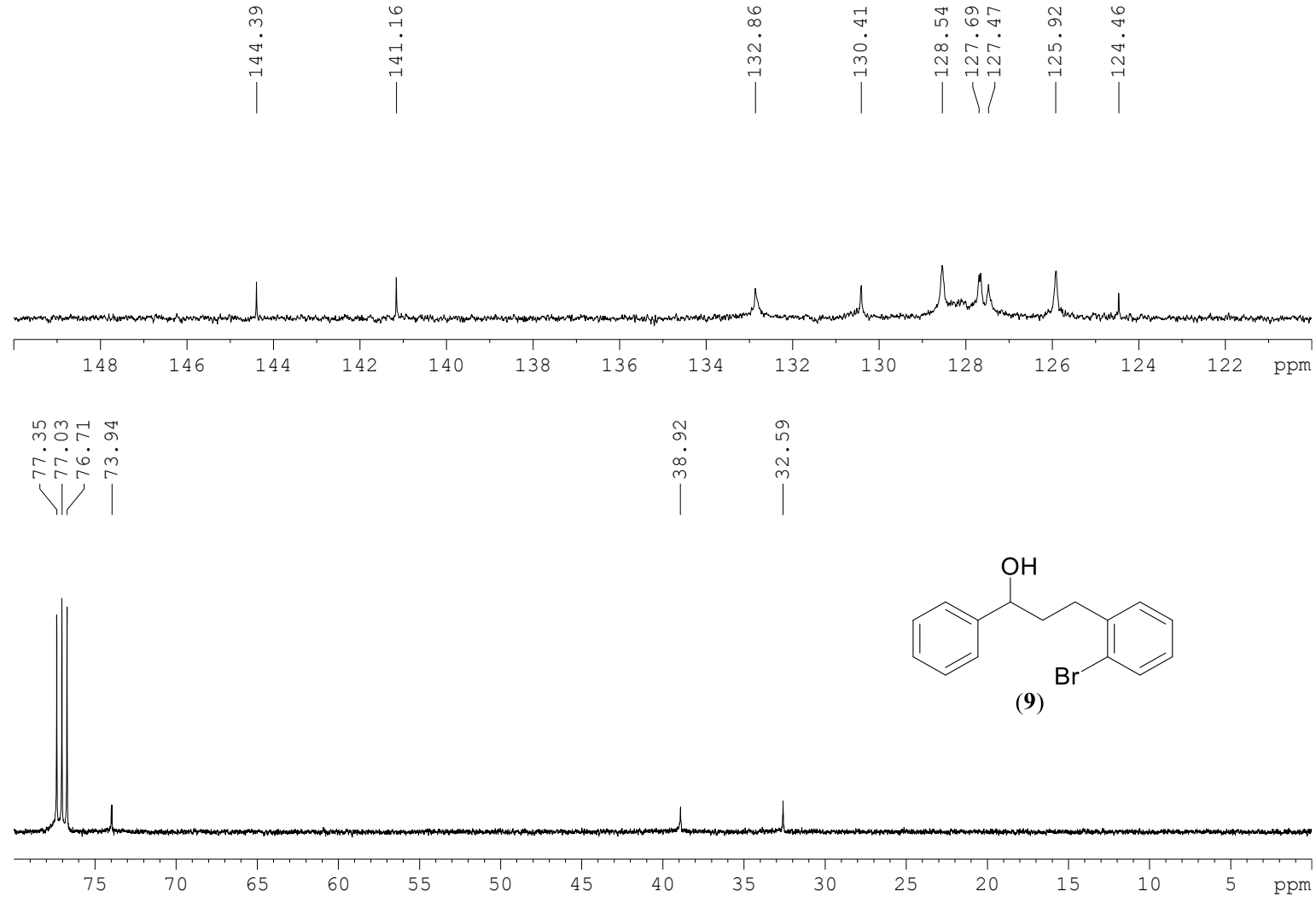

Figure S70. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**9**) in $CDCl_3$.

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Acquired   : 10 Nov 2021  18:33     using AcqMethod COMMONMETHOD-2010.M
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Sample Name: PG-ST-02-186-03
Misc Info  :
Vial Number: 2
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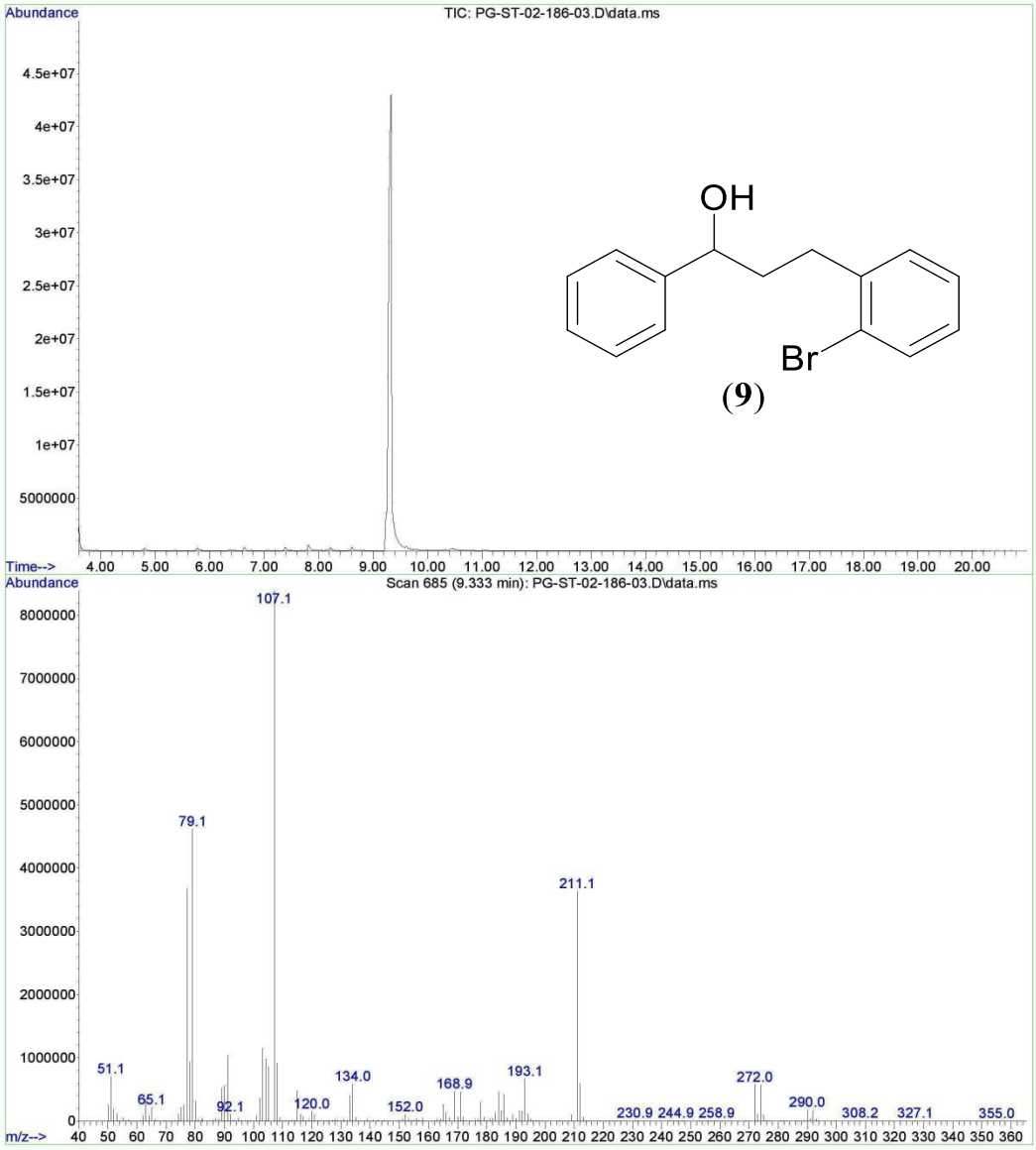

Figure S71. GCMS trace in EtOAc of (**9**) showing the M^+ peak at *m/z* 272.

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date Time	Info
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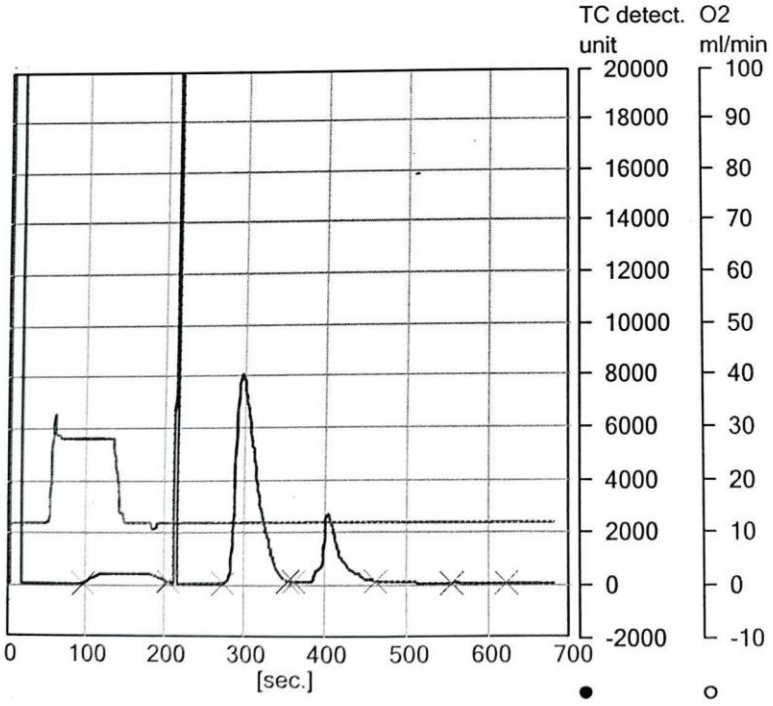

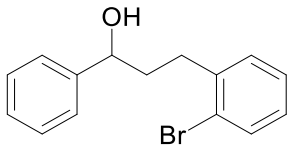

(**9**)

Name: eassuperuser, Access: VarioMICRO administrator 12-11-2021 10:05:02

varioMICRO V4.0.1 (aeb1e0e)2015-10-12, CHNS Mode, Ser. No.: 15154051
Elementar Analysensysteme GmbH

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Figure S72. Elemental analysis data of (**9**).

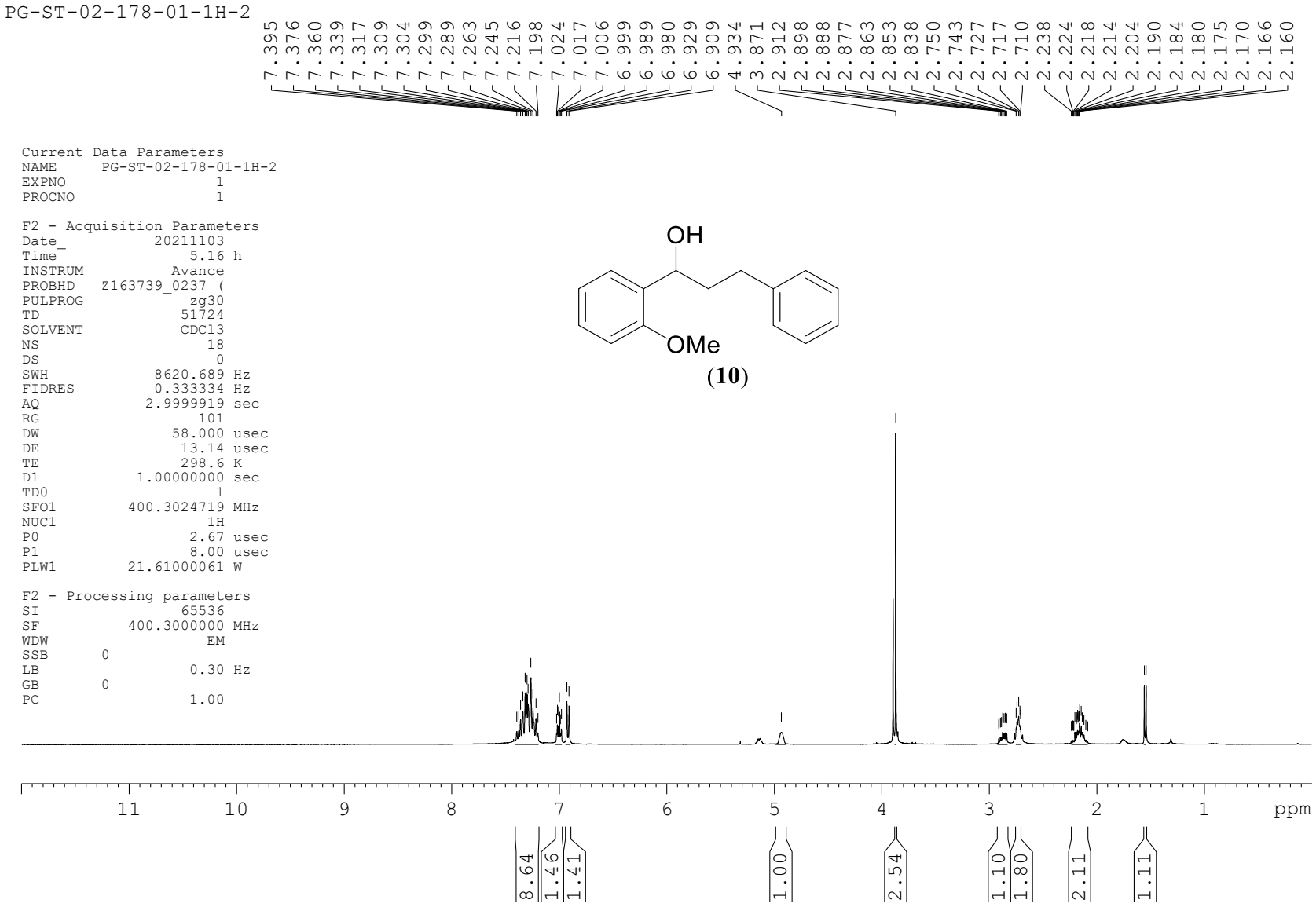

Figure S73. ^{1}H NMR spectrum of (**10**) in $CDCl_3$.

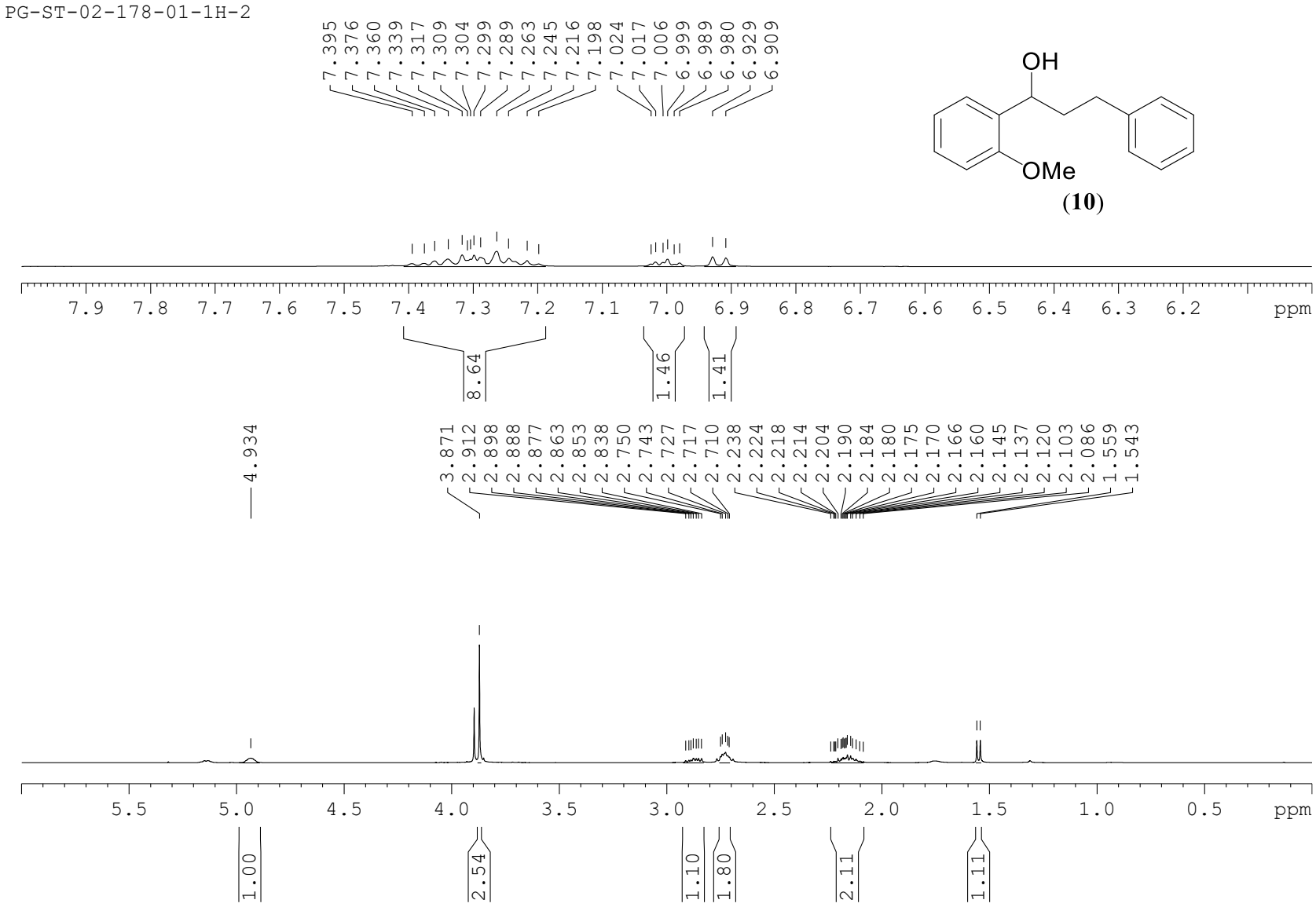

Figure S74. Expanded ^{1}H NMR spectrum of (**10**) in $CDCl_3$.

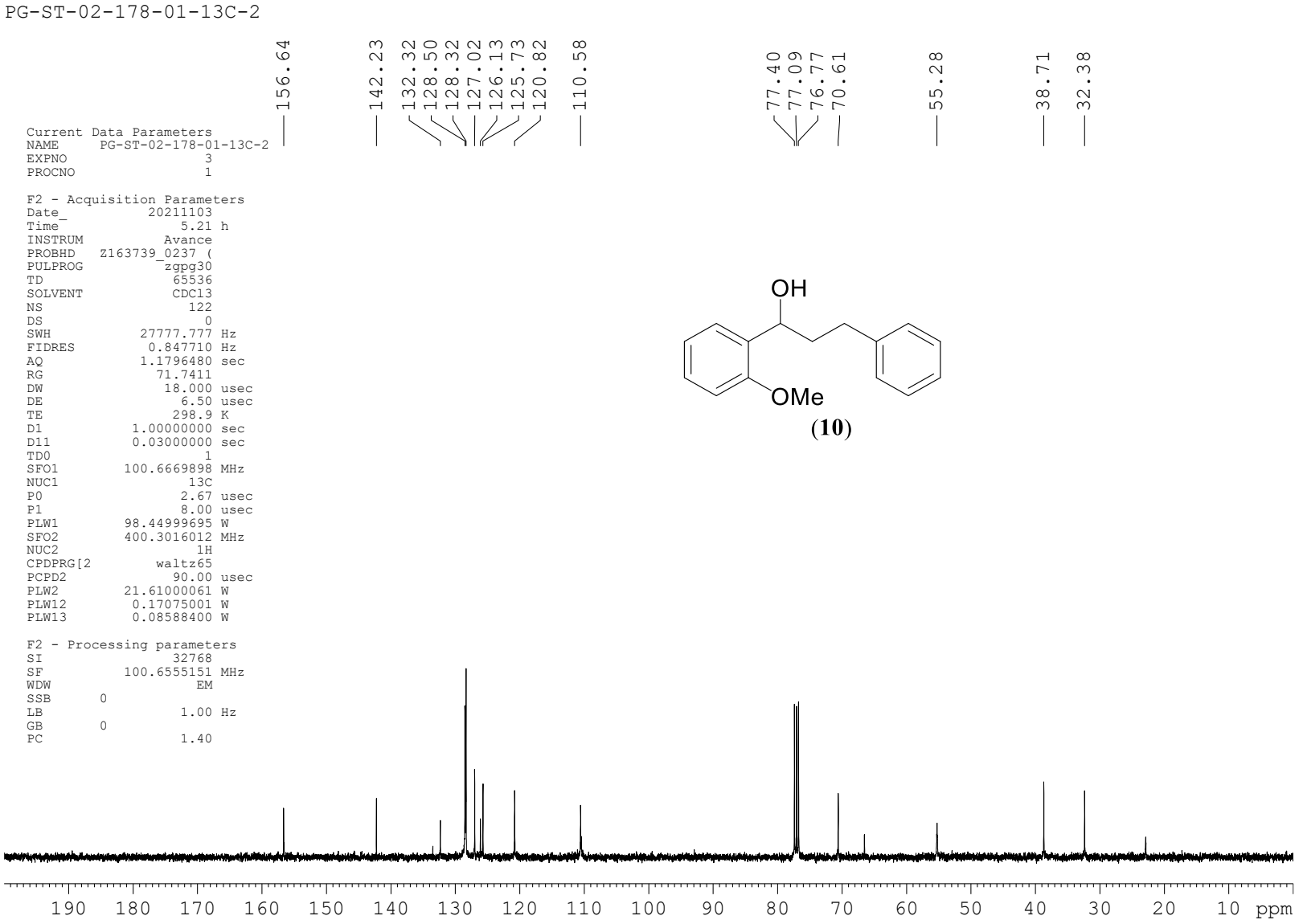

Figure S75. $^{13}C\{^{1}H\}$ NMR spectrum of (**10**) in $CDCl_3$.

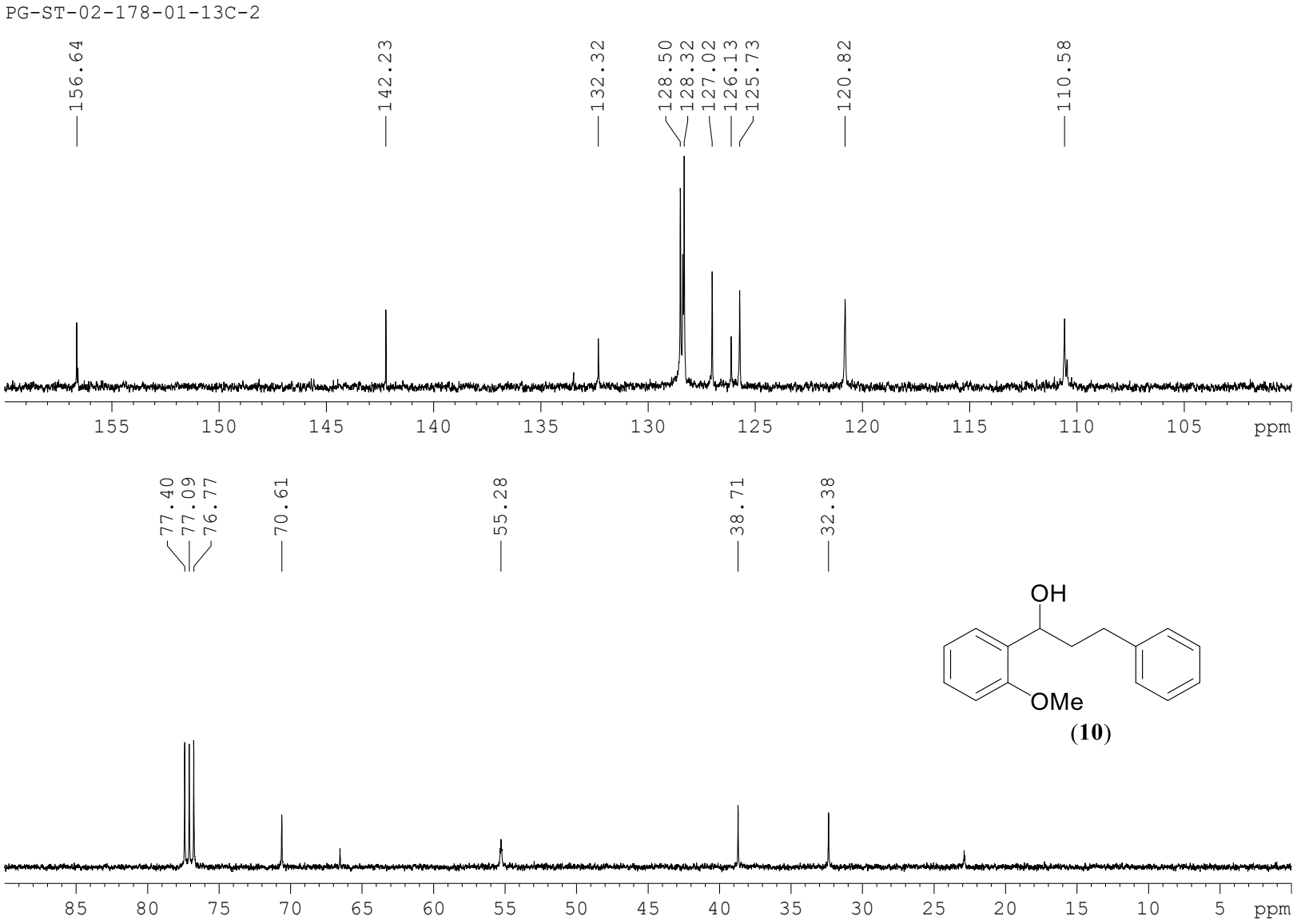

Figure S76. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**10**) in $CDCl_3$.

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Vial Number: 3
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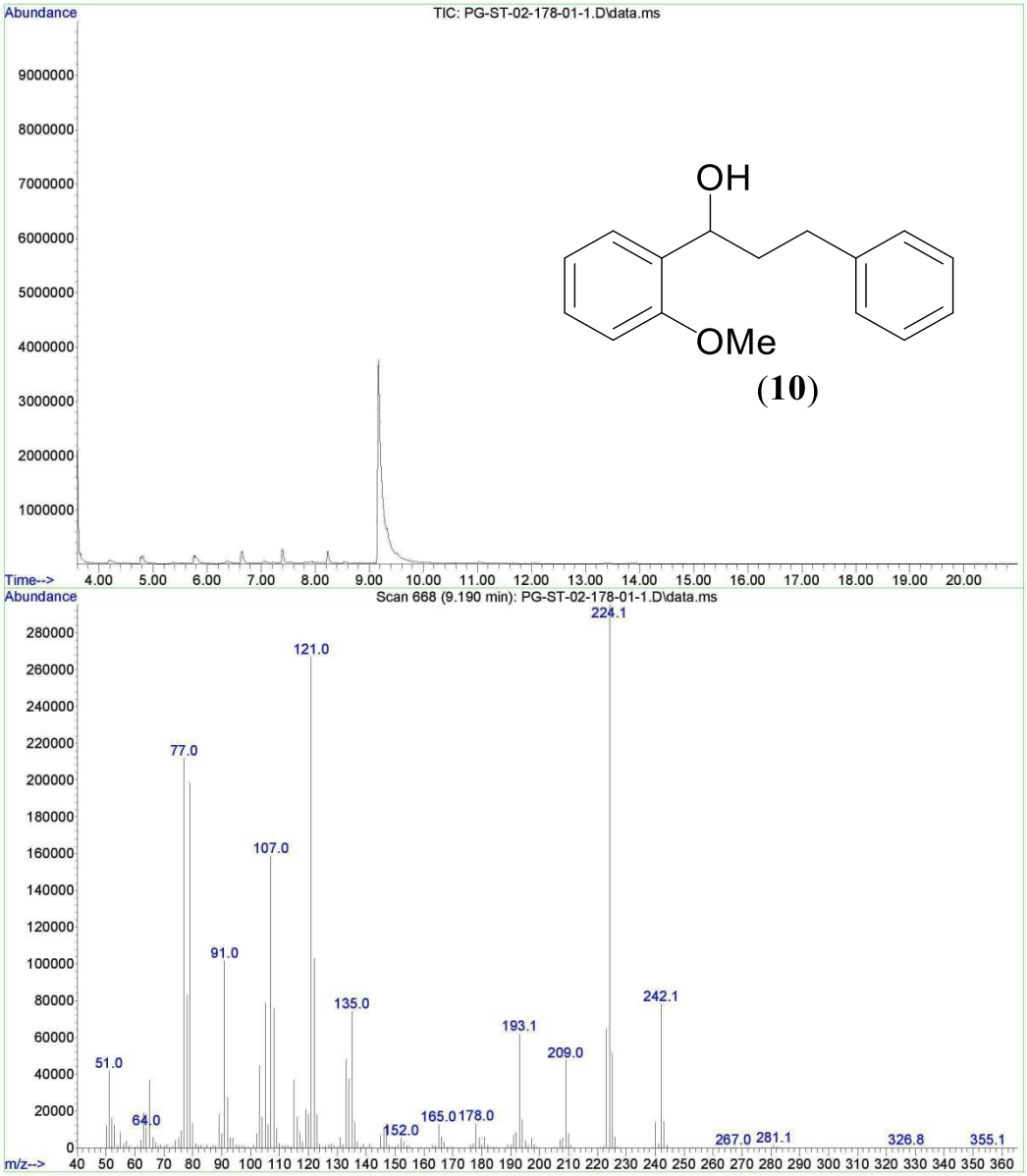

Figure S77. GCMS trace in EtOAc of (**10**) showing the M^+ peak at *m/z* 242.

Document: CHNS16112021 (varioMICRO) from: --.--.-- (modified)

SP18022016
varioMICRO CHNS
serial number: 15154051

Graphic report

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date	Time	Info
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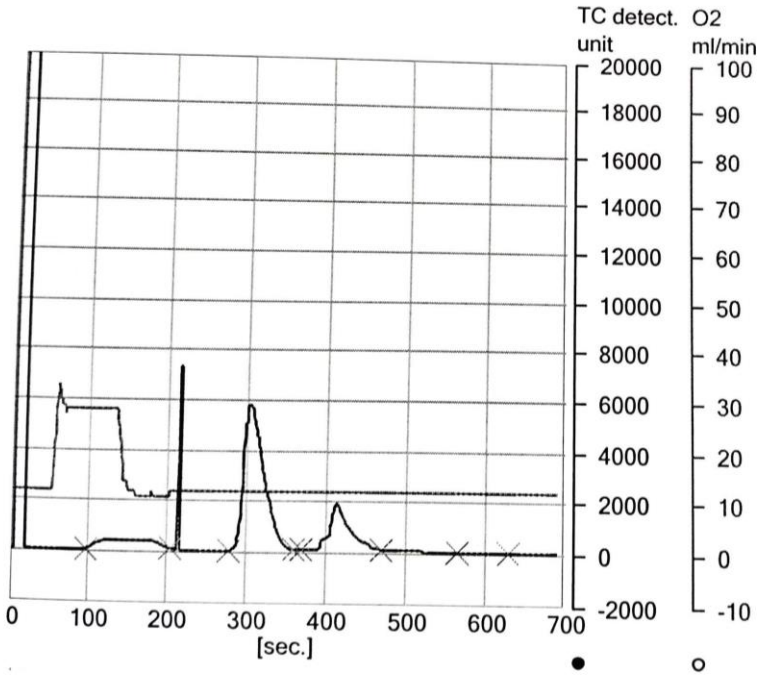

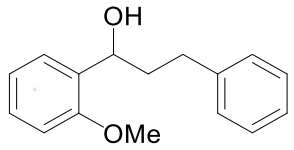

(**10**)

Figure S78. Elemental analysis data of (**10**).

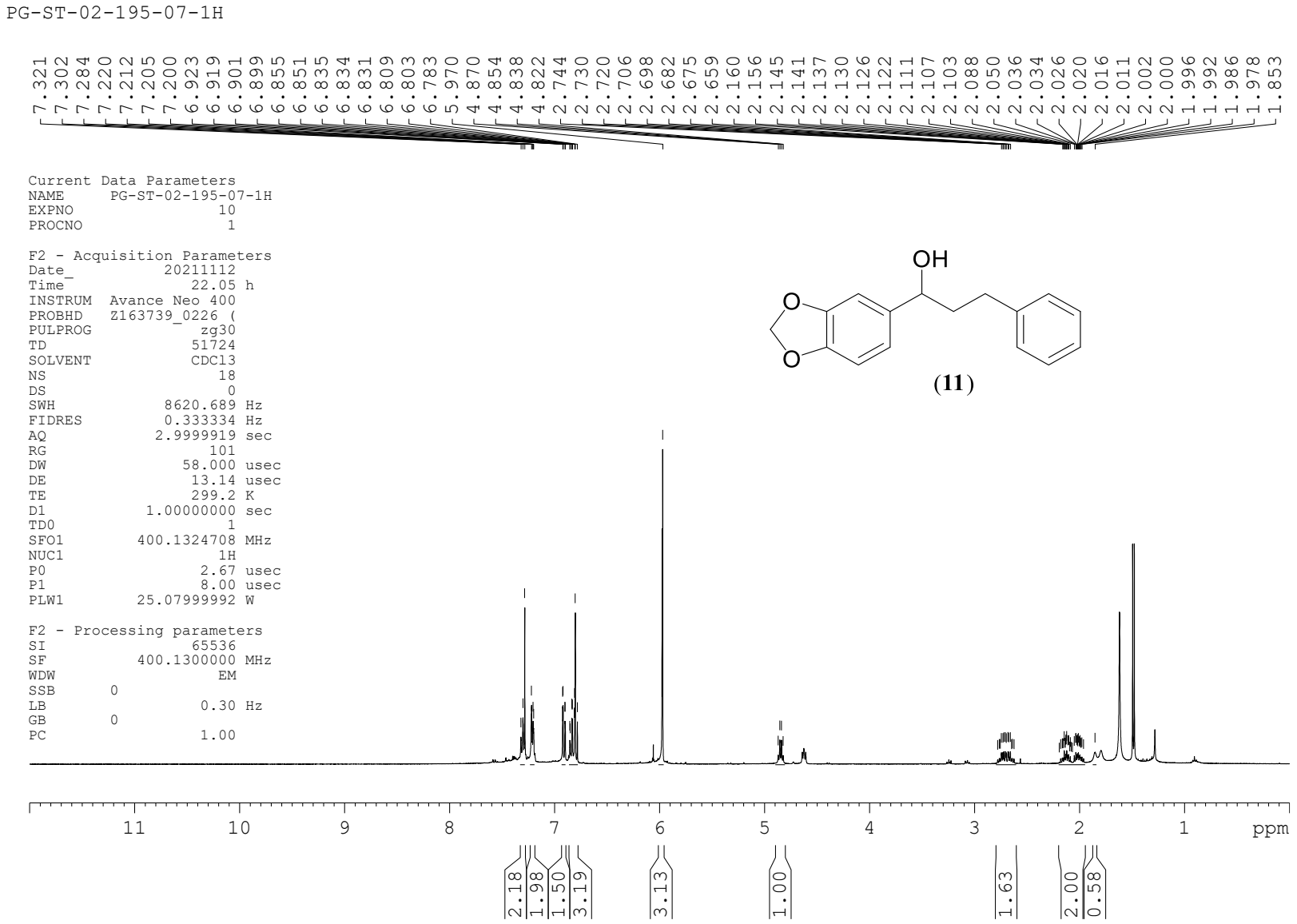

Figure S79. ^{1}H NMR spectrum of (**11**) in $CDCl_3$.

PG-ST-02-195-07-1H

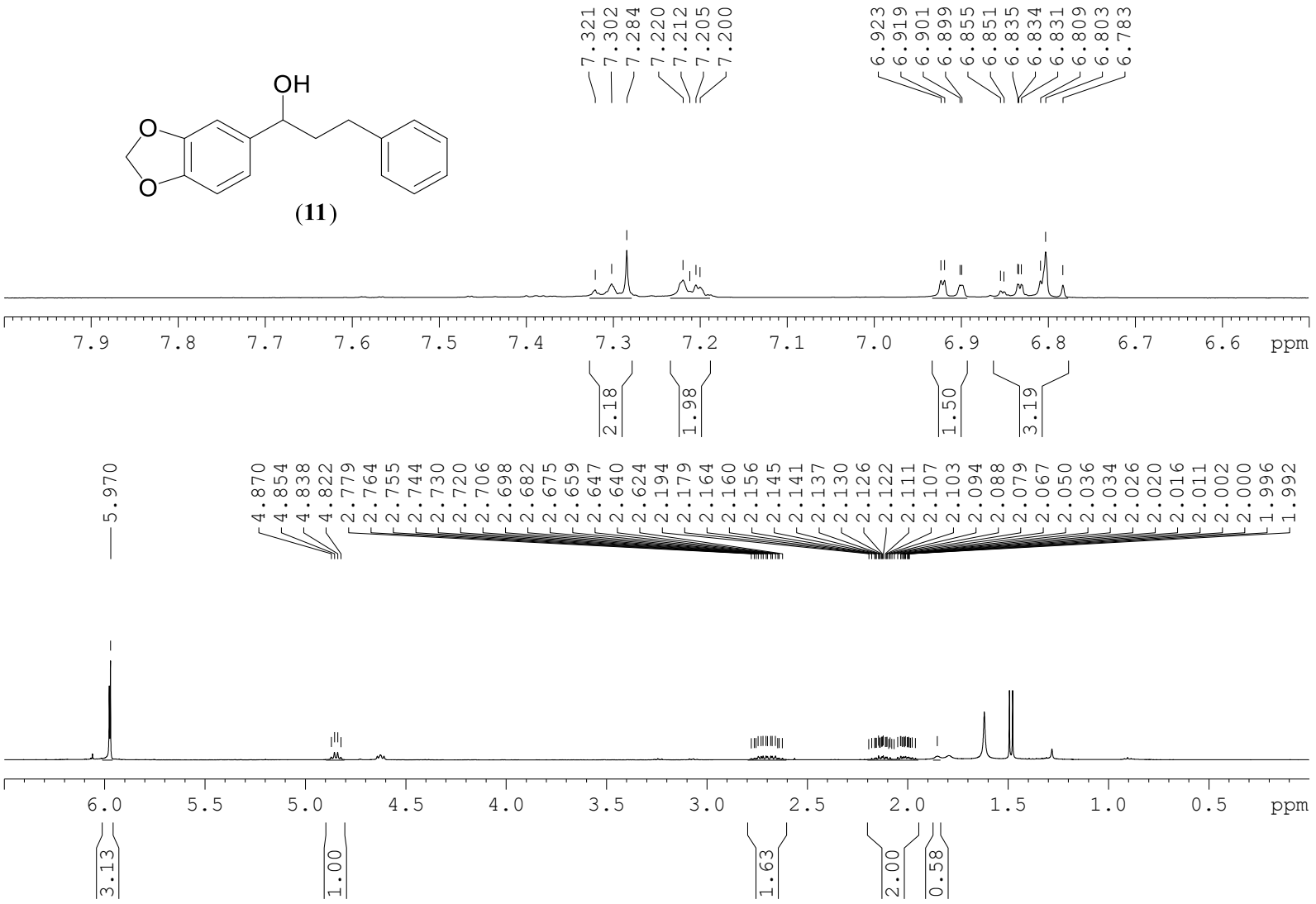

Figure S80. Expanded ^{1}H NMR spectrum of (**11**) in $CDCl_3$.

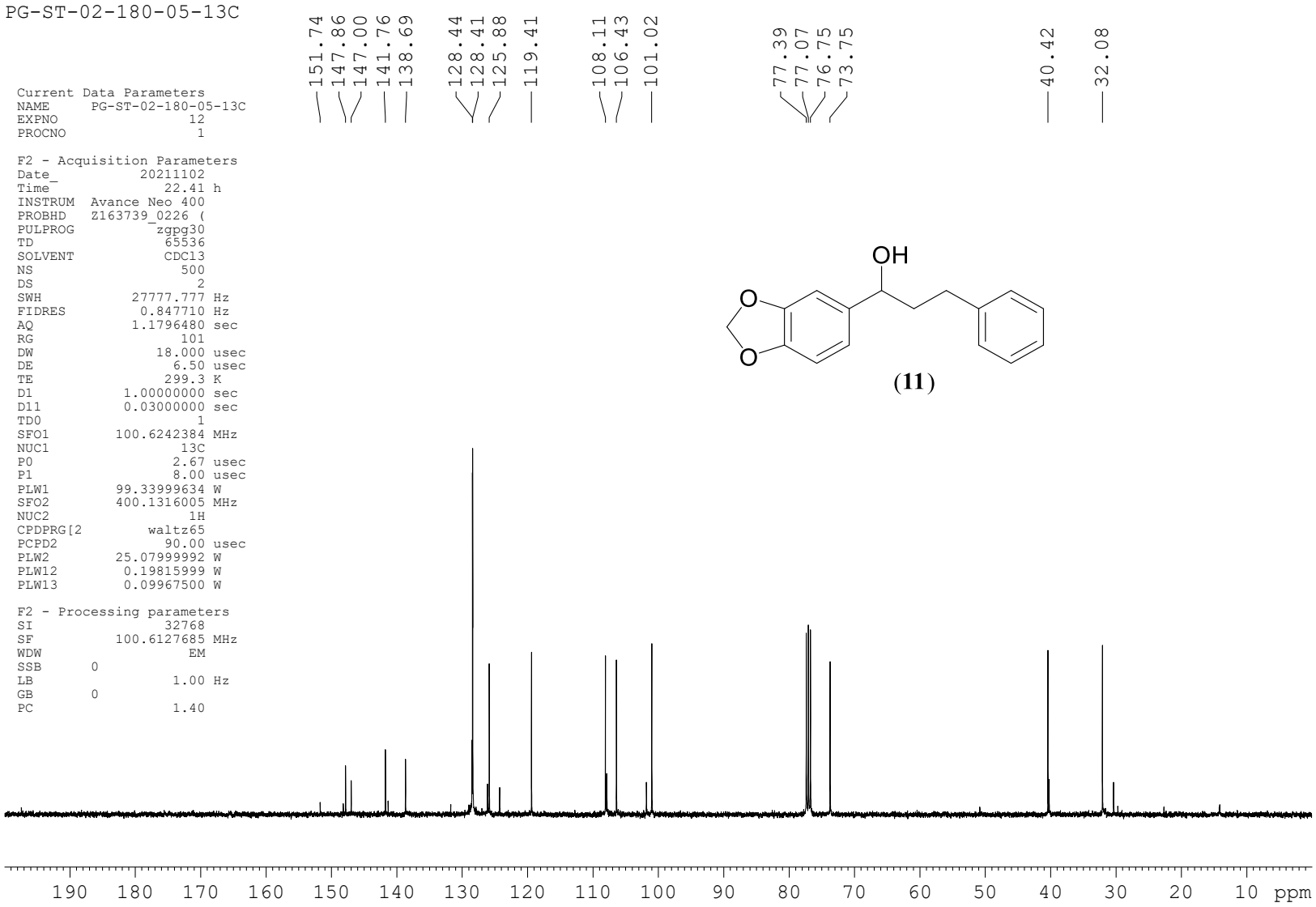

Figure S81. $^{13}C\{^{1}H\}$ NMR spectrum of (**11**) in $CDCl_3$.

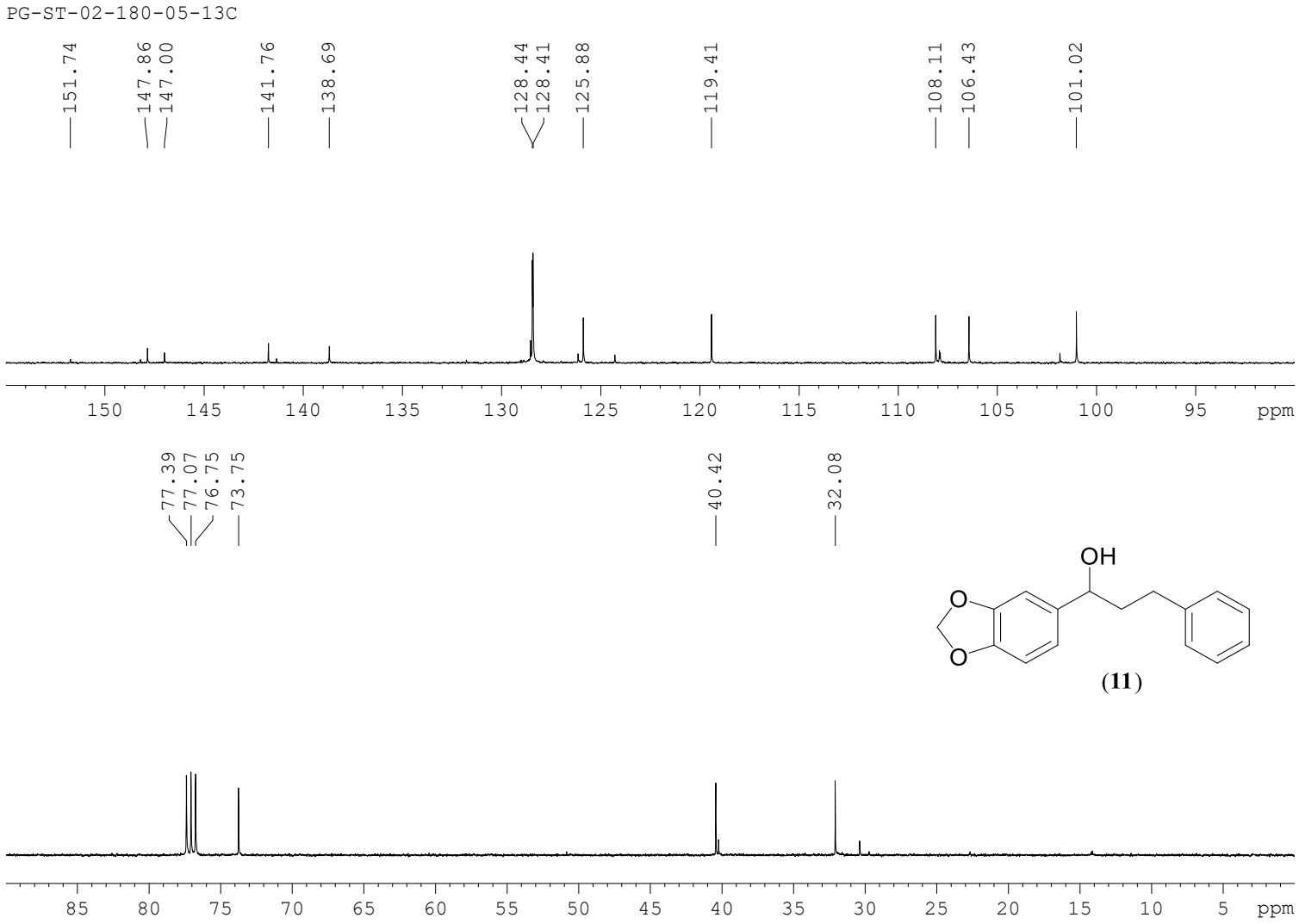

Figure S82. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**11**) in $CDCl_3$.

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Vial Number: 2
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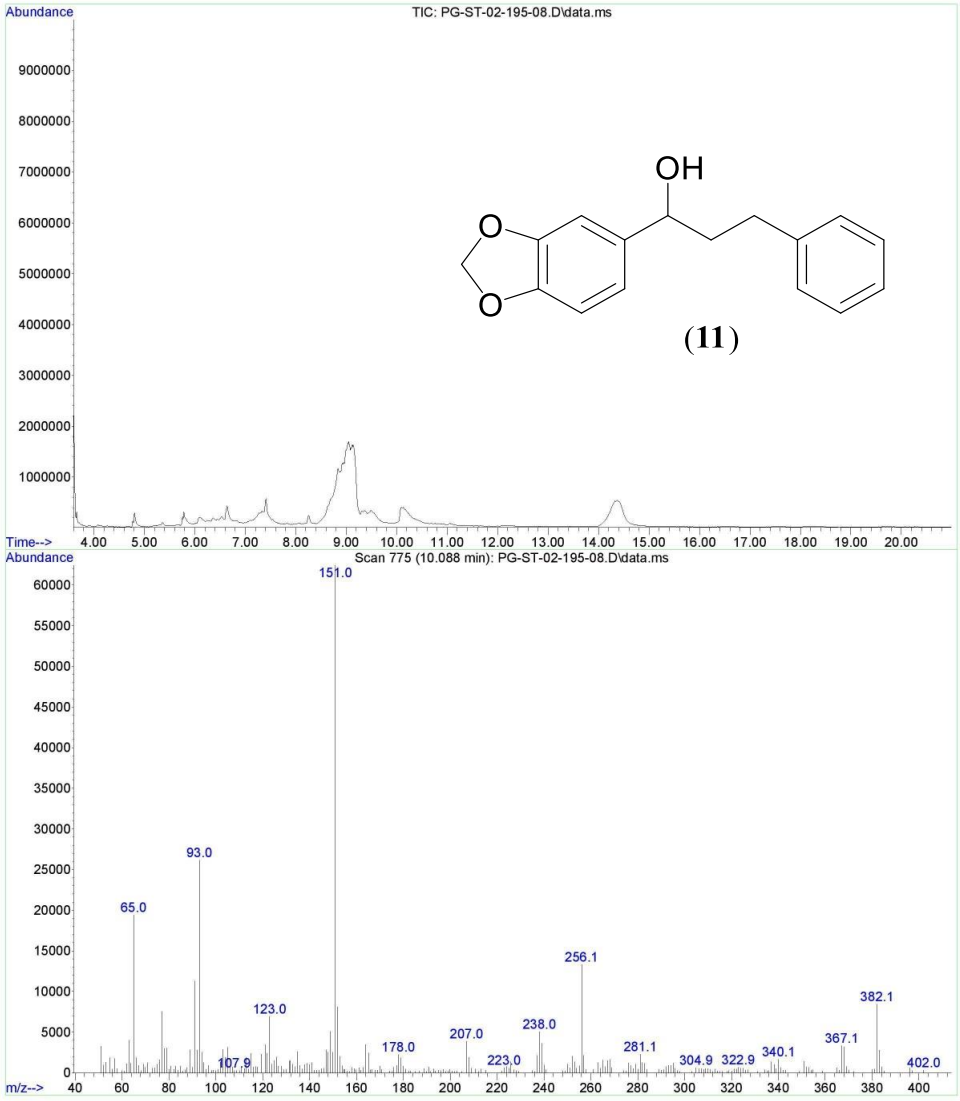

Figure S83. GCMS trace in EtOAc of (**11**) showing the M^+ peak at *m/z* 256.

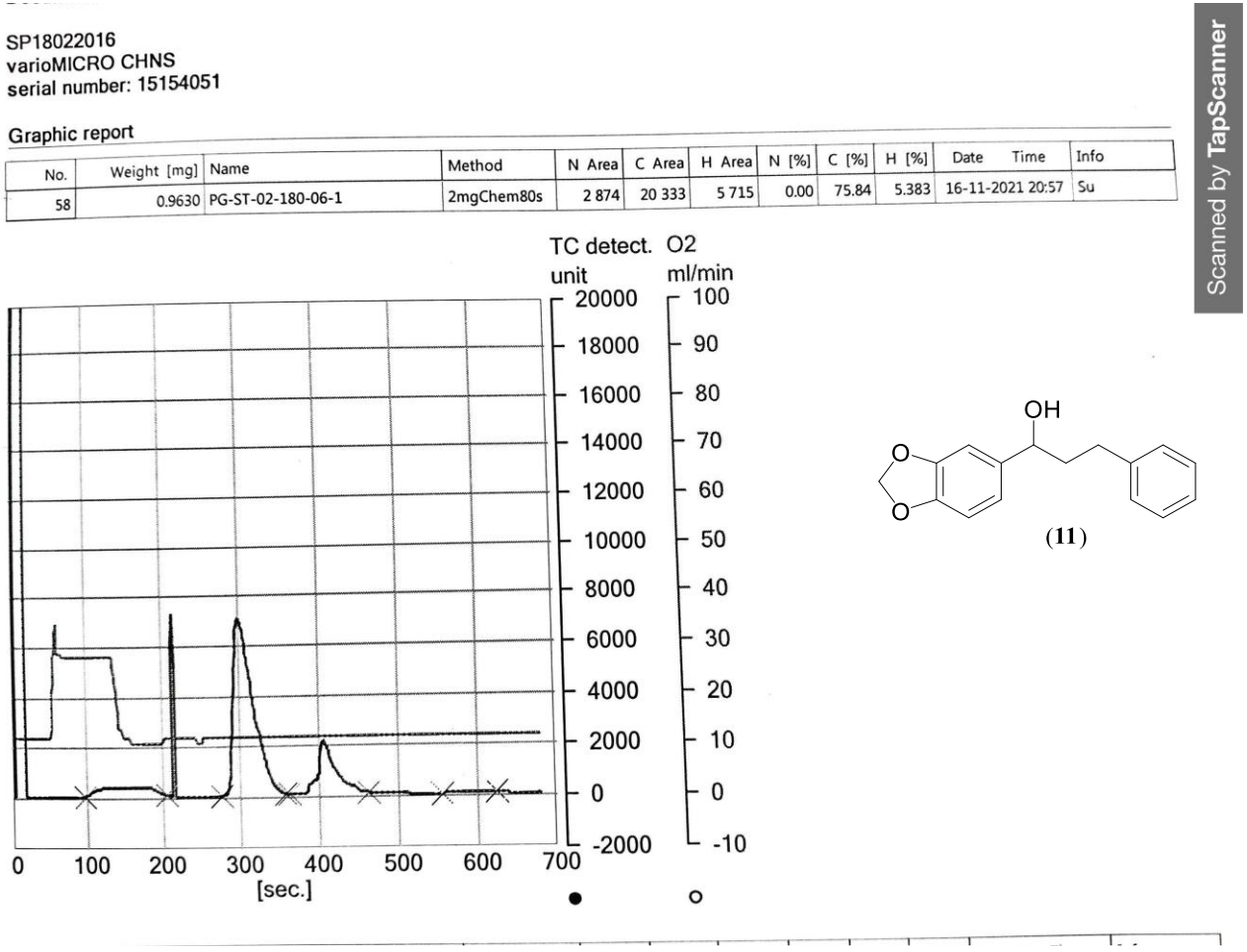

Figure S84. Elemental analysis data of (**11**).

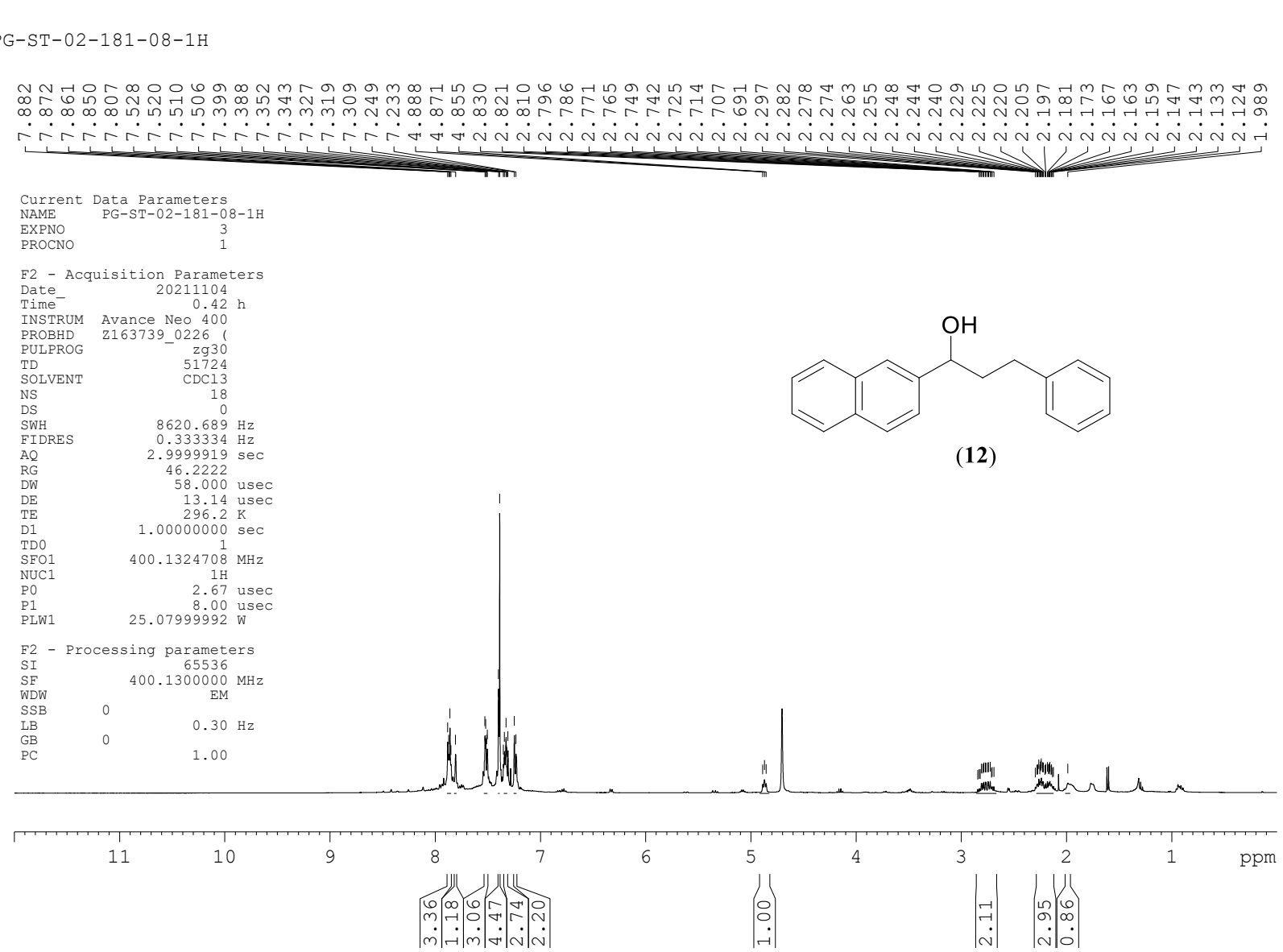

Figure S85. ^{1}H NMR spectrum of (**12**) in $CDCl_3$.

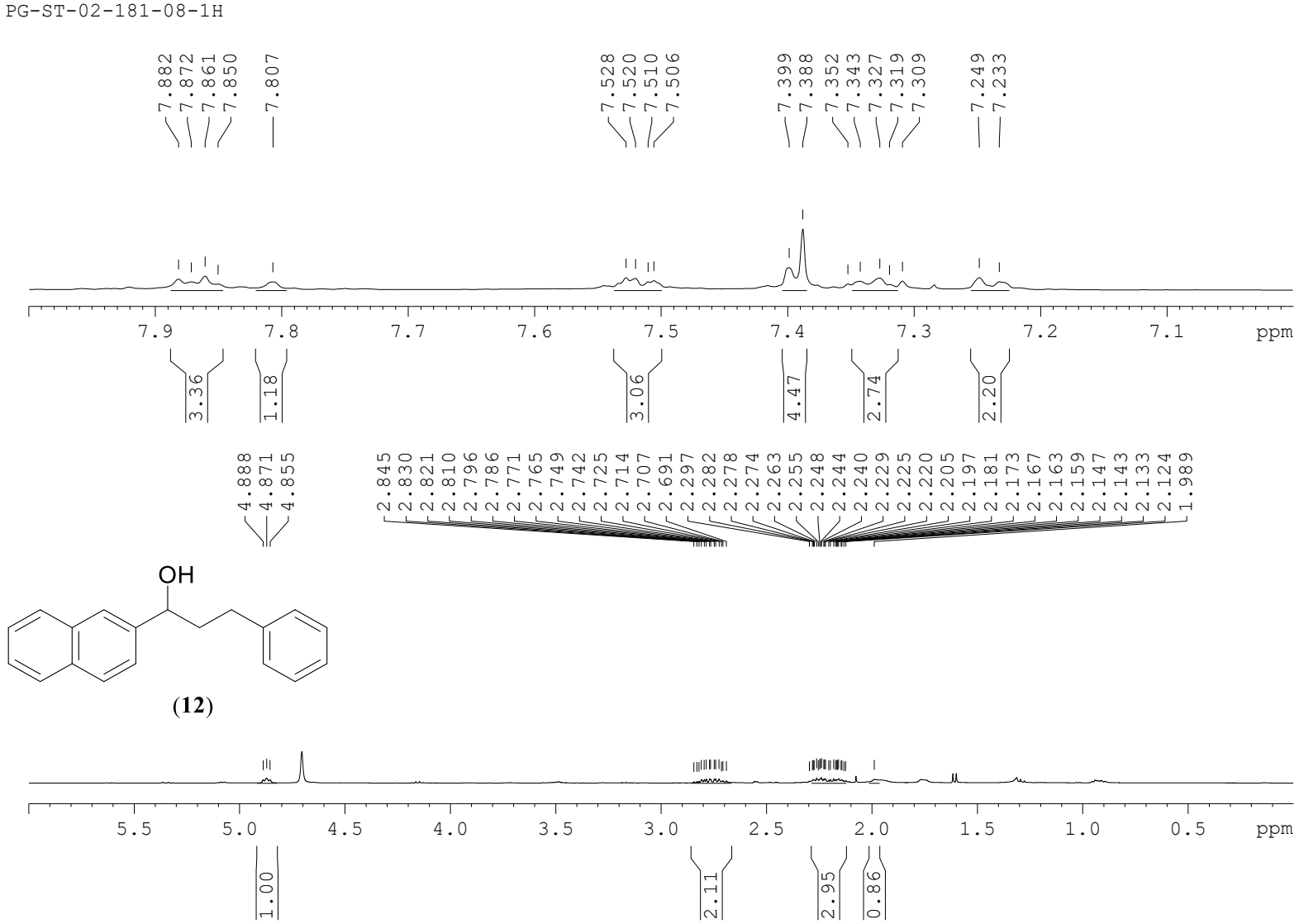

Figure S86. Expanded ^{1}H NMR spectrum of (**12**) in $CDCl_3$.

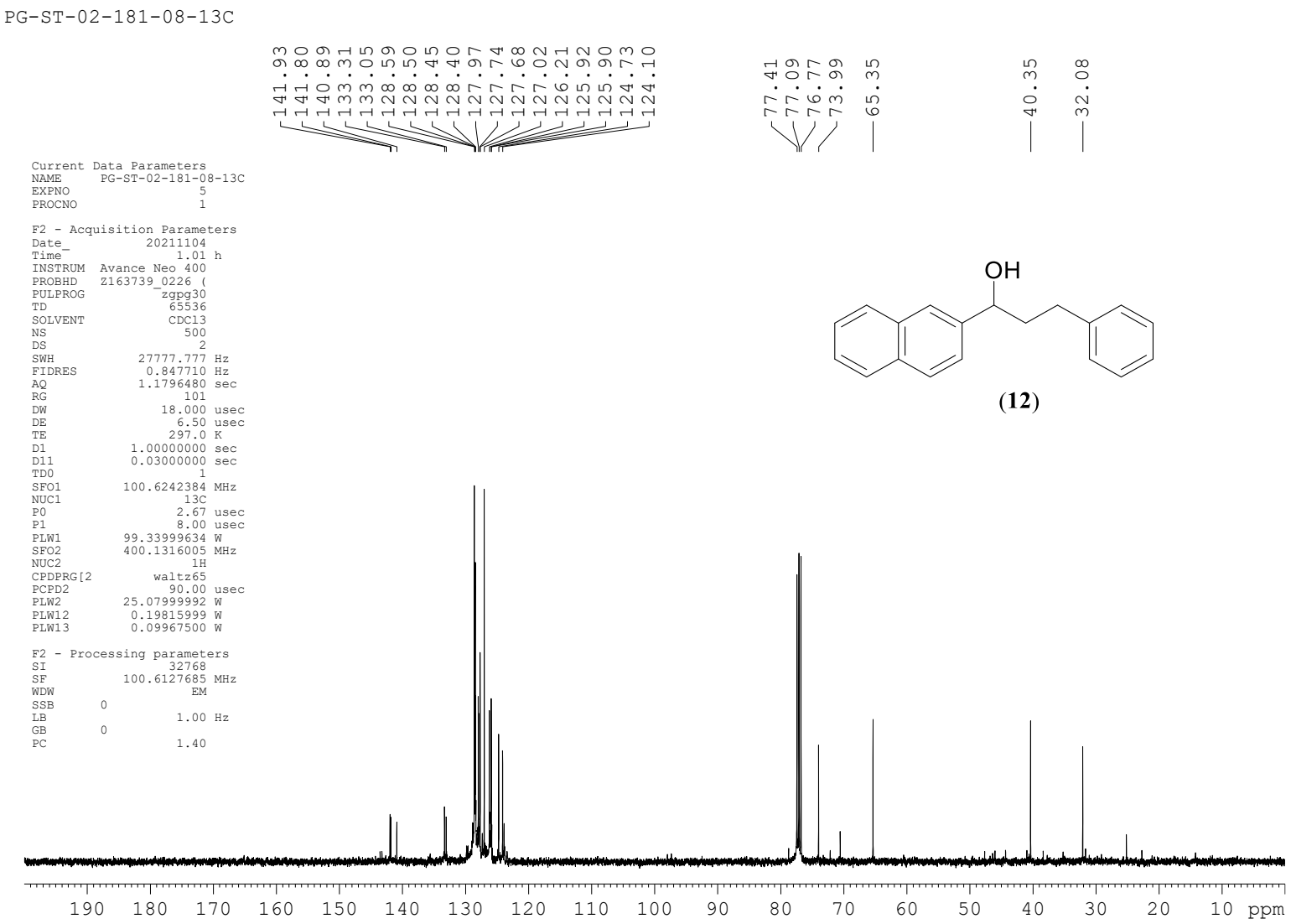

Figure S87. $^{13}C\{^{1}H\}$ NMR spectrum of (**12**) in $CDCl_3$.

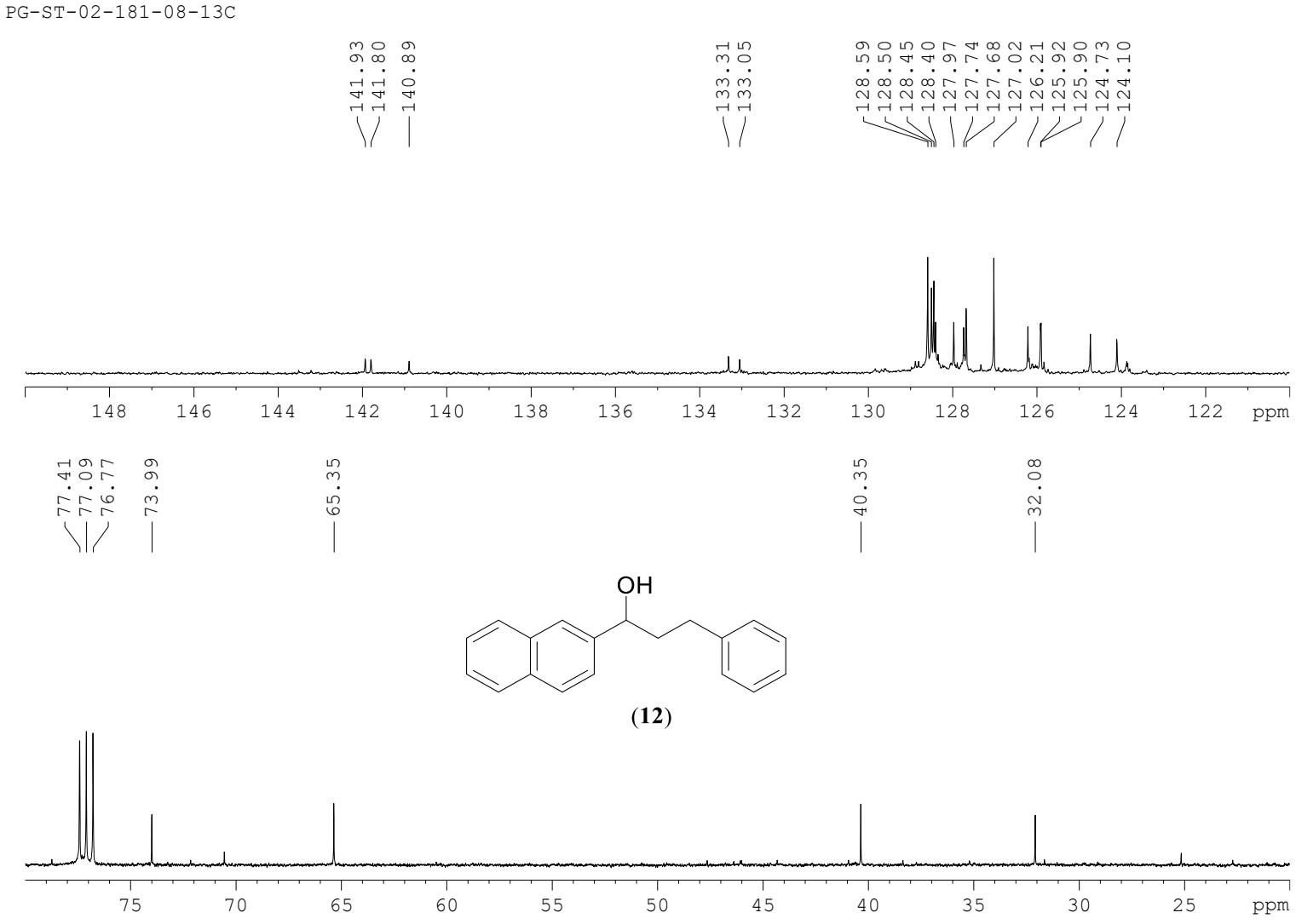

Figure S88. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**12**) in $CDCl_3$.

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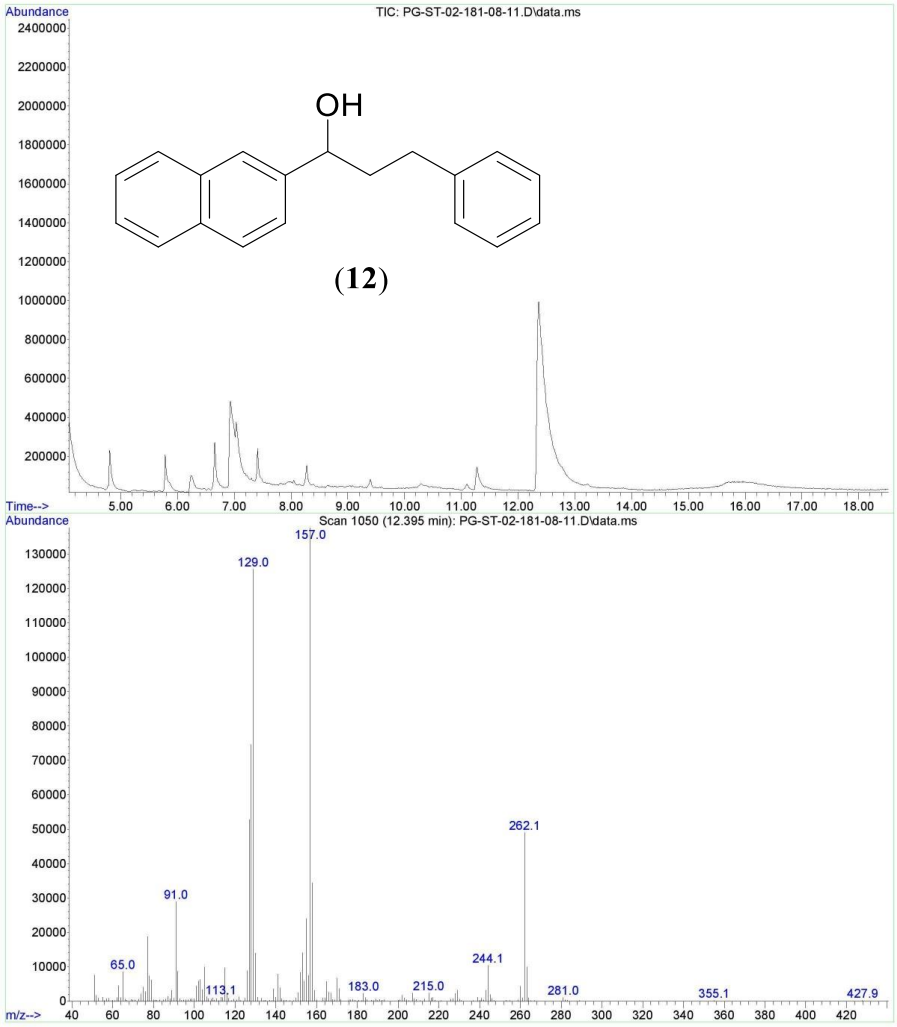

Figure S89. GCMS trace in EtOAc of (**12**) showing the M^+ peak at *m/z* 262.

Document: CHNS01022022 (varioMICRO) from: --.--.-- (modified)

SP18022016
varioMICRO CHNS
serial number: 15154051

Graphic report

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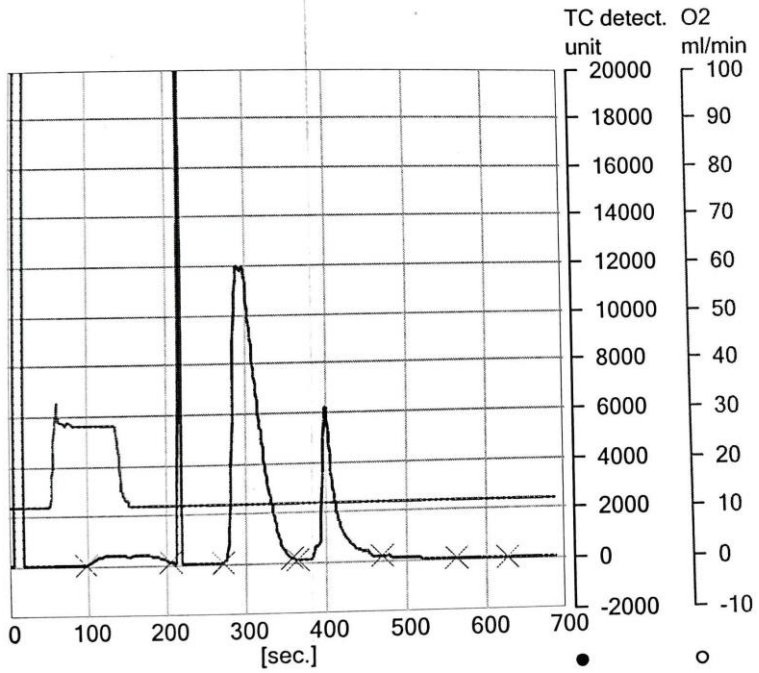

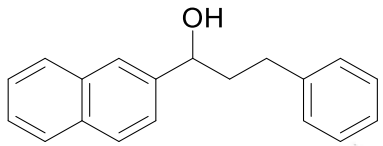

(**12**)

Figure S90. Elemental analysis data of (**12**).

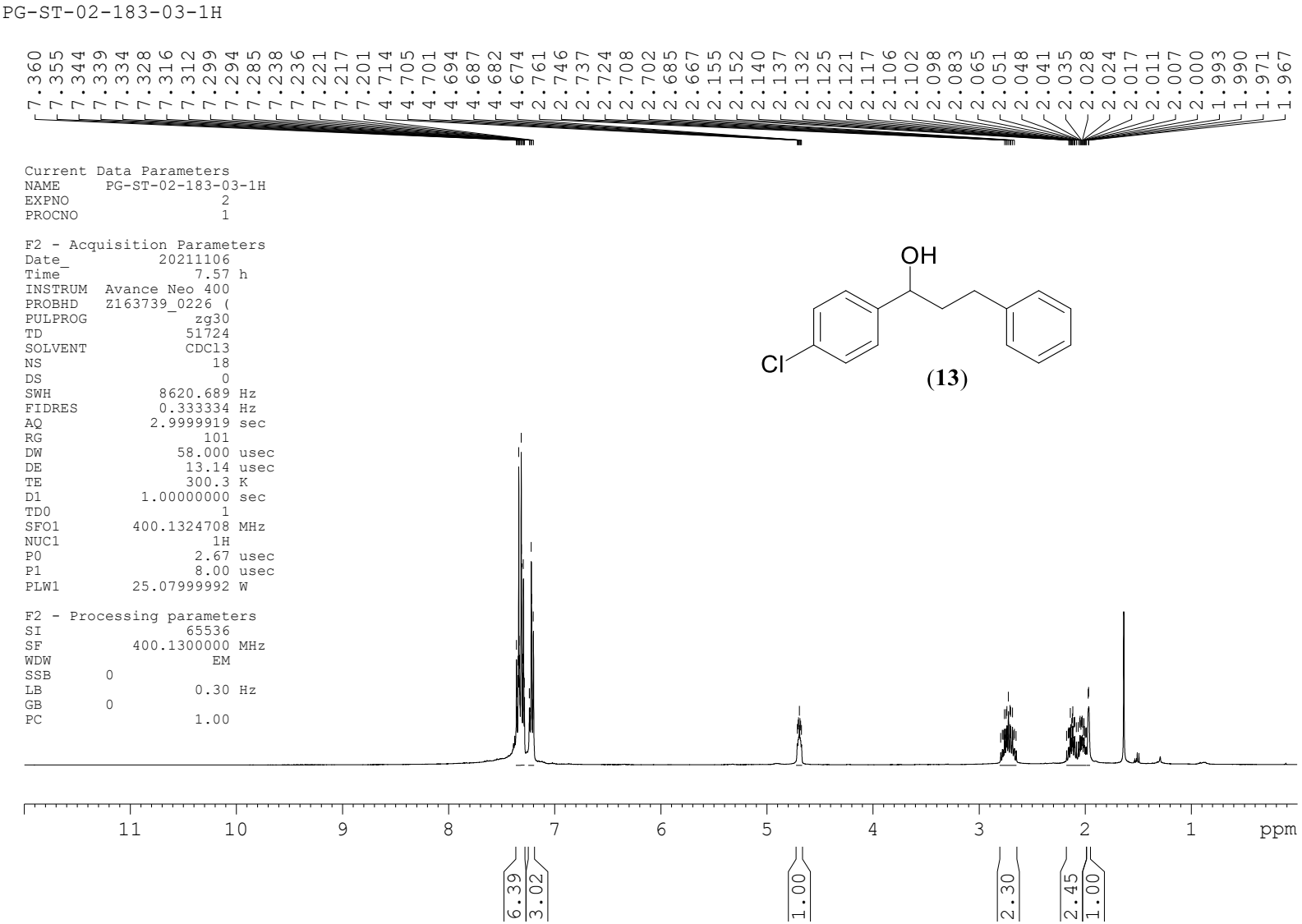

Figure S91. ^{1}H NMR spectrum of (**13**) in $CDCl_3$.

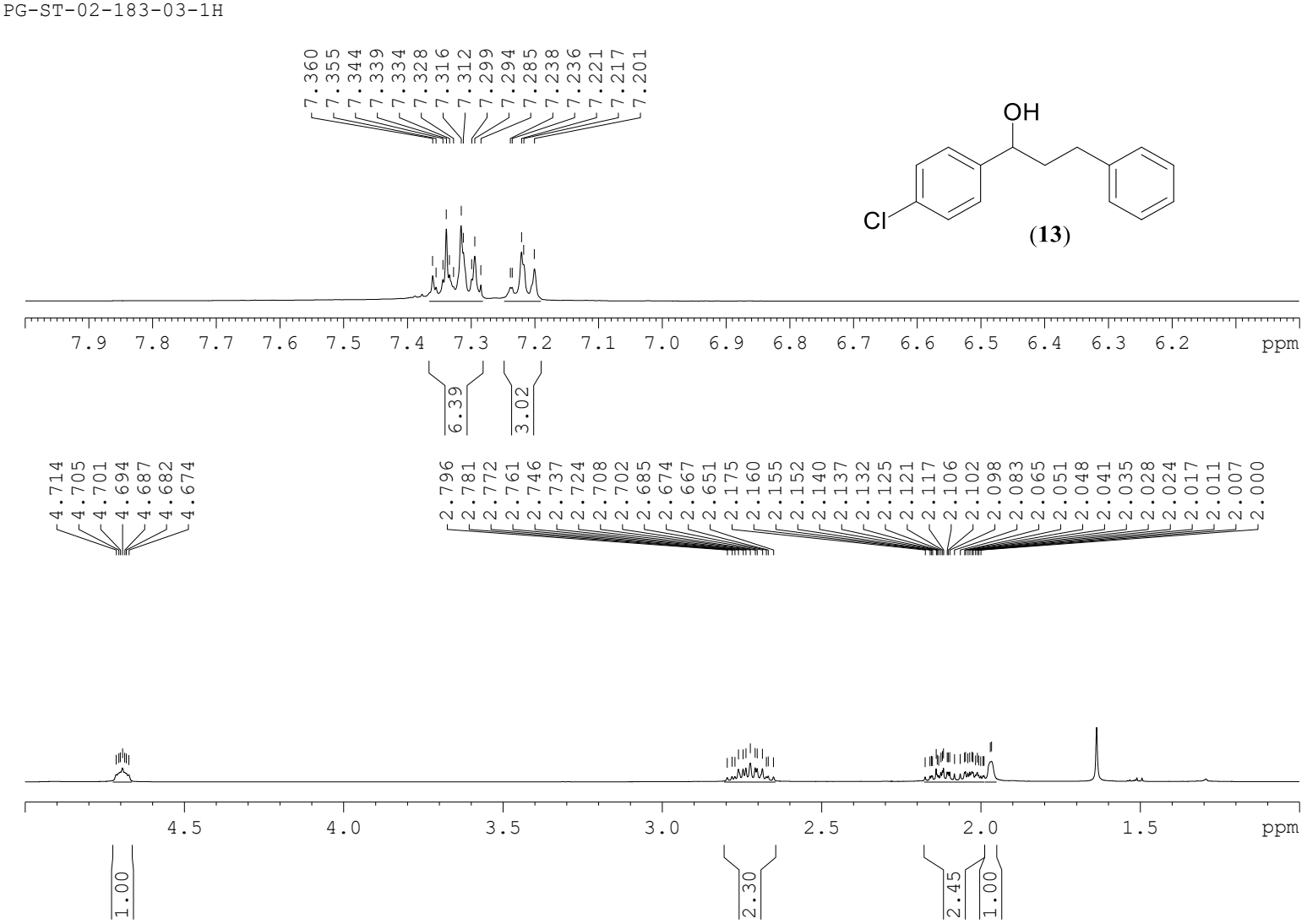

Figure S92. Expanded ^{1}H NMR spectrum of (**13**) in $CDCl_3$.

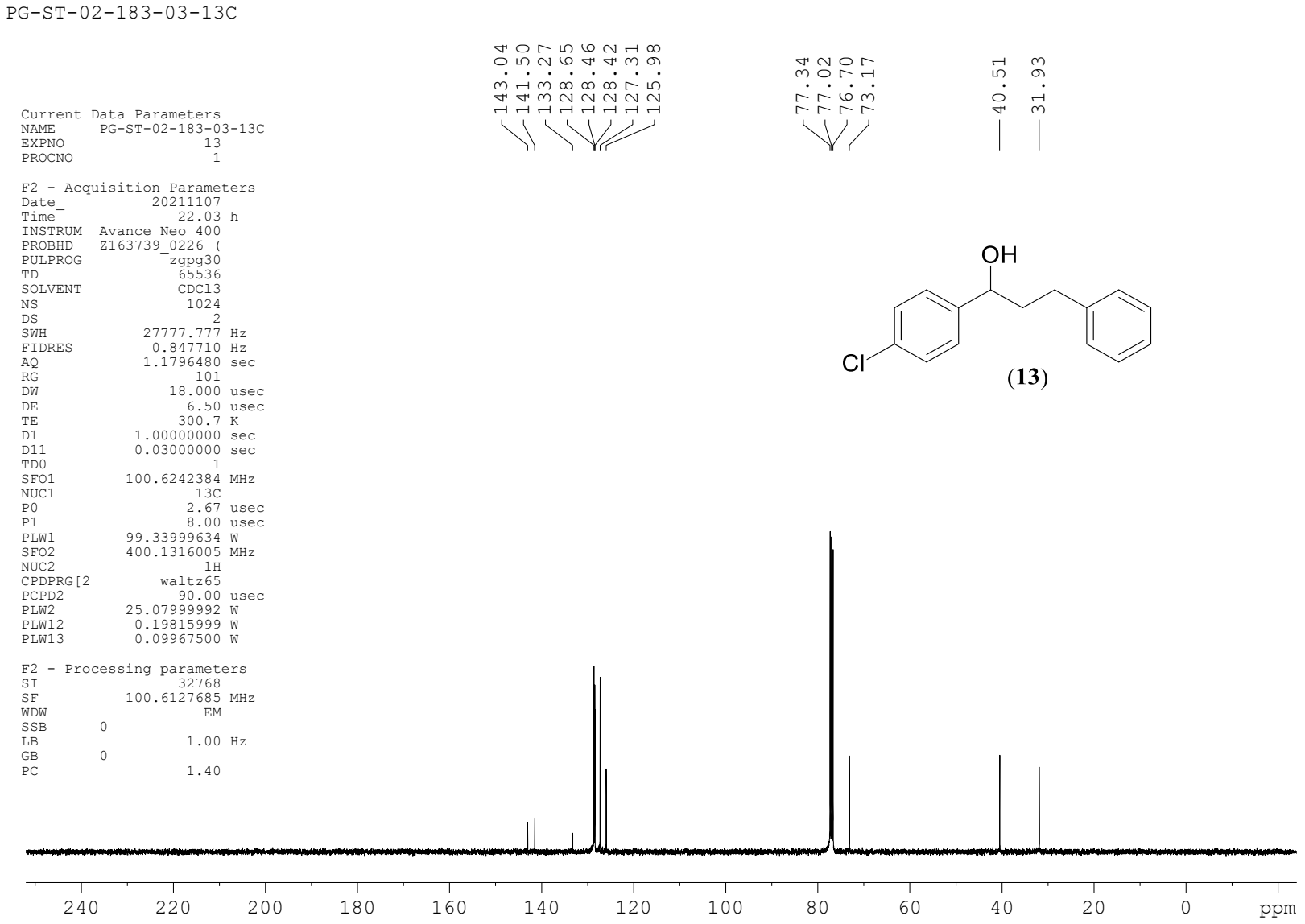

Figure S93. $^{13}C\{^{1}H\}$ NMR spectrum of (**13**) in $CDCl_3$.

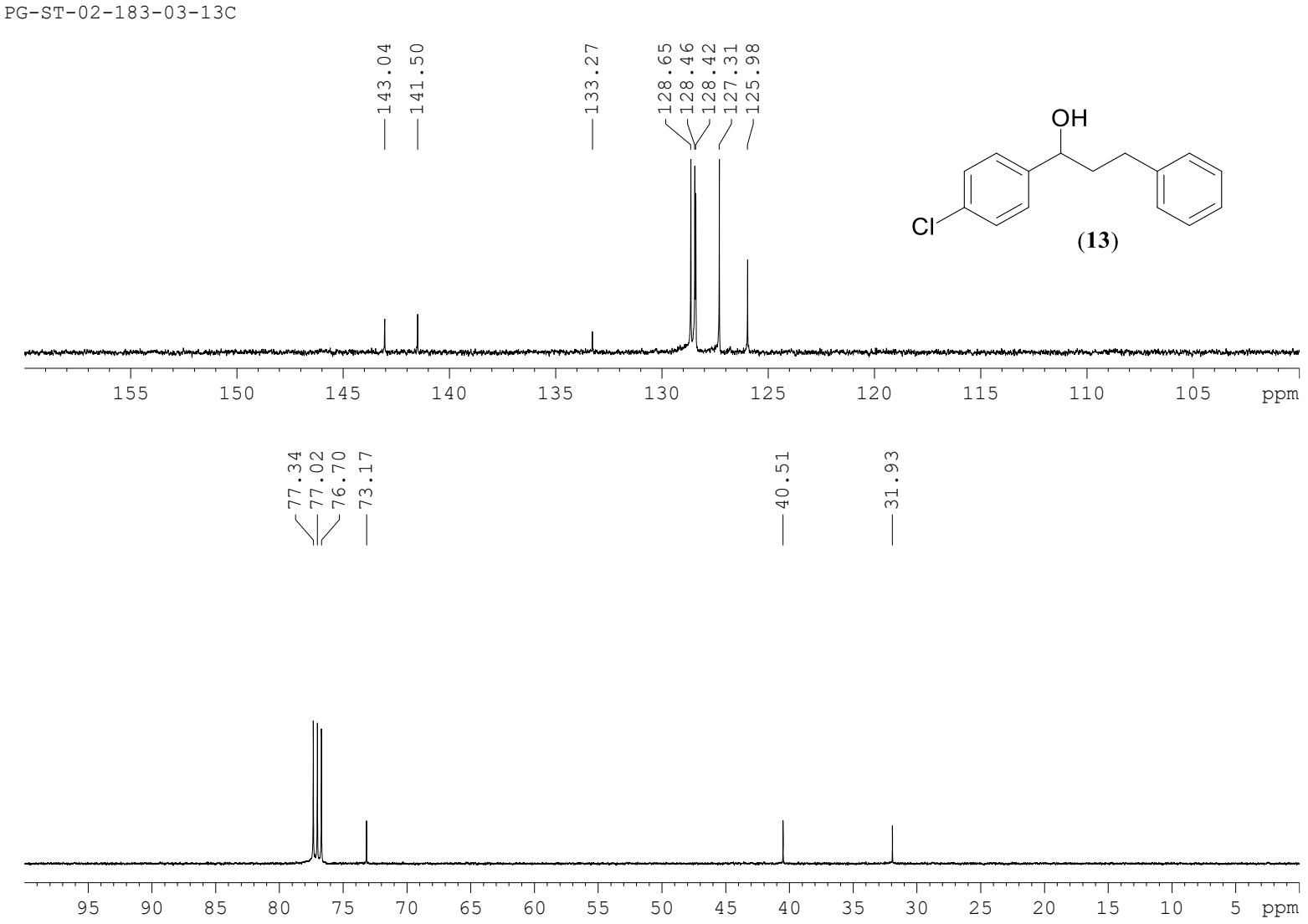

Figure S94. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**13**) in $CDCl_3$.

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Sample Name: PG-ST-02-183-03
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Vial Number: 1
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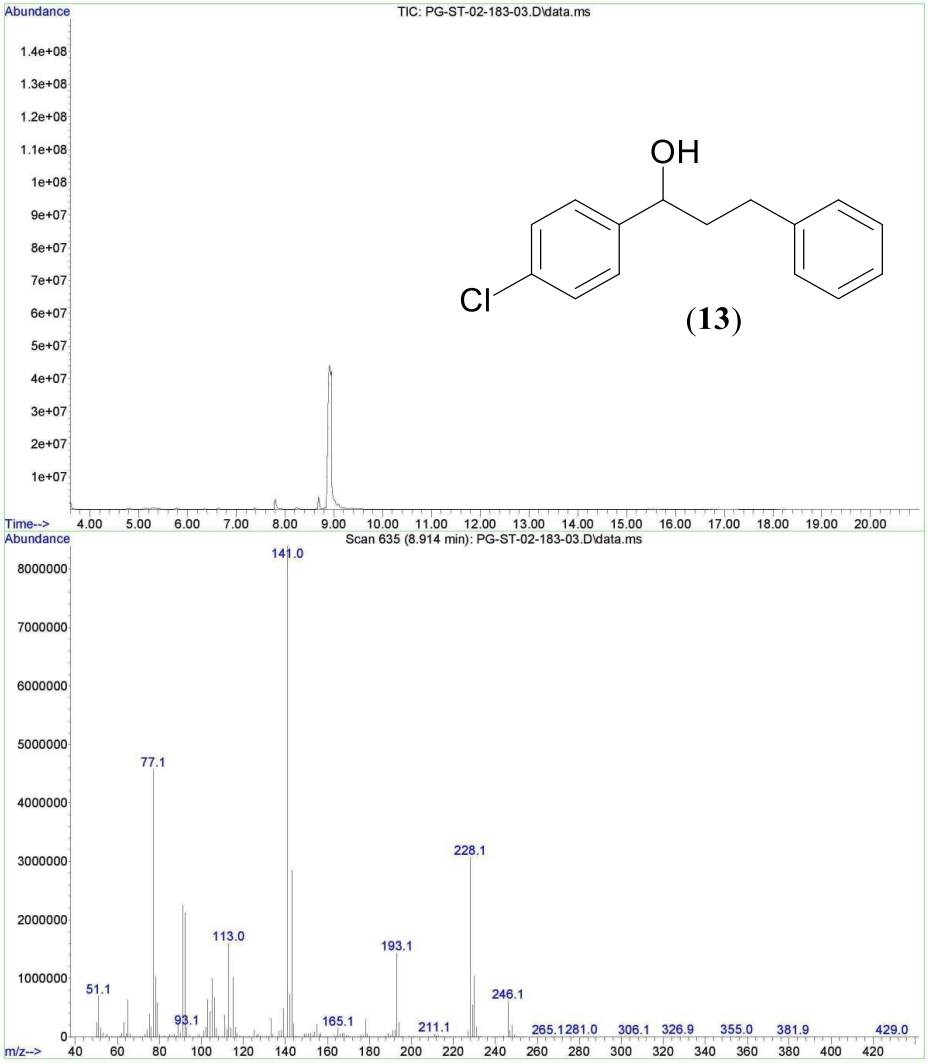

Figure S95. GCMS trace in EtOAc of (**13**) showing the M^+ peak at *m/z* 246.

Document: CHNS11112021 (varioMICRO) from: 12-11-2021 10:04:06

SP18022016
varioMICRO CHNS
serial number: 15154051

Graphic report

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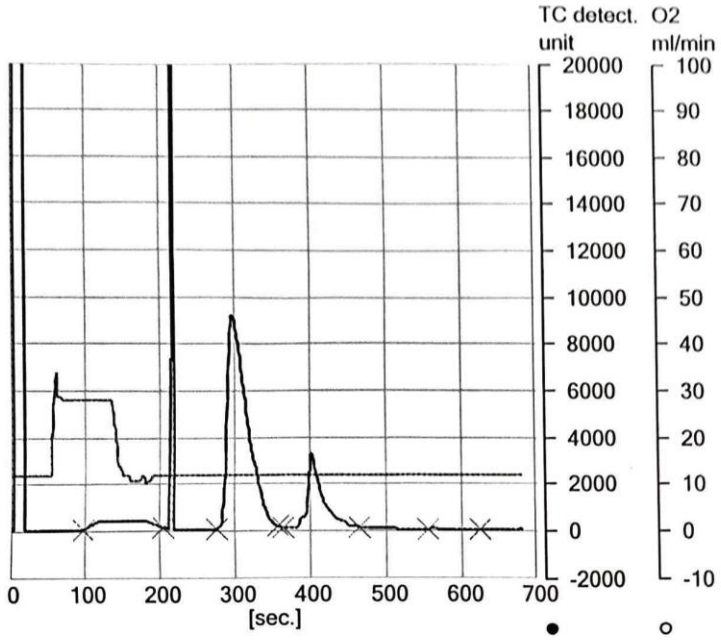
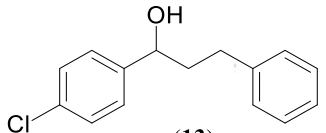




(**13**)

Figure S96. Elemental analysis data of (**13**).

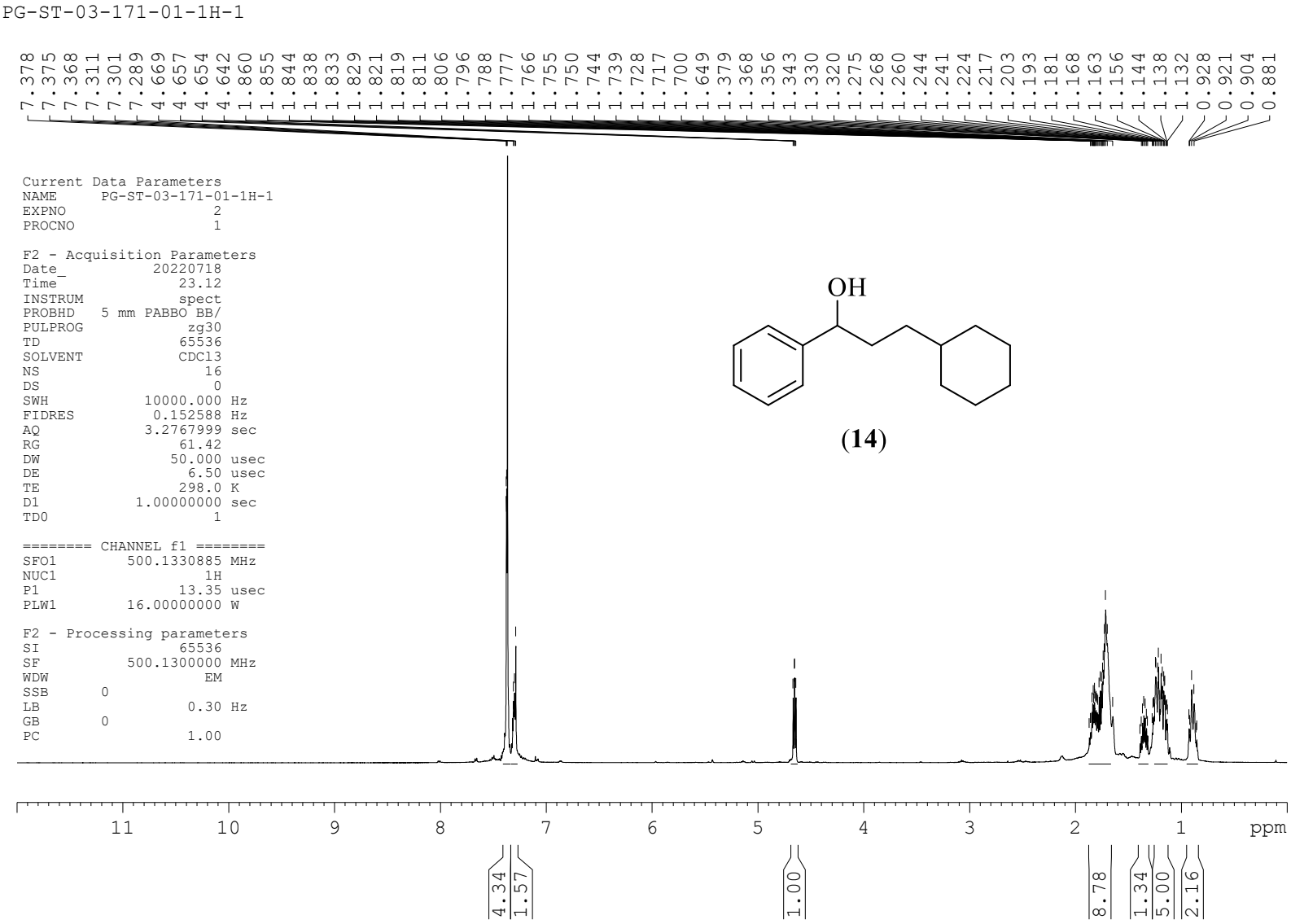


Figure S97. ^{1}H NMR spectrum of (**14**) in $CDCl_3$.

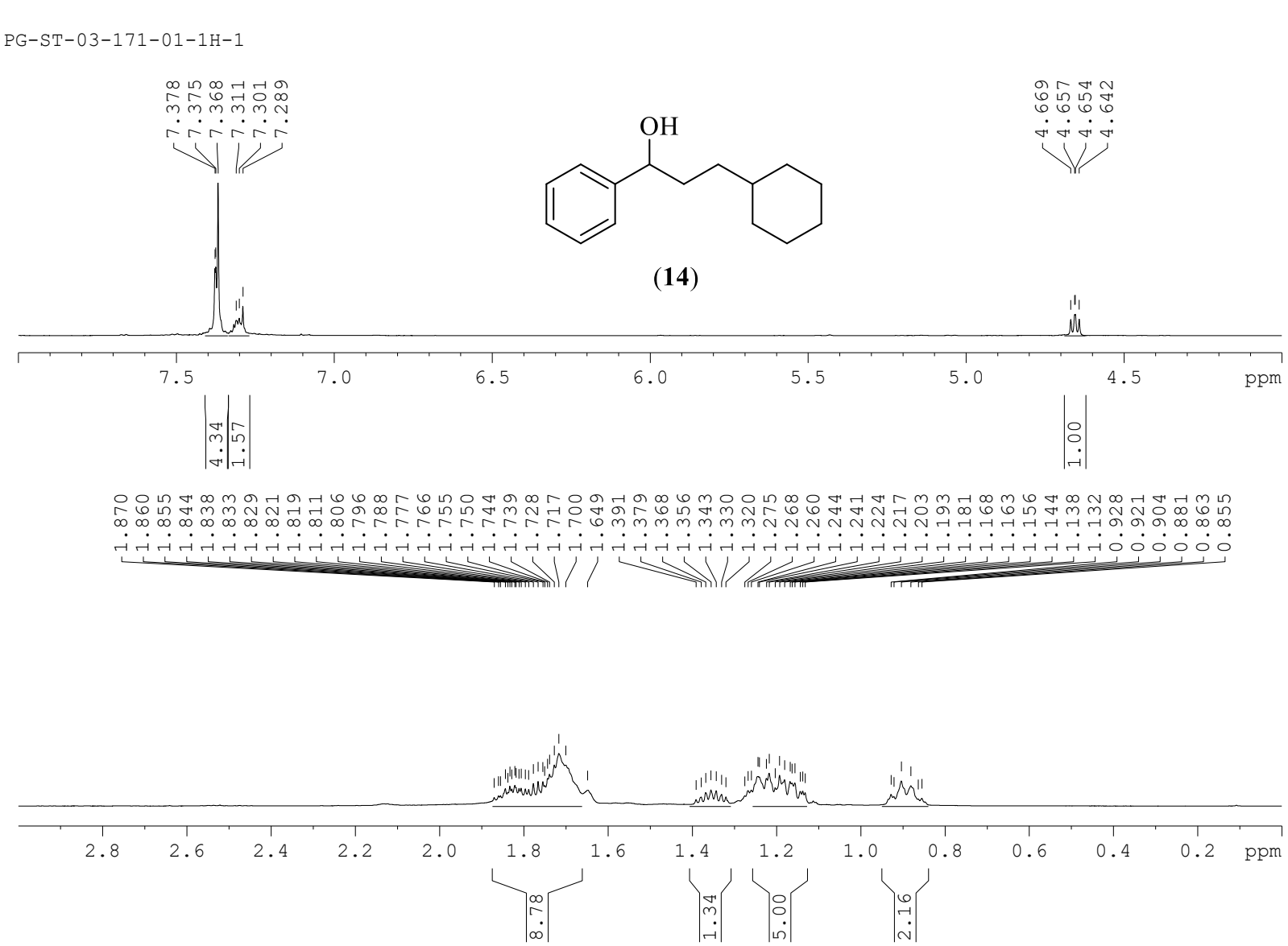


Figure S98. Expanded ^{1}H NMR spectrum of (**14**) in $CDCl_3$.

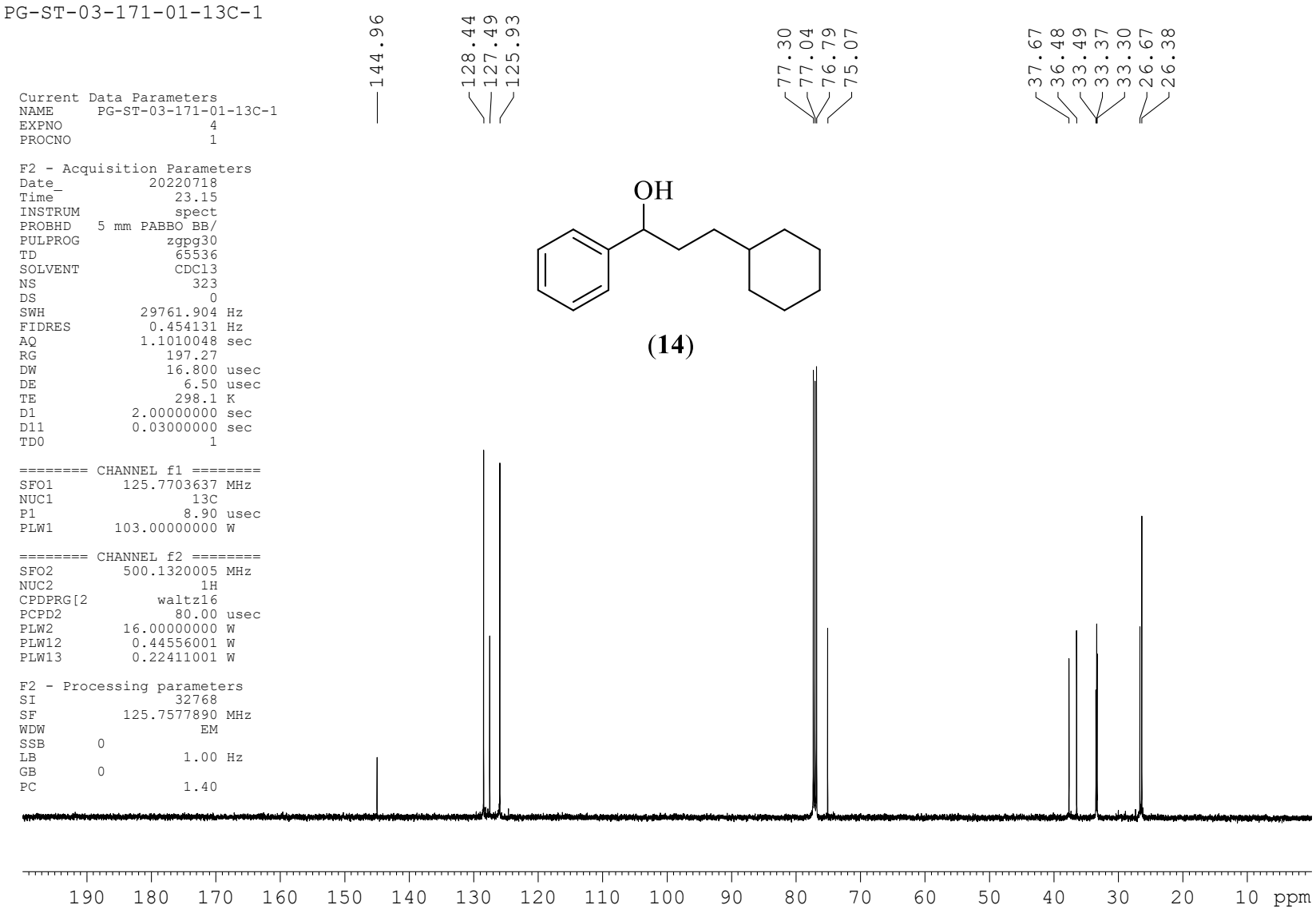


Figure S99. $^{13}C\{^{1}H\}$ NMR spectrum of (**14**) in $CDCl_3$.

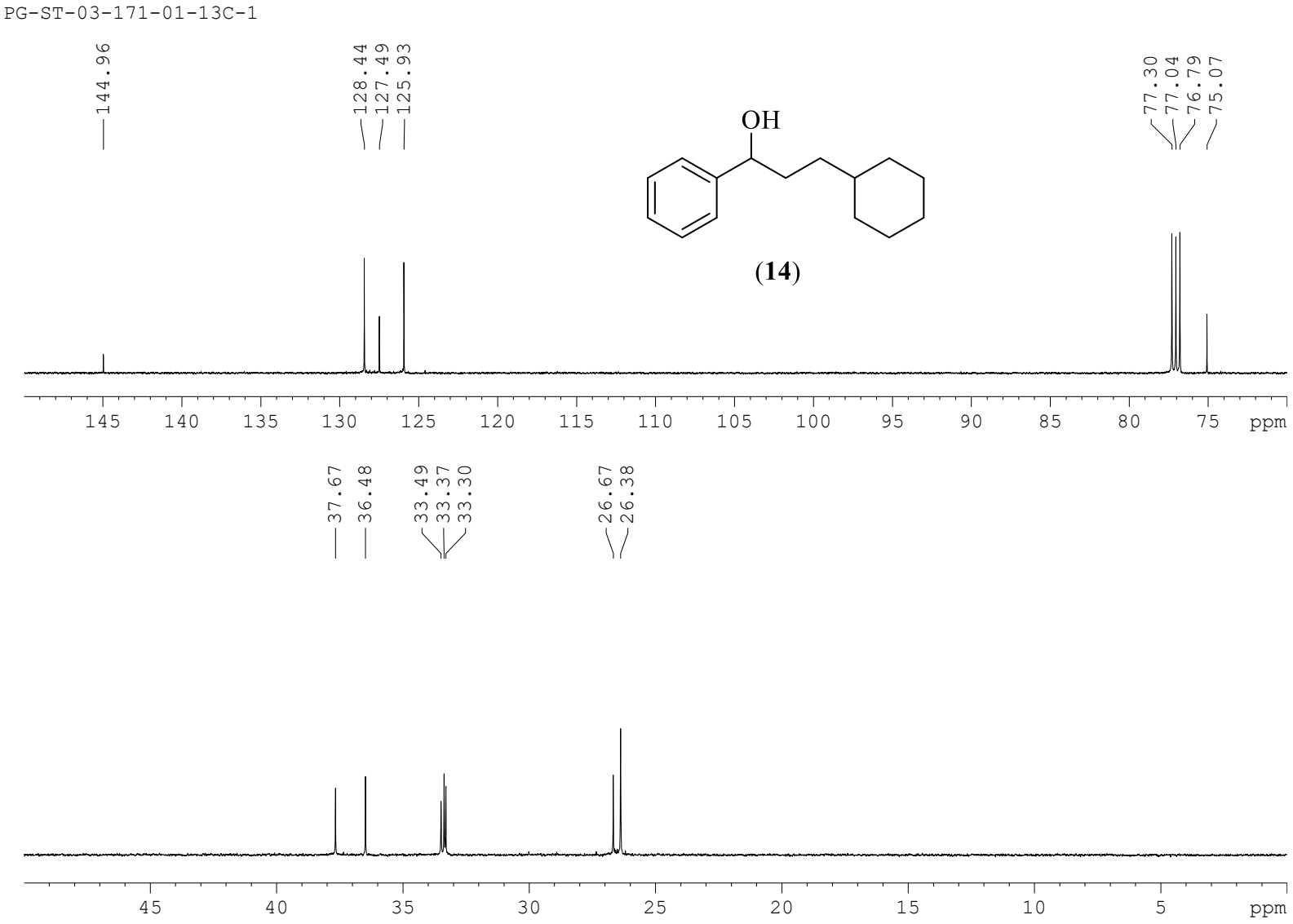


Figure S100. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**14**) in $CDCl_3$.

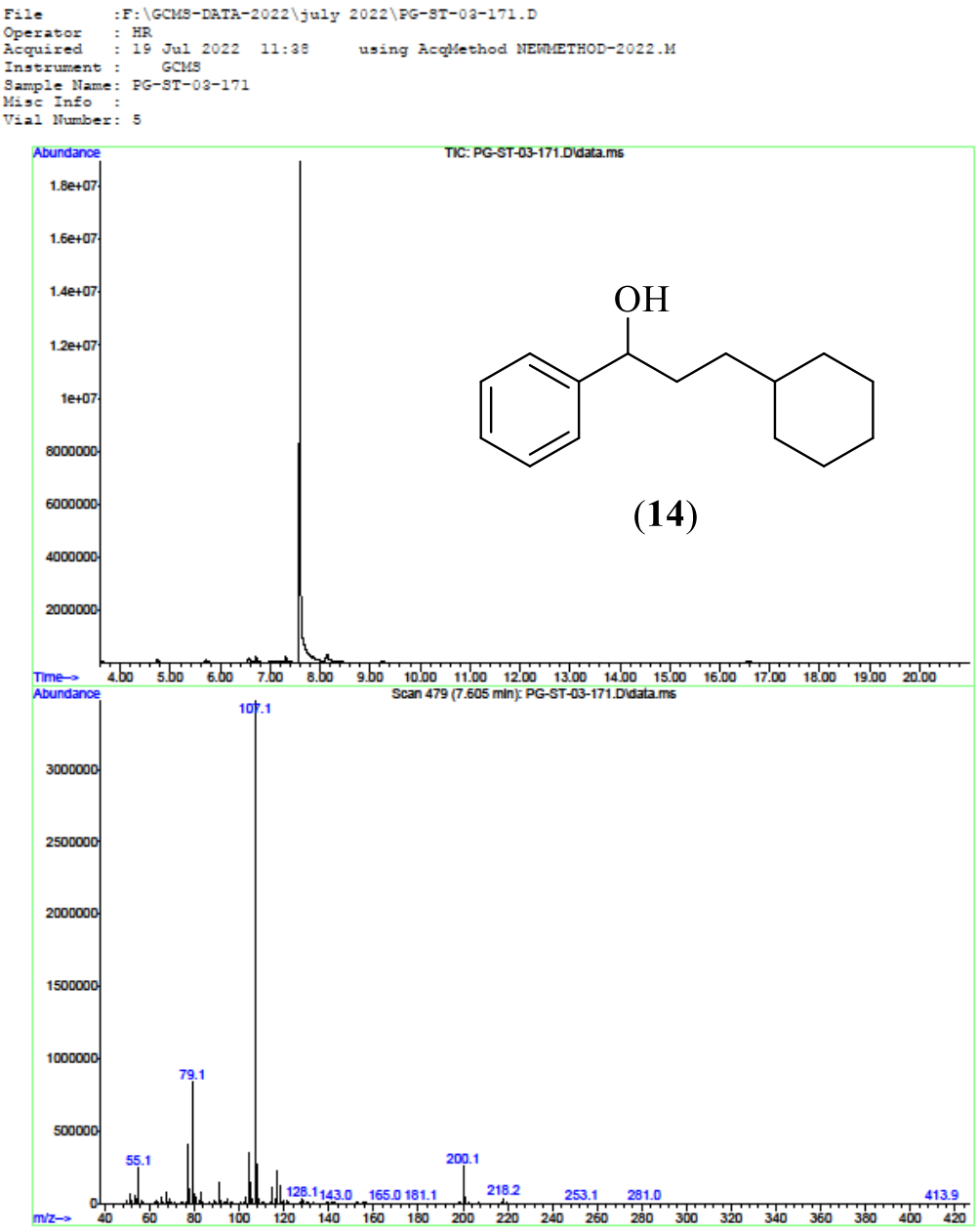
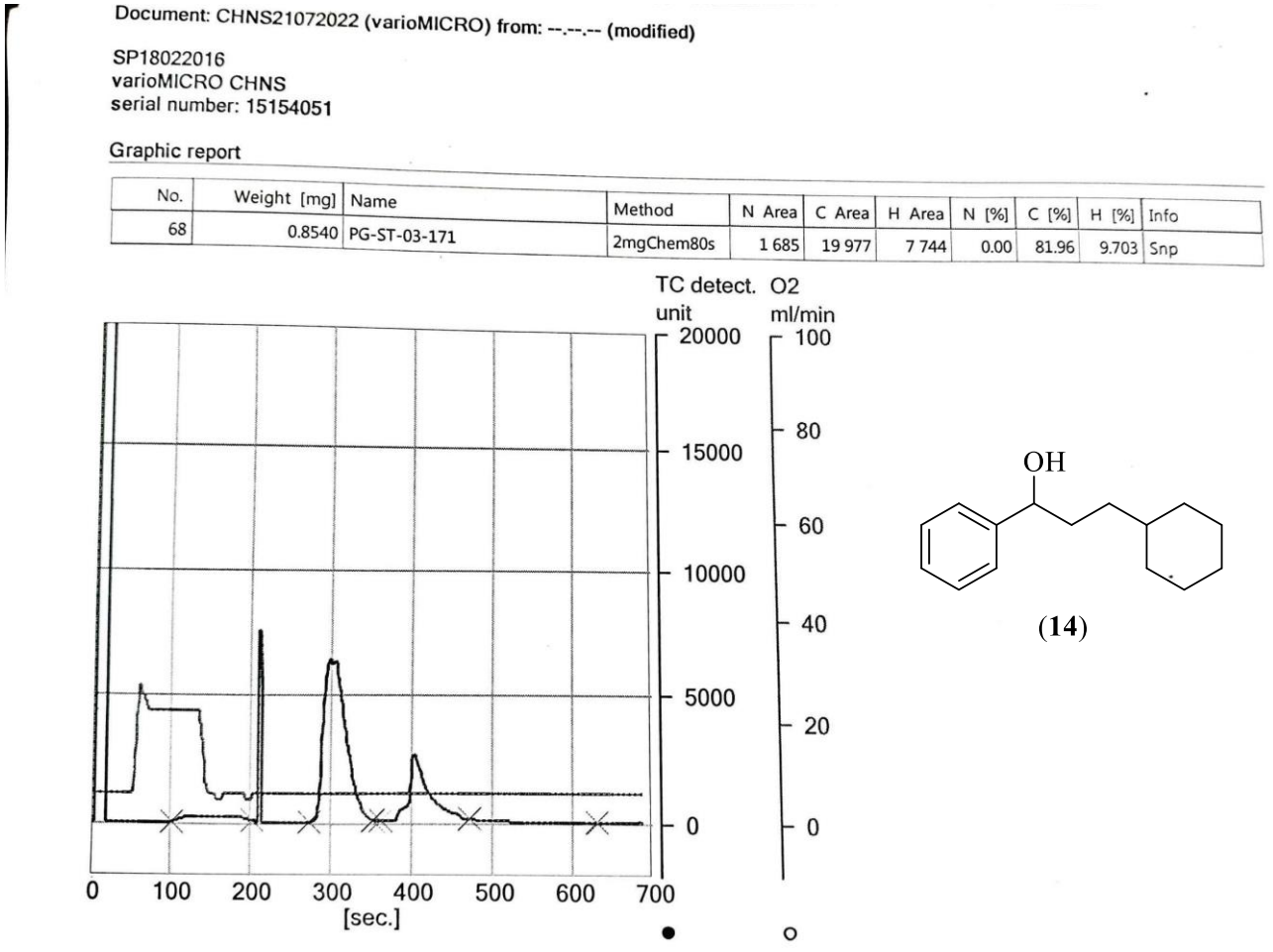


Figure S101. GCMS trace in EtOAc of (**14**) showing the M^+ peak at *m/z* 218.



(**14**)

Figure S102. Elemental analysis data of (**14**).

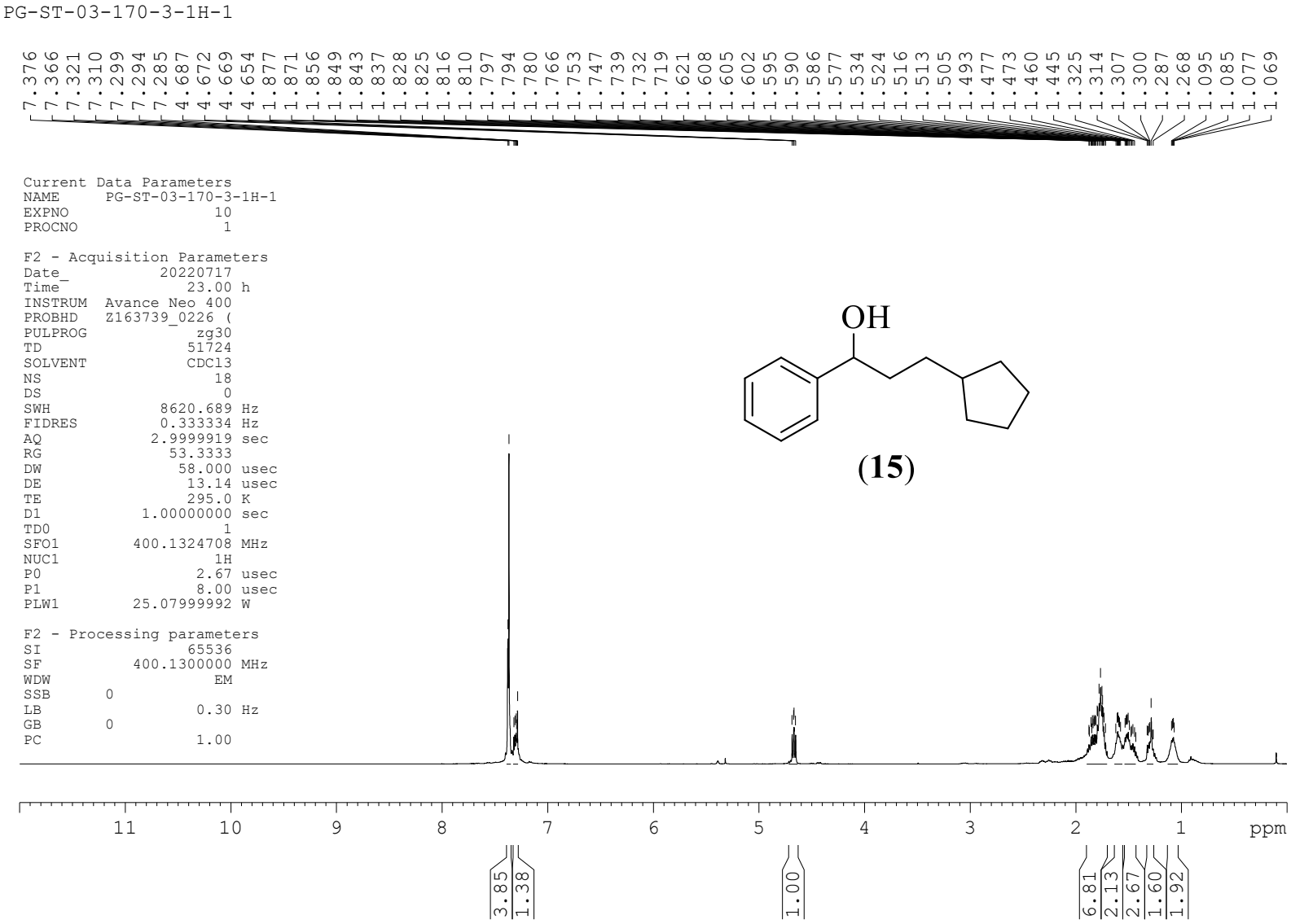


Figure S103. ^{1}H NMR spectrum of (**15**) in $CDCl_3$.

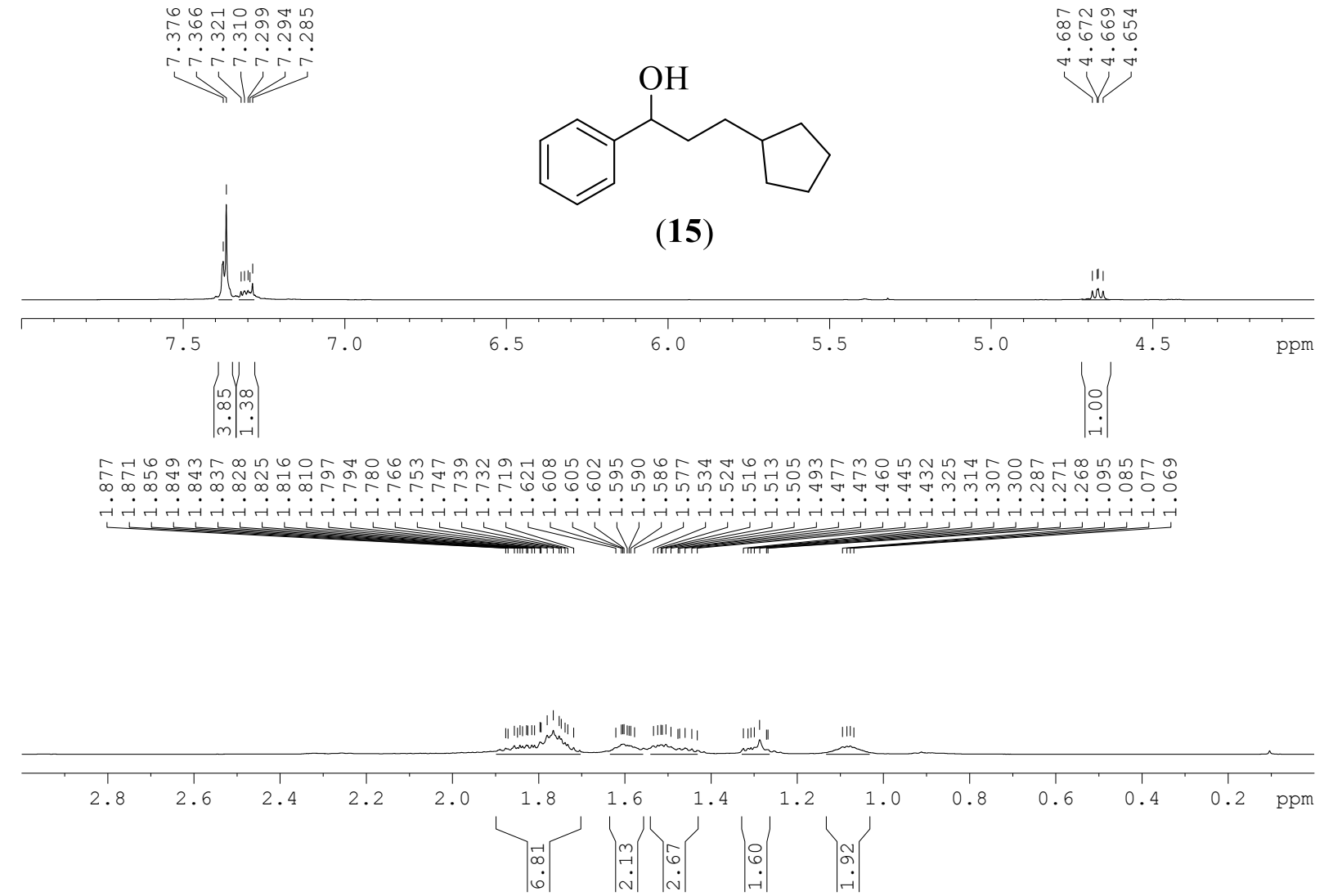


Figure S104. Expanded ^{1}H NMR spectrum of (**15**) in $CDCl_3$.

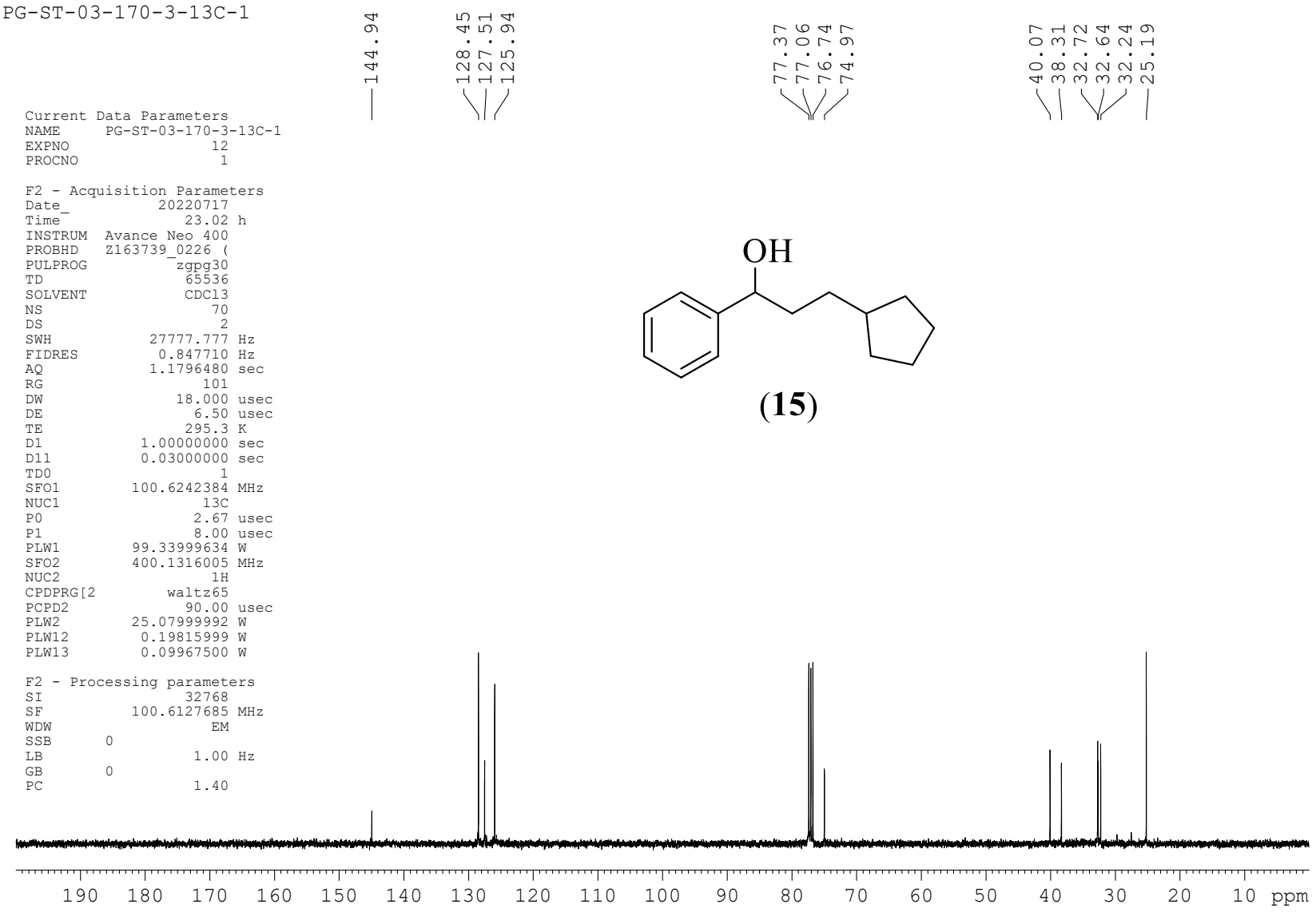


Figure S105. $^{13}C\{^{1}H\}$ NMR spectrum of (**15**) in $CDCl_3$.

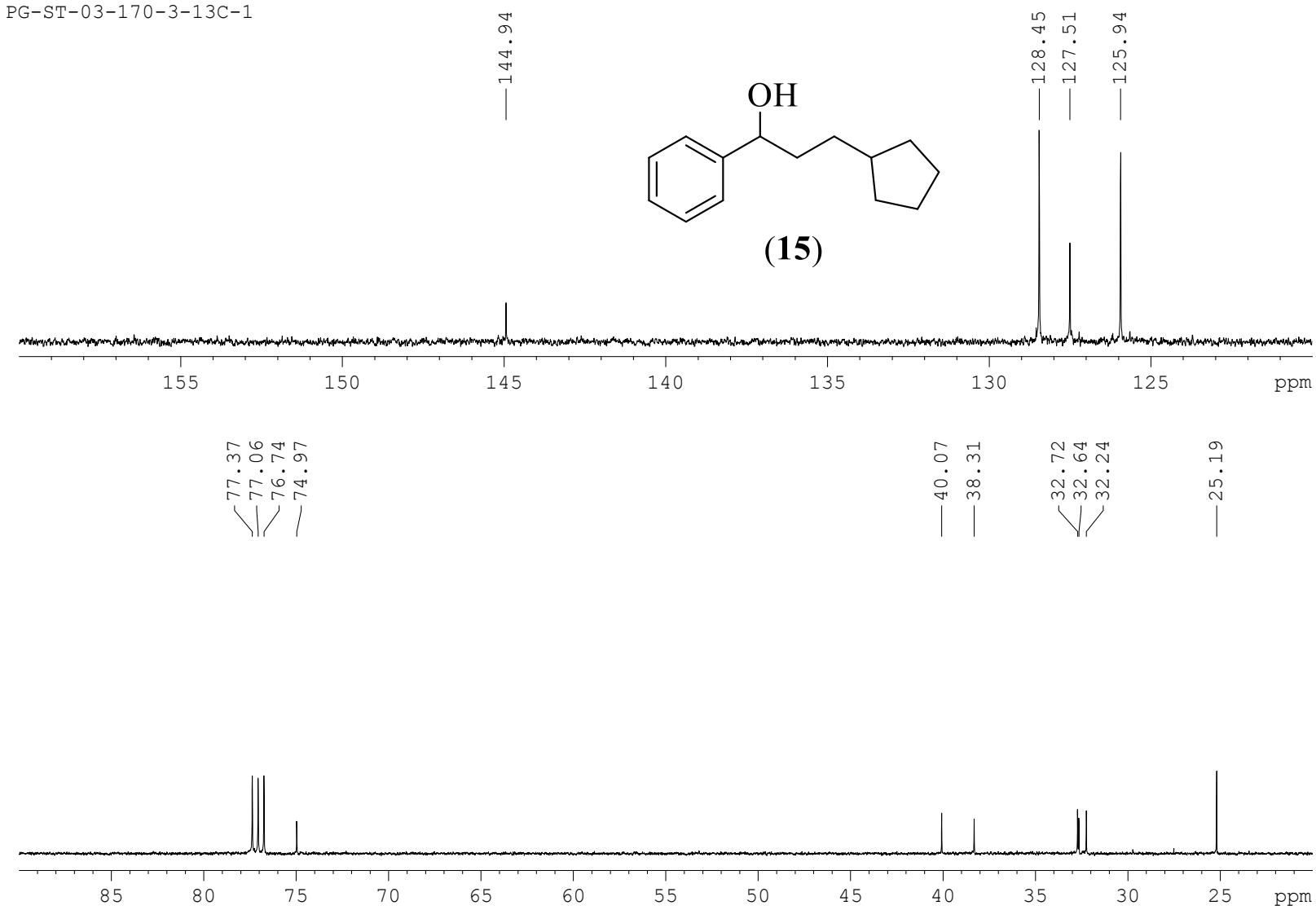


Figure S106. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**15**) in $CDCl_3$.

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Instrument :    GCMS
Sample Name: PG-ST-03-170-2
Misc Info  :
Vial Number: 6
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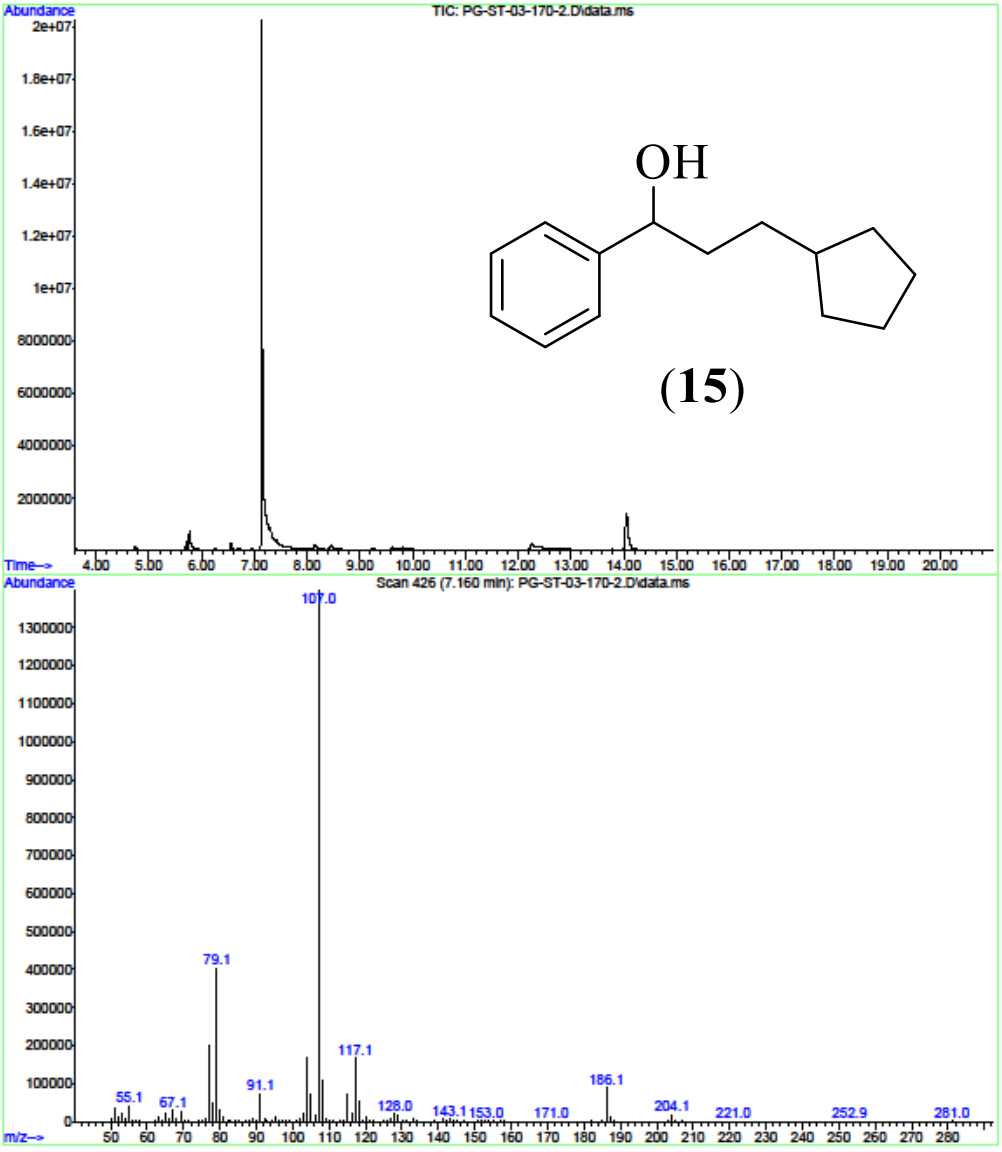

Figure S107. GCMS trace in EtOAc of (**15**) showing the M^+ peak at *m/z* 186.

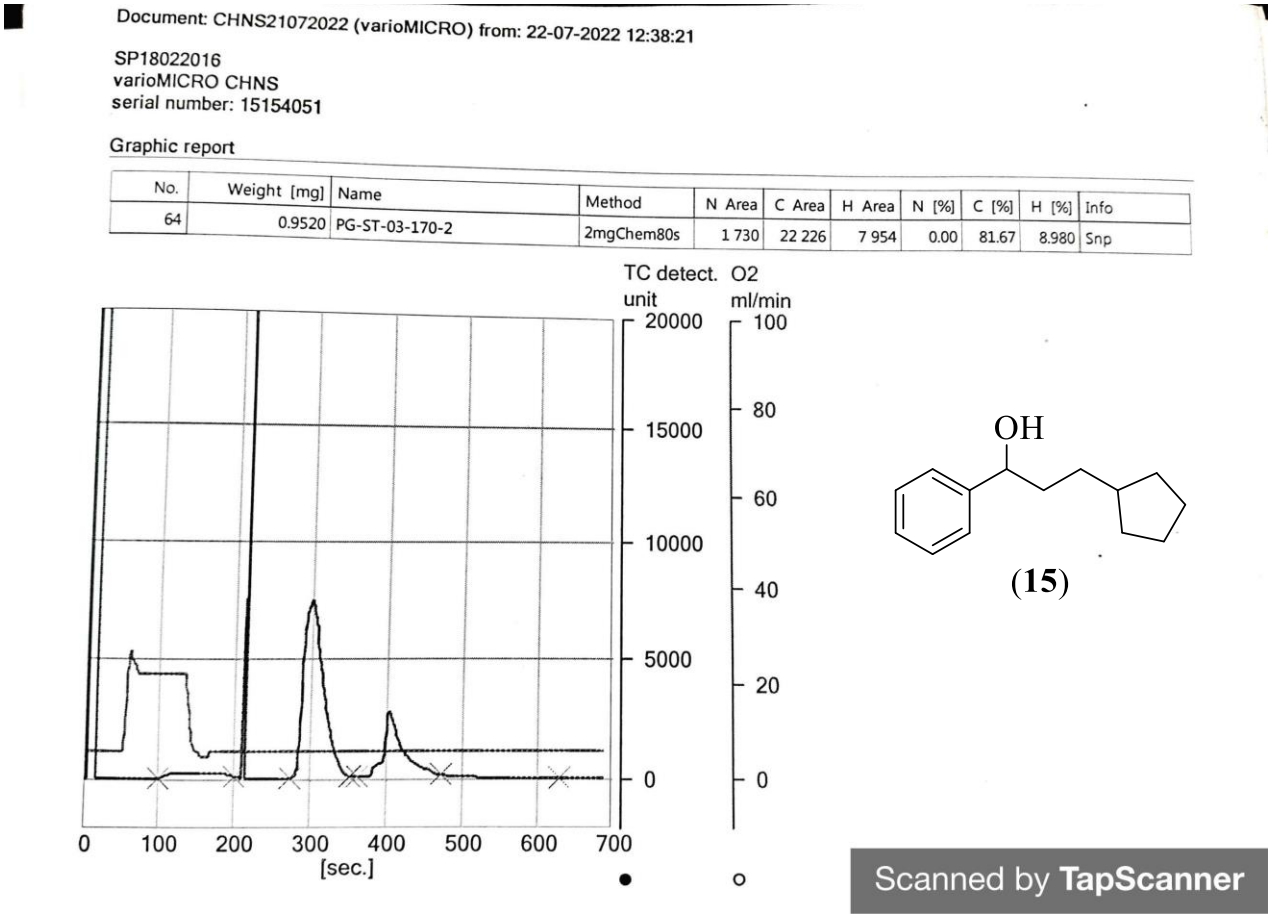

Figure S108. Elemental analysis data of (**15**).

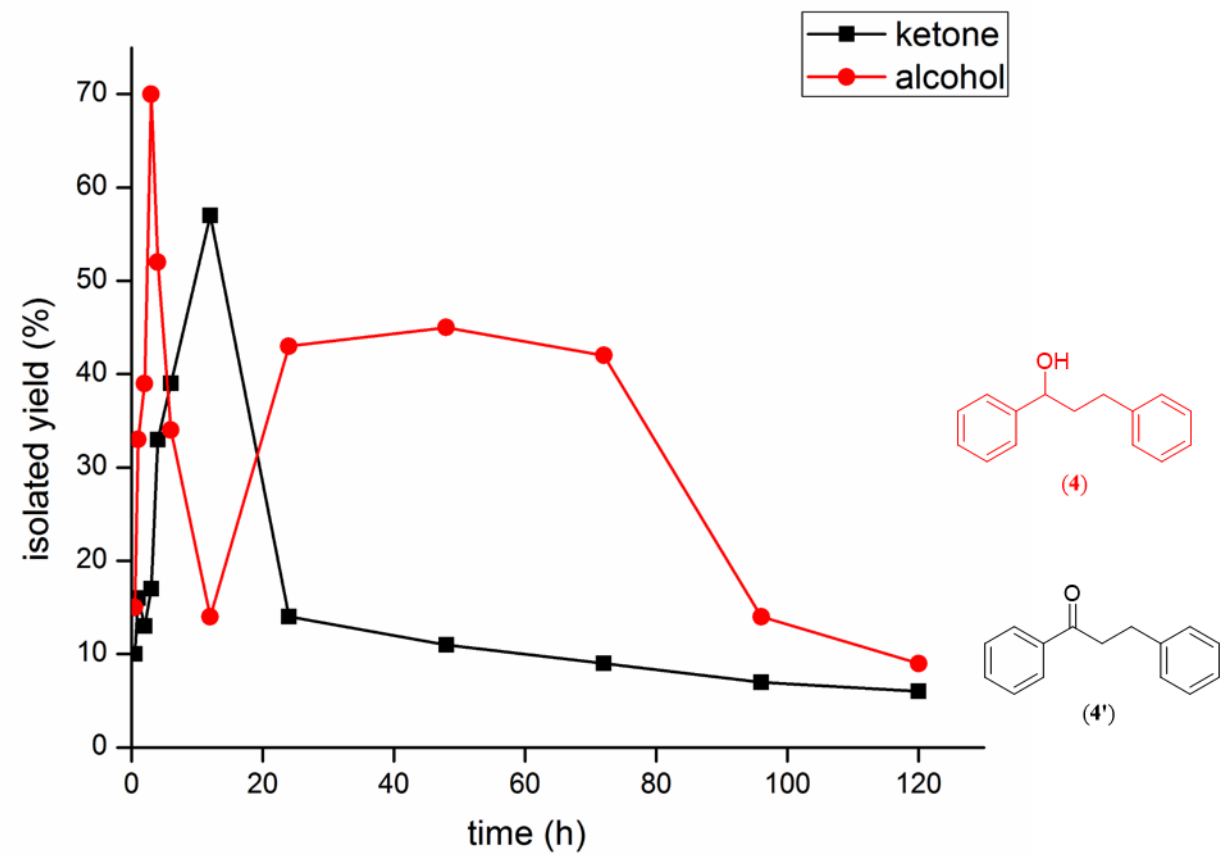

Figure S109. An overlay of the formation of (**4**) and (**4'**) as a function of time in the reaction of 1-phenylethanol and benzyl alcohol as catalyzed by the Ru−NHC complex (**1b**).

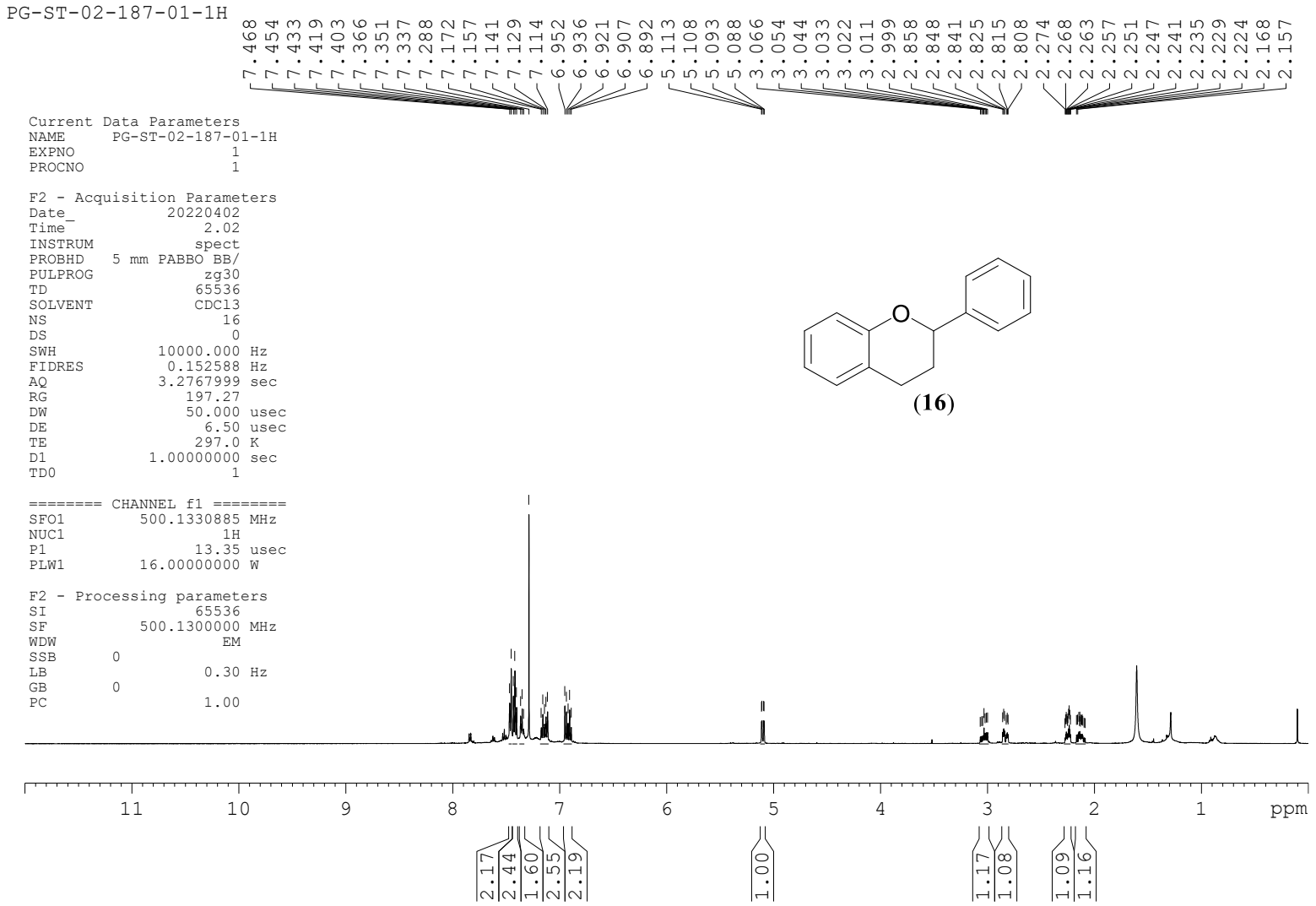

Figure S110. ^{1}H NMR spectrum of (**16**) in $CDCl_3$.

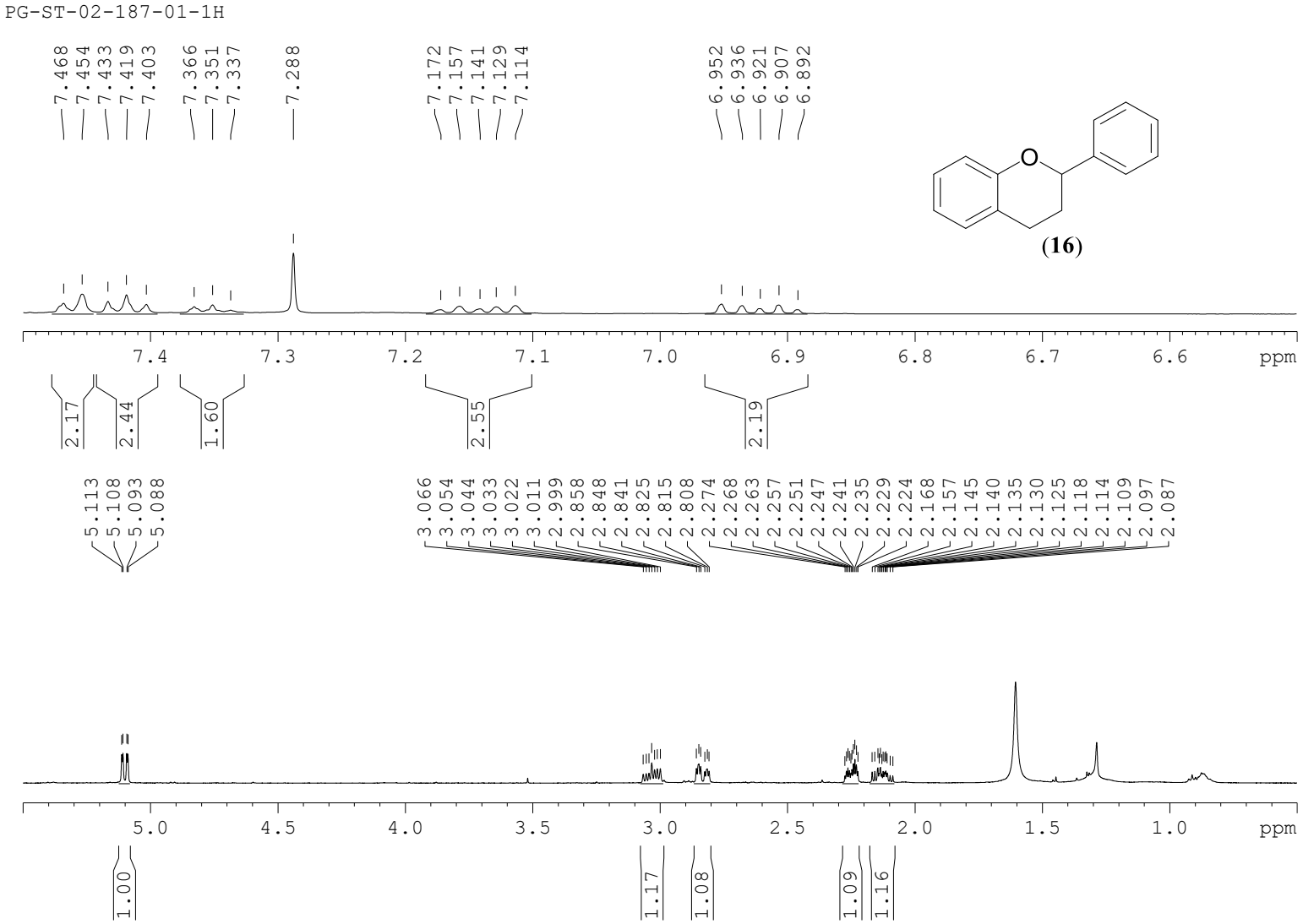

Figure S111. Expanded ^{1}H NMR spectrum of (**16**) in $CDCl_3$.

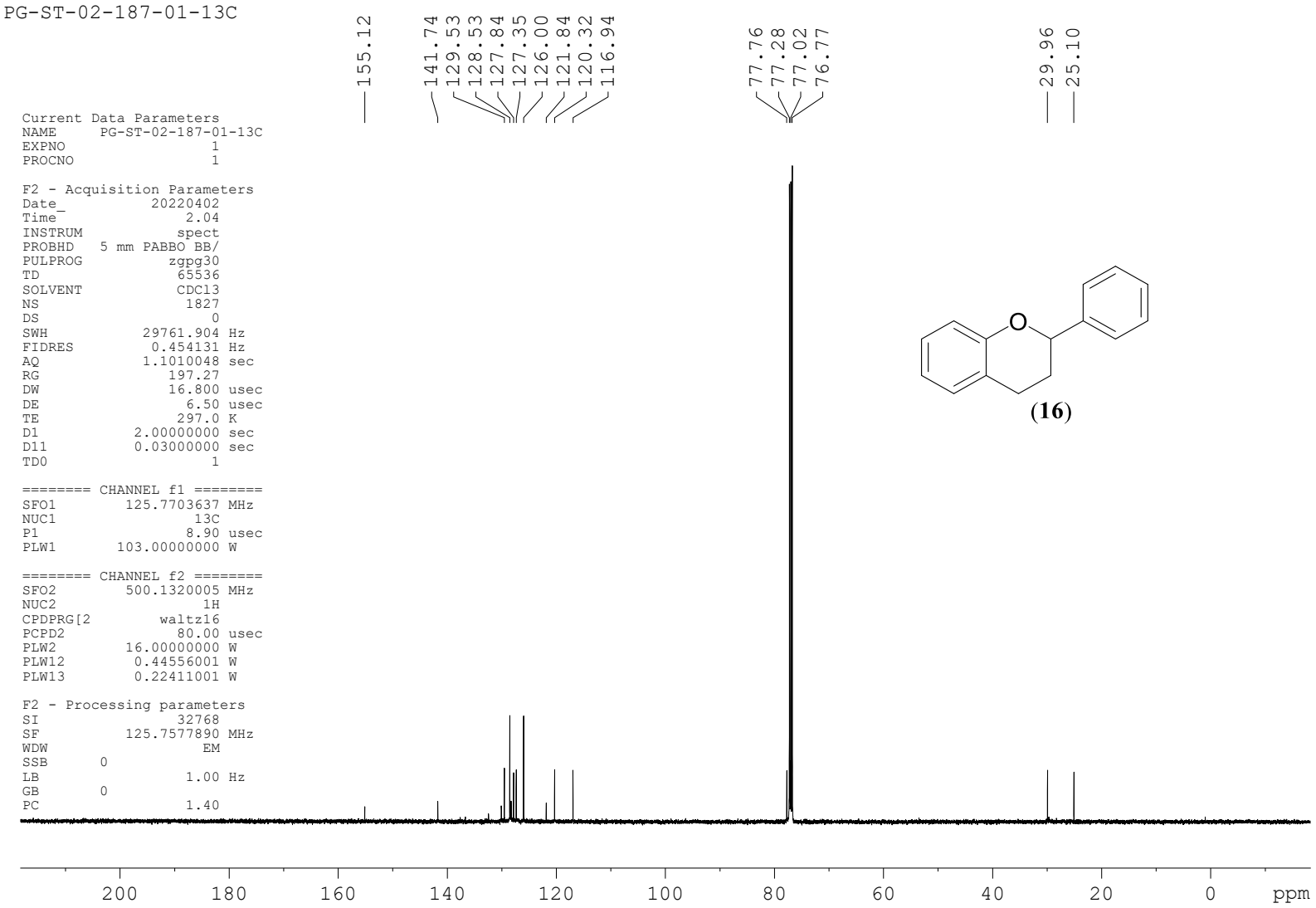

Figure S112. $^{13}C\{^{1}H\}$ NMR spectrum of (**16**) in $CDCl_3$.

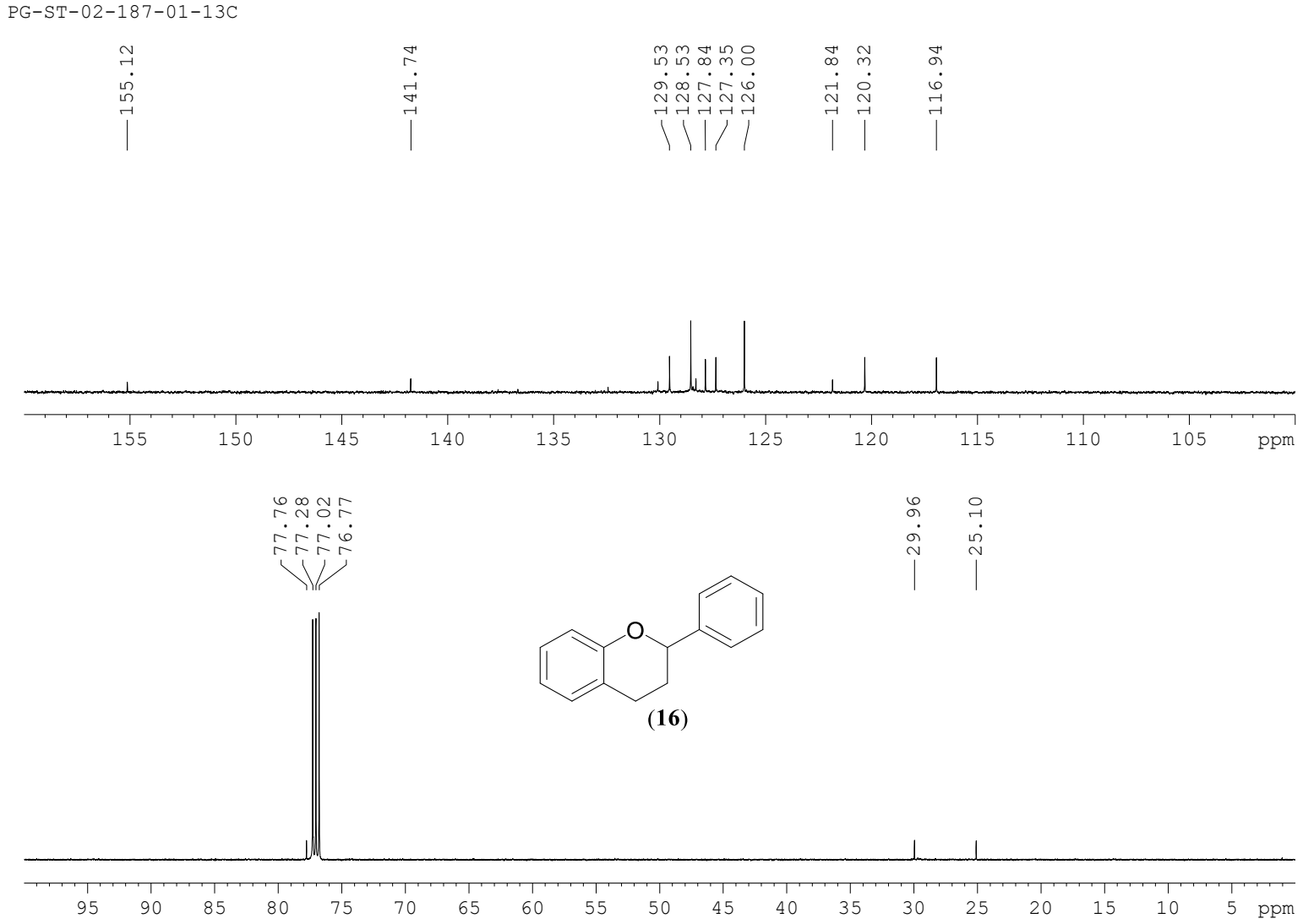

Figure S113. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**16**) in $CDCl_3$.

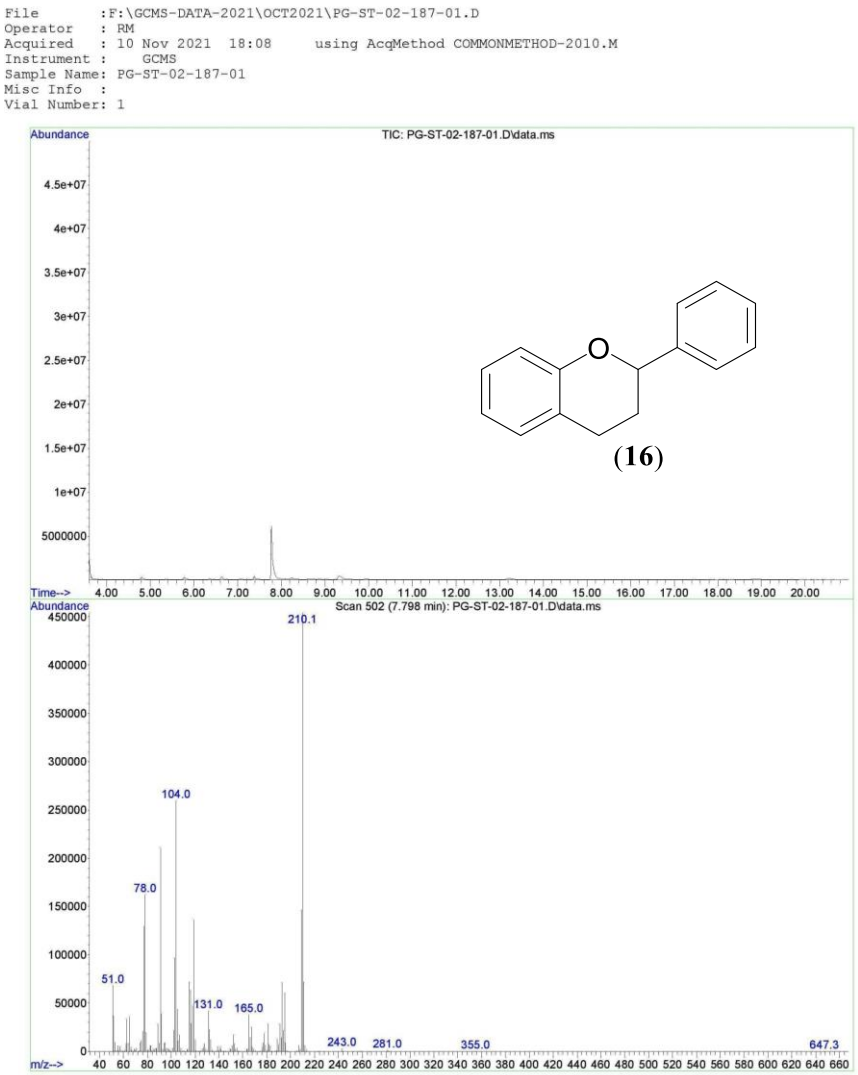

Figure S114. GCMS trace in EtOAc of (**16**) showing the M^+ peak at *m/z* 210.

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date Time	Info
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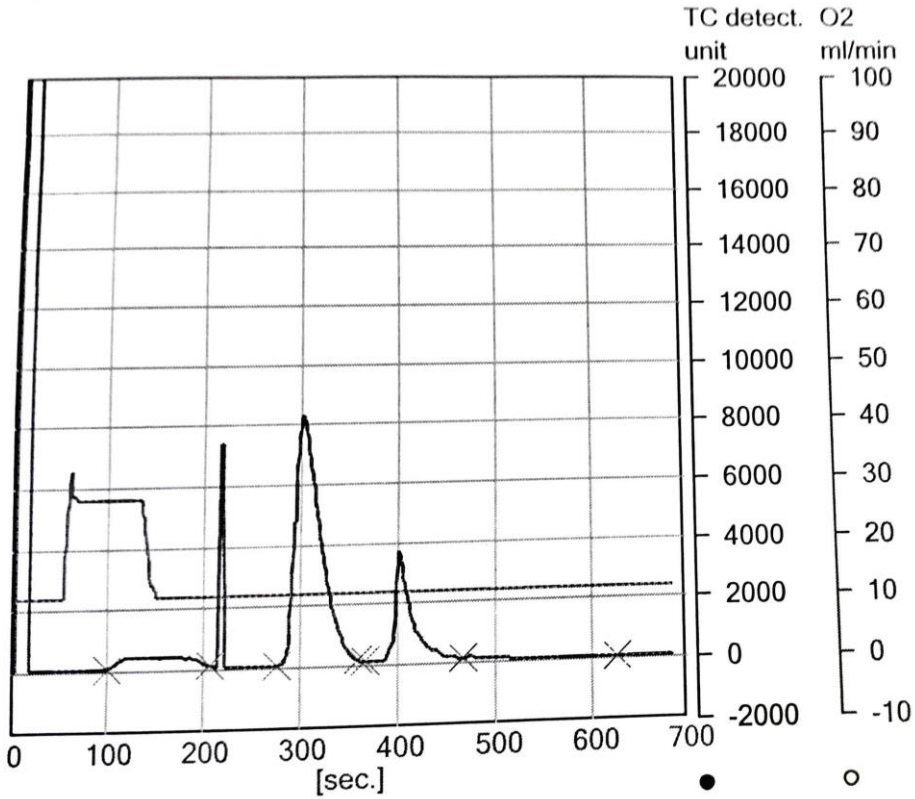

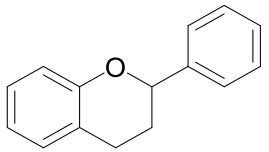

(**16**)

Figure S115. Elemental analysis data of (**16**).

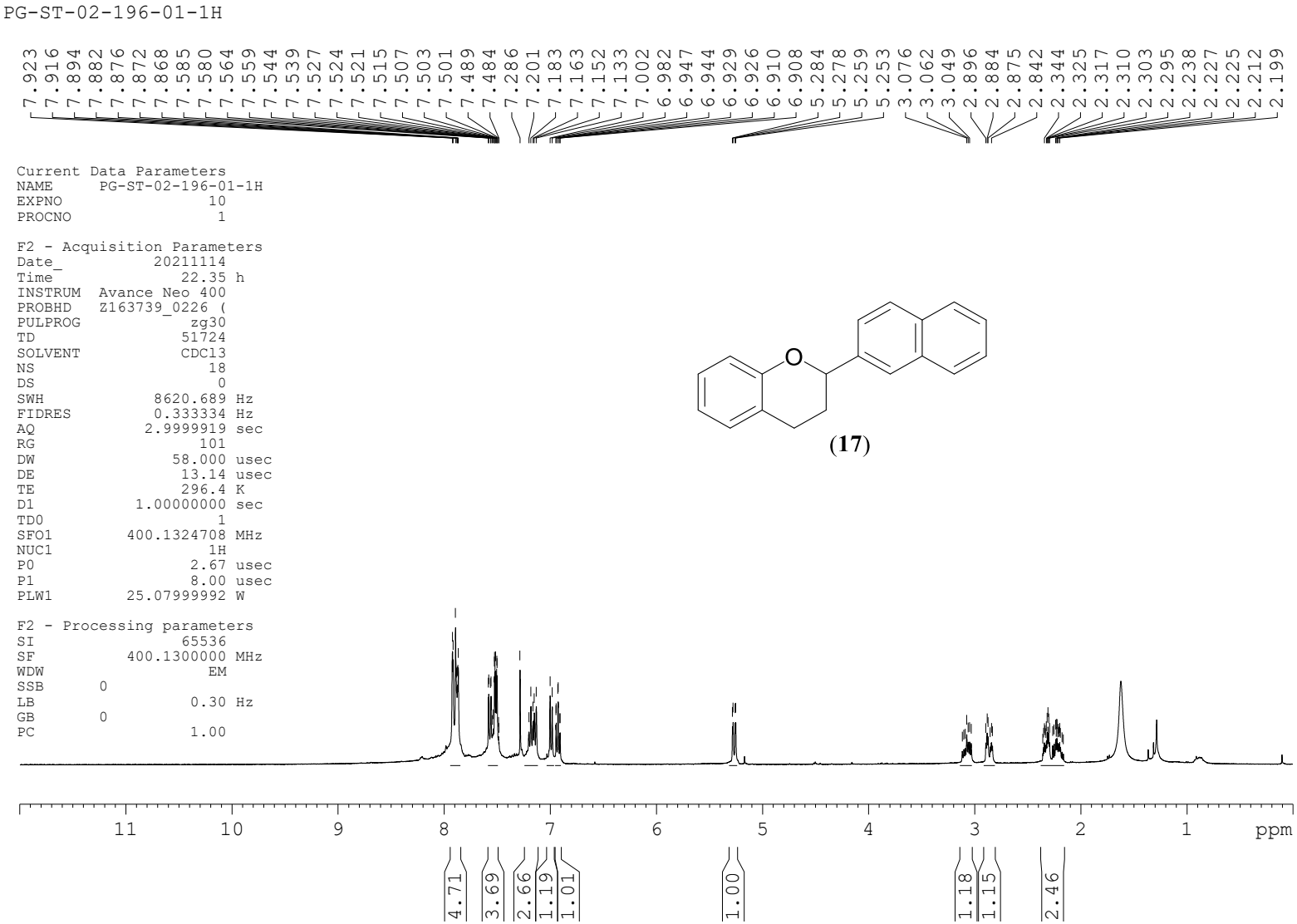

Figure S116. ^{1}H NMR spectrum of (**17**) in $CDCl_3$.

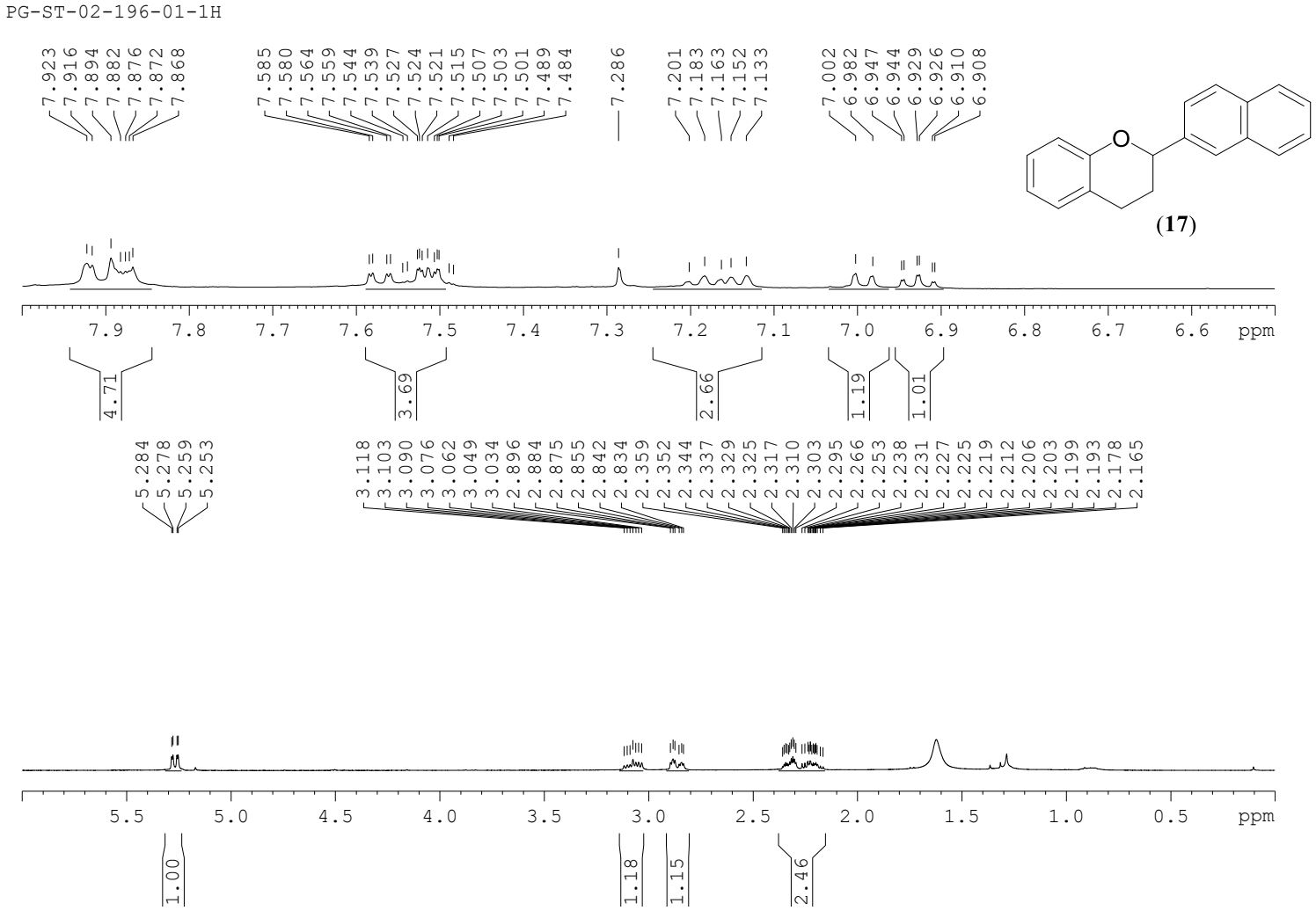

Figure S117. Expanded ^{1}H NMR spectrum of (**17**) in $CDCl_3$.

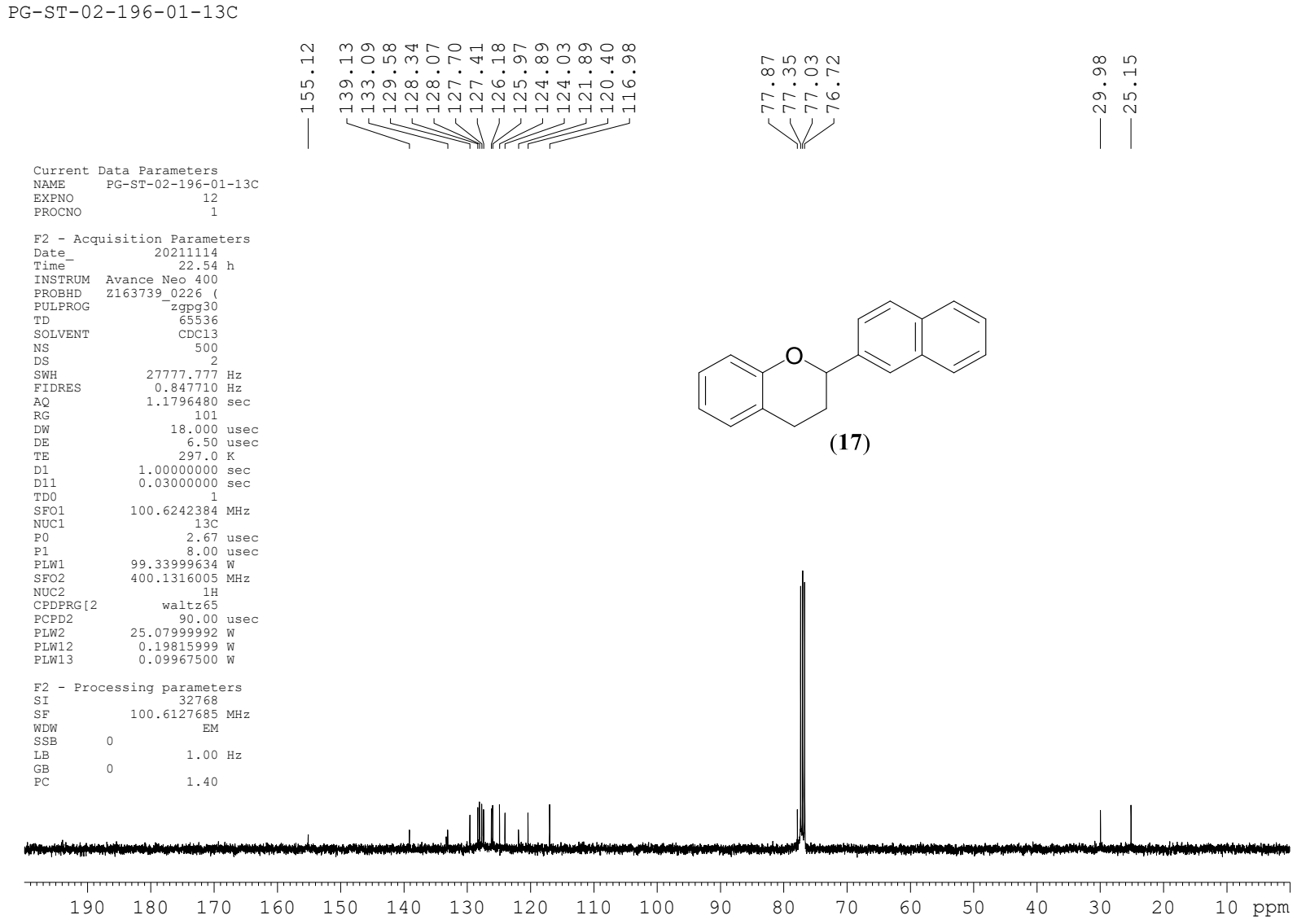

Figure S118. $^{13}C\{^{1}H\}$ NMR spectrum of (**17**) in $CDCl_3$.

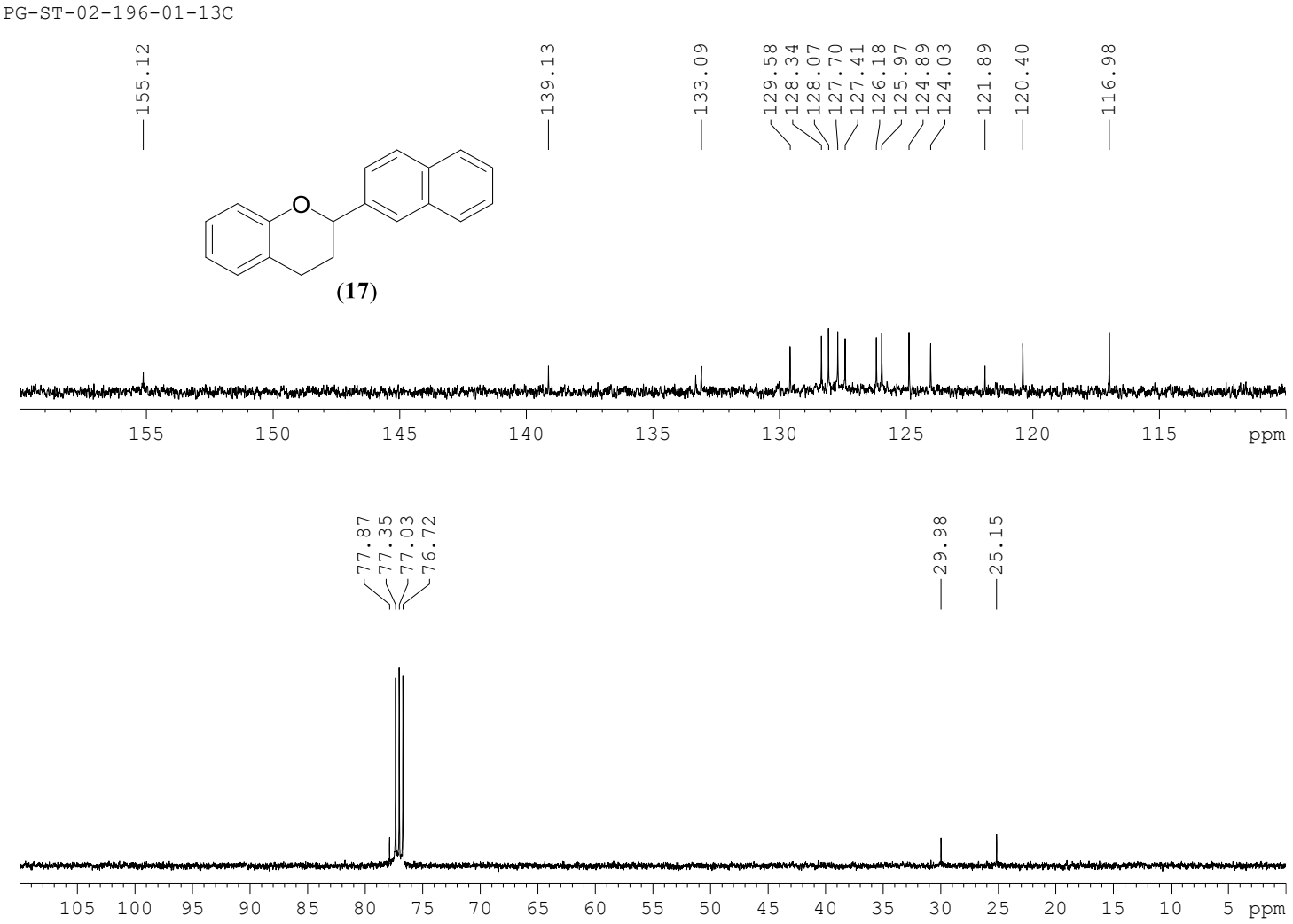

Figure S119. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**17**) in $CDCl_3$.

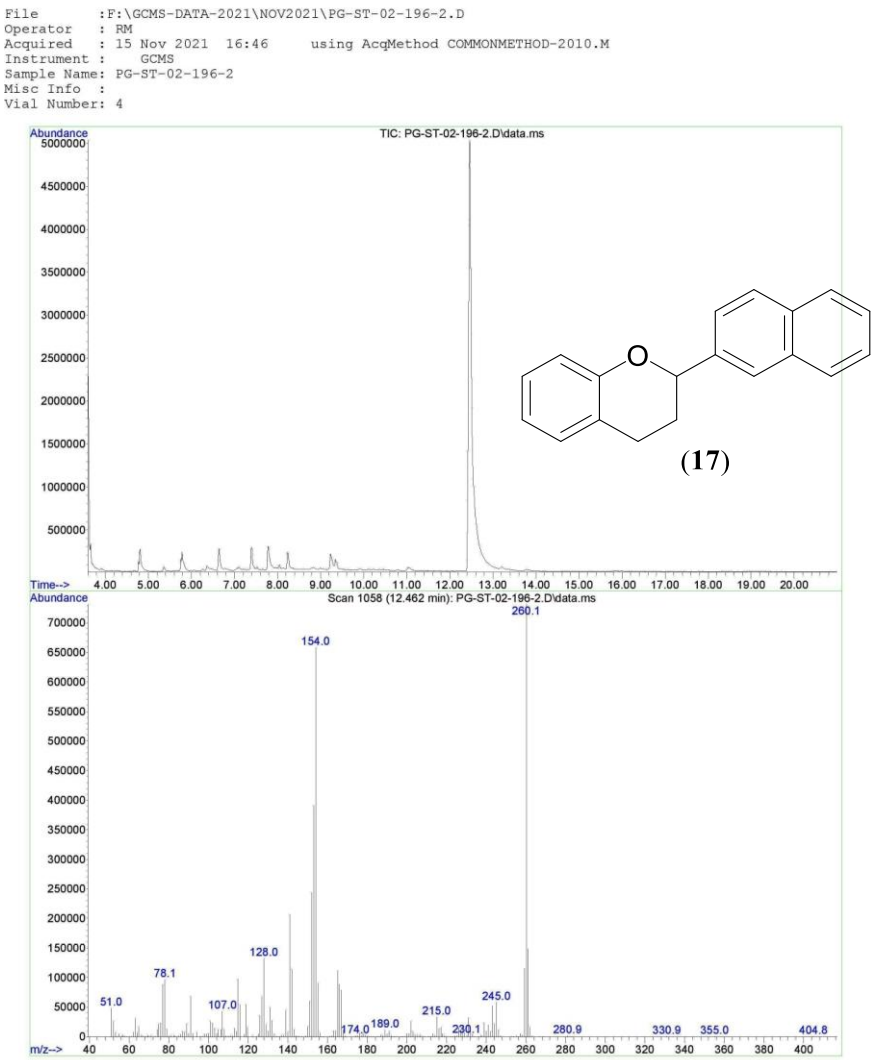

Figure S120. GCMS trace in EtOAc of (**17**) showing the M^+ peak at *m/z* 260.

Document: CHNS01022022 (varioMICRO) from: --.--.-- (modified)

SP18022016
varioMICRO CHNS
serial number: 15154051

Graphic report

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date Time	Info
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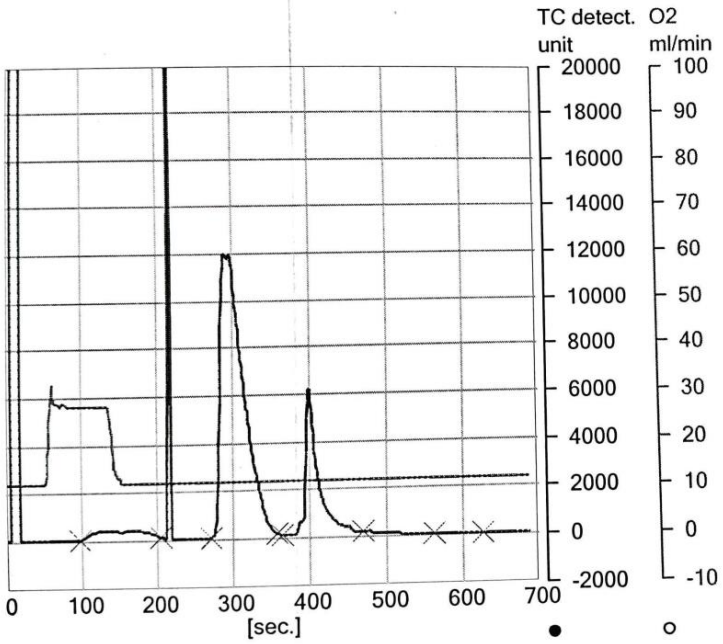
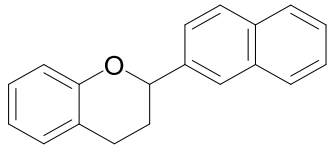




(**17**)

Figure S121. Elemental analysis data (**17**).

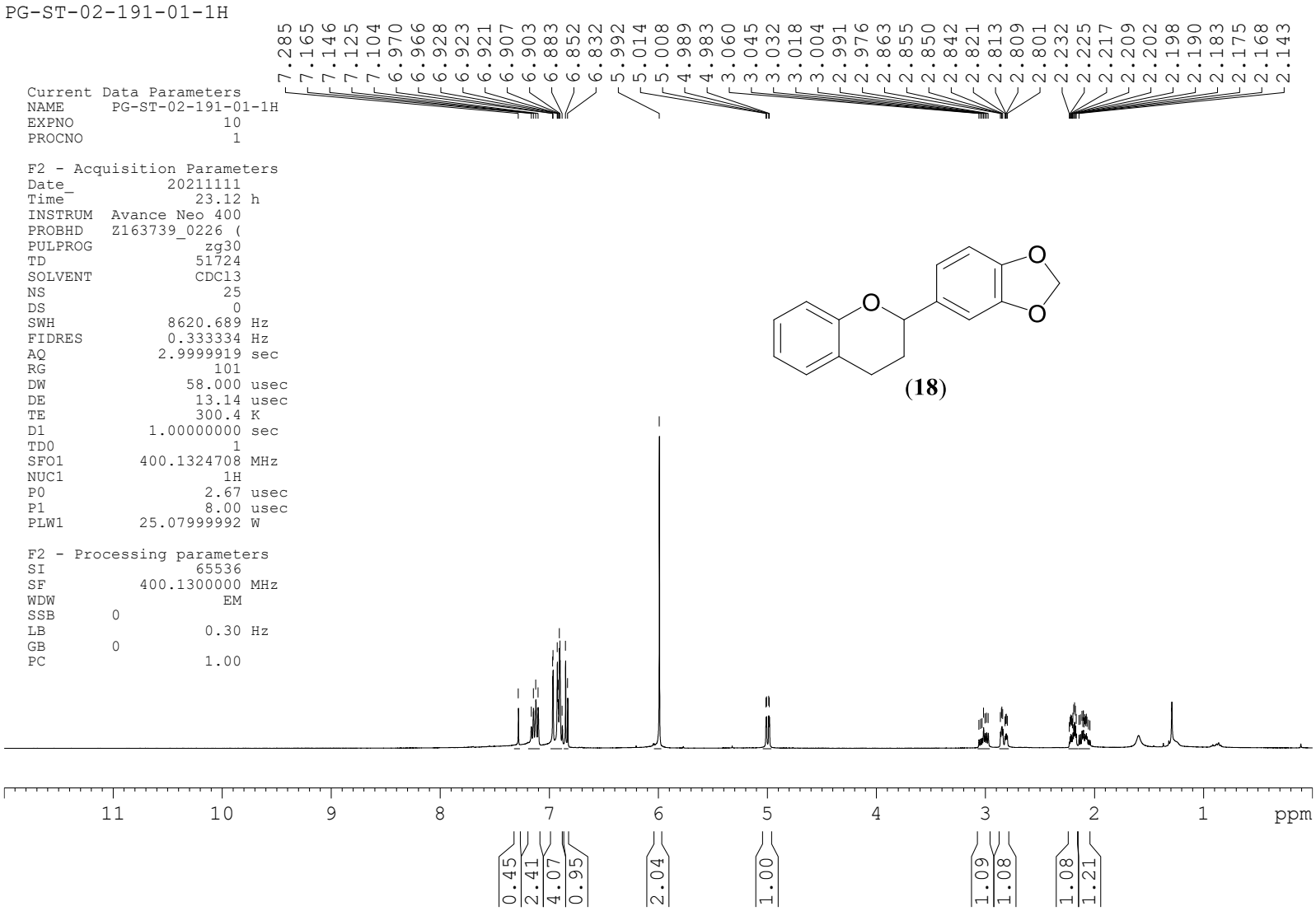


Figure S122. ^{1}H NMR spectrum of (**18**) in $CDCl_3$.

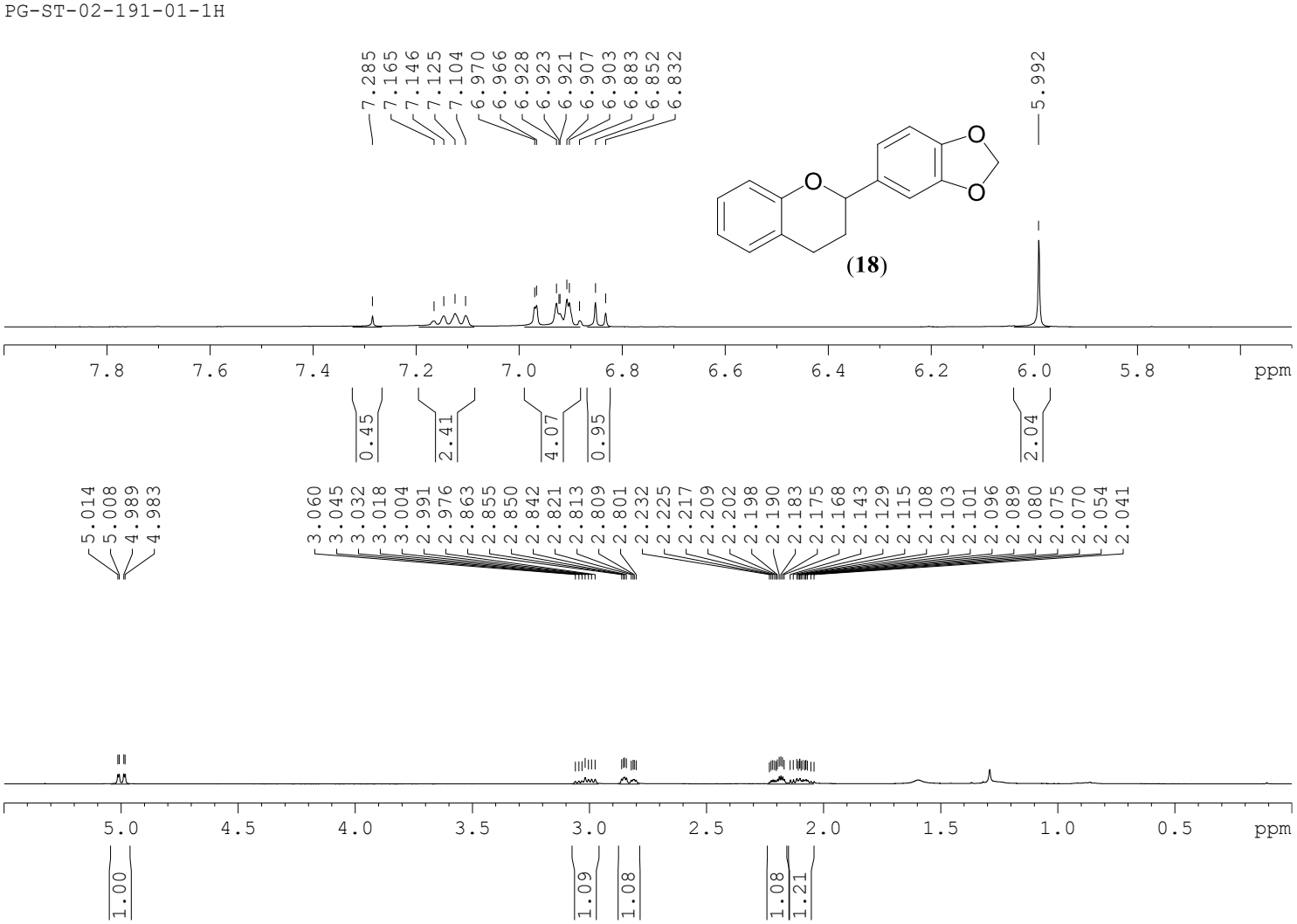
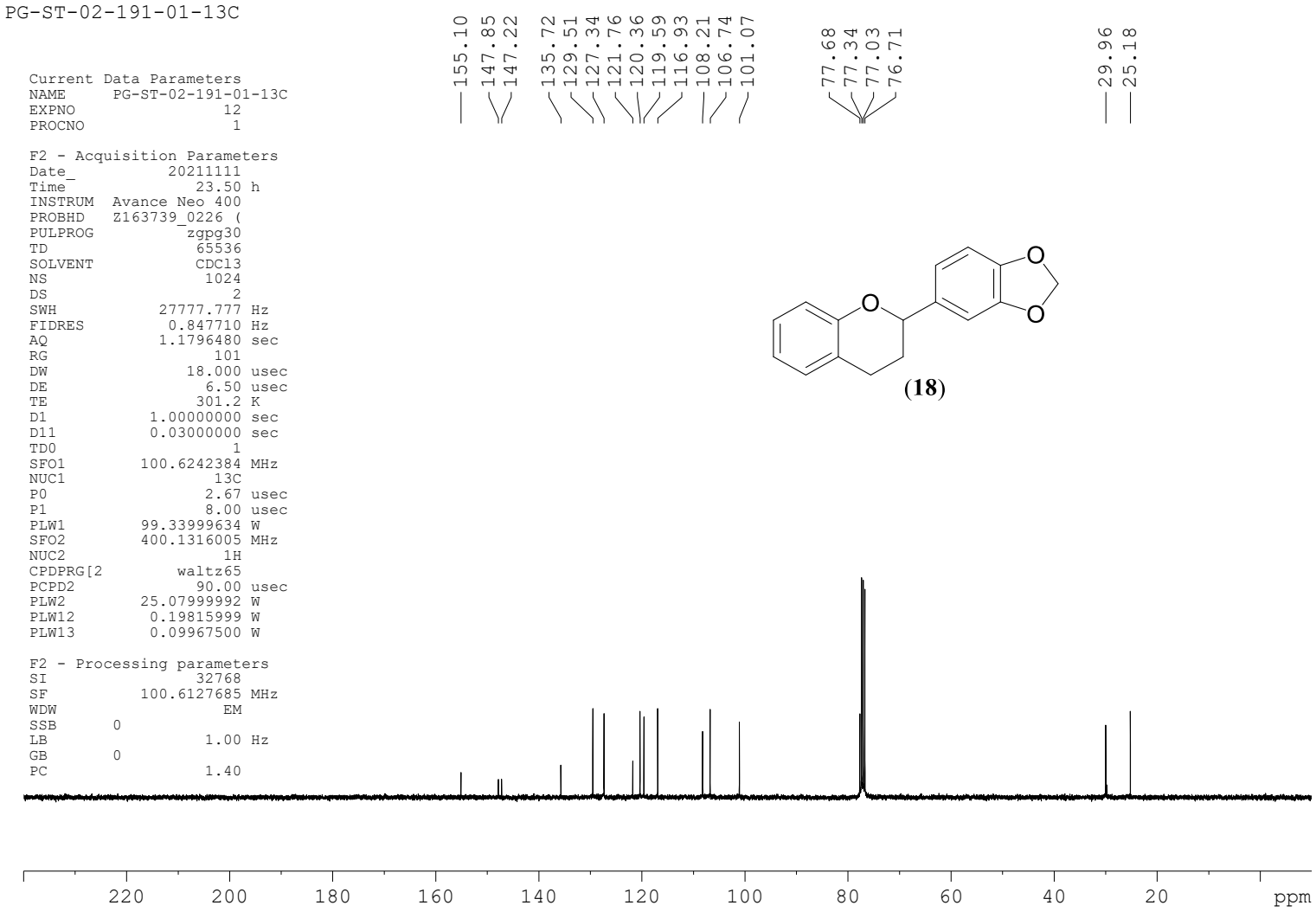


Figure S123. Expanded ^{1}H NMR spectrum of (**18**) in $CDCl_3$.



(**18**)

Figure S124. $^{13}C\{^{1}H\}$ NMR spectrum of (**18**) in $CDCl_3$.

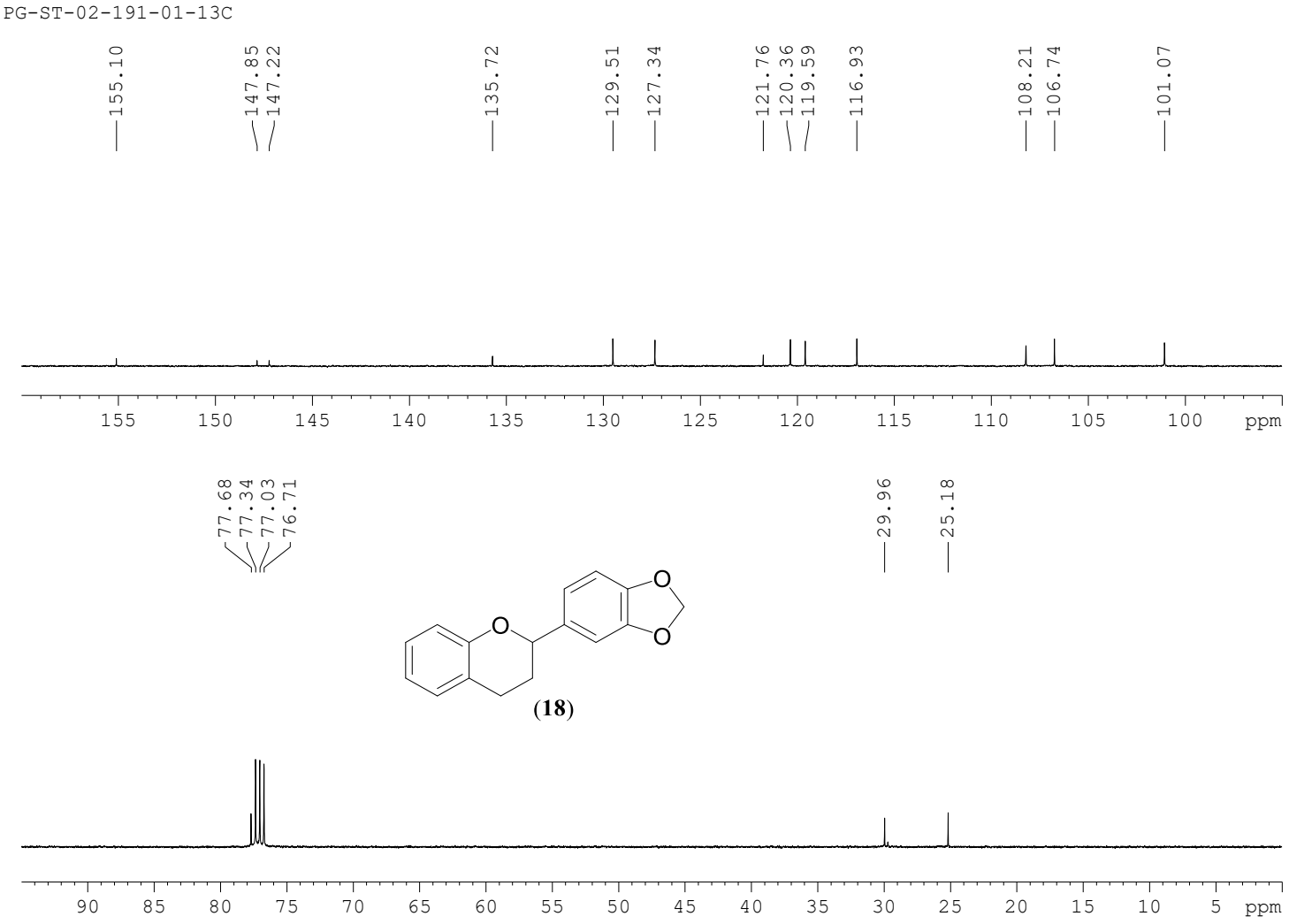


Figure S125. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**18**) in $CDCl_3$.

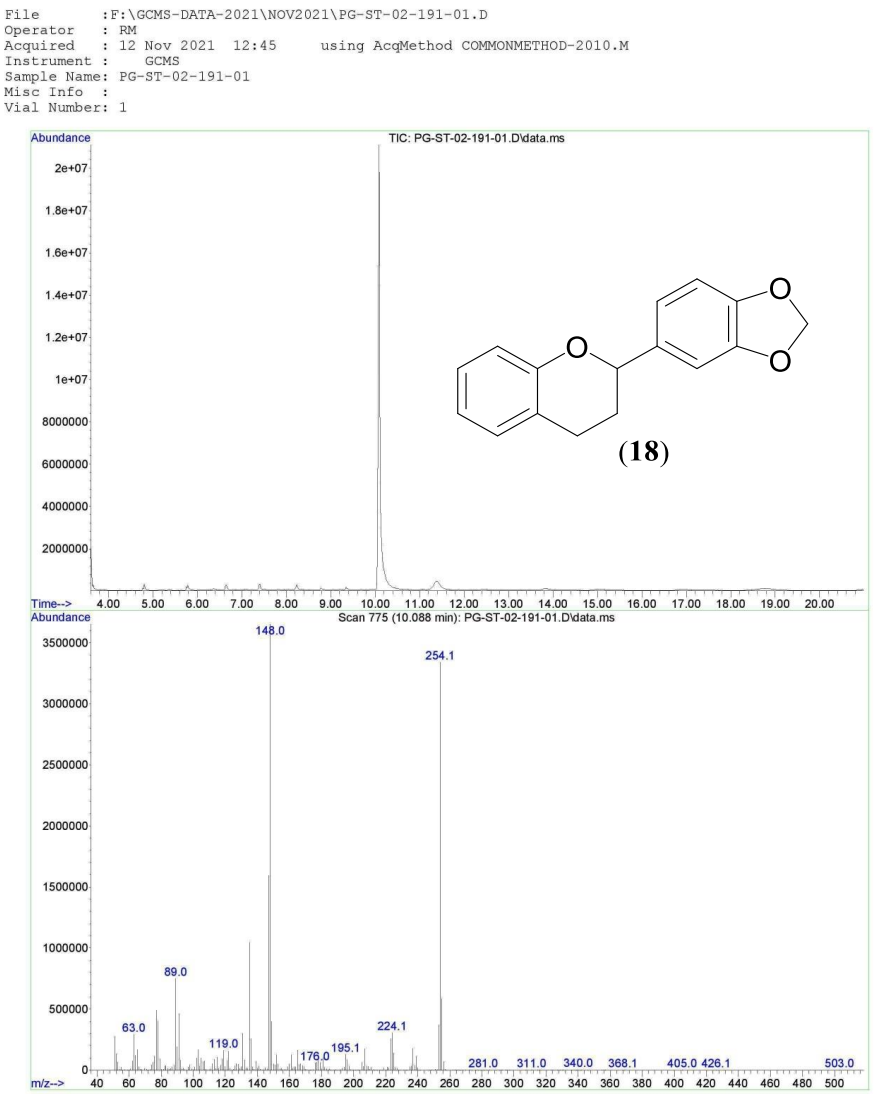


Figure S126. GCMS trace in EtOAc of (**18**) showing the M^+ peak at *m/z* 254.

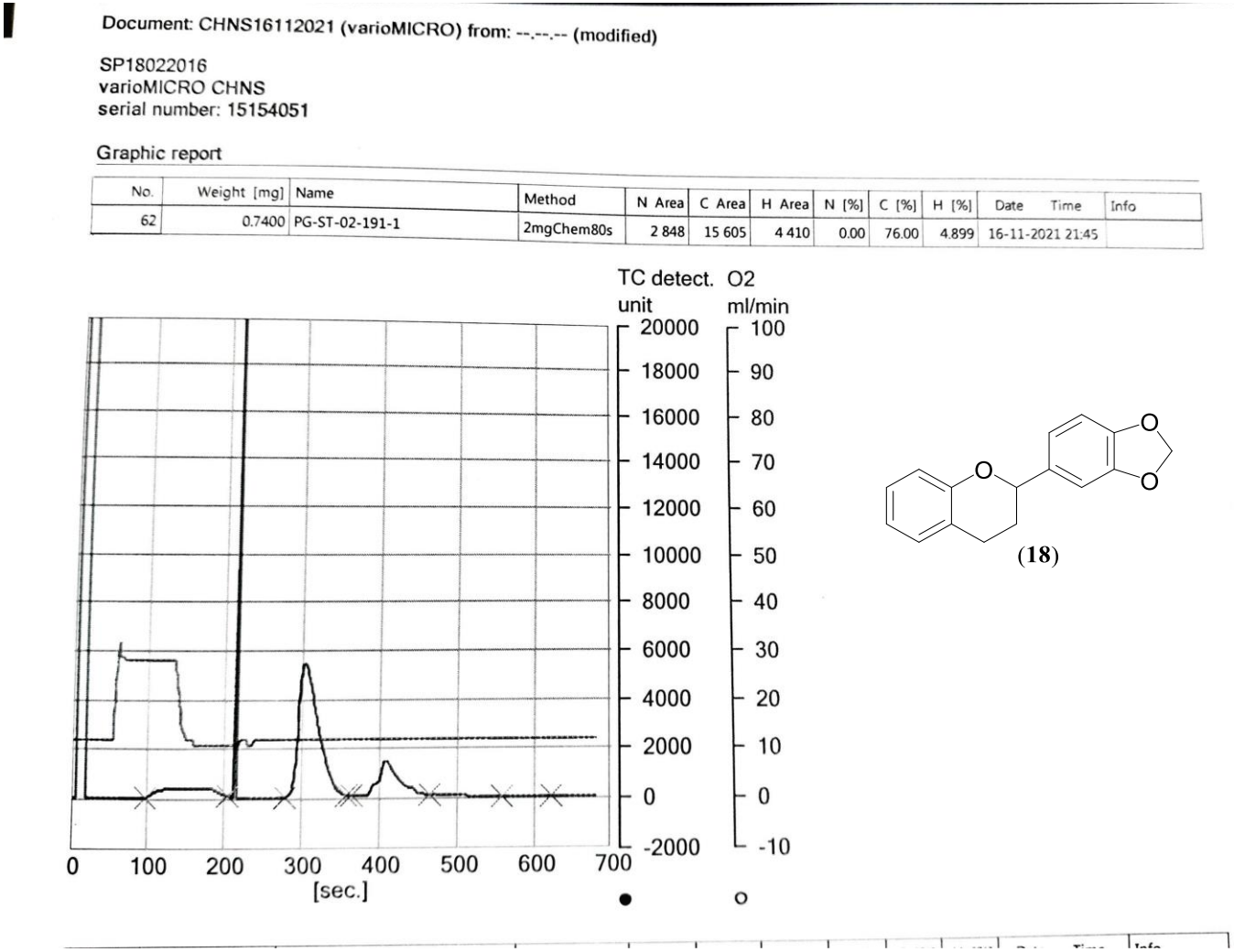


Figure S127. Elemental analysis data (**18**)..

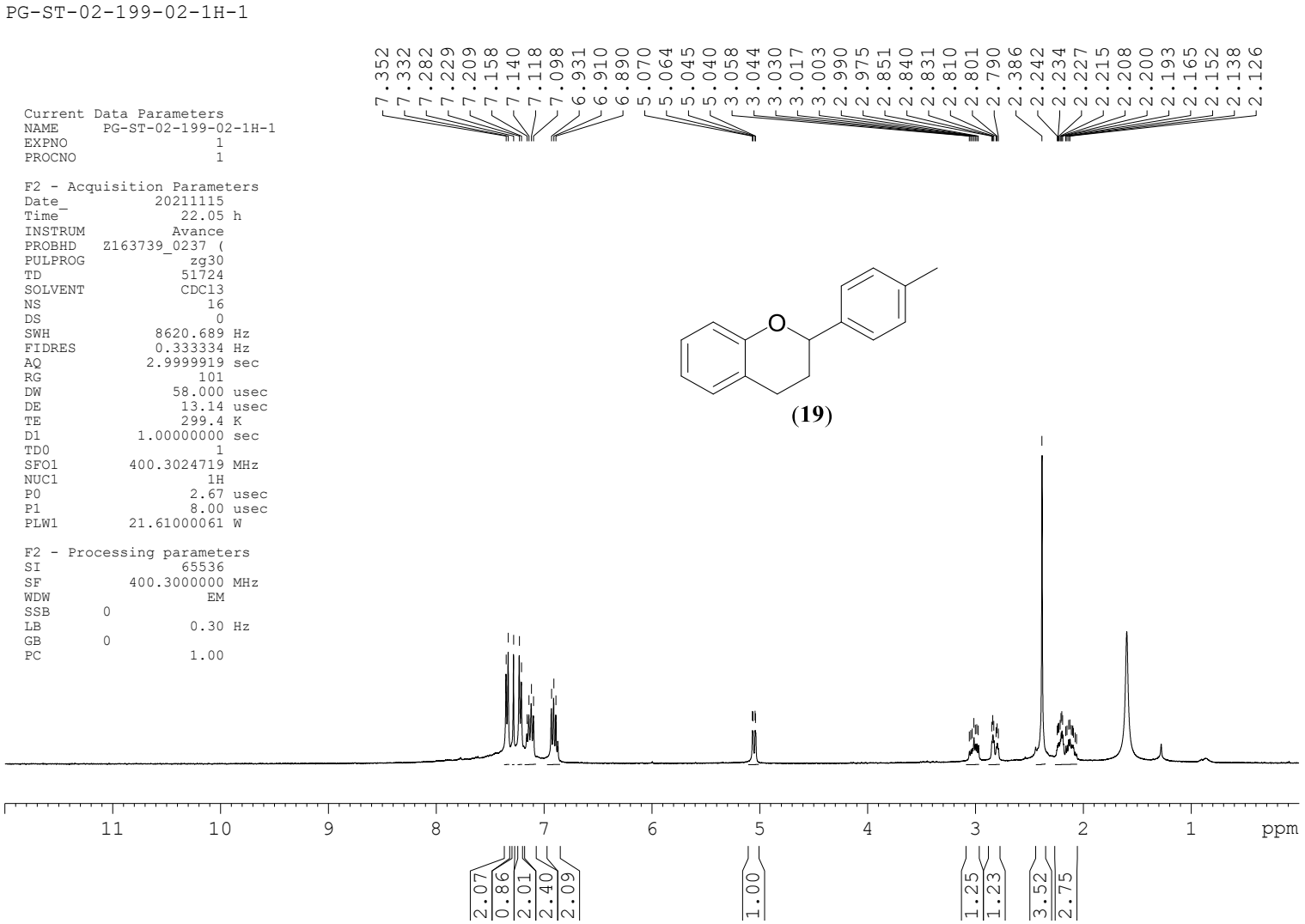


Figure S128. ^{1}H NMR spectrum of (**19**) in $CDCl_3$.

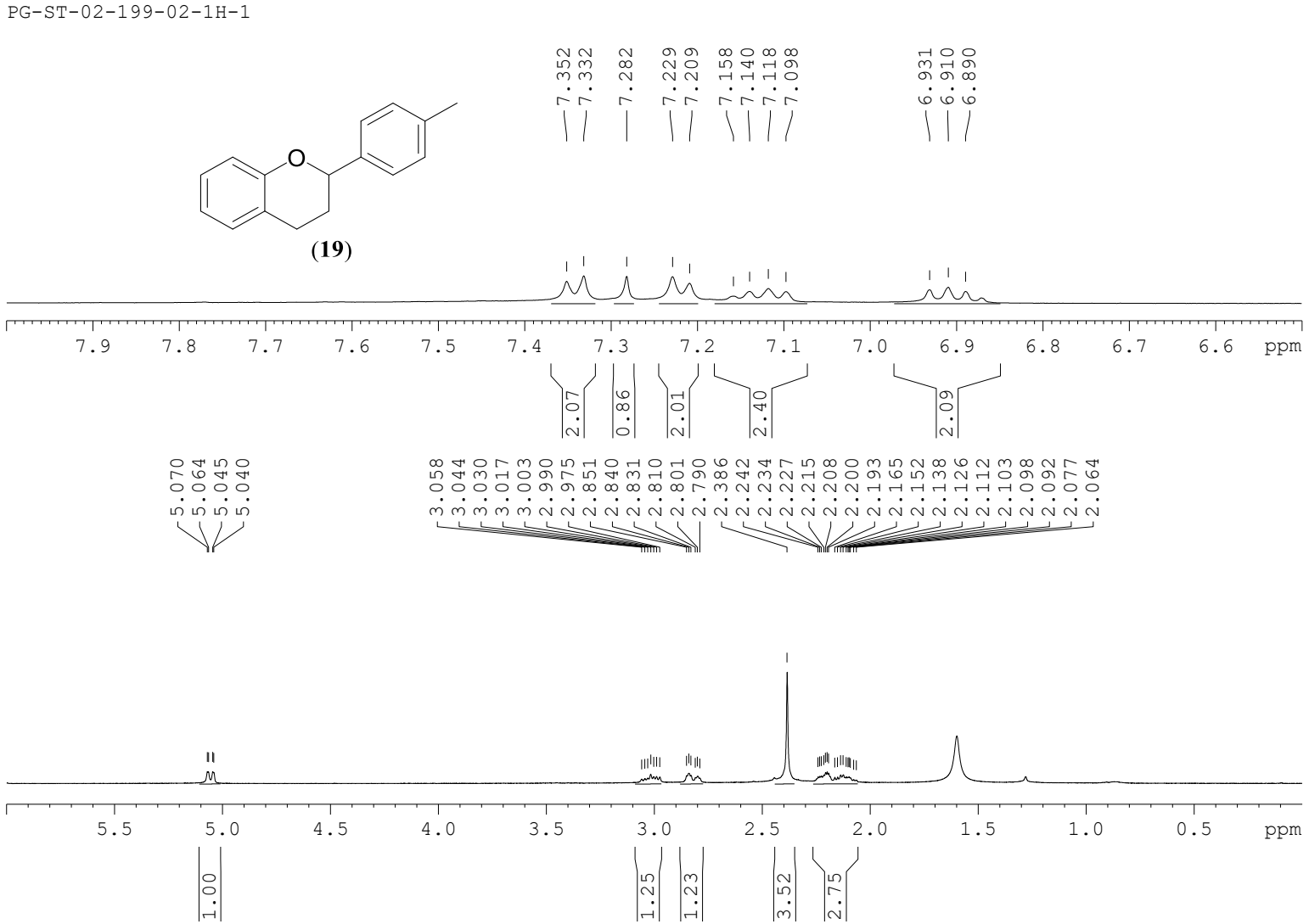


Figure S129. Expanded ^{1}H NMR spectrum of (**19**) in $CDCl_3$.

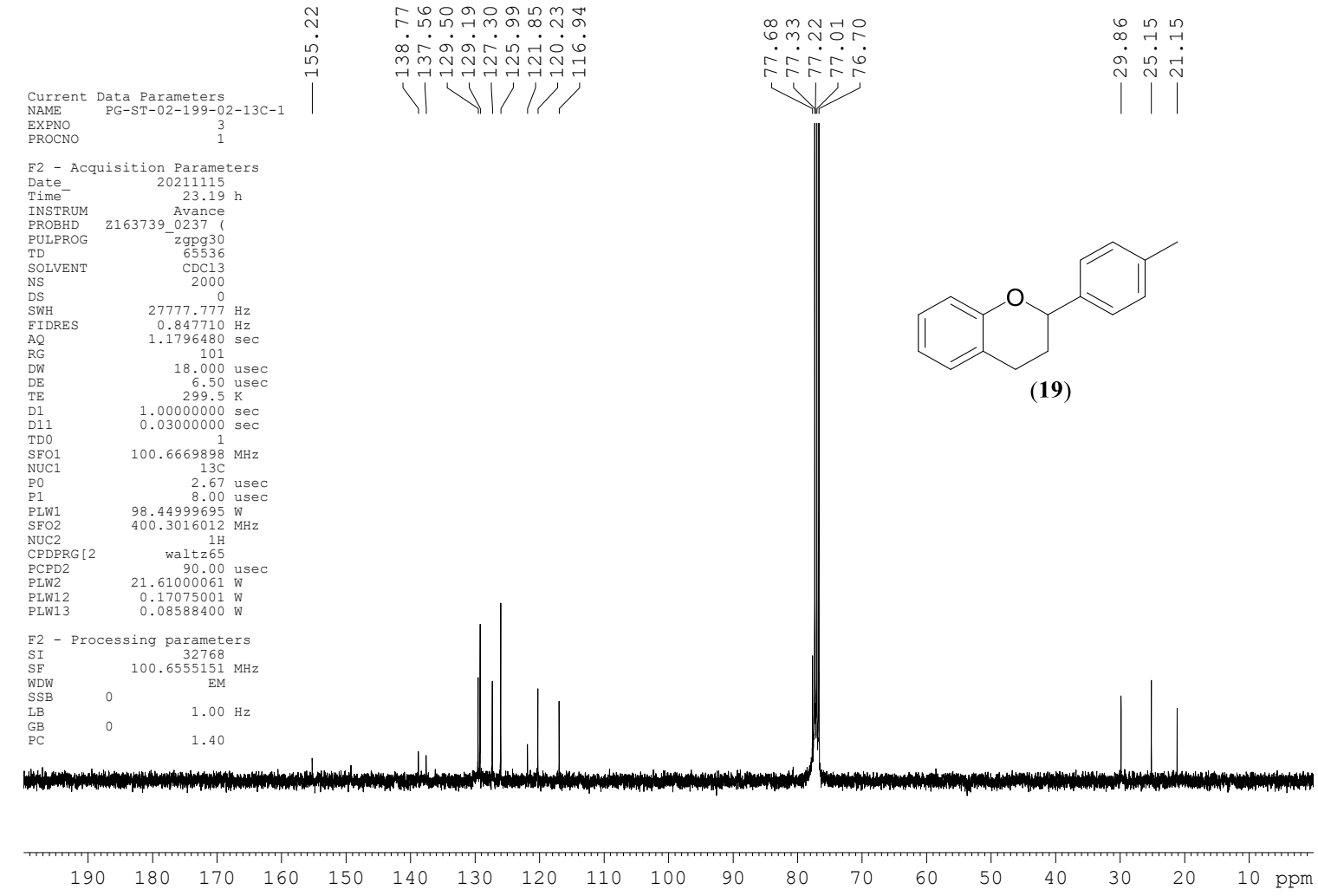


Figure S130. $^{13}C\{^{1}H\}$ NMR spectrum of (**19**) in $CDCl_3$.

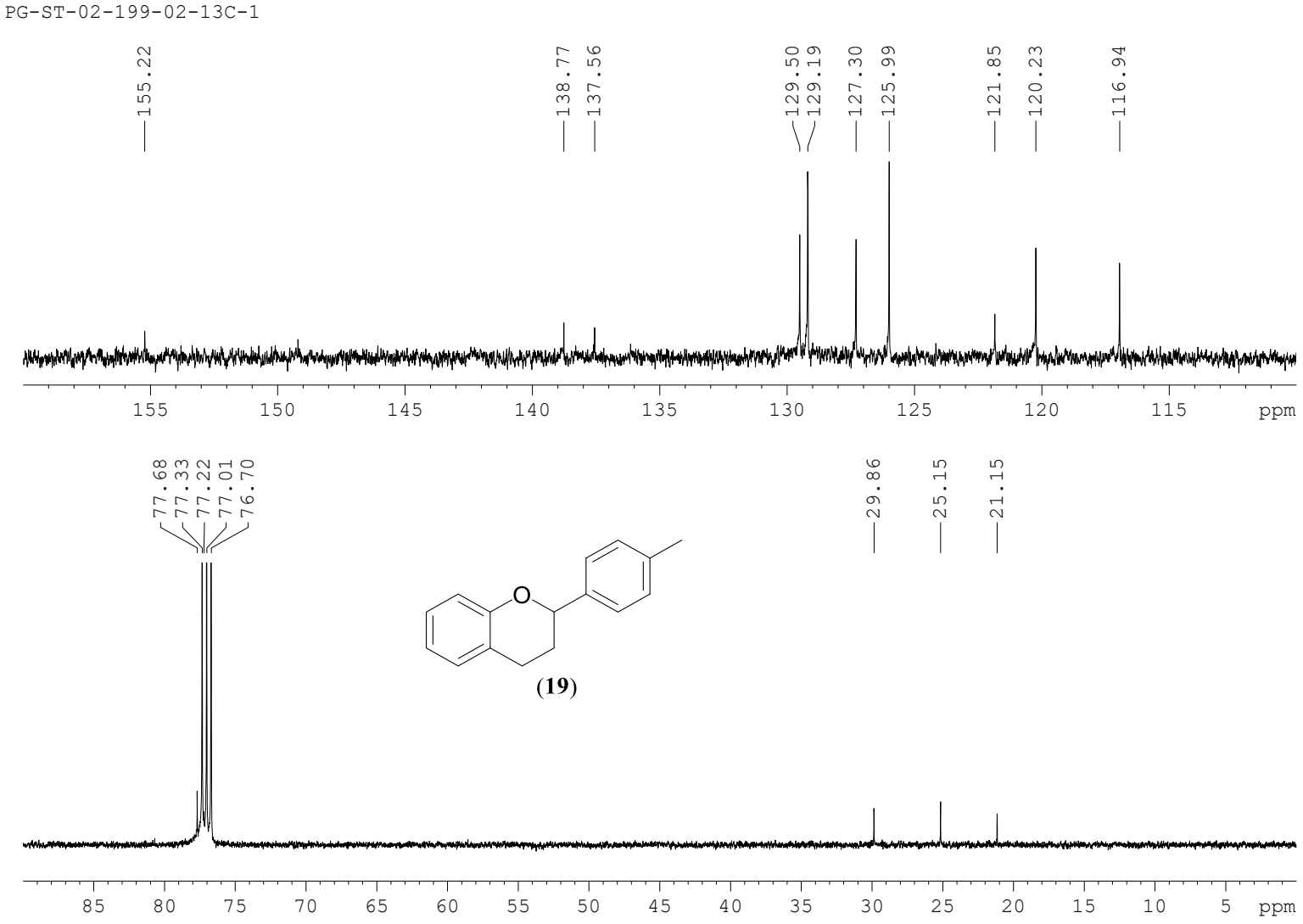


Figure S131. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**19**) in $CDCl_3$.

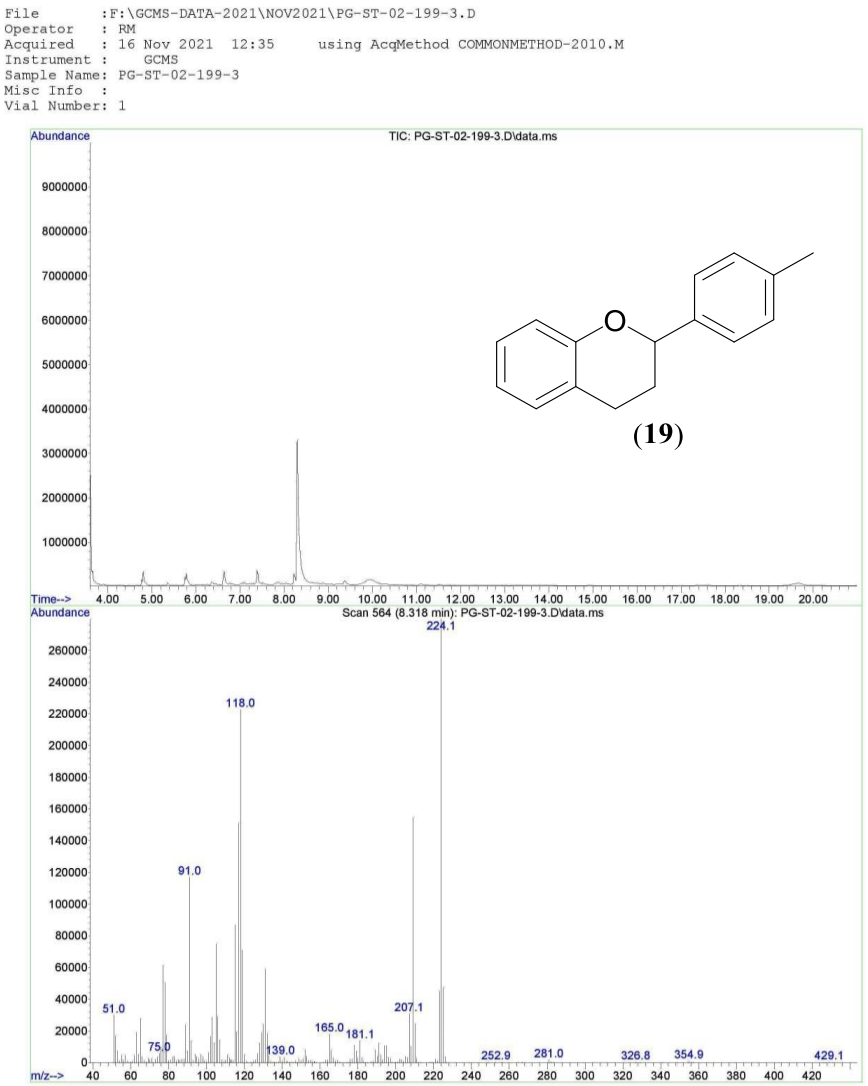


Figure S132. GCMS trace in EtOAc of (**19**) showing the M^+ peak at *m/z* 224.

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date Time	Info
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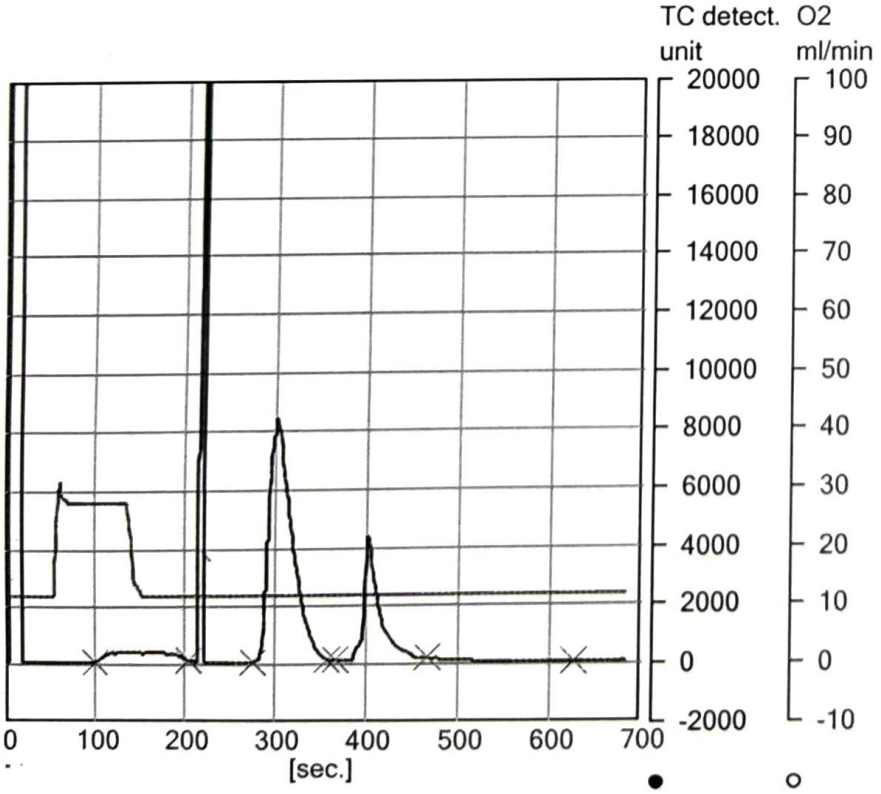

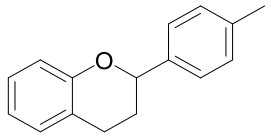

(**19**)

Figure S133. Elemental analysis data (**19**).

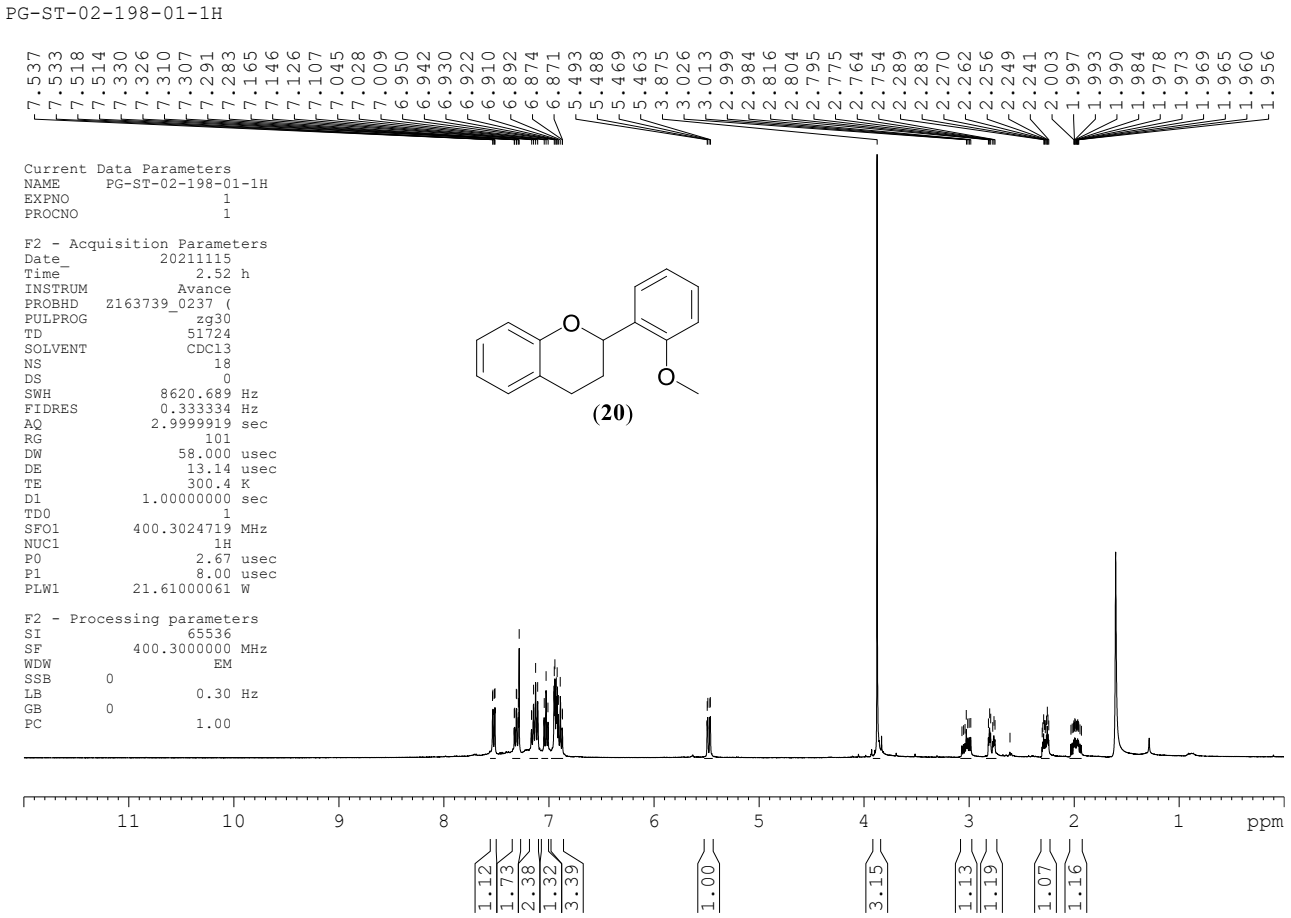

Figure S134. ^{1}H NMR spectrum of (**20**) in $CDCl_3$.

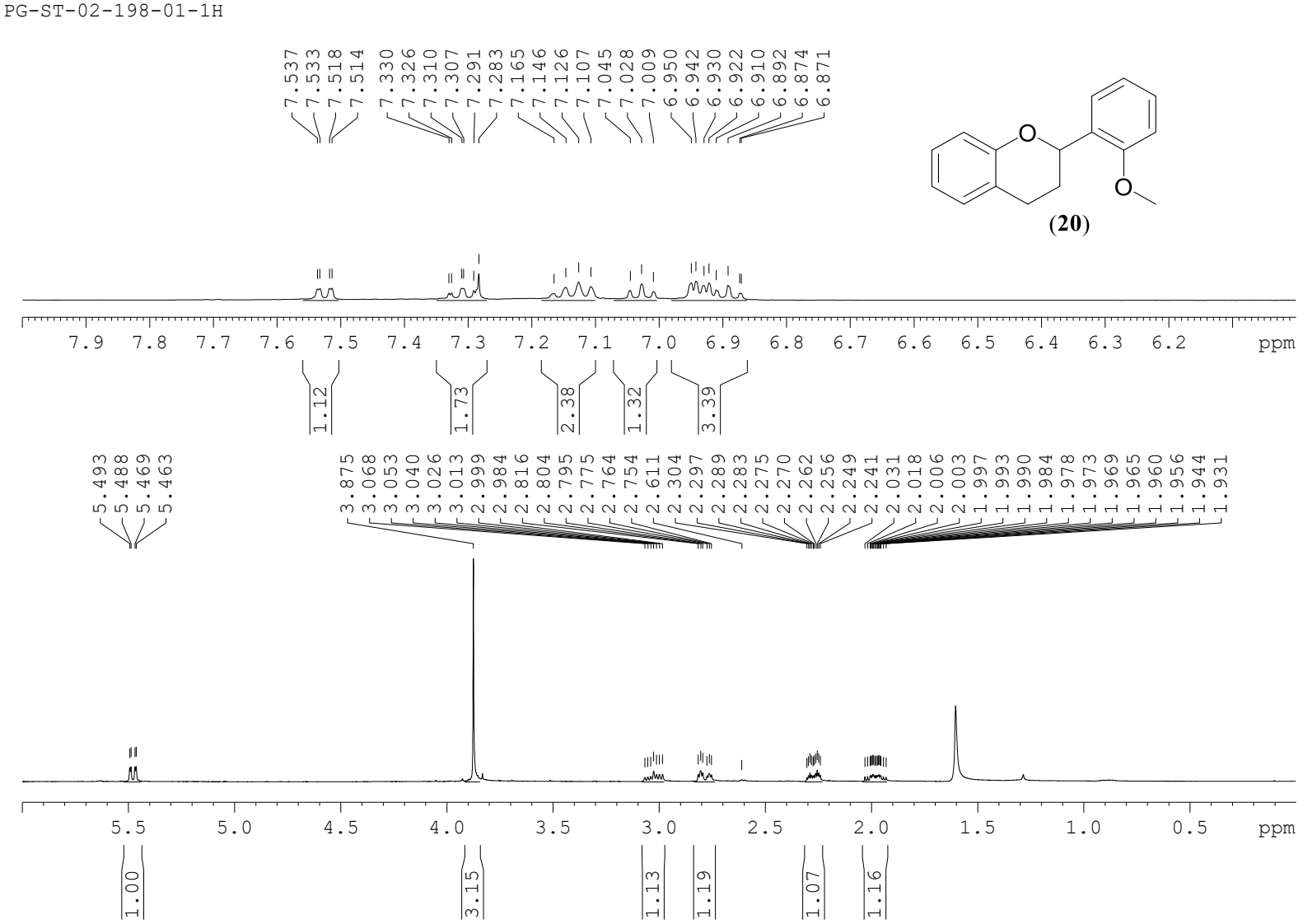

Figure S135. Expanded ^{1}H NMR spectrum of (**20**) in $CDCl_3$.

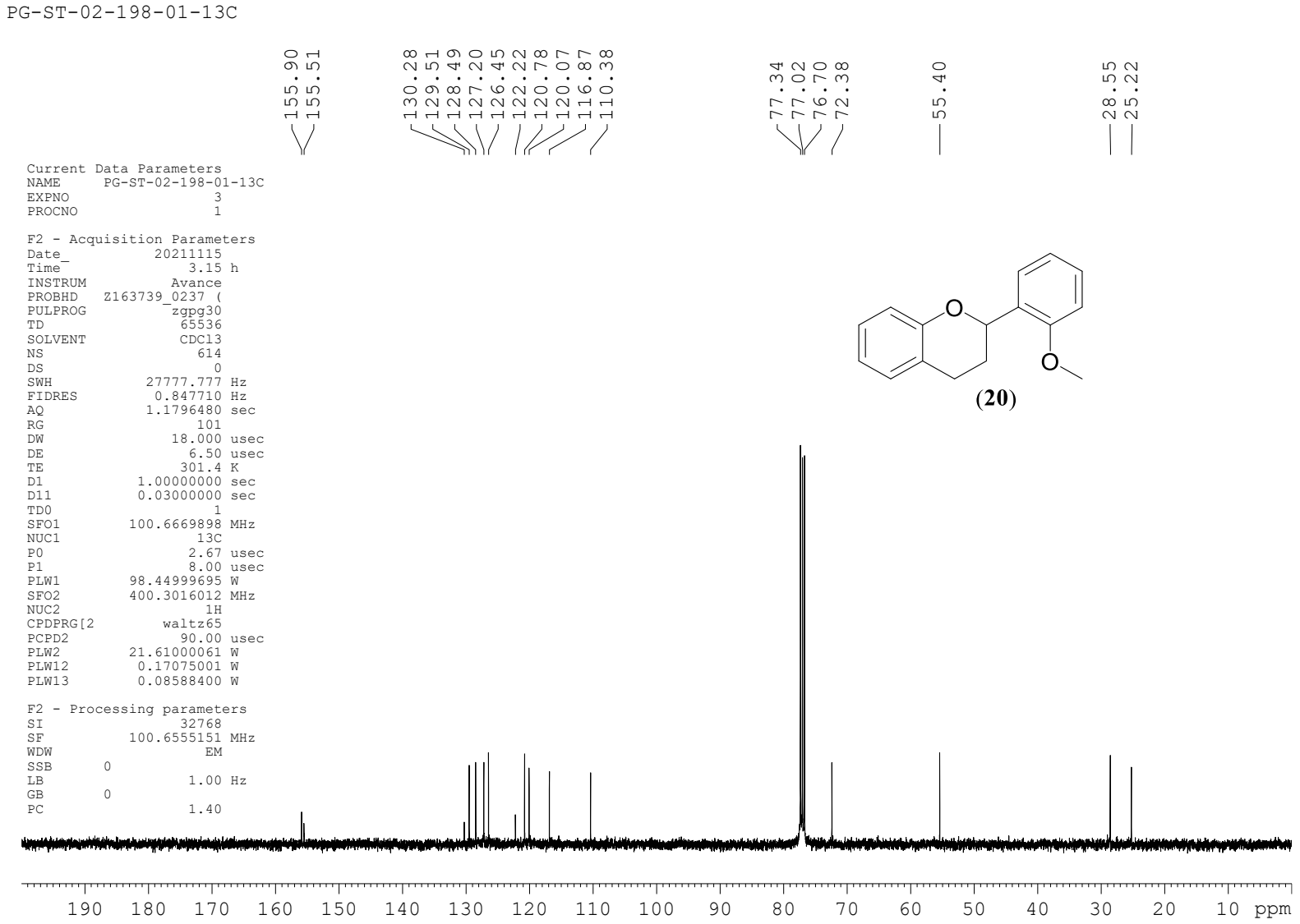

Figure S136. $^{13}C\{^{1}H\}$ NMR spectrum of (**20**) in $CDCl_3$.

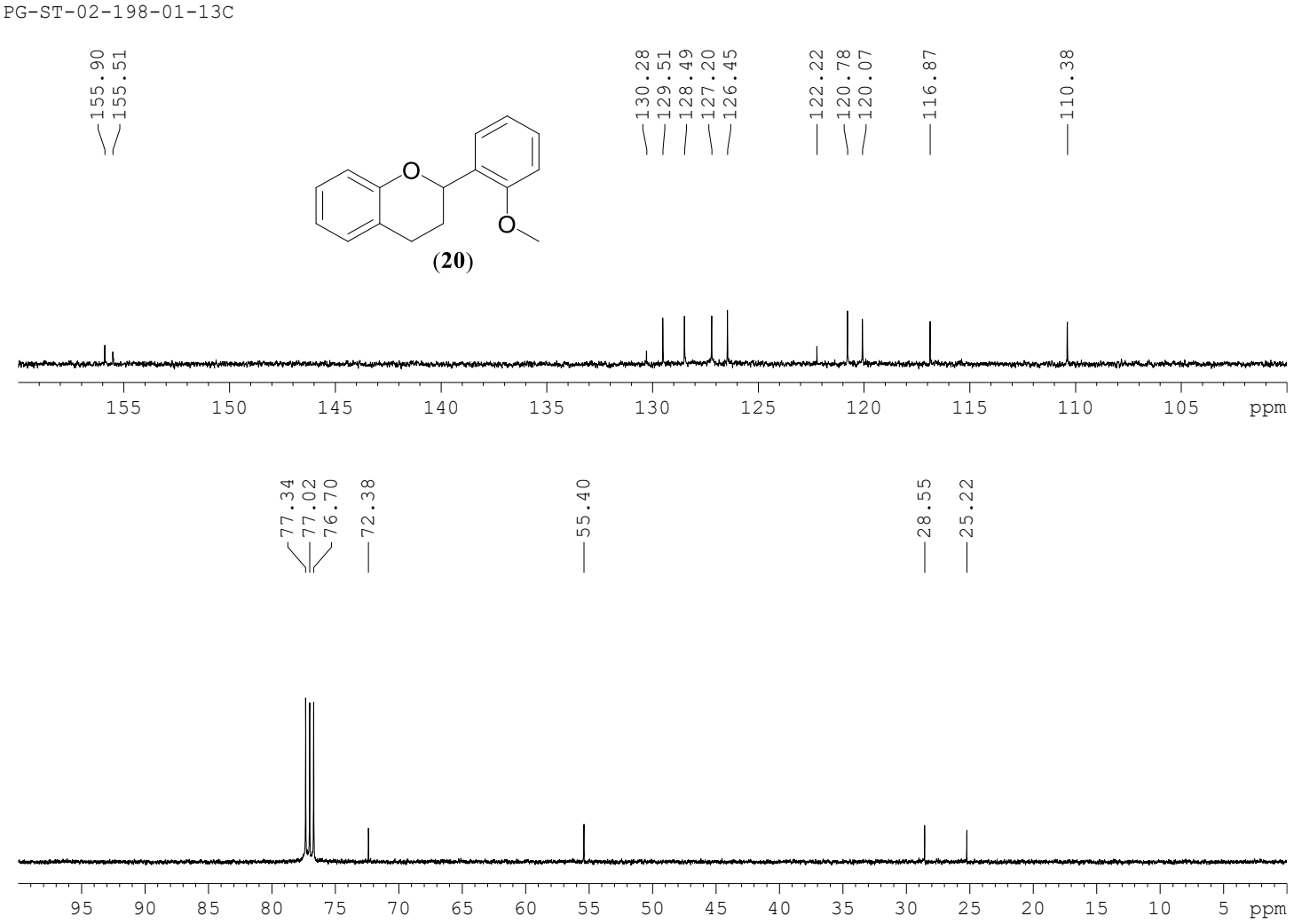

Figure S137. Expanded $^{13}C\{^{1}H\}$ NMR spectrum of (**20**) in $CDCl_3$.

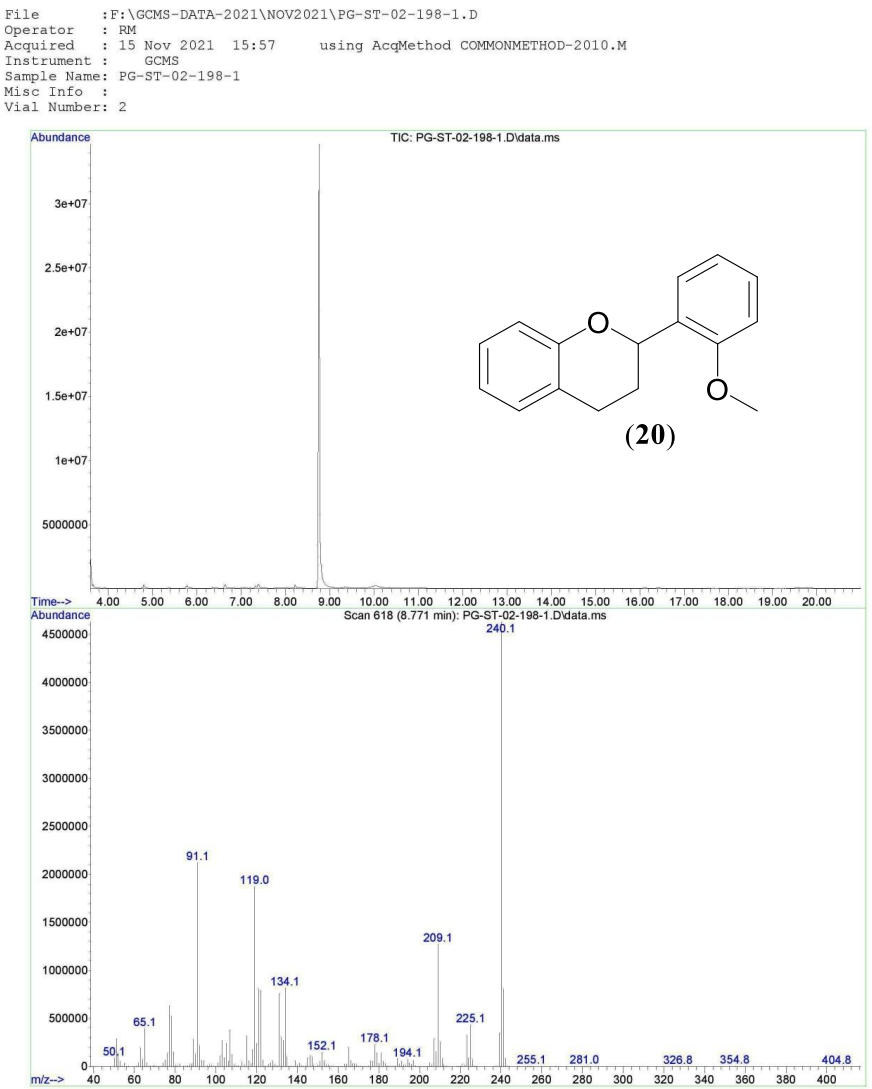

Figure S138. GCMS trace in EtOAc of (**20**) showing the M^+ peak at *m/z* 240.

No.	Weight [mg]	Name	Method	N Area	C Area	H Area	N [%]	C [%]	H [%]	Date Time	Info
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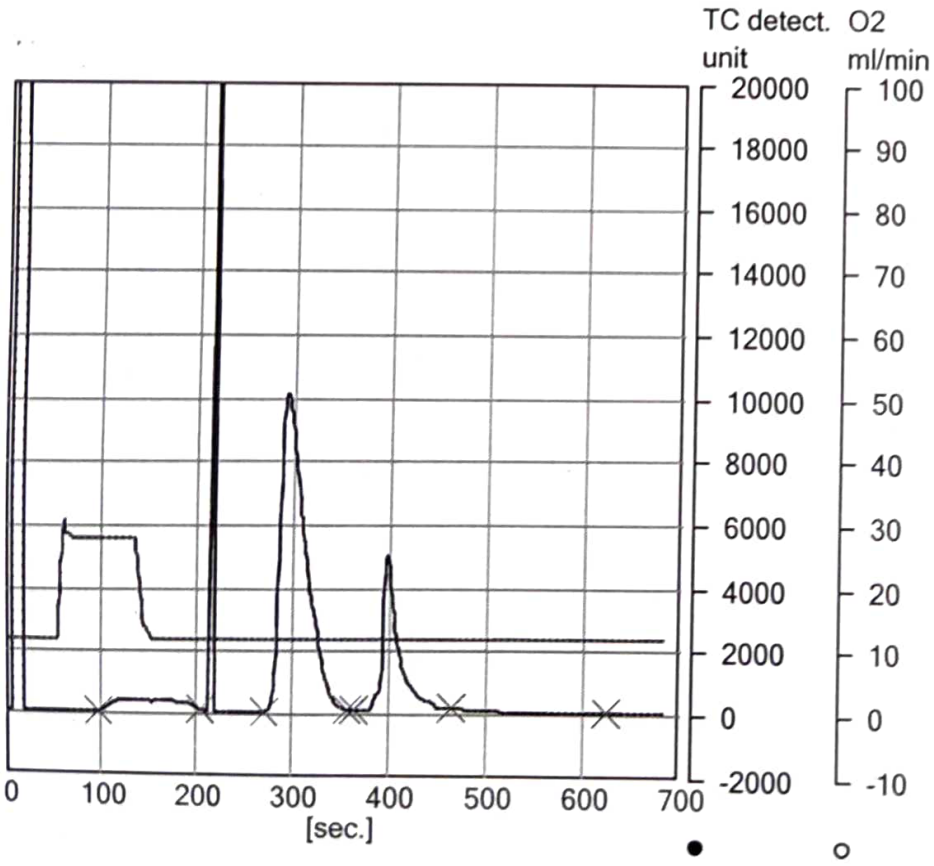
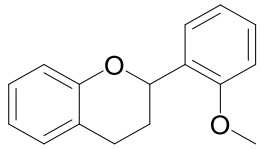
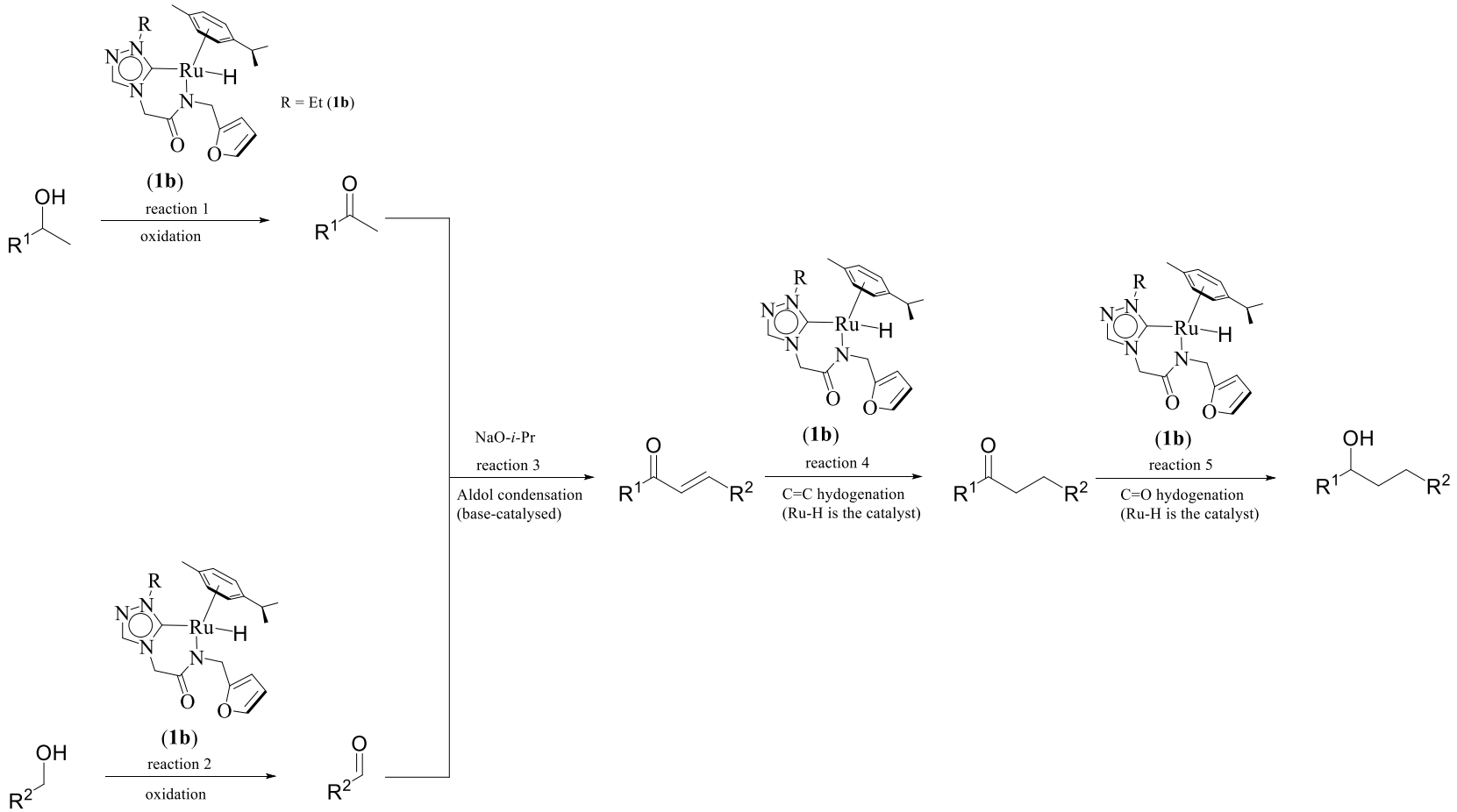


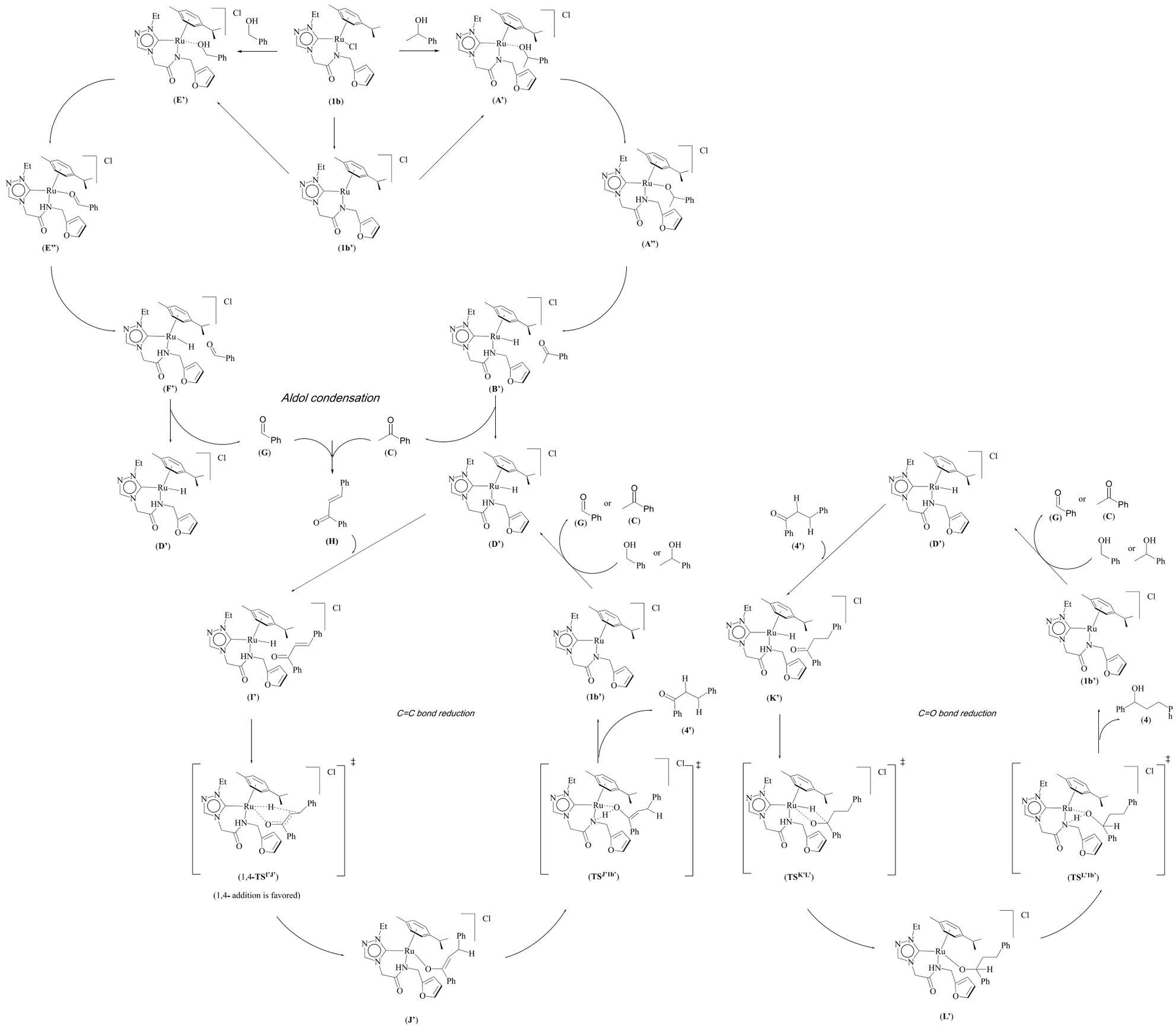


(**20**)

Figure S139. Elemental analysis data (**20**).



Scheme S1. One pot tandem β-alkylation reaction of secondary alcohol involving five sequential reactions.



Scheme S2. A proposed ionic mechanistic pathway for the Ru−NHC (**1b**) catalyzed one pot tandem β-alkylation reaction for representative substrates namely 1-phenylethanol and benzyl alcohol is shown.

Table S1. X−ray crystallographic data for Ru−NHC complexes **(1**−**3)b**.

Compound	**1b**	**2b**	**3b**
Lattice	Monoclinic	Monoclinic	Triclinic
Formula	$C_{21}H_{27}RuClN_4O_2$	$2(C_{22}H_{29}ClN_4O_2Ru),C_7H_8$	$C_{26}H_{29}RuClN_4O_2$
Formula weight	503.99	1128.16	566.05
Space group	$P2_1/n$	$P2_1/n$	$P1$
a/Å	12.9792(4)	14.6902(9)	9.7727(4)
b/Å	13.3677(5)	13.7174(9)	10.5843(4)
c/Å	13.2454(4)	24.6811(15	11.9045(5)
α/°	90	90	92.434(10)
β/°	113.95	93.8260(10)	93.6720(10)
γ/°	90	90	95.5490(10)
V/Å^3	2100.19(12)	4962.4(5)	1221.61(9)
Z	4	4	2
Temperature (K)	125(2)	125(2)	125(2)
Radiation (λ,Å)	0.71073	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.594	1.510	1.539
θ max, deg.	30.53	30.03	30.52
No. of data	6410	14511	7604
No. of parameters	266	645	311
R_1	0.0210	0.0311	0.0418
wR_2	0.0530	0.0698	0.0937
GOF	1.033	1.036	1.071

Table S2. A comparison of the metrical data of the neutral (amido-N functionalized NHC)Ru(*p*-cymene)Cl type complexes known in the literature is shown.

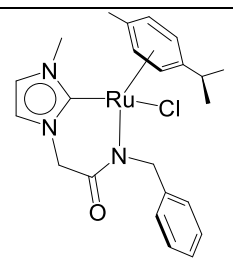
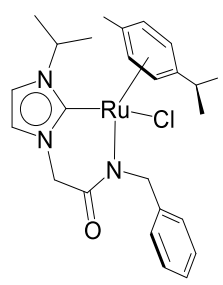
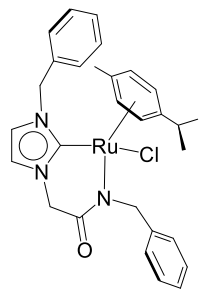
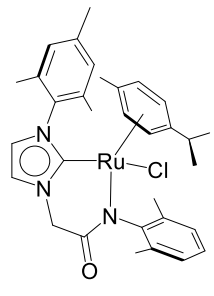
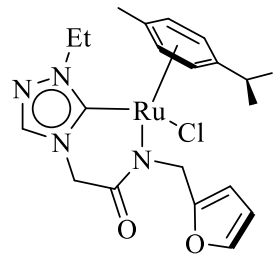
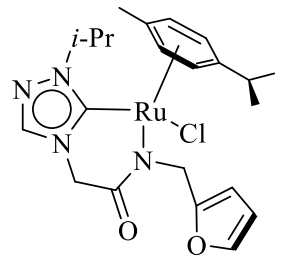
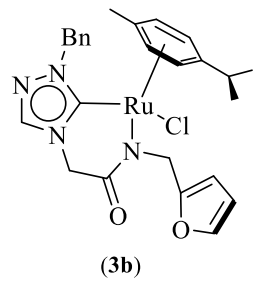
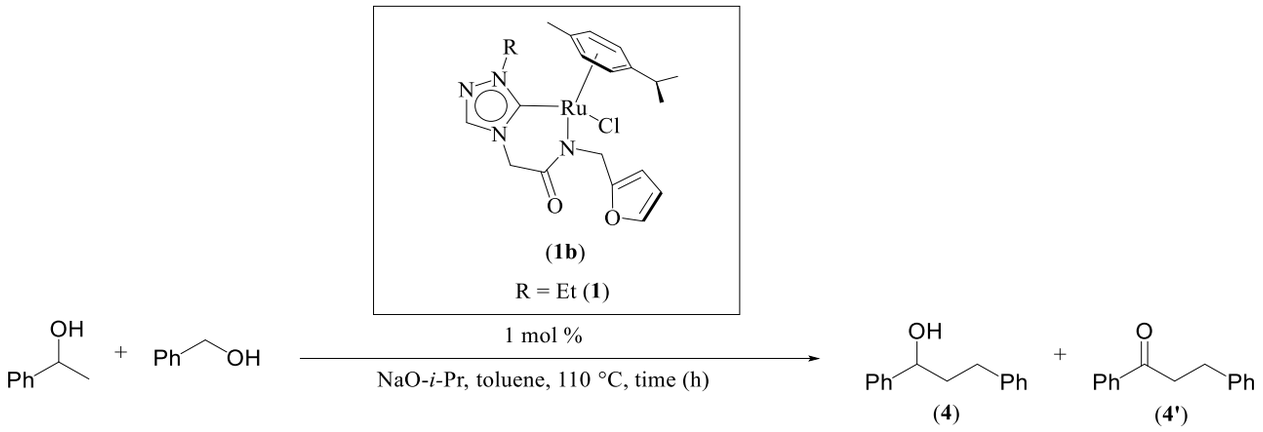
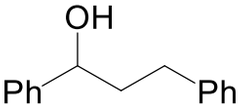
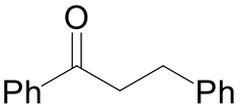
S. No.	complex	*d*(Ru–$C_{carbene}$)/ (Å)	*d*(Ru–N)/ (Å)	*d*(Ru–Cl)/ (Å)	*d*(Ru–$C_{centroid}$)/ (Å)	Reference
1.		2.0172(19)	2.1074(16)	2.4404(7)	1.706	[3]
2.		2.033(5)	2.125(5)	2.4256(14)	1.712	[3]
3.		2.019(3)	2.1074(16)	2.4325(8)	1.719	[3]
4.		2.087(5)	2.153(4)	2.4299(14)	1.736	[4]
5.	 (**1b**)	2.0193(13)	2.1226(11)	2.4095(3)	1.716	present work
6.	 (**2b**)	2.0384(19)	2.1230(16)	2.4319(5)	1.724	present work
7.	 (**3b**)	2.016(3)	2.131(2)	2.4347(7)	1.714	present work

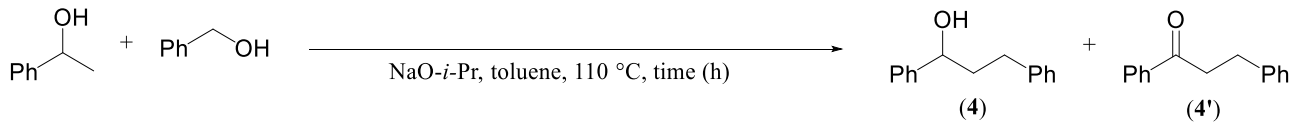
Table S3. Time variation study for the Ru−NHC (**1b**) catalyzed one pot tandem β-alkylation reaction for two representative substrates namely 1-phenylethanol and benzyl alcohol[a].

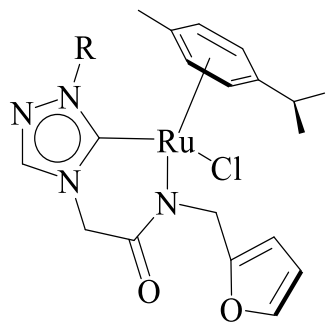
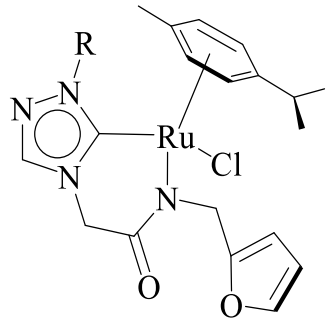


S.No	time (h)	yield[b]	
			
		(**4**)	(**4'**)
1	0.5	15	10
2	1	33	16
3	2	39	13
4	3	70	17
5	4	52	33
6	6	34	39
7	12	14	57
8	24	43	14
9	48	45	11
10	72	42	9
11	96	14	7
12	120	9	6

(*a*). Reaction conditions: 1:1:1 ratio of 1°-alcohol:2°-alcohol:NaO*i*Pr 1.00 mmol, 1 mol % of (**1b**), 2.0 mL of toluene at 110 °C for T hour. (*b*) Isolated yields (%).

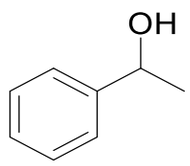
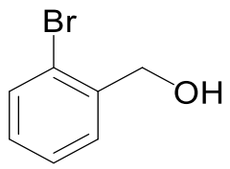
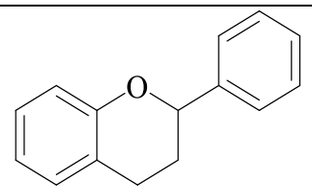
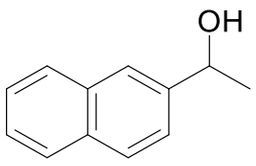
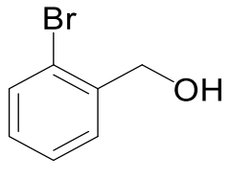
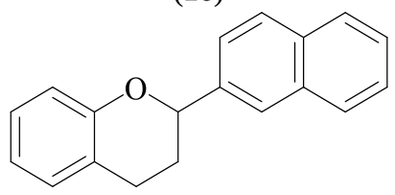
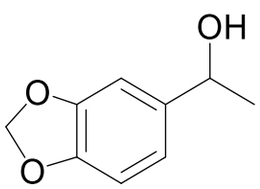
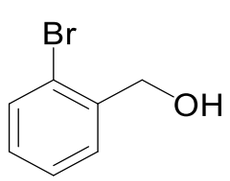
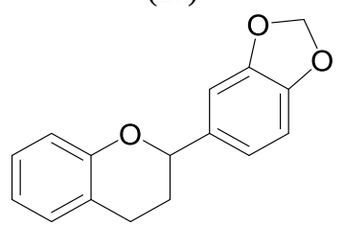
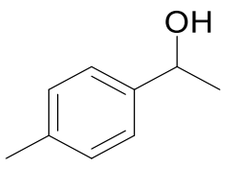
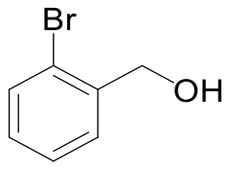
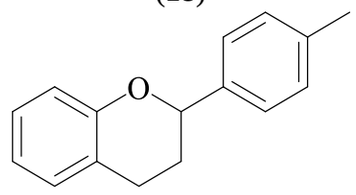
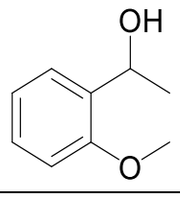
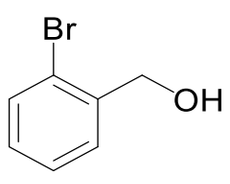
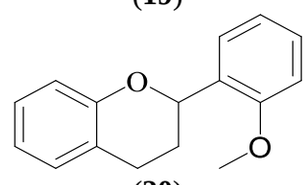
Table S4. Selected results of blank, control and Hg drop experiments for the one pot tandem β-alkylation reaction for two representative substrates namely 1-phenylethanol and benzyl alcohol[a].



S. No	metal complex	Hg	yield[b] (4)	yield[b] (4')
1	-		ND	ND
2	[(*p*-cymene)$RuCl_2$]$_2$		23	6
3	 (**1b**) R = Et (**1**)		70	17
4	 (**1b**) R = Et (**1**)	Hg	61	14

(*a*). Reaction conditions: 1:1:1 ratio of 1°-alcohol:2°-alcohol:NaO*i*Pr 1.00 mmol, 1 mol % of (**1b**), 2.0 mL of toluene at 110 °C for 3 hours. (*b*). Isolated yields (%).

Table S5. Selected results for the Ru−NHC (**1-3)b** catalyzed one pot synthesis of flavan derivatives (**16-20**).

S. No.	2° alcohol	1° alcohol	product	Ru−NHC (**1b**)	Ru−NHC (**2b**)	Ru−NHC (**3b**)
				yield[b]	yield[b]	yield[b]
11			 (**16**)	26	28	31
12			 (**17**)	40	33	37
13			 (**18**)	34	33	28
14			 (**19**)	30	28	32
15			 (**20**)	37	29	33

Reaction conditions: (*a*). Reaction conditions: 1:1:1 ratio of 1°-alcohol:2°-alcohol:base 1.00 mmol, 1 mol % of (**1b**/**2b**/**3b**), 2.0 mL of toluene at 110 °C for 3 hours. (*a*). Reaction conditions: 20 mol % CuI, 20 mol % 2,2′-bipyridine, base 1.00 mmol, 1.0 mL of toluene at 110 °C for 24 hours. (*c*) Isolated yields (%).

Density Functional Theory Data

Co-ordinates of Optimized Geometries and Transition States

Dehydrogenation of alcohols

Primary alcohols

(**1b**)

Ru	0.347238000	0.325521000	0.165767000
Cl	0.701533000	1.014693000	-2.161698000
O	-0.276603000	-3.861260000	-0.458958000
O	-3.618149000	-0.777095000	-1.067733000
N	-0.231007000	-1.558553000	-0.592037000
N	2.481149000	-1.763430000	0.325545000
N	3.412441000	0.072775000	-0.215803000
N	4.430954000	-0.849313000	-0.160996000
C	2.201264000	-0.449645000	0.074249000
C	3.827952000	-1.956382000	0.166573000
H	4.318733000	-2.909530000	0.299368000
C	3.742623000	1.446703000	-0.608060000
H	4.412747000	1.853589000	0.158239000
H	2.801452000	1.995428000	-0.599138000
C	4.387247000	1.509978000	-1.990253000
H	4.639174000	2.550433000	-2.222761000
H	3.685773000	1.145094000	-2.745041000
H	5.303568000	0.914064000	-2.023975000
C	1.481774000	-2.766918000	0.688123000
H	1.204205000	-2.628872000	1.739931000
H	1.935810000	-3.752697000	0.582050000
C	0.222717000	-2.753548000	-0.197643000
C	-1.361419000	-1.617099000	-1.534869000
H	-1.187409000	-2.459024000	-2.215172000
H	-1.361218000	-0.697489000	-2.122151000
C	-2.703680000	-1.791356000	-0.887807000
C	-3.263889000	-2.771684000	-0.118375000
H	-2.767731000	-3.688839000	0.162754000
C	-4.594193000	-2.341723000	0.200502000
H	-5.332532000	-2.872165000	0.786739000
C	-4.758464000	-1.131225000	-0.401608000
H	-5.580520000	-0.435262000	-0.475213000
C	0.463322000	0.715050000	2.416213000
C	-0.773521000	0.089558000	2.128533000
H	-1.013857000	-0.864872000	2.585288000
C	-1.738479000	0.711888000	1.271829000

H	-2.679798000	0.205033000	1.091486000
C	-1.460227000	1.913344000	0.609950000
C	-0.154323000	2.488377000	0.819637000
H	0.132175000	3.370302000	0.259518000
C	0.754526000	1.950506000	1.745058000
H	1.710380000	2.438212000	1.908714000
C	1.425690000	0.142185000	3.424542000
H	1.293089000	0.637148000	4.395354000
H	2.465621000	0.290322000	3.116858000
H	1.257853000	-0.928536000	3.573789000
C	-2.519022000	2.566504000	-0.269137000
H	-3.036172000	1.750277000	-0.787210000
C	-1.957976000	3.520020000	-1.333635000
H	-1.193885000	3.030311000	-1.944273000
H	-1.525655000	4.423471000	-0.883830000
H	-2.770115000	3.848006000	-1.991749000
C	-3.550726000	3.288578000	0.625806000
H	-4.013091000	2.604133000	1.345779000
H	-4.346760000	3.722207000	0.009608000
H	-3.080285000	4.104361000	1.188964000

(E')

Ru	0.439394000	-0.734381000	-0.387611000
O	0.985237000	-0.514073000	3.824754000
O	2.608150000	2.649874000	1.005597000
N	0.458976000	-0.088944000	1.623843000
N	-0.637649000	-2.761269000	1.558380000
N	-1.829944000	-2.838534000	-0.203425000
N	-2.372953000	-3.772158000	0.643557000
C	-0.762396000	-2.203171000	0.320615000
C	-1.626203000	-3.701450000	1.708130000
H	-1.760414000	-4.300648000	2.597175000
C	-2.488777000	-2.621517000	-1.497455000
H	-2.440212000	-3.565620000	-2.049552000
H	-1.888945000	-1.876421000	-2.021267000
C	-3.935231000	-2.161258000	-1.332743000
H	-4.389079000	-2.032863000	-2.320936000
H	-3.979257000	-1.207367000	-0.798939000
H	-4.518300000	-2.902844000	-0.780975000
C	0.381141000	-2.395925000	2.541861000
H	1.326534000	-2.884780000	2.279440000
H	0.068094000	-2.776220000	3.514730000
C	0.624971000	-0.887609000	2.706657000
C	0.763942000	1.334824000	1.902227000
H	0.309146000	1.583011000	2.868144000
H	0.285585000	1.949162000	1.134436000

C	2.213894000	1.709506000	1.931942000
C	3.285155000	1.347620000	2.697749000
H	3.255815000	0.649183000	3.520876000
C	4.408900000	2.096699000	2.216282000
H	5.420849000	2.073666000	2.596436000
C	3.945195000	2.872719000	1.198069000
H	4.394174000	3.619138000	0.560543000
C	1.872580000	-2.275273000	-1.257650000
C	2.601318000	-1.311976000	-0.514185000
H	3.188966000	-1.626940000	0.341409000
C	2.654961000	0.057754000	-0.926128000
H	3.283296000	0.744532000	-0.371427000
C	1.882584000	0.526893000	-1.995048000
C	1.018701000	-0.428852000	-2.642294000
H	0.354986000	-0.093884000	-3.431630000
C	1.070738000	-1.800578000	-2.346046000
H	0.465906000	-2.500272000	-2.913370000
C	1.966887000	-3.745804000	-0.948719000
H	2.724591000	-4.205092000	-1.595981000
H	1.020301000	-4.262938000	-1.130206000
H	2.270670000	-3.921318000	0.086912000
C	2.029776000	1.970751000	-2.466986000
H	1.978514000	2.603843000	-1.572829000
C	0.955182000	2.433676000	-3.460463000
H	-0.060631000	2.309588000	-3.072560000
H	1.026975000	1.897707000	-4.414535000
H	1.094401000	3.496746000	-3.679164000
C	3.434206000	2.156820000	-3.089004000
H	4.230053000	1.912151000	-2.378523000
H	3.568773000	3.197933000	-3.400441000
H	3.559913000	1.521526000	-3.973586000
C	-1.789264000	1.685794000	-0.888171000
O	-1.465377000	0.398710000	-0.261273000
C	-3.022446000	2.284485000	-0.275012000
C	-4.297515000	1.912174000	-0.726447000
C	-2.910439000	3.201100000	0.780553000
C	-5.439890000	2.441775000	-0.128488000
H	-4.392721000	1.215759000	-1.556205000
C	-4.053726000	3.730147000	1.380952000
H	-1.926867000	3.514233000	1.124808000
C	-5.318372000	3.349312000	0.927733000
H	-6.423179000	2.154780000	-0.489318000
H	-3.957288000	4.443871000	2.193660000
H	-6.208505000	3.765304000	1.390447000
H	-0.926477000	2.352324000	-0.788008000
H	-1.506349000	0.501842000	0.711267000

H	-1.930961000	1.442127000	-1.942628000

($TS^{E'E''}$)

Ru	-0.637222000	-0.728745000	-0.023848000
O	-0.589400000	1.991492000	-3.282444000
O	-2.106231000	3.069906000	0.754421000
N	-0.073324000	1.042613000	-1.243181000
N	0.485832000	-1.418688000	-2.758119000
N	1.190290000	-2.867021000	-1.373196000
N	1.796733000	-3.178959000	-2.564526000
C	0.375108000	-1.797739000	-1.451451000
C	1.349982000	-2.280961000	-3.390872000
H	1.611385000	-2.217191000	-4.437378000
C	1.584762000	-3.652198000	-0.196654000
H	1.371144000	-4.700663000	-0.425337000
H	0.938910000	-3.329437000	0.618020000
C	3.057792000	-3.453424000	0.154208000
H	3.308946000	-4.064835000	1.027005000
H	3.256342000	-2.404109000	0.390197000
H	3.699881000	-3.759863000	-0.675697000
C	-0.233823000	-0.319313000	-3.383353000
H	-1.271944000	-0.619800000	-3.567759000
H	0.223929000	-0.115764000	-4.352954000
C	-0.283789000	1.011525000	-2.627802000
C	-0.258798000	2.426861000	-0.682843000
H	0.308224000	3.107118000	-1.324902000
H	0.210450000	2.429034000	0.301232000
C	-1.660184000	2.920180000	-0.540643000
C	-2.638716000	3.323439000	-1.405505000
H	-2.558066000	3.340939000	-2.481888000
C	-3.755160000	3.733941000	-0.606311000
H	-4.701189000	4.123186000	-0.956047000
C	-3.377769000	3.566005000	0.691398000
H	-3.853061000	3.764013000	1.640192000
C	-2.894839000	-1.207753000	-0.250423000
C	-2.759345000	-0.010897000	0.510352000
H	-3.218092000	0.898134000	0.137535000
C	-2.036321000	0.032996000	1.725696000
H	-1.958139000	0.974512000	2.256259000
C	-1.389120000	-1.128031000	2.229733000
C	-1.458757000	-2.314327000	1.451853000
H	-0.970365000	-3.217467000	1.793991000
C	-2.189592000	-2.342086000	0.229716000
H	-2.208767000	-3.260592000	-0.349436000
C	-3.759206000	-1.264639000	-1.482705000
H	-4.787821000	-1.529860000	-1.207377000

H	-3.403885000	-2.020877000	-2.189520000
H	-3.795481000	-0.295915000	-1.989652000
C	-0.694575000	-1.071802000	3.579718000
H	-0.213899000	-0.087246000	3.648607000
C	0.380203000	-2.146065000	3.793651000
H	1.125825000	-2.142998000	2.991490000
H	-0.054386000	-3.150148000	3.863235000
H	0.902874000	-1.958513000	4.736535000
C	-1.770146000	-1.141650000	4.690560000
H	-2.510072000	-0.340679000	4.592537000
H	-1.294197000	-1.044751000	5.671648000
H	-2.300122000	-2.100586000	4.664715000
C	1.910272000	0.504033000	1.421434000
O	1.400931000	-0.136360000	0.247472000
C	3.008653000	1.484545000	1.070497000
C	4.091370000	1.083659000	0.273332000
C	2.967964000	2.801057000	1.545305000
C	5.109151000	1.982657000	-0.041317000
H	4.133034000	0.064356000	-0.101412000
C	3.991307000	3.701193000	1.237684000
H	2.136829000	3.124803000	2.168940000
C	5.062179000	3.293986000	0.441715000
H	5.943673000	1.660453000	-0.657969000
H	3.948759000	4.718225000	1.617007000
H	5.857843000	3.992480000	0.199190000
H	1.111062000	1.025066000	1.968828000
H	0.940753000	0.629055000	-0.709366000
H	2.296647000	-0.282389000	2.084563000

(**E’’**)

Ru	0.947703000	0.059965000	0.031023000
O	0.396096000	-1.886951000	-3.308881000
O	-1.329160000	-3.168348000	0.525681000
N	-0.508834000	-0.623496000	-1.610570000
N	1.039674000	1.610930000	-2.588231000
N	1.216336000	3.004677000	-0.993607000
N	1.177539000	3.763094000	-2.138105000
C	1.142492000	1.682039000	-1.221628000
C	1.071469000	2.891261000	-3.094434000
H	1.021459000	3.129425000	-4.147380000
C	1.252535000	3.722160000	0.288380000
H	2.126378000	4.379881000	0.255359000
H	1.403700000	2.964847000	1.054241000
C	-0.028647000	4.512361000	0.540314000
H	0.061214000	5.051780000	1.488898000
H	-0.881938000	3.832373000	0.600151000

H	-0.199285000	5.244556000	-0.253735000
C	1.022048000	0.386014000	-3.372788000
H	2.042108000	0.048258000	-3.579680000
H	0.550600000	0.601686000	-4.337324000
C	0.277875000	-0.807397000	-2.769895000
C	-1.560381000	-1.687864000	-1.388617000
H	-2.037950000	-1.863600000	-2.357024000
H	-2.293114000	-1.232349000	-0.720908000
C	-1.116143000	-2.989251000	-0.821650000
C	-0.619552000	-4.142487000	-1.361482000
H	-0.366496000	-4.294117000	-2.400399000
C	-0.507524000	-5.085640000	-0.290405000
H	-0.160227000	-6.107534000	-0.351081000
C	-0.953655000	-4.444533000	0.826702000
H	-1.087793000	-4.744396000	1.855192000
C	2.804365000	-1.376702000	-0.126635000
C	1.752459000	-2.043024000	0.576415000
H	1.376102000	-2.981939000	0.183778000
C	1.191438000	-1.522224000	1.760485000
H	0.398848000	-2.069030000	2.256328000
C	1.623462000	-0.268762000	2.286164000
C	2.605067000	0.444235000	1.554526000
H	2.947226000	1.410949000	1.902316000
C	3.184849000	-0.109570000	0.367798000
H	3.933115000	0.467712000	-0.166734000
C	3.456822000	-2.007809000	-1.328978000
H	4.169561000	-2.778719000	-1.010419000
H	4.013162000	-1.269674000	-1.915067000
H	2.718561000	-2.488592000	-1.978792000
C	1.067752000	0.213678000	3.614380000
H	0.045147000	-0.176540000	3.689993000
C	1.004073000	1.738472000	3.771813000
H	0.420519000	2.198141000	2.968401000
H	2.001840000	2.192954000	3.790896000
H	0.522721000	1.987711000	4.722643000
C	1.898501000	-0.428694000	4.750858000
H	1.910097000	-1.521461000	4.680046000
H	1.469547000	-0.156859000	5.720756000
H	2.935621000	-0.074905000	4.728301000
C	-1.725888000	0.646339000	1.340577000
O	-0.792046000	1.107572000	0.390003000
C	-3.153984000	0.756619000	0.821461000
C	-3.514784000	1.744442000	-0.104902000
C	-4.142719000	-0.118596000	1.292861000
C	-4.834862000	1.856162000	-0.546581000
H	-2.755122000	2.426337000	-0.474829000

C	-5.463961000	-0.005275000	0.855716000
H	-3.877530000	-0.894454000	2.008640000
C	-5.813677000	0.983099000	-0.066830000
H	-5.101314000	2.630010000	-1.261816000
H	-6.217754000	-0.691997000	1.230974000
H	-6.840722000	1.071716000	-0.409307000
H	-1.545631000	-0.403611000	1.623271000
H	-0.950038000	0.298084000	-1.494484000
H	-1.640263000	1.235959000	2.271196000

(**TS**$^{\mathbf{E''F'}}$)

Ru	0.347102000	-0.618432000	0.473464000
O	-1.068324000	-3.329358000	-1.661252000
O	-3.581465000	-0.078733000	-0.253650000
N	-0.517207000	-1.084058000	-1.524372000
N	2.253547000	-1.924387000	-1.487654000
N	3.372454000	-0.509848000	-0.363623000
N	4.266149000	-1.060948000	-1.249172000
C	2.122871000	-1.013398000	-0.467583000
C	3.556755000	-1.912542000	-1.924433000
H	3.935051000	-2.535477000	-2.722312000
C	3.880727000	0.495125000	0.580405000
H	4.445969000	-0.033215000	1.356889000
H	3.000691000	0.942951000	1.041009000
C	4.758178000	1.545794000	-0.095293000
H	5.100471000	2.261445000	0.659035000
H	4.205319000	2.093036000	-0.865598000
H	5.633815000	1.087690000	-0.559905000
C	1.231504000	-2.855124000	-1.945992000
H	1.381460000	-3.839116000	-1.492744000
H	1.333443000	-2.971691000	-3.031733000
C	-0.220109000	-2.462206000	-1.675365000
C	-1.925682000	-0.689646000	-1.916030000
H	-2.085837000	-1.092164000	-2.921735000
H	-1.897679000	0.398046000	-1.982354000
C	-3.065587000	-1.081003000	-1.043419000
C	-3.840487000	-2.200214000	-0.918714000
H	-3.679013000	-3.138984000	-1.426887000
C	-4.882505000	-1.881801000	0.008993000
H	-5.683024000	-2.527724000	0.341400000
C	-4.678794000	-0.585174000	0.376792000
H	-5.207041000	0.098765000	1.023916000
C	-0.323824000	-2.328564000	1.984376000
C	-1.419364000	-1.438968000	1.757742000
H	-2.347465000	-1.844427000	1.369722000
C	-1.330858000	-0.056225000	2.011570000

H	-2.188184000	0.575265000	1.814064000
C	-0.118049000	0.525546000	2.488862000
C	0.996627000	-0.335245000	2.656967000
H	1.942665000	0.062531000	3.001511000
C	0.891420000	-1.735987000	2.397974000
H	1.770716000	-2.359762000	2.528301000
C	-0.474321000	-3.813734000	1.789352000
H	-1.019660000	-4.252286000	2.634586000
H	0.500073000	-4.308211000	1.732087000
H	-1.036240000	-4.041596000	0.877949000
C	-0.108455000	1.999779000	2.862239000
H	-0.669114000	2.526671000	2.079559000
C	1.283283000	2.635421000	2.960676000
H	1.847030000	2.533625000	2.027528000
H	1.876641000	2.203126000	3.774905000
H	1.183676000	3.704716000	3.172116000
C	-0.876476000	2.175371000	4.194006000
H	-1.897315000	1.785042000	4.131353000
H	-0.937058000	3.238187000	4.450211000
H	-0.364949000	1.658636000	5.014275000
C	0.922465000	1.759731000	-1.740285000
O	0.871001000	0.927953000	-2.679324000
C	-0.063656000	2.873384000	-1.604655000
C	-1.115989000	2.996334000	-2.523654000
C	0.099067000	3.843906000	-0.605267000
C	-2.007044000	4.063141000	-2.427708000
H	-1.196724000	2.270496000	-3.326829000
C	-0.792771000	4.910459000	-0.508578000
H	0.934186000	3.766987000	0.087750000
C	-1.851065000	5.017014000	-1.416768000
H	-2.814124000	4.162378000	-3.147790000
H	-0.659127000	5.664926000	0.261445000
H	-2.543112000	5.851288000	-1.346629000
H	0.573126000	0.961013000	-0.449386000
H	0.111528000	-0.471263000	-2.092584000
H	1.895857000	1.968855000	-1.255240000

(**F'**)

Ru	-1.259585000	-0.593095000	-0.113642000
O	-0.526325000	1.663033000	-2.889495000
O	-1.947516000	3.249957000	1.059174000
N	0.094506000	1.077132000	-0.730942000
N	1.104138000	-1.370809000	-1.780483000
N	0.959783000	-2.779254000	-0.193095000
N	2.076659000	-3.147003000	-0.907033000
C	0.329745000	-1.694592000	-0.689486000

C	2.140358000	-2.270275000	-1.863907000
H	2.900243000	-2.250965000	-2.631779000
C	0.640558000	-3.531969000	1.023841000
H	0.551686000	-4.584764000	0.739538000
H	-0.332678000	-3.169637000	1.355174000
C	1.698761000	-3.344945000	2.109089000
H	1.436616000	-3.948848000	2.983709000
H	1.755063000	-2.296119000	2.418729000
H	2.681950000	-3.664135000	1.752478000
C	0.822014000	-0.289453000	-2.714962000
H	0.259825000	-0.658424000	-3.577119000
H	1.777143000	0.105534000	-3.079151000
C	0.039874000	0.896904000	-2.139605000
C	-0.062458000	2.501045000	-0.261684000
H	0.571550000	3.117497000	-0.907607000
H	0.356004000	2.514142000	0.746435000
C	-1.429654000	3.085382000	-0.202784000
C	-2.277929000	3.637433000	-1.121216000
H	-2.117859000	3.665267000	-2.188865000
C	-3.389315000	4.164487000	-0.389124000
H	-4.250899000	4.681138000	-0.788509000
C	-3.134091000	3.906467000	0.925603000
H	-3.652978000	4.131473000	1.845143000
C	-3.048934000	-1.379805000	-1.574426000
C	-3.302160000	-0.034789000	-1.263789000
H	-3.420444000	0.688249000	-2.065152000
C	-3.425472000	0.419398000	0.087360000
H	-3.663378000	1.461580000	0.264947000
C	-3.267645000	-0.451248000	1.179403000
C	-2.879899000	-1.799583000	0.879500000
H	-2.710198000	-2.506929000	1.682370000
C	-2.766284000	-2.239867000	-0.463518000
H	-2.489292000	-3.272721000	-0.653975000
C	-3.048307000	-1.896629000	-2.989595000
H	-4.025093000	-2.332407000	-3.236047000
H	-2.297903000	-2.680976000	-3.133214000
H	-2.856680000	-1.093171000	-3.707154000
C	-3.540816000	0.026944000	2.595794000
H	-3.406226000	1.115207000	2.587299000
C	-2.594486000	-0.553216000	3.657287000
H	-1.547088000	-0.364812000	3.401782000
H	-2.731678000	-1.633795000	3.783895000
H	-2.802028000	-0.089454000	4.627165000
C	-5.015943000	-0.268200000	2.950366000
H	-5.703726000	0.190284000	2.231883000
H	-5.249353000	0.126934000	3.944701000

H	-5.210622000	-1.347256000	2.964458000
C	3.637714000	0.672674000	0.794575000
O	2.891520000	0.672342000	-0.184374000
C	5.089609000	0.833699000	0.740994000
C	5.750697000	1.027925000	-0.486127000
C	5.825483000	0.799097000	1.937642000
C	7.130727000	1.183446000	-0.509922000
H	5.165389000	1.058300000	-1.399688000
C	7.209199000	0.954232000	1.909937000
H	5.309254000	0.651472000	2.883562000
C	7.858853000	1.145828000	0.687256000
H	7.646618000	1.336204000	-1.453112000
H	7.780313000	0.928052000	2.832767000
H	8.937937000	1.268613000	0.664382000
H	-0.385720000	-0.494255000	1.221462000
H	1.005355000	0.753450000	-0.372784000
H	3.212394000	0.545967000	1.809914000

Dehydrogenation of Seconadary alcohols

(**A'**)

Ru	-0.400443000	-0.889608000	0.266402000
O	-0.508850000	-0.036468000	-3.895925000
O	-2.636314000	2.564094000	-0.846391000
N	-0.237775000	0.071921000	-1.611120000
N	1.037885000	-2.515164000	-1.818132000
N	2.015962000	-2.819111000	0.048297000
N	2.713230000	-3.581491000	-0.855391000
C	0.978778000	-2.157447000	-0.504016000
C	2.095275000	-3.374499000	-1.982828000
H	2.372953000	-3.816585000	-2.928842000
C	2.484136000	-2.797072000	1.440244000
H	2.333726000	-3.799645000	1.854944000
H	1.832993000	-2.097821000	1.965511000
C	3.949776000	-2.384605000	1.546695000
H	4.251914000	-2.390010000	2.598792000
H	4.098707000	-1.377080000	1.146445000
H	4.591976000	-3.078366000	0.999086000
C	0.116069000	-2.052538000	-2.854915000
H	-0.810215000	-2.636195000	-2.798969000
H	0.571613000	-2.245413000	-3.826778000
C	-0.231976000	-0.556079000	-2.813325000
C	-0.618391000	1.502972000	-1.706572000
H	-0.086685000	1.922911000	-2.567892000
H	-0.262855000	2.019225000	-0.811273000
C	-2.081294000	1.793491000	-1.844237000

C	-3.039414000	1.486669000	-2.768036000
H	-2.874511000	0.919465000	-3.672013000
C	-4.258383000	2.091141000	-2.316072000
H	-5.221487000	2.066205000	-2.806924000
C	-3.959222000	2.735516000	-1.154431000
H	-4.524475000	3.353773000	-0.473703000
C	-1.787596000	-2.637207000	0.711635000
C	-2.502292000	-1.625180000	0.020836000
H	-2.950110000	-1.847801000	-0.941780000
C	-2.723210000	-0.339843000	0.609808000
H	-3.333979000	0.378870000	0.076234000
C	-2.134115000	0.012932000	1.829892000
C	-1.279160000	-0.970099000	2.446624000
H	-0.752099000	-0.715468000	3.359130000
C	-1.172061000	-2.281202000	1.954571000
H	-0.584587000	-3.016213000	2.494694000
C	-1.714382000	-4.046462000	0.186442000
H	-2.509583000	-4.646744000	0.646155000
H	-0.759843000	-4.523287000	0.427089000
H	-1.861931000	-4.081383000	-0.896473000
C	-2.464686000	1.356183000	2.474164000
H	-2.366635000	2.115532000	1.689154000
C	-1.556899000	1.745407000	3.648474000
H	-0.497134000	1.761586000	3.375017000
H	-1.680689000	1.067217000	4.501450000
H	-1.821345000	2.748593000	3.996545000
C	-3.942834000	1.346600000	2.930405000
H	-4.624138000	1.148240000	2.096963000
H	-4.207357000	2.319690000	3.357330000
H	-4.113846000	0.583958000	3.699200000
C	1.668793000	1.584549000	1.307367000
O	1.434687000	0.358154000	0.516977000
C	2.566864000	2.515484000	0.522897000
C	3.839397000	2.102411000	0.096663000
C	2.131541000	3.809971000	0.210668000
C	4.656439000	2.969291000	-0.627709000
H	4.194749000	1.102287000	0.332069000
C	2.953863000	4.681288000	-0.506028000
H	1.147988000	4.142083000	0.535487000
C	4.216111000	4.261298000	-0.927916000
H	5.638786000	2.639573000	-0.953198000
H	2.606258000	5.683798000	-0.737235000
H	4.855464000	4.936872000	-1.488437000
H	0.696646000	2.068370000	1.452530000
C	2.239790000	1.149210000	2.650711000
H	3.221375000	0.683144000	2.526238000

H	2.356429000	2.020926000	3.302091000
H	1.573843000	0.435660000	3.147818000
H	1.510819000	0.584389000	-0.433070000

(**TS**$^{\mathbf{A'A''}}$)

Ru	-0.793620000	-0.564605000	-0.063325000
O	1.672423000	-0.477372000	3.460752000
O	3.039516000	-2.216532000	-0.364160000
N	0.859338000	-0.083196000	1.335783000
N	-1.757967000	0.320811000	2.672733000
N	-3.160016000	0.989505000	1.222764000
N	-3.620306000	1.471658000	2.422117000
C	-2.025302000	0.270447000	1.334320000
C	-2.746650000	1.051955000	3.287365000
H	-2.785959000	1.243767000	4.350045000
C	-3.915714000	1.348624000	0.013983000
H	-4.870162000	0.812090000	0.050351000
H	-3.333514000	0.975425000	-0.827530000
C	-4.144374000	2.854234000	-0.095201000
H	-4.707004000	3.065191000	-1.010302000
H	-3.192037000	3.389585000	-0.140988000
H	-4.718913000	3.225533000	0.756353000
C	-0.661697000	-0.353182000	3.353143000
H	-0.899579000	-1.418955000	3.456328000
H	-0.575691000	0.061092000	4.358836000
C	0.729132000	-0.274638000	2.719550000
C	2.283488000	-0.269159000	0.881021000
H	2.908097000	0.361042000	1.520244000
H	2.338195000	0.130620000	-0.131567000
C	2.807452000	-1.667972000	0.879511000
C	3.183375000	-2.562983000	1.841837000
H	3.141336000	-2.395986000	2.907356000
C	3.660227000	-3.730875000	1.162201000
H	4.047764000	-4.635057000	1.610455000
C	3.556656000	-3.466060000	-0.168707000
H	3.814112000	-4.013576000	-1.062736000
C	-1.480089000	-2.769957000	-0.036467000
C	-0.135213000	-2.698422000	-0.481243000
H	0.635417000	-3.210885000	0.084851000
C	0.233898000	-2.009755000	-1.674292000
H	1.273060000	-2.021393000	-1.979029000
C	-0.721619000	-1.299605000	-2.426029000
C	-2.049827000	-1.229234000	-1.903597000
H	-2.805380000	-0.652749000	-2.422174000
C	-2.417767000	-1.969285000	-0.750954000
H	-3.443898000	-1.918724000	-0.398676000

C	-1.891437000	-3.633261000	1.127069000
H	-2.194721000	-4.625518000	0.770098000
H	-2.741119000	-3.204523000	1.667210000
H	-1.063830000	-3.776193000	1.828194000
C	-0.326059000	-0.678128000	-3.756474000
H	0.655618000	-0.207310000	-3.611380000
C	-1.299449000	0.382269000	-4.286922000
H	-1.479177000	1.180299000	-3.560598000
H	-2.263850000	-0.058107000	-4.566437000
H	-0.883964000	0.841641000	-5.188950000
C	-0.146441000	-1.813200000	-4.794091000
H	0.599597000	-2.546575000	-4.472349000
H	0.182196000	-1.391082000	-5.749195000
H	-1.092031000	-2.340267000	-4.965201000
C	0.426099000	2.193285000	-1.185190000
O	-0.237632000	1.506730000	-0.110625000
C	1.737924000	2.801391000	-0.710105000
C	1.797280000	3.535648000	0.483928000
C	2.902493000	2.663881000	-1.475629000
C	2.997771000	4.107771000	0.905819000
H	0.899060000	3.658946000	1.083638000
C	4.103546000	3.243860000	-1.059953000
H	2.871076000	2.103915000	-2.408573000
C	4.154461000	3.963851000	0.134511000
H	3.030144000	4.672656000	1.833406000
H	4.997408000	3.129198000	-1.666657000
H	5.087789000	4.412459000	0.462094000
H	0.657328000	1.477858000	-1.986988000
C	-0.519019000	3.267036000	-1.735450000
H	-0.731011000	4.014537000	-0.963956000
H	-0.067584000	3.780261000	-2.591468000
H	-1.467879000	2.822901000	-2.055548000
H	0.497743000	0.955217000	0.841915000

(**A”**)

Ru	-0.746106000	-0.624164000	-0.144445000
O	-0.228059000	-1.033666000	3.694931000
O	3.231002000	-0.878081000	0.844836000
N	0.074966000	0.258374000	1.815660000
N	-2.806873000	0.588250000	1.725134000
N	-3.334148000	1.071128000	-0.278746000
N	-4.270999000	1.696857000	0.505353000
C	-2.428479000	0.370655000	0.425020000
C	-3.927300000	1.389294000	1.719477000
H	-4.447322000	1.711483000	2.610393000
C	-3.388224000	1.280868000	-1.734421000

H	-4.237727000	0.706734000	-2.120870000
H	-2.460199000	0.864764000	-2.123665000
C	-3.520054000	2.757532000	-2.094906000
H	-3.537356000	2.857079000	-3.184803000
H	-2.667532000	3.322830000	-1.709191000
H	-4.442606000	3.183495000	-1.694014000
C	-2.205548000	-0.020118000	2.904215000
H	-2.699013000	-0.968594000	3.136417000
H	-2.368014000	0.648541000	3.756453000
C	-0.703785000	-0.311983000	2.845084000
C	1.553475000	0.327514000	2.106179000
H	1.655235000	0.667017000	3.141717000
H	1.940584000	1.102672000	1.444496000
C	2.356333000	-0.911105000	1.905254000
C	2.539358000	-2.068195000	2.610729000
H	2.005867000	-2.351077000	3.506104000
C	3.576659000	-2.796876000	1.945532000
H	3.991824000	-3.753209000	2.231704000
C	3.962942000	-2.026842000	0.888240000
H	4.721417000	-2.130645000	0.126955000
C	-1.697105000	-2.746593000	-0.109823000
C	-0.357683000	-2.826153000	0.327707000
H	-0.137742000	-3.207503000	1.319655000
C	0.736976000	-2.504883000	-0.542441000
H	1.745909000	-2.685237000	-0.189467000
C	0.528018000	-1.971250000	-1.817671000
C	-0.832352000	-1.652847000	-2.166731000
H	-1.047154000	-1.154869000	-3.104091000
C	-1.913337000	-2.092408000	-1.362604000
H	-2.929761000	-1.908185000	-1.696641000
C	-2.842889000	-3.280754000	0.708400000
H	-3.101838000	-4.291723000	0.369535000
H	-3.740591000	-2.662795000	0.605699000
H	-2.579676000	-3.350362000	1.768117000
C	1.706207000	-1.773294000	-2.765326000
H	2.470663000	-1.211996000	-2.211461000
C	1.371100000	-1.003415000	-4.049478000
H	0.954883000	-0.012681000	-3.849174000
H	0.662552000	-1.558209000	-4.676460000
H	2.282257000	-0.864765000	-4.639497000
C	2.305932000	-3.154899000	-3.119980000
H	2.629646000	-3.703317000	-2.229888000
H	3.175961000	-3.024490000	-3.771829000
H	1.575643000	-3.773788000	-3.653990000
C	0.808761000	1.746734000	-1.367943000
O	-0.304154000	1.346331000	-0.586180000

C	1.699037000	2.702139000	-0.575433000
C	1.132141000	3.742040000	0.177768000
C	3.094065000	2.580912000	-0.607224000
C	1.941263000	4.634850000	0.881577000
H	0.051006000	3.849776000	0.204259000
C	3.907327000	3.475778000	0.093745000
H	3.550116000	1.778760000	-1.183675000
C	3.332524000	4.504665000	0.841227000
H	1.487941000	5.438227000	1.456415000
H	4.987765000	3.366348000	0.057060000
H	3.962490000	5.201496000	1.386707000
H	1.425744000	0.876885000	-1.641879000
C	0.323900000	2.422610000	-2.662438000
H	-0.245052000	3.327586000	-2.425218000
H	1.166455000	2.712359000	-3.300808000
H	-0.327432000	1.748828000	-3.231796000
H	-0.232767000	1.169008000	1.449402000

(**TS**$^{\mathbf{A''B'}}$)

Ru	0.420917000	-0.502406000	0.430453000
O	-0.667026000	-3.313127000	-1.733645000
O	-3.703511000	-0.724753000	0.037012000
N	-0.570831000	-1.007446000	-1.502867000
N	2.383840000	-1.538918000	-1.672782000
N	3.452082000	-0.338651000	-0.283202000
N	4.392186000	-0.782965000	-1.178703000
C	2.197741000	-0.784087000	-0.542346000
C	3.712760000	-1.503612000	-2.017614000
H	4.130440000	-2.013641000	-2.873790000
C	3.901594000	0.512890000	0.831068000
H	4.091078000	-0.131424000	1.697814000
H	3.062230000	1.167328000	1.068950000
C	5.150548000	1.320854000	0.493145000
H	5.398867000	1.951015000	1.353194000
H	4.985639000	1.968745000	-0.372485000
H	6.002681000	0.673312000	0.279525000
C	1.377838000	-2.301014000	-2.402818000
H	1.680983000	-3.348716000	-2.455576000
H	1.311016000	-1.903715000	-3.424026000
C	-0.031569000	-2.283324000	-1.811174000
C	-2.062919000	-0.880808000	-1.738637000
H	-2.233752000	-1.233815000	-2.761853000
H	-2.259975000	0.191239000	-1.714019000
C	-3.025219000	-1.556458000	-0.825806000
C	-3.521883000	-2.825154000	-0.714164000
H	-3.184368000	-3.685425000	-1.271904000

C	-4.548039000	-2.783065000	0.282336000
H	-5.160348000	-3.604783000	0.626497000
C	-4.617493000	-1.487614000	0.700725000
H	-5.242211000	-0.963977000	1.408557000
C	0.065830000	-2.301714000	1.976842000
C	-1.157047000	-1.602211000	1.791123000
H	-2.023068000	-2.158467000	1.452501000
C	-1.290226000	-0.217000000	2.046828000
H	-2.250536000	0.258724000	1.889990000
C	-0.183191000	0.547784000	2.498705000
C	1.066809000	-0.117424000	2.610567000
H	1.940371000	0.428252000	2.940686000
C	1.186218000	-1.510448000	2.334983000
H	2.159116000	-1.983210000	2.435677000
C	0.161142000	-3.797274000	1.787038000
H	-0.829755000	-4.256623000	1.831837000
H	0.778939000	-4.248192000	2.570482000
H	0.598542000	-4.061819000	0.818646000
C	-0.390931000	1.996538000	2.907353000
H	-1.078567000	2.434970000	2.173278000
C	0.887414000	2.844215000	2.936260000
H	1.425473000	2.805428000	1.982826000
H	1.571321000	2.525833000	3.731929000
H	0.632460000	3.889800000	3.136056000
C	-1.090972000	2.028436000	4.286704000
H	-2.040273000	1.483363000	4.274370000
H	-1.299824000	3.064115000	4.574370000
H	-0.454346000	1.584907000	5.061004000
C	0.629781000	1.945521000	-1.784495000
O	0.680487000	1.075410000	-2.694874000
C	-0.655123000	2.718096000	-1.577744000
C	-1.658226000	2.604098000	-2.553261000
C	-0.847839000	3.607040000	-0.508603000
C	-2.835027000	3.345665000	-2.451997000
H	-1.483610000	1.954781000	-3.404985000
C	-2.026084000	4.345375000	-0.404826000
H	-0.077751000	3.726648000	0.246449000
C	-3.024787000	4.213589000	-1.374124000
H	-3.596548000	3.259145000	-3.221839000
H	-2.162036000	5.032936000	0.425338000
H	-3.938417000	4.795828000	-1.296745000
H	0.555407000	1.067773000	-0.468511000
C	1.924809000	2.669543000	-1.421547000
H	2.044673000	3.490863000	-2.139893000
H	1.923828000	3.102166000	-0.418885000
H	2.769811000	1.990077000	-1.537788000

H	-0.123855000	-0.262579000	-2.089795000

(**B'**)

Ru	-1.398480000	-0.465507000	-0.033891000
O	-0.485801000	0.993495000	-3.208378000
O	-0.657161000	3.489260000	0.539668000
N	0.300345000	0.566632000	-1.067970000
N	0.349672000	-2.199204000	-1.731426000
N	0.046706000	-3.224070000	0.107577000
N	0.891796000	-4.026481000	-0.623595000
C	-0.310777000	-2.090582000	-0.529025000
C	1.060991000	-3.374184000	-1.735423000
H	1.671405000	-3.711939000	-2.560574000
C	-0.313006000	-3.649339000	1.464066000
H	-0.776563000	-4.637317000	1.382421000
H	-1.058840000	-2.934984000	1.812720000
C	0.893128000	-3.687230000	2.399548000
H	0.574126000	-4.025936000	3.390503000
H	1.337317000	-2.691818000	2.500732000
H	1.652606000	-4.380734000	2.028287000
C	0.248642000	-1.239154000	-2.822204000
H	-0.534611000	-1.532483000	-3.526798000
H	1.201483000	-1.231518000	-3.364010000
C	-0.044468000	0.204890000	-2.398725000
C	0.655253000	2.017807000	-0.867206000
H	1.295093000	2.304121000	-1.708662000
H	1.253118000	2.038618000	0.045643000
C	-0.444094000	3.010380000	-0.729490000
C	-1.237253000	3.686922000	-1.613564000
H	-1.266320000	3.528795000	-2.681755000
C	-1.993697000	4.630367000	-0.847638000
H	-2.718812000	5.342422000	-1.216315000
C	-1.598540000	4.469704000	0.448031000
H	-1.856229000	4.961845000	1.373715000
C	-3.515218000	-0.731690000	-1.212090000
C	-3.276810000	0.640864000	-1.020016000
H	-3.246648000	1.304065000	-1.878918000
C	-3.085758000	1.204412000	0.278949000
H	-2.955335000	2.276471000	0.367580000
C	-3.072705000	0.403698000	1.435605000
C	-3.173341000	-1.013003000	1.243335000
H	-3.134998000	-1.681728000	2.094735000
C	-3.380378000	-1.556850000	-0.051936000
H	-3.469289000	-2.634448000	-0.156934000
C	-3.860405000	-1.308768000	-2.560239000
H	-4.949506000	-1.363304000	-2.684931000

H	-3.469498000	-2.324894000	-2.676201000
H	-3.468097000	-0.687577000	-3.371192000
C	-2.998828000	1.039351000	2.813554000
H	-2.533129000	2.023350000	2.678845000
C	-2.156893000	0.256677000	3.831871000
H	-1.142271000	0.083761000	3.459696000
H	-2.607209000	-0.712519000	4.077901000
H	-2.089477000	0.823754000	4.766004000
C	-4.435947000	1.261278000	3.337875000
H	-5.030234000	1.866014000	2.644609000
H	-4.407955000	1.778712000	4.302631000
H	-4.954325000	0.306179000	3.484441000
C	3.937378000	-0.838745000	0.134470000
O	2.865210000	-0.687915000	-0.458474000
C	4.864264000	0.303598000	0.351856000
C	4.611973000	1.523387000	-0.301026000
C	5.986557000	0.199729000	1.192448000
C	5.456237000	2.612726000	-0.116329000
H	3.757526000	1.592922000	-0.965462000
C	6.826226000	1.295109000	1.385497000
H	6.204297000	-0.730791000	1.706403000
C	6.563322000	2.501102000	0.731668000
H	5.258895000	3.547937000	-0.632143000
H	7.686016000	1.207647000	2.042812000
H	7.222125000	3.352159000	0.878507000
H	-0.356232000	-0.464642000	1.178308000
C	4.323403000	-2.212649000	0.644446000
H	5.309510000	-2.510268000	0.270957000
H	4.379094000	-2.216370000	1.739789000
H	3.575315000	-2.940232000	0.325773000
H	1.107622000	0.021350000	-0.742380000

(**D'**)

Ru	0.305984000	0.220333000	0.113556000
O	-0.351486000	-3.388095000	0.521028000
O	-3.220584000	-0.742360000	-1.680213000
N	0.042050000	-1.711155000	-1.026328000
N	2.713948000	-1.554872000	-0.089801000
N	3.363609000	0.434947000	-0.477745000
N	4.486629000	-0.348751000	-0.605747000
C	2.251790000	-0.255247000	-0.152808000
C	4.065088000	-1.552436000	-0.361244000
H	4.686686000	-2.436679000	-0.364488000
C	3.486602000	1.866476000	-0.782188000
H	4.283481000	2.261912000	-0.145593000
H	2.539332000	2.319354000	-0.489155000

C	3.787840000	2.114441000	-2.258868000
H	3.899050000	3.189571000	-2.431398000
H	2.973121000	1.746932000	-2.891361000
H	4.717732000	1.621394000	-2.554916000
C	1.918289000	-2.691516000	0.355517000
H	1.973234000	-2.801390000	1.442486000
H	2.333467000	-3.603674000	-0.088426000
C	0.432019000	-2.636949000	-0.013713000
C	-1.207994000	-2.078597000	-1.793959000
H	-1.130873000	-3.144306000	-2.032648000
H	-1.151923000	-1.504773000	-2.720953000
C	-2.521404000	-1.801207000	-1.154921000
C	-3.290199000	-2.443073000	-0.224485000
H	-3.001094000	-3.318399000	0.338218000
C	-4.532182000	-1.735330000	-0.161123000
H	-5.386300000	-1.966241000	0.460000000
C	-4.436610000	-0.719860000	-1.067051000
H	-5.115912000	0.050897000	-1.398619000
C	0.105053000	0.358609000	2.541915000
C	-1.126987000	-0.075980000	2.030242000
H	-1.559874000	-1.006006000	2.386474000
C	-1.850288000	0.682263000	1.054583000
H	-2.816521000	0.315461000	0.727157000
C	-1.355918000	1.891137000	0.536333000
C	-0.036054000	2.275152000	0.950159000
H	0.416721000	3.174614000	0.550438000
C	0.671247000	1.519922000	1.919455000
H	1.658797000	1.853955000	2.224133000
C	0.815570000	-0.354995000	3.662203000
H	0.615012000	0.145627000	4.618040000
H	1.901032000	-0.354041000	3.517955000
H	0.474831000	-1.390321000	3.756448000
C	-2.207398000	2.753698000	-0.379523000
H	-2.945353000	2.086251000	-0.840271000
C	-1.428612000	3.443693000	-1.509589000
H	-0.878370000	2.717924000	-2.116535000
H	-0.717407000	4.185198000	-1.126288000
H	-2.126414000	3.978589000	-2.161861000
C	-2.970097000	3.789302000	0.478326000
H	-3.572914000	3.306849000	1.255056000
H	-3.640661000	4.379281000	-0.155083000
H	-2.276685000	4.482727000	0.969032000
H	0.505140000	0.786448000	-1.369697000
H	0.793758000	-1.566361000	-1.699348000

Hydrogenation of olefine

(I')

Ru	2.035887000	-0.753180000	-0.249594000
O	0.640376000	-1.540545000	2.960248000
O	2.625616000	2.436526000	2.182840000
N	0.453363000	-0.068488000	1.173128000
N	-0.552939000	-2.244328000	-0.375281000
N	0.021794000	-1.818689000	-2.378574000
N	-1.182171000	-2.476383000	-2.475667000
C	0.448335000	-1.653541000	-1.109397000
C	-1.509796000	-2.714937000	-1.241303000
H	-2.410968000	-3.223519000	-0.931559000
C	0.648538000	-1.339639000	-3.615047000
H	0.842736000	-2.214429000	-4.243836000
H	1.600575000	-0.899953000	-3.316605000
C	-0.225921000	-0.324834000	-4.348713000
H	0.274154000	-0.015118000	-5.272052000
H	-0.396282000	0.564307000	-3.733097000
H	-1.193343000	-0.761379000	-4.610370000
C	-0.567755000	-2.362021000	1.076977000
H	-0.206457000	-3.345144000	1.390493000
H	-1.603655000	-2.250770000	1.415371000
C	0.259997000	-1.313378000	1.830042000
C	0.591308000	1.126753000	2.081348000
H	-0.171909000	1.020927000	2.859196000
H	0.331550000	1.984742000	1.458227000
C	1.910337000	1.392085000	2.715508000
C	2.551817000	0.916622000	3.824714000
H	2.207732000	0.106863000	4.451505000
C	3.737915000	1.702552000	3.982047000
H	4.484160000	1.614685000	4.759362000
C	3.728793000	2.609708000	2.963425000
H	4.383107000	3.420154000	2.679624000
C	3.476534000	-2.589763000	0.432884000
C	3.716076000	-1.492006000	1.280017000
H	3.587107000	-1.605994000	2.351764000
C	4.136886000	-0.222504000	0.779768000
H	4.357778000	0.569012000	1.486473000
C	4.275532000	0.014870000	-0.600059000
C	3.904472000	-1.050687000	-1.483234000
H	3.963275000	-0.913567000	-2.556231000
C	3.509970000	-2.314310000	-0.969485000
H	3.250520000	-3.104022000	-1.668869000
C	3.166855000	-3.963679000	0.967618000
H	2.678748000	-3.906847000	1.945609000
H	4.090048000	-4.543825000	1.093179000

H	2.520741000	-4.524718000	0.284587000
C	4.841499000	1.333381000	-1.100259000
H	4.642013000	2.075857000	-0.317772000
C	4.209976000	1.844089000	-2.403688000
H	3.121588000	1.919607000	-2.314697000
H	4.444172000	1.194595000	-3.255673000
H	4.607389000	2.836535000	-2.640202000
C	6.374220000	1.196878000	-1.246222000
H	6.843508000	0.888290000	-0.306062000
H	6.810304000	2.155955000	-1.545261000
H	6.632921000	0.456847000	-2.012869000
C	-2.965185000	1.204887000	-0.169639000
O	-2.177103000	0.280470000	0.112964000
C	-2.439814000	2.532627000	-0.604093000
C	-1.154471000	2.606470000	-1.170183000
C	-3.178081000	3.717345000	-0.439808000
C	-0.626776000	3.830590000	-1.571793000
H	-0.582280000	1.694584000	-1.309168000
C	-2.641256000	4.944505000	-0.827281000
H	-4.160292000	3.691369000	0.021059000
C	-1.368731000	5.003446000	-1.399162000
H	0.361387000	3.872297000	-2.021227000
H	-3.216129000	5.854222000	-0.681720000
H	-0.956273000	5.959174000	-1.709538000
H	1.485727000	0.481601000	-1.104479000
C	-4.418683000	1.015437000	-0.103944000
H	-0.357681000	0.127848000	0.564803000
C	-4.961384000	-0.111555000	0.415122000
C	-6.370000000	-0.458985000	0.534462000
C	-6.712619000	-1.664009000	1.179939000
C	-7.410321000	0.352162000	0.033962000
C	-8.043194000	-2.046690000	1.326916000
H	-5.921322000	-2.298528000	1.572216000
C	-8.738088000	-0.030845000	0.179541000
H	-7.177808000	1.282816000	-0.474642000
C	-9.059535000	-1.230223000	0.826677000
H	-8.288031000	-2.977642000	1.829587000
H	-9.528318000	0.602881000	-0.212050000
H	-10.098949000	-1.524921000	0.938086000
H	-4.260170000	-0.850603000	0.800699000
H	-5.046534000	1.804546000	-0.501344000

1,4-TS$^{I'J'}$

Ru	-0.923307000	-0.593067000	0.642185000
O	-1.029812000	-3.717439000	-1.373781000
O	-3.191748000	-0.089603000	-2.693502000

N	-0.329975000	-1.506107000	-1.316037000
N	1.503505000	-2.370349000	0.797612000
N	1.793864000	-0.742553000	2.137161000
N	2.903020000	-1.538411000	2.284097000
C	0.899905000	-1.216814000	1.238626000
C	2.704449000	-2.512541000	1.448629000
H	3.389041000	-3.332068000	1.283859000
C	1.684696000	0.451824000	2.986869000
H	1.315988000	0.134313000	3.969445000
H	0.922964000	1.079170000	2.521913000
C	3.013201000	1.186557000	3.142051000
H	2.853140000	2.083520000	3.749115000
H	3.415332000	1.487420000	2.171174000
H	3.754275000	0.559162000	3.641320000
C	0.977471000	-3.322196000	-0.174846000
H	0.712000000	-4.259301000	0.320594000
H	1.766995000	-3.529710000	-0.907106000
C	-0.247704000	-2.880168000	-0.977220000
C	-1.060891000	-1.237816000	-2.606500000
H	-0.660449000	-1.941401000	-3.343798000
H	-0.761052000	-0.232683000	-2.908519000
C	-2.548628000	-1.302744000	-2.622249000
C	-3.464058000	-2.311573000	-2.732991000
H	-3.241585000	-3.367977000	-2.721232000
C	-4.746416000	-1.690817000	-2.870934000
H	-5.701737000	-2.181878000	-2.993424000
C	-4.521474000	-0.346076000	-2.845408000
H	-5.158835000	0.519376000	-2.945188000
C	-1.986463000	-1.715527000	2.459707000
C	-2.760693000	-1.956862000	1.310146000
H	-2.950790000	-2.976142000	0.988568000
C	-3.370772000	-0.880677000	0.594350000
H	-4.026040000	-1.119407000	-0.236550000
C	-3.190098000	0.458841000	0.963789000
C	-2.224547000	0.712012000	1.995804000
H	-1.984218000	1.734148000	2.268238000
C	-1.684402000	-0.348168000	2.761713000
H	-1.051425000	-0.121817000	3.612271000
C	-1.462705000	-2.840989000	3.320906000
H	-2.196797000	-3.649165000	3.390191000
H	-1.249249000	-2.490411000	4.335009000
H	-0.538695000	-3.268618000	2.917085000
C	-4.065877000	1.555485000	0.382049000
H	-4.671964000	1.085347000	-0.400465000
C	-3.289855000	2.712575000	-0.255891000
H	-2.677589000	2.358450000	-1.087985000

H	-2.631905000	3.215776000	0.460412000
H	-3.989696000	3.462149000	-0.641330000
C	-5.030348000	2.060879000	1.478445000
H	-5.611127000	1.242265000	1.917303000
H	-5.733439000	2.783948000	1.051636000
H	-4.486783000	2.563993000	2.287084000
C	2.905413000	0.260531000	-1.188979000
O	2.260172000	-0.719410000	-1.658862000
C	4.397149000	0.208298000	-1.216742000
C	5.208796000	1.308808000	-0.887305000
C	5.015759000	-0.990170000	-1.614205000
C	6.597616000	1.204863000	-0.937553000
H	4.764887000	2.260744000	-0.615491000
C	6.402519000	-1.094146000	-1.662386000
H	4.386274000	-1.827717000	-1.894386000
C	7.198291000	0.003206000	-1.320007000
H	7.211599000	2.064753000	-0.686106000
H	6.866252000	-2.026458000	-1.972141000
H	8.281024000	-0.075169000	-1.359398000
C	2.230652000	1.397952000	-0.632620000
C	0.860879000	1.622759000	-0.843143000
C	0.319704000	2.989317000	-0.569749000
C	-0.286751000	3.705052000	-1.612328000
C	0.475100000	3.615919000	0.675797000
C	-0.713632000	5.019549000	-1.420035000
H	-0.406039000	3.237147000	-2.586576000
C	0.036463000	4.925089000	0.874219000
H	0.953057000	3.080043000	1.491672000
C	-0.557864000	5.632092000	-0.174979000
H	-1.166457000	5.564568000	-2.243299000
H	0.165303000	5.397540000	1.844181000
H	-0.893180000	6.653841000	-0.022931000
H	0.464692000	1.167764000	-1.750380000
H	2.785318000	2.114559000	-0.040236000
H	0.077714000	0.761690000	-0.011512000
H	0.637614000	-1.109196000	-1.421999000

(**J'**)

Ru	-1.033285000	0.904437000	-0.415526000
O	-3.989889000	1.105890000	2.222308000
O	-2.964595000	-2.710341000	0.166819000
N	-1.914051000	0.307201000	1.620012000
N	-0.943038000	3.031364000	1.749750000
N	0.847206000	3.166608000	0.607444000
N	0.974452000	4.107479000	1.599410000
C	-0.314736000	2.490801000	0.654506000

C	-0.126124000	4.005440000	2.279467000
H	-0.378226000	4.604309000	3.143113000
C	1.997163000	2.978787000	-0.292777000
H	2.136517000	3.921244000	-0.832366000
H	1.703083000	2.204221000	-0.998996000
C	3.260124000	2.584634000	0.467277000
H	4.084746000	2.460702000	-0.241139000
H	3.115346000	1.633557000	0.985134000
H	3.535285000	3.357253000	1.189810000
C	-2.299630000	2.748506000	2.198161000
H	-3.013378000	3.402316000	1.687396000
H	-2.360951000	2.978818000	3.266925000
C	-2.814555000	1.318064000	2.022391000
C	-2.380032000	-1.104572000	1.875432000
H	-2.750602000	-1.131232000	2.905599000
H	-1.478220000	-1.714547000	1.812640000
C	-3.405094000	-1.673227000	0.955198000
C	-4.750372000	-1.505047000	0.774704000
H	-5.368763000	-0.779304000	1.280679000
C	-5.162884000	-2.482293000	-0.186392000
H	-6.162703000	-2.648144000	-0.562731000
C	-4.043449000	-3.188563000	-0.514368000
H	-3.855065000	-4.032217000	-1.160912000
C	-2.134058000	2.240282000	-1.935975000
C	-2.968833000	1.154434000	-1.592574000
H	-3.940815000	1.343299000	-1.147916000
C	-2.597558000	-0.197790000	-1.888914000
H	-3.311406000	-0.983769000	-1.672505000
C	-1.347134000	-0.521055000	-2.426971000
C	-0.420794000	0.570959000	-2.583903000
H	0.594070000	0.367108000	-2.901526000
C	-0.822025000	1.915021000	-2.412011000
H	-0.116333000	2.713610000	-2.616318000
C	-2.584488000	3.670455000	-1.800168000
H	-2.949825000	4.036711000	-2.767779000
H	-1.766261000	4.326898000	-1.488493000
H	-3.405684000	3.765679000	-1.083493000
C	-1.032022000	-1.958960000	-2.830129000
H	-1.223169000	-2.582848000	-1.947972000
C	0.418255000	-2.185583000	-3.273400000
H	1.128720000	-1.907879000	-2.489943000
H	0.655625000	-1.621820000	-4.184506000
H	0.566950000	-3.245415000	-3.503542000
C	-2.005680000	-2.402681000	-3.946691000
H	-3.053282000	-2.327720000	-3.637945000
H	-1.808818000	-3.445723000	-4.215839000

H	-1.872763000	-1.793734000	-4.848575000
C	1.398543000	-0.954204000	0.416981000
O	0.508541000	0.027649000	0.701473000
C	1.295987000	-2.117431000	1.355212000
C	1.254587000	-1.889836000	2.742826000
C	1.205102000	-3.439377000	0.892639000
C	1.140399000	-2.952377000	3.638736000
H	1.337603000	-0.871791000	3.114404000
C	1.085731000	-4.503971000	1.789409000
H	1.221793000	-3.632420000	-0.176231000
C	1.053987000	-4.264333000	3.163963000
H	1.128237000	-2.759530000	4.708231000
H	1.015716000	-5.520582000	1.412364000
H	0.965657000	-5.092629000	3.861117000
C	2.346079000	-0.842117000	-0.542545000
H	2.316134000	0.056305000	-1.157974000
H	-0.954220000	0.389533000	1.979374000
C	3.537942000	-1.739967000	-0.788208000
H	3.532988000	-2.579000000	-0.086091000
H	3.494099000	-2.174747000	-1.797771000
C	4.837349000	-0.958573000	-0.649287000
C	5.486790000	-0.430625000	-1.771851000
C	5.385227000	-0.713863000	0.618234000
C	6.653009000	0.327413000	-1.635178000
H	5.083792000	-0.624468000	-2.764221000
C	6.551893000	0.037915000	0.759418000
H	4.893712000	-1.121718000	1.498896000
C	7.188521000	0.564552000	-0.368065000
H	7.148154000	0.721845000	-2.518662000
H	6.969202000	0.207531000	1.748540000
H	8.099840000	1.146021000	-0.259598000

$TS^{J'1b'}$

Ru	-0.941333000	0.766814000	-0.686675000
O	-3.600306000	-1.878672000	1.562782000
O	-1.738343000	-3.209418000	-1.779857000
N	-1.790129000	-0.887127000	0.515035000
N	-3.464011000	1.549280000	0.822848000
N	-2.092676000	3.169863000	0.917141000
N	-3.175175000	3.564990000	1.663504000
C	-2.234995000	1.941737000	0.379130000
C	-3.993559000	2.557191000	1.592397000
H	-4.964274000	2.511786000	2.064736000
C	-0.917670000	4.053196000	0.920165000
H	-1.252963000	5.031995000	0.564605000
H	-0.217706000	3.633469000	0.198838000

C	-0.286124000	4.156633000	2.306969000
H	0.557460000	4.853435000	2.267242000
H	0.081520000	3.180780000	2.635393000
H	-1.008885000	4.535453000	3.034456000
C	-4.047349000	0.234642000	0.593263000
H	-4.320556000	0.132811000	-0.463482000
H	-4.951930000	0.146428000	1.195394000
C	-3.125673000	-0.931506000	0.969299000
C	-1.192339000	-2.274798000	0.435135000
H	-1.146240000	-2.677715000	1.449973000
H	-0.166688000	-2.138864000	0.086536000
C	-1.918859000	-3.261707000	-0.413470000
C	-2.733784000	-4.312355000	-0.108525000
H	-3.057748000	-4.588793000	0.884217000
C	-3.078878000	-4.950314000	-1.343517000
H	-3.707612000	-5.818986000	-1.478543000
C	-2.452756000	-4.244106000	-2.321472000
H	-2.401621000	-4.337674000	-3.395643000
C	-1.045899000	2.220711000	-2.537927000
C	-1.713061000	0.993612000	-2.822157000
H	-2.754737000	1.002014000	-3.124586000
C	-1.017751000	-0.237536000	-2.723250000
H	-1.556205000	-1.161442000	-2.902189000
C	0.380932000	-0.305791000	-2.424376000
C	0.988172000	0.902880000	-2.031847000
H	2.011685000	0.899046000	-1.672054000
C	0.292940000	2.148260000	-2.079208000
H	0.820200000	3.058821000	-1.815169000
C	-1.752920000	3.544814000	-2.700560000
H	-2.564898000	3.461961000	-3.428450000
H	-1.056627000	4.311500000	-3.053286000
H	-2.186169000	3.895983000	-1.759093000
C	1.141988000	-1.612028000	-2.584225000
H	0.464306000	-2.417423000	-2.283262000
C	2.419622000	-1.703597000	-1.739679000
H	2.226399000	-1.498690000	-0.681724000
H	3.194609000	-1.007643000	-2.079837000
H	2.837464000	-2.712309000	-1.818226000
C	1.460307000	-1.819047000	-4.083669000
H	0.552930000	-1.813312000	-4.697828000
H	1.959009000	-2.783118000	-4.228457000
H	2.128379000	-1.033937000	-4.456780000
C	1.172228000	0.374085000	1.717148000
O	-0.120321000	0.671556000	1.320745000
C	1.254109000	-0.797369000	2.632708000
C	0.332543000	-0.921962000	3.688507000

C	2.212209000	-1.809084000	2.455054000
C	0.377923000	-2.019132000	4.547642000
H	-0.407936000	-0.142651000	3.845601000
C	2.255535000	-2.907403000	3.315810000
H	2.915035000	-1.743314000	1.630514000
C	1.340284000	-3.015793000	4.364104000
H	-0.333646000	-2.093086000	5.365170000
H	3.000965000	-3.682586000	3.161546000
H	1.375225000	-3.870419000	5.033462000
C	2.187481000	1.175649000	1.343607000
H	1.931063000	1.991208000	0.669015000
H	-0.996533000	-0.262316000	1.260249000
C	3.635550000	1.116804000	1.767569000
H	3.909232000	2.095286000	2.189732000
H	3.774978000	0.385271000	2.567693000
C	4.575903000	0.805444000	0.608548000
C	5.314915000	-0.383341000	0.574808000
C	4.716960000	1.706202000	-0.459057000
C	6.161087000	-0.674280000	-0.499134000
H	5.242671000	-1.081983000	1.405054000
C	5.558325000	1.419271000	-1.535544000
H	4.183587000	2.655270000	-0.435450000
C	6.281003000	0.222968000	-1.561264000
H	6.732313000	-1.598653000	-0.499709000
H	5.664747000	2.136399000	-2.345447000
H	6.943159000	0.001714000	-2.393455000

(**1b'**)

Ru	0.290536000	0.177983000	0.285251000
O	-1.703593000	-2.995625000	-1.599223000
O	-3.720167000	0.474472000	0.133659000
N	-0.924983000	-0.983585000	-0.789293000
N	1.411493000	-2.649559000	0.016517000
N	3.089732000	-1.356651000	0.112679000
N	3.610097000	-2.616714000	-0.021041000
C	1.737042000	-1.329770000	0.142477000
C	2.562240000	-3.387185000	-0.072666000
H	2.588438000	-4.462867000	-0.171032000
C	4.059513000	-0.254530000	0.079341000
H	4.847359000	-0.513771000	0.791356000
H	3.546151000	0.633315000	0.439261000
C	4.634574000	-0.041769000	-1.320292000
H	5.374648000	0.764411000	-1.292588000
H	3.848855000	0.231312000	-2.032444000
H	5.130265000	-0.949317000	-1.674935000
C	0.052420000	-3.172373000	-0.039553000

H	-0.361054000	-3.226048000	0.974714000
H	0.088617000	-4.181837000	-0.449269000
C	-0.908717000	-2.365849000	-0.915229000
C	-2.107196000	-0.392860000	-1.490629000
H	-2.200634000	-0.892047000	-2.457640000
H	-1.889212000	0.659432000	-1.673881000
C	-3.397139000	-0.531884000	-0.751912000
C	-4.385220000	-1.472037000	-0.752993000
H	-4.395979000	-2.372442000	-1.349676000
C	-5.380466000	-1.029375000	0.178771000
H	-6.309620000	-1.522816000	0.426778000
C	-4.931133000	0.150054000	0.684192000
H	-5.332156000	0.862287000	1.389347000
C	0.221691000	1.030245000	2.387623000
C	-1.005745000	1.336783000	1.714661000
H	-1.940046000	0.948934000	2.106378000
C	-1.025892000	2.077028000	0.515973000
H	-1.978653000	2.255468000	0.032237000
C	0.185711000	2.451272000	-0.127857000
C	1.414002000	2.168170000	0.552389000
H	2.351528000	2.456110000	0.092205000
C	1.422054000	1.513185000	1.801505000
H	2.367325000	1.279418000	2.279920000
C	0.223140000	0.284069000	3.694049000
H	0.087621000	0.991242000	4.522820000
H	1.167029000	-0.243523000	3.856078000
H	-0.594712000	-0.440572000	3.739882000
C	0.146593000	3.207731000	-1.443229000
H	-0.813122000	2.967081000	-1.918556000
C	1.266697000	2.830089000	-2.424860000
H	1.283130000	1.753551000	-2.626251000
H	2.254796000	3.131331000	-2.058209000
H	1.107606000	3.348190000	-3.375570000
C	0.150946000	4.725370000	-1.144350000
H	-0.676938000	5.012646000	-0.487839000
H	0.051583000	5.284740000	-2.080071000
H	1.088608000	5.031109000	-0.666042000

1,2-TS$^{I'J'}$

Ru	-0.837006000	-0.785219000	0.470418000
O	-2.856918000	-2.346093000	-2.243330000
O	-4.263821000	1.348783000	-0.467803000
N	-1.553206000	-0.530441000	-1.632109000
N	0.654125000	-2.483944000	-1.573295000
N	1.967379000	-2.123499000	0.058461000
N	2.709465000	-2.820092000	-0.861207000

C	0.698786000	-1.874198000	-0.343766000
C	1.885129000	-3.027287000	-1.842424000
H	2.125413000	-3.565466000	-2.748052000
C	2.624157000	-1.707085000	1.311840000
H	1.864855000	-1.766107000	2.088753000
H	2.919647000	-0.660727000	1.203441000
C	3.826353000	-2.576857000	1.662634000
H	4.224174000	-2.239983000	2.625354000
H	4.615263000	-2.489000000	0.913864000
H	3.549120000	-3.631510000	1.752857000
C	-0.519371000	-2.682729000	-2.412453000
H	-0.820428000	-3.733109000	-2.391090000
H	-0.253651000	-2.425796000	-3.445910000
C	-1.758094000	-1.865988000	-2.055410000
C	-2.657145000	0.427152000	-2.035079000
H	-2.784450000	0.295416000	-3.115311000
H	-2.242317000	1.420162000	-1.863920000
C	-3.993040000	0.353211000	-1.380533000
C	-5.115746000	-0.404703000	-1.566263000
H	-5.200697000	-1.253156000	-2.228119000
C	-6.128867000	0.135401000	-0.712247000
H	-7.146497000	-0.212462000	-0.602885000
C	-5.559591000	1.195921000	-0.073168000
H	-5.923126000	1.921420000	0.638845000
C	-2.330613000	-2.240801000	1.609349000
C	-2.975534000	-0.994954000	1.374502000
H	-3.895470000	-0.987500000	0.800885000
C	-2.462196000	0.231650000	1.861382000
H	-2.999512000	1.148250000	1.652775000
C	-1.249936000	0.271360000	2.596416000
C	-0.545277000	-0.950268000	2.760098000
H	0.388987000	-0.959352000	3.305523000
C	-1.073691000	-2.176370000	2.263192000
H	-0.504128000	-3.089950000	2.407916000
C	-2.950380000	-3.541107000	1.170942000
H	-3.723577000	-3.852664000	1.884631000
H	-2.205362000	-4.340844000	1.120389000
H	-3.423664000	-3.443491000	0.189005000
C	-0.796418000	1.574673000	3.229814000
H	-1.047839000	2.372040000	2.520051000
C	0.706600000	1.648501000	3.531144000
H	1.311734000	1.408961000	2.650136000
H	0.993720000	0.966238000	4.339984000
H	0.968481000	2.659058000	3.860802000
C	-1.621830000	1.815710000	4.515849000
H	-2.697151000	1.831591000	4.310859000

H	-1.347238000	2.778635000	4.959059000
H	-1.428718000	1.034215000	5.259818000
C	0.978461000	1.342819000	-1.250624000
O	0.794945000	0.626915000	-2.282228000
C	0.192342000	2.639045000	-1.120922000
C	-0.399477000	3.155255000	-2.283584000
C	0.116345000	3.384591000	0.064971000
C	-1.067154000	4.380395000	-2.257074000
H	-0.303718000	2.594471000	-3.207537000
C	-0.556259000	4.605288000	0.093563000
H	0.579731000	3.011580000	0.972532000
C	-1.152628000	5.106273000	-1.067499000
H	-1.508793000	4.773768000	-3.168334000
H	-0.607625000	5.172903000	1.018713000
H	-1.668960000	6.061585000	-1.046103000
H	0.264397000	0.538592000	-0.146652000
C	2.316765000	1.358255000	-0.592556000
H	2.423156000	1.963801000	0.301701000
H	-0.662644000	-0.129677000	-2.028046000
C	3.374296000	0.739173000	-1.156243000
H	3.177752000	0.178758000	-2.068580000
C	4.761196000	0.735006000	-0.691458000
C	5.693158000	-0.076290000	-1.367785000
C	5.214493000	1.499730000	0.403380000
C	7.024812000	-0.133862000	-0.961152000
H	5.361358000	-0.666215000	-2.218418000
C	6.544415000	1.444727000	0.806807000
H	4.527128000	2.155869000	0.929841000
C	7.454657000	0.626353000	0.128148000
H	7.727090000	-0.765943000	-1.496820000
H	6.878258000	2.046969000	1.647030000
H	8.493246000	0.589327000	0.443822000

(**1,2-J'**)

Ru	-1.243438000	-0.407513000	-0.755181000
O	-4.289590000	-0.394994000	1.412662000
O	-0.520638000	-2.105824000	2.766451000
N	-2.145247000	0.419976000	1.163420000
N	-3.140675000	1.936327000	-1.093398000
N	-1.502644000	2.213958000	-2.420126000
N	-2.293227000	3.326623000	-2.576739000
C	-1.988499000	1.331446000	-1.529547000
C	-3.283448000	3.133520000	-1.758862000
H	-4.112599000	3.812233000	-1.618347000
C	-0.250999000	2.147827000	-3.189385000
H	-0.528021000	2.134260000	-4.248646000

H	0.212161000	1.201447000	-2.921408000
C	0.679465000	3.316115000	-2.878364000
H	1.575634000	3.233955000	-3.501978000
H	0.982110000	3.287265000	-1.828574000
H	0.198775000	4.273935000	-3.094135000
C	-4.102844000	1.336857000	-0.183208000
H	-4.872163000	0.791193000	-0.737139000
H	-4.604453000	2.138348000	0.371763000
C	-3.531518000	0.364392000	0.848412000
C	-1.829826000	-0.064794000	2.567473000
H	-2.592138000	0.366726000	3.222305000
H	-0.870920000	0.388676000	2.816955000
C	-1.768559000	-1.529359000	2.806166000
C	-2.688269000	-2.461630000	3.197439000
H	-3.746972000	-2.288724000	3.323877000
C	-1.976040000	-3.686676000	3.398507000
H	-2.381637000	-4.635553000	3.720385000
C	-0.668808000	-3.412862000	3.125352000
H	0.238631000	-3.996790000	3.160287000
C	-2.600415000	-2.271355000	-1.334604000
C	-1.669901000	-2.662018000	-0.322300000
H	-2.053422000	-3.058693000	0.611798000
C	-0.275224000	-2.563597000	-0.503375000
H	0.388579000	-2.887367000	0.289099000
C	0.270563000	-2.029248000	-1.706147000
C	-0.639031000	-1.532695000	-2.670679000
H	-0.269599000	-1.083503000	-3.584045000
C	-2.051887000	-1.655426000	-2.480951000
H	-2.718258000	-1.277522000	-3.250872000
C	-4.075747000	-2.530752000	-1.182888000
H	-4.293584000	-3.584114000	-1.399798000
H	-4.661848000	-1.924977000	-1.881201000
H	-4.419667000	-2.323272000	-0.165275000
C	1.771506000	-2.054908000	-1.923674000
H	2.237125000	-1.936247000	-0.939307000
C	2.310753000	-0.937643000	-2.823872000
H	2.034391000	0.043236000	-2.428214000
H	1.954969000	-1.029136000	-3.857469000
H	3.403339000	-0.991098000	-2.852206000
C	2.156859000	-3.450938000	-2.468877000
H	1.824889000	-4.256075000	-1.804336000
H	3.245391000	-3.518477000	-2.564747000
H	1.718654000	-3.624850000	-3.458635000
C	1.116021000	0.791149000	0.800396000
O	0.296628000	0.920043000	-0.341995000
C	0.854268000	1.925565000	1.808731000

C	0.142540000	3.075013000	1.440015000
C	1.348008000	1.834873000	3.119991000
C	-0.083594000	4.103207000	2.362494000
H	-0.208302000	3.166743000	0.416690000
C	1.118845000	2.856045000	4.041965000
H	1.924109000	0.960743000	3.415521000
C	0.398953000	3.994886000	3.666595000
H	-0.625640000	4.994474000	2.056097000
H	1.505664000	2.766459000	5.053396000
H	0.225696000	4.792413000	4.383353000
C	2.570992000	0.819407000	0.381653000
H	2.847155000	1.674195000	-0.233714000
H	-1.735103000	1.353939000	1.052258000
C	3.477587000	-0.104129000	0.741885000
H	3.138081000	-0.926495000	1.375608000
C	4.905384000	-0.158981000	0.392396000
C	5.678114000	-1.232341000	0.870836000
C	5.542773000	0.809262000	-0.407312000
C	7.034123000	-1.340498000	0.564603000
H	5.206293000	-1.987987000	1.495555000
C	6.895942000	0.701704000	-0.714959000
H	4.978382000	1.656321000	-0.786618000
C	7.648954000	-0.373429000	-0.231580000
H	7.609734000	-2.177721000	0.949539000
H	7.368716000	1.461521000	-1.331301000
H	8.705327000	-0.452245000	-0.471702000
H	0.940906000	-0.166564000	1.318154000

Ketone hydrogenation
(**K'**)

Ru	2.044637000	-0.620931000	-0.472374000
O	0.751406000	-2.417429000	2.441721000
O	2.850055000	1.523727000	2.873920000
N	0.555800000	-0.469625000	1.197274000
N	-0.555203000	-2.039597000	-0.912346000
N	-0.106340000	-0.977376000	-2.699930000
N	-1.311650000	-1.596020000	-2.935414000
C	0.398421000	-1.222005000	-1.473072000
C	-1.560955000	-2.230445000	-1.829016000
H	-2.436146000	-2.838318000	-1.650525000
C	0.440133000	-0.104639000	-3.744500000
H	0.583941000	-0.716975000	-4.640310000
H	1.413448000	0.222982000	-3.378428000
C	-0.472149000	1.084979000	-4.036268000
H	-0.030929000	1.693993000	-4.831860000
H	-0.594720000	1.712199000	-3.147452000

H	-1.457441000	0.747082000	-4.368365000
C	-0.475970000	-2.632243000	0.416110000
H	-0.059414000	-3.642097000	0.365894000
H	-1.492561000	-2.705026000	0.818217000
C	0.355146000	-1.855266000	1.443347000
C	0.766158000	0.373182000	2.429058000
H	0.019809000	0.052049000	3.163056000
H	0.528749000	1.392630000	2.119151000
C	2.113211000	0.379274000	3.061002000
C	2.771688000	-0.453871000	3.921196000
H	2.418690000	-1.417291000	4.258171000
C	3.990151000	0.205986000	4.280188000
H	4.756272000	-0.153672000	4.952887000
C	3.982757000	1.400219000	3.621458000
H	4.657093000	2.242857000	3.595795000
C	3.518871000	-2.549540000	-0.671475000
C	3.818620000	-1.899831000	0.536526000
H	3.770134000	-2.452150000	1.470075000
C	4.201732000	-0.522400000	0.579894000
H	4.461660000	-0.087017000	1.537923000
C	4.265930000	0.266553000	-0.581471000
C	3.839120000	-0.348948000	-1.804870000
H	3.832273000	0.220678000	-2.726230000
C	3.469335000	-1.717699000	-1.837382000
H	3.167388000	-2.154428000	-2.785086000
C	3.237470000	-4.027606000	-0.746750000
H	2.909901000	-4.419517000	0.220869000
H	4.144065000	-4.575004000	-1.034777000
H	2.470213000	-4.254148000	-1.494467000
C	4.801261000	1.687516000	-0.518766000
H	4.598081000	2.051025000	0.495735000
C	4.141775000	2.659602000	-1.507779000
H	3.052444000	2.661959000	-1.398848000
H	4.386268000	2.414373000	-2.548349000
H	4.508928000	3.674794000	-1.324987000
C	6.333931000	1.657307000	-0.716783000
H	6.824287000	1.015899000	0.023171000
H	6.746130000	2.667180000	-0.618117000
H	6.595085000	1.284417000	-1.714342000
C	-2.909763000	1.274150000	0.213061000
O	-2.058095000	0.387899000	0.333786000
C	-2.517770000	2.690366000	-0.033516000
C	-1.167875000	2.991864000	-0.292224000
C	-3.457476000	3.736246000	-0.018092000
C	-0.768618000	4.303844000	-0.527233000
H	-0.440829000	2.186649000	-0.320662000

C	-3.054322000	5.050795000	-0.247043000
H	-4.504725000	3.533146000	0.178862000
C	-1.711456000	5.336803000	-0.502530000
H	0.275446000	4.524455000	-0.730509000
H	-3.787901000	5.851031000	-0.226870000
H	-1.400077000	6.361561000	-0.683764000
H	1.440627000	0.818005000	-0.824484000
C	-4.384856000	0.919769000	0.312413000
H	-4.905486000	1.314791000	-0.569956000
H	-0.258872000	-0.074286000	0.707648000
C	-4.662195000	-0.585037000	0.462100000
H	-4.139770000	-0.956218000	1.351140000
C	-6.144013000	-0.883973000	0.561674000
C	-6.913626000	-1.080570000	-0.593119000
C	-6.780950000	-0.939648000	1.808469000
C	-8.285234000	-1.323490000	-0.505884000
H	-6.434383000	-1.049279000	-1.570066000
C	-8.152616000	-1.181958000	1.900507000
H	-6.197380000	-0.798875000	2.716290000
C	-8.908803000	-1.373845000	0.742589000
H	-8.865243000	-1.478455000	-1.411548000
H	-8.628931000	-1.226595000	2.876055000
H	-9.975537000	-1.566514000	0.812626000
H	-4.229010000	-1.108823000	-0.398757000
H	-4.813183000	1.463975000	1.166199000

TS$^{K'L'}$

Ru	-0.989817000	-0.731634000	0.444080000
O	-3.169980000	-2.030950000	-2.293081000
O	-4.121744000	1.831707000	-0.491543000
N	-1.669303000	-0.383844000	-1.649013000
N	0.169139000	-2.786917000	-1.504898000
N	1.416414000	-2.708744000	0.213526000
N	1.964620000	-3.675216000	-0.590601000
C	0.300791000	-2.137072000	-0.304584000
C	1.190535000	-3.695529000	-1.632451000
H	1.323225000	-4.341014000	-2.488815000
C	2.064455000	-2.439760000	1.509536000
H	1.598649000	-3.087266000	2.262311000
H	1.827112000	-1.404443000	1.754519000
C	3.572867000	-2.666203000	1.478901000
H	3.977449000	-2.422900000	2.466700000
H	4.063548000	-2.024229000	0.741709000
H	3.815736000	-3.705852000	1.251847000
C	-0.863755000	-2.586768000	-2.515277000
H	-1.299901000	-3.551832000	-2.779712000

H	-0.398771000	-2.149549000	-3.408271000
C	-2.024421000	-1.677946000	-2.107745000
C	-2.639621000	0.710747000	-2.048555000
H	-2.777442000	0.603748000	-3.130348000
H	-2.100773000	1.641620000	-1.869917000
C	-3.975560000	0.806015000	-1.399246000
C	-5.180883000	0.185943000	-1.577491000
H	-5.369262000	-0.648942000	-2.235278000
C	-6.119095000	0.847989000	-0.723436000
H	-7.170718000	0.625169000	-0.609485000
C	-5.425225000	1.836739000	-0.092152000
H	-5.697502000	2.605568000	0.615125000
C	-2.704819000	-1.901176000	1.602008000
C	-3.137986000	-0.565478000	1.375629000
H	-4.056859000	-0.407630000	0.823049000
C	-2.417205000	0.557115000	1.845378000
H	-2.794084000	1.550919000	1.636926000
C	-1.209326000	0.394235000	2.573227000
C	-0.721583000	-0.928525000	2.740246000
H	0.200693000	-1.098746000	3.278771000
C	-1.452121000	-2.047764000	2.249171000
H	-1.046178000	-3.044636000	2.393340000
C	-3.536998000	-3.079603000	1.170175000
H	-4.343539000	-3.258727000	1.892397000
H	-2.936385000	-3.992160000	1.111192000
H	-3.997271000	-2.902977000	0.193150000
C	-0.543484000	1.605731000	3.202779000
H	-0.607111000	2.418709000	2.469148000
C	0.930399000	1.403022000	3.577997000
H	1.526202000	1.044714000	2.731404000
H	1.045829000	0.692240000	4.404778000
H	1.360541000	2.352216000	3.912659000
C	-1.363297000	2.030129000	4.444908000
H	-2.405854000	2.246234000	4.190313000
H	-0.928823000	2.933306000	4.885914000
H	-1.355157000	1.243942000	5.208636000
C	1.102570000	0.962373000	-1.199591000
O	0.804929000	0.349071000	-2.276929000
C	0.644832000	2.407547000	-1.058461000
C	0.093133000	3.041557000	-2.182043000
C	0.829723000	3.154784000	0.114964000
C	-0.287553000	4.382857000	-2.127307000
H	-0.000198000	2.474489000	-3.102428000
C	0.448981000	4.495418000	0.171183000
H	1.278883000	2.693109000	0.988195000
C	-0.116974000	5.111935000	-0.948438000

H	-0.702194000	4.863137000	-3.009154000
H	0.603110000	5.063767000	1.084407000
H	-0.407776000	6.157575000	-0.905848000
H	0.269721000	0.344306000	-0.181559000
C	2.462290000	0.622591000	-0.570410000
H	2.530412000	0.966487000	0.466560000
H	-0.732611000	-0.095764000	-2.047863000
C	3.616316000	1.245121000	-1.399241000
H	3.513758000	2.336107000	-1.401441000
C	4.969359000	0.849493000	-0.848963000
C	5.592030000	-0.336564000	-1.265395000
C	5.615424000	1.641522000	0.110450000
C	6.825281000	-0.722426000	-0.736208000
H	5.113553000	-0.953620000	-2.023570000
C	6.848678000	1.259804000	0.641651000
H	5.154689000	2.572985000	0.433583000
C	7.456510000	0.075038000	0.221160000
H	7.298190000	-1.638436000	-1.080003000
H	7.339335000	1.892279000	1.376574000
H	8.419626000	-0.219359000	0.628390000
H	3.510810000	0.908102000	-2.436328000
H	2.571965000	-0.463682000	-0.576014000

(**L'**)

Ru	-1.257884000	0.725450000	-0.517980000
O	-4.398882000	0.201374000	1.703325000
O	-2.058960000	-3.244129000	0.046020000
N	-2.126720000	-0.059483000	1.458035000
N	-1.911165000	2.836631000	1.565433000
N	-0.107286000	3.383889000	0.577777000
N	-0.308783000	4.350601000	1.531144000
C	-1.070558000	2.447143000	0.554620000
C	-1.410427000	3.993985000	2.119391000
H	-1.879009000	4.529851000	2.932544000
C	1.116362000	3.444674000	-0.239531000
H	0.973079000	4.224185000	-0.996556000
H	1.188975000	2.473124000	-0.726088000
C	2.355803000	3.728117000	0.603202000
H	3.234187000	3.734067000	-0.049561000
H	2.493771000	2.948833000	1.357698000
H	2.285547000	4.697618000	1.101267000
C	-3.177738000	2.208739000	1.916929000
H	-3.999779000	2.674879000	1.366222000
H	-3.361954000	2.380087000	2.983197000
C	-3.294332000	0.700367000	1.681533000
C	-2.266884000	-1.533381000	1.747779000

H	-2.825954000	-1.617441000	2.684824000
H	-1.250594000	-1.891419000	1.914220000
C	-2.906750000	-2.387440000	0.708834000
C	-4.195057000	-2.631842000	0.321694000
H	-5.071645000	-2.123194000	0.694738000
C	-4.142923000	-3.690859000	-0.640196000
H	-4.976166000	-4.152485000	-1.151487000
C	-2.826923000	-4.026937000	-0.763406000
H	-2.298133000	-4.777299000	-1.331677000
C	-2.667032000	1.630191000	-2.125741000
C	-3.060574000	0.302079000	-1.856527000
H	-4.062968000	0.101410000	-1.492618000
C	-2.198041000	-0.808433000	-2.139818000
H	-2.588426000	-1.810163000	-2.002305000
C	-0.881092000	-0.625208000	-2.573306000
C	-0.403148000	0.733230000	-2.617849000
H	0.633001000	0.933878000	-2.860105000
C	-1.290920000	1.826175000	-2.465366000
H	-0.911810000	2.836300000	-2.584522000
C	-3.626047000	2.787041000	-2.027939000
H	-4.032513000	3.017294000	-3.020768000
H	-3.135486000	3.692888000	-1.657896000
H	-4.472520000	2.551749000	-1.375724000
C	-0.032161000	-1.826324000	-2.977003000
H	-0.056682000	-2.530676000	-2.134795000
C	1.432086000	-1.489701000	-3.287379000
H	1.935667000	-0.998639000	-2.450238000
H	1.516977000	-0.844545000	-4.170391000
H	1.979759000	-2.411361000	-3.507271000
C	-0.680866000	-2.527771000	-4.193367000
H	-1.704281000	-2.853889000	-3.983185000
H	-0.095487000	-3.411670000	-4.467411000
H	-0.708145000	-1.860246000	-5.062369000
C	1.282711000	-0.724521000	0.568040000
O	0.388874000	0.370722000	0.688273000
C	1.321422000	-1.497152000	1.884327000
C	1.434217000	-0.807615000	3.102462000
C	1.261108000	-2.896823000	1.911323000
C	1.482826000	-1.500069000	4.312696000
H	1.485486000	0.277810000	3.093882000
C	1.312031000	-3.593712000	3.122547000
H	1.170380000	-3.447845000	0.977829000
C	1.421748000	-2.896864000	4.326515000
H	1.575230000	-0.951632000	5.246568000
H	1.264679000	-4.679250000	3.123184000
H	1.462085000	-3.436232000	5.268560000

C	2.680051000	-0.182509000	0.190071000
H	2.986274000	0.527449000	0.968495000
H	-1.258154000	0.282164000	1.891299000
C	3.785940000	-1.241846000	0.008362000
H	3.890470000	-1.814678000	0.936881000
H	3.485053000	-1.959039000	-0.767290000
C	5.115740000	-0.617214000	-0.362789000
C	5.495780000	-0.466815000	-1.703236000
C	5.981790000	-0.140554000	0.631639000
C	6.704078000	0.144548000	-2.043777000
H	4.844668000	-0.844755000	-2.489602000
C	7.190426000	0.471640000	0.297015000
H	5.709696000	-0.259209000	1.678575000
C	7.555110000	0.617559000	-1.043317000
H	6.984595000	0.243206000	-3.089180000
H	7.851427000	0.827252000	1.082945000
H	8.498660000	1.088100000	-1.305191000
H	0.950659000	-1.422750000	-0.217453000
H	2.579156000	0.399887000	-0.736362000

$TS^{L'1b'}$

Ru	1.156925000	-0.777034000	-0.547523000
O	3.845772000	-0.075645000	2.638710000
O	2.889966000	3.113542000	-0.373329000
N	1.973475000	0.110152000	1.300653000
N	1.683718000	-2.796536000	1.629946000
N	-0.104851000	-3.358829000	0.624110000
N	0.058347000	-4.285736000	1.622786000
C	0.877190000	-2.437537000	0.588442000
C	1.152186000	-3.917850000	2.221318000
H	1.592729000	-4.421866000	3.069547000
C	-1.314120000	-3.449324000	-0.209527000
H	-1.188088000	-4.300196000	-0.888404000
H	-1.343896000	-2.530812000	-0.795035000
C	-2.579423000	-3.610251000	0.628461000
H	-3.446450000	-3.645693000	-0.038468000
H	-2.703256000	-2.763961000	1.310004000
H	-2.550938000	-4.532729000	1.212420000
C	2.921718000	-2.130454000	2.014409000
H	3.730152000	-2.449712000	1.346087000
H	3.186170000	-2.455159000	3.022273000
C	2.929897000	-0.597465000	2.025203000
C	2.201308000	1.590496000	1.376635000
H	2.383711000	1.827783000	2.429594000
H	1.266312000	2.072964000	1.089379000
C	3.294373000	2.159253000	0.532683000

C	4.651689000	2.015477000	0.464580000
H	5.247625000	1.364925000	1.086957000
C	5.113160000	2.920021000	-0.546881000
H	6.134830000	3.082897000	-0.860946000
C	4.009025000	3.565358000	-1.015617000
H	3.851312000	4.350182000	-1.739761000
C	2.224595000	-1.976307000	-2.209307000
C	2.954455000	-0.795418000	-1.944011000
H	3.989693000	-0.861880000	-1.626140000
C	2.385794000	0.496761000	-2.179359000
H	3.011868000	1.369510000	-2.036981000
C	1.049079000	0.655812000	-2.567130000
C	0.259455000	-0.544008000	-2.657116000
H	-0.798930000	-0.473407000	-2.879387000
C	0.843580000	-1.823246000	-2.554722000
H	0.233528000	-2.705125000	-2.717914000
C	2.863881000	-3.343499000	-2.120963000
H	2.322614000	-4.064194000	-2.740869000
H	2.870830000	-3.729121000	-1.096345000
H	3.899374000	-3.308546000	-2.471875000
C	0.515110000	2.040155000	-2.919487000
H	0.831864000	2.717075000	-2.116334000
C	-1.011448000	2.116075000	-3.050224000
H	-1.525535000	1.762678000	-2.151489000
H	-1.373835000	1.533822000	-3.906238000
H	-1.313220000	3.154658000	-3.217144000
C	1.184692000	2.523808000	-4.227290000
H	2.275790000	2.550089000	-4.141366000
H	0.841282000	3.534932000	-4.469678000
H	0.925568000	1.869652000	-5.068002000
C	-1.298613000	0.919603000	0.772913000
O	-0.375850000	-0.187140000	0.859312000
C	-1.438700000	1.562870000	2.142028000
C	-1.712739000	0.780846000	3.274853000
C	-1.315712000	2.949877000	2.292923000
C	-1.858405000	1.375633000	4.527728000
H	-1.806511000	-0.297016000	3.173307000
C	-1.467913000	3.547974000	3.546373000
H	-1.106500000	3.570161000	1.423660000
C	-1.738054000	2.761437000	4.666630000
H	-2.069773000	0.759014000	5.397036000
H	-1.373020000	4.625567000	3.645539000
H	-1.854466000	3.223556000	5.642649000
C	-2.629239000	0.381448000	0.222022000
H	-2.996840000	-0.394208000	0.904358000
H	0.700020000	0.001494000	1.459365000

C	-3.725260000	1.448961000	0.027456000
H	-3.945768000	1.915052000	0.994527000
H	-3.349011000	2.248677000	-0.624462000
C	-4.989280000	0.860504000	-0.565913000
C	-5.223790000	0.898076000	-1.946884000
C	-5.937745000	0.233392000	0.254584000
C	-6.371202000	0.322590000	-2.496522000
H	-4.507901000	1.396908000	-2.597933000
C	-7.085622000	-0.344089000	-0.289740000
H	-5.780681000	0.207886000	1.331099000
C	-7.305252000	-0.302558000	-1.668528000
H	-6.540209000	0.371297000	-3.569000000
H	-7.813598000	-0.817680000	0.363450000
H	-8.202173000	-0.745072000	-2.092635000
H	-2.432068000	-0.113567000	-0.738843000
H	-0.903246000	1.672700000	0.074888000

Deprotonated alcohol pathway or neutral Pathway

Dehydrogenation of alcohols

(**E**)

Ru	-0.438175000	0.467512000	-0.603191000
O	-1.679398000	1.756406000	3.294406000
O	-3.294881000	-2.080422000	1.432884000
N	-1.017312000	0.585886000	1.420726000
N	0.482413000	2.972176000	0.749200000
N	2.024109000	2.319205000	-0.568065000
N	2.503440000	3.472325000	0.008731000
C	0.784658000	1.984734000	-0.146342000
C	1.542320000	3.838927000	0.808661000
H	1.570404000	4.712545000	1.443625000
C	2.872296000	1.568148000	-1.503832000
H	2.820742000	2.060256000	-2.483236000
H	2.419300000	0.577524000	-1.567711000
C	4.319648000	1.473294000	-1.027605000
H	4.897402000	0.906782000	-1.765426000
H	4.383041000	0.943834000	-0.072885000
H	4.768411000	2.463521000	-0.916942000
C	-0.759403000	3.030621000	1.520611000
H	-1.562751000	3.401782000	0.872897000
H	-0.619649000	3.741701000	2.335454000
C	-1.183343000	1.691058000	2.156543000
C	-1.408752000	-0.662882000	2.094540000
H	-1.058310000	-0.617682000	3.133141000

H	-0.898419000	-1.487885000	1.592966000
C	-2.882776000	-0.947040000	2.099413000
C	-3.968744000	-0.325669000	2.646964000
H	-3.926611000	0.579446000	3.234216000
C	-5.116951000	-1.110608000	2.297707000
H	-6.147165000	-0.921660000	2.567934000
C	-4.653390000	-2.161564000	1.567117000
H	-5.119873000	-3.019785000	1.107391000
C	-1.500460000	1.639741000	-2.272356000
C	-2.491444000	1.008778000	-1.487004000
H	-3.244192000	1.606730000	-0.984145000
C	-2.536568000	-0.417716000	-1.364187000
H	-3.312821000	-0.864417000	-0.752966000
C	-1.563768000	-1.237701000	-1.946453000
C	-0.506228000	-0.582065000	-2.674986000
H	0.310147000	-1.174255000	-3.072395000
C	-0.504263000	0.803995000	-2.887472000
H	0.288907000	1.259632000	-3.472051000
C	-1.512861000	3.126537000	-2.519347000
H	-1.989779000	3.347480000	-3.483340000
H	-0.498973000	3.538417000	-2.551729000
H	-2.075305000	3.654703000	-1.743497000
C	-1.638478000	-2.750536000	-1.807372000
H	-2.196008000	-2.947016000	-0.883754000
C	-0.261798000	-3.422436000	-1.674655000
H	0.345947000	-2.924665000	-0.912902000
H	0.289947000	-3.403432000	-2.623696000
H	-0.390057000	-4.475558000	-1.400356000
C	-2.441802000	-3.348405000	-2.981899000
H	-3.450842000	-2.924305000	-3.039689000
H	-2.534819000	-4.434441000	-2.864349000
H	-1.940462000	-3.157393000	-3.939143000
C	1.801728000	-0.706029000	1.151086000
O	1.093910000	-0.807578000	-0.042188000
C	3.111999000	-1.488507000	1.100463000
C	3.486246000	-2.226418000	-0.026713000
C	3.972074000	-1.475213000	2.208935000
C	4.690430000	-2.936878000	-0.047176000
H	2.818311000	-2.235717000	-0.881099000
C	5.174761000	-2.180714000	2.191198000
H	3.693132000	-0.907243000	3.095451000
C	5.539530000	-2.916889000	1.059543000
H	4.964109000	-3.508882000	-0.931085000
H	5.828360000	-2.157595000	3.060029000
H	6.475838000	-3.469052000	1.044314000
H	2.051993000	0.340092000	1.409591000

H	1.226205000	-1.079761000	2.018515000

(**A**)

Ru	-0.600928000	-0.539998000	-0.407119000
O	1.215067000	-1.850799000	3.263445000
O	3.617565000	-1.240870000	-0.511338000
N	0.653636000	-0.825856000	1.275120000
N	-2.119235000	-1.282120000	2.086914000
N	-3.338358000	-0.021046000	0.882157000
N	-4.100526000	-0.308921000	1.988842000
C	-2.120200000	-0.606915000	0.901299000
C	-3.325700000	-1.074675000	2.704140000
H	-3.589919000	-1.491834000	3.664916000
C	-3.868986000	0.838478000	-0.187088000
H	-4.245646000	0.191801000	-0.989776000
H	-3.006095000	1.396503000	-0.557159000
C	-4.976720000	1.766781000	0.298073000
H	-5.302442000	2.388659000	-0.542615000
H	-4.622256000	2.427055000	1.094758000
H	-5.837709000	1.209193000	0.674163000
C	-1.017991000	-2.113779000	2.567628000
H	-1.070962000	-3.089054000	2.068877000
H	-1.154745000	-2.271851000	3.638041000
C	0.398049000	-1.541093000	2.378148000
C	2.060543000	-0.383722000	1.174660000
H	2.379341000	-0.023728000	2.158767000
H	2.108666000	0.453898000	0.479141000
C	3.021047000	-1.442105000	0.715072000
C	3.466426000	-2.621721000	1.242127000
H	3.165307000	-3.018221000	2.200026000
C	4.381305000	-3.184456000	0.291497000
H	4.931589000	-4.111526000	0.380161000
C	4.437975000	-2.307312000	-0.748257000
H	4.991703000	-2.277122000	-1.674583000
C	-0.677299000	-2.625632000	-1.468191000
C	0.632168000	-2.098562000	-1.575253000
H	1.459043000	-2.654935000	-1.146821000
C	0.907336000	-0.870914000	-2.246645000
H	1.931354000	-0.521526000	-2.299247000
C	-0.144635000	-0.083770000	-2.760419000
C	-1.480701000	-0.543158000	-2.582750000
H	-2.314078000	0.051006000	-2.934594000
C	-1.730162000	-1.775020000	-1.919789000
H	-2.759074000	-2.098084000	-1.783338000
C	-0.943654000	-3.996206000	-0.900963000
H	-0.943102000	-4.752573000	-1.697430000

H	-1.919724000	-4.043520000	-0.405822000
H	-0.173345000	-4.280800000	-0.177377000
C	0.171662000	1.212767000	-3.487705000
H	1.101822000	1.594931000	-3.048625000
C	-0.901663000	2.299097000	-3.321980000
H	-1.113693000	2.463813000	-2.261607000
H	-1.832478000	2.033629000	-3.839348000
H	-0.547380000	3.237548000	-3.763510000
C	0.442702000	0.910907000	-4.977479000
H	1.249198000	0.179975000	-5.102584000
H	0.730474000	1.829246000	-5.502094000
H	-0.454555000	0.511475000	-5.466003000
C	-0.342545000	2.173669000	1.100292000
O	-0.674228000	1.516313000	-0.093544000
C	1.034373000	2.845758000	1.053642000
C	1.580527000	3.290255000	-0.156021000
C	1.755050000	3.075849000	2.233529000
C	2.814833000	3.943558000	-0.187913000
H	1.027148000	3.109828000	-1.071764000
C	2.989358000	3.727311000	2.207850000
H	1.348665000	2.730726000	3.182850000
C	3.525300000	4.163990000	0.993944000
H	3.224268000	4.280261000	-1.137878000
H	3.536454000	3.886680000	3.134002000
H	4.488536000	4.667272000	0.969748000
H	-0.332056000	1.473261000	1.949265000
C	-1.408801000	3.251403000	1.396282000
H	-2.388067000	2.785872000	1.550814000
H	-1.157100000	3.830327000	2.292936000
H	-1.481770000	3.945474000	0.550853000

(**TS**$^{\mathbf{EF}}$)

Ru	0.307269000	-0.533382000	0.523771000
O	0.695254000	3.701330000	1.124839000
O	3.690540000	1.387820000	-1.431876000
N	0.623255000	1.552759000	0.286111000
N	-1.566781000	1.142080000	2.137585000
N	-2.646031000	-0.567094000	1.466404000
N	-3.540555000	0.155536000	2.219480000
C	-1.419000000	0.000170000	1.397438000
C	-2.853370000	1.192011000	2.606123000
H	-3.242334000	1.996107000	3.213697000
C	-3.066407000	-1.841867000	0.862169000
H	-2.777634000	-2.652197000	1.543296000
H	-2.499267000	-1.955072000	-0.064805000
C	-4.567222000	-1.895120000	0.596366000

H	-4.799442000	-2.850387000	0.113552000
H	-4.873723000	-1.086542000	-0.071971000
H	-5.143962000	-1.820218000	1.521144000
C	-0.495448000	2.101557000	2.403011000
H	0.175031000	1.680173000	3.162798000
H	-0.944623000	3.009382000	2.807322000
C	0.331245000	2.512957000	1.172303000
C	1.395723000	2.032640000	-0.871131000
H	1.002718000	3.014788000	-1.164149000
H	1.243998000	1.339423000	-1.702952000
C	2.873375000	2.164305000	-0.641514000
C	3.639876000	2.910963000	0.206785000
H	3.250585000	3.617810000	0.924323000
C	5.007175000	2.575222000	-0.066661000
H	5.889448000	2.978983000	0.411449000
C	4.982031000	1.653074000	-1.068089000
H	5.743310000	1.125412000	-1.622470000
C	1.091501000	-1.901846000	2.304641000
C	2.161863000	-1.083685000	1.896712000
H	2.658512000	-0.438430000	2.614126000
C	2.615320000	-1.096757000	0.540281000
H	3.441898000	-0.451051000	0.266804000
C	2.031844000	-1.921349000	-0.439732000
C	0.863113000	-2.657851000	-0.044636000
H	0.300987000	-3.213268000	-0.786049000
C	0.431121000	-2.682105000	1.299848000
H	-0.421024000	-3.294240000	1.574974000
C	0.629797000	-1.942364000	3.744420000
H	1.484937000	-1.944503000	4.428253000
H	0.038041000	-2.841706000	3.941167000
H	0.007802000	-1.075922000	3.993500000
C	2.635701000	-2.001997000	-1.840174000
H	2.753669000	-0.971107000	-2.196338000
C	1.775281000	-2.773295000	-2.852183000
H	0.740637000	-2.417943000	-2.895626000
H	1.749764000	-3.844174000	-2.610071000
H	2.216808000	-2.679893000	-3.850605000
C	4.047689000	-2.624070000	-1.762388000
H	4.712921000	-2.049469000	-1.109018000
H	4.500419000	-2.656697000	-2.760033000
H	4.002048000	-3.651468000	-1.380162000
C	-1.244498000	-0.628747000	-2.233773000
O	-1.461045000	-1.857402000	-2.355764000
C	-2.395125000	0.355387000	-2.195698000
C	-3.687023000	-0.113543000	-2.463884000
C	-2.191225000	1.726056000	-1.991525000

C	-4.762313000	0.774345000	-2.519610000
H	-3.819179000	-1.175156000	-2.648011000
C	-3.266321000	2.613318000	-2.039816000
H	-1.192242000	2.095515000	-1.782165000
C	-4.554998000	2.139169000	-2.302905000
H	-5.760176000	0.404264000	-2.742072000
H	-3.098402000	3.674736000	-1.876516000
H	-5.391433000	2.831927000	-2.347853000
H	-0.691117000	-0.396439000	-0.915018000
H	-0.324266000	-0.190254000	-2.679376000

(**F**)

Ru	-1.386320000	-0.636917000	-0.109095000
O	1.716461000	1.752112000	-1.911240000
O	-1.629276000	3.643671000	0.530965000
N	0.052910000	0.863354000	-0.574639000
N	0.836705000	-1.623405000	-1.829604000
N	0.438474000	-3.141581000	-0.394110000
N	1.470652000	-3.630844000	-1.161904000
C	0.015079000	-1.911661000	-0.769183000
C	1.689288000	-2.678525000	-2.023436000
H	2.442244000	-2.710170000	-2.797627000
C	0.000505000	-3.916749000	0.767052000
H	-0.393825000	-4.873057000	0.404576000
H	-0.815639000	-3.342783000	1.208454000
C	1.131602000	-4.133627000	1.771607000
H	0.743912000	-4.671779000	2.644008000
H	1.554256000	-3.179222000	2.100380000
H	1.933928000	-4.729725000	1.327413000
C	0.797215000	-0.355059000	-2.555648000
H	-0.125509000	-0.314930000	-3.146380000
H	1.653053000	-0.318828000	-3.230647000
C	0.885434000	0.865253000	-1.617699000
C	0.204878000	2.024380000	0.320549000
H	1.272609000	2.250487000	0.427792000
H	-0.189733000	1.750274000	1.300629000
C	-0.489958000	3.268682000	-0.147440000
C	-0.243189000	4.166495000	-1.145823000
H	0.586829000	4.107612000	-1.834061000
C	-1.284819000	5.150449000	-1.087968000
H	-1.406259000	6.015695000	-1.725620000
C	-2.093975000	4.788465000	-0.055408000
H	-2.982502000	5.214077000	0.386060000
C	-3.291250000	-1.284878000	-1.510886000
C	-3.289237000	0.111776000	-1.453410000
H	-3.288096000	0.694358000	-2.369427000

C	-3.264627000	0.795645000	-0.193258000
H	-3.221848000	1.879162000	-0.189632000
C	-3.308002000	0.112337000	1.035531000
C	-3.231383000	-1.322541000	0.977915000
H	-3.216949000	-1.902204000	1.893726000
C	-3.205277000	-1.997077000	-0.264577000
H	-3.161604000	-3.082189000	-0.277763000
C	-3.368691000	-2.036594000	-2.815068000
H	-4.379095000	-2.438549000	-2.968478000
H	-2.675440000	-2.884526000	-2.830112000
H	-3.135947000	-1.387113000	-3.664448000
C	-3.457521000	0.880463000	2.340164000
H	-3.066581000	1.887977000	2.152676000
C	-2.670634000	0.285166000	3.517816000
H	-1.613278000	0.160567000	3.265420000
H	-3.065893000	-0.692053000	3.821786000
H	-2.745927000	0.947440000	4.387619000
C	-4.954942000	1.012526000	2.693583000
H	-5.516914000	1.492985000	1.884987000
H	-5.082535000	1.613643000	3.601336000
H	-5.404073000	0.028344000	2.876880000
H	-0.518378000	-0.773235000	1.218908000
C	3.343512000	-0.490379000	1.245059000
O	3.258494000	-1.333578000	2.124519000
C	4.590139000	0.221324000	0.888022000
C	4.582736000	1.160071000	-0.155429000
C	5.777886000	-0.046073000	1.589141000
C	5.762494000	1.827154000	-0.490632000
H	3.664080000	1.368510000	-0.703229000
C	6.949110000	0.622056000	1.250466000
H	5.753067000	-0.777939000	2.391009000
C	6.940931000	1.559941000	0.209495000
H	5.759902000	2.555102000	-1.297190000
H	7.869630000	0.418765000	1.791281000
H	7.857588000	2.081978000	-0.053673000
H	2.452564000	-0.208739000	0.648188000

(**B**)

Ru	-2.058973000	-0.401723000	-0.149778000
O	2.151227000	0.460746000	-0.028701000
O	-0.999683000	3.621995000	0.979820000
N	-0.122327000	0.329178000	0.349894000
N	0.128884000	-2.360031000	-0.627034000
N	-1.497042000	-3.433755000	0.223782000
N	-0.496923000	-4.365690000	0.055613000
C	-1.154094000	-2.185784000	-0.174350000

C	0.477918000	-3.675084000	-0.464022000
H	1.440133000	-4.081870000	-0.739868000
C	-2.726312000	-3.848123000	0.895338000
H	-3.094636000	-4.741939000	0.381661000
H	-3.438796000	-3.034912000	0.750087000
C	-2.504305000	-4.122844000	2.382178000
H	-3.442232000	-4.452071000	2.842779000
H	-2.165503000	-3.215718000	2.892558000
H	-1.755233000	-4.907539000	2.523191000
C	0.954496000	-1.272155000	-1.148383000
H	0.557353000	-0.963159000	-2.122666000
H	1.968214000	-1.649689000	-1.287240000
C	1.027227000	-0.063058000	-0.196853000
C	0.015124000	1.415684000	1.335368000
H	0.931561000	1.244423000	1.912912000
H	-0.836948000	1.365257000	2.016151000
C	0.078299000	2.795526000	0.749926000
C	1.008041000	3.462331000	0.004866000
H	1.952271000	3.047447000	-0.315200000
C	0.479884000	4.771858000	-0.244911000
H	0.949715000	5.574076000	-0.797753000
C	-0.734117000	4.816681000	0.369003000
H	-1.489284000	5.579810000	0.482614000
C	-3.012893000	-0.303445000	-2.407354000
C	-2.530639000	0.975398000	-2.116173000
H	-1.826512000	1.456947000	-2.787595000
C	-2.936234000	1.665526000	-0.926222000
H	-2.517645000	2.644519000	-0.722591000
C	-3.865569000	1.120781000	-0.023231000
C	-4.301658000	-0.225668000	-0.276038000
H	-4.990806000	-0.710526000	0.405743000
C	-3.864766000	-0.921434000	-1.426706000
H	-4.220521000	-1.932883000	-1.600903000
C	-2.650277000	-1.034691000	-3.674347000
H	-3.491324000	-1.026967000	-4.380369000
H	-2.403128000	-2.082703000	-3.472749000
H	-1.793838000	-0.569198000	-4.171609000
C	-4.395830000	1.955948000	1.132187000
H	-3.637896000	2.722841000	1.333064000
C	-4.619677000	1.168456000	2.432074000
H	-3.710987000	0.639977000	2.735352000
H	-5.426457000	0.431794000	2.331106000
H	-4.908847000	1.854389000	3.236221000
C	-5.692333000	2.672781000	0.696200000
H	-5.529462000	3.288846000	-0.194972000
H	-6.057800000	3.323895000	1.498649000

H	-6.483739000	1.948830000	0.464800000
H	-2.120464000	-0.749163000	1.404525000
C	5.944355000	-0.490775000	1.789125000
O	6.781114000	-0.596487000	2.675826000
C	6.352027000	-0.080718000	0.403463000
C	5.421881000	0.175334000	-0.617008000
C	7.724544000	0.051788000	0.135121000
C	5.869567000	0.555202000	-1.884623000
H	4.352927000	0.105929000	-0.432112000
C	8.165022000	0.425212000	-1.130647000
H	8.424393000	-0.144620000	0.941090000
C	7.235473000	0.677799000	-2.145364000
H	5.145209000	0.762150000	-2.668381000
H	9.229236000	0.522310000	-1.329819000
H	7.577090000	0.973204000	-3.134498000
C	4.484553000	-0.803612000	2.063085000
H	3.810235000	-0.007312000	1.732482000
H	4.187956000	-1.704402000	1.509456000
H	4.362936000	-0.987566000	3.132571000

(**D**)

Ru	0.407464000	-0.379281000	-0.109518000
O	-0.285218000	3.829747000	0.351882000
O	-3.612306000	0.734689000	1.017405000
N	-0.247868000	1.528279000	0.562057000
N	2.490712000	1.741387000	-0.243778000
N	3.430359000	-0.010290000	0.510656000
N	4.414357000	0.953611000	0.506294000
C	2.229751000	0.431819000	0.067191000
C	3.803872000	2.006956000	0.040917000
H	4.269125000	2.970364000	-0.109606000
C	3.737747000	-1.318500000	1.081461000
H	4.654998000	-1.677540000	0.603659000
H	2.909749000	-1.971085000	0.800219000
C	3.897550000	-1.259292000	2.600191000
H	4.150590000	-2.252738000	2.986821000
H	2.965140000	-0.929747000	3.069402000
H	4.696580000	-0.565493000	2.877851000
C	1.475589000	2.665299000	-0.748336000
H	1.217285000	2.376390000	-1.774049000
H	1.900440000	3.669633000	-0.762055000
C	0.208283000	2.709255000	0.129382000
C	-1.376635000	1.630943000	1.499734000
H	-1.210326000	2.504532000	2.142353000
H	-1.385368000	0.735300000	2.124891000
C	-2.723536000	1.774285000	0.853040000

C	-3.304901000	2.750351000	0.095490000
H	-2.826404000	3.678915000	-0.178734000
C	-4.623526000	2.291986000	-0.232812000
H	-5.372278000	2.810686000	-0.816368000
C	-4.759490000	1.070008000	0.351838000
H	-5.563015000	0.351280000	0.410000000
C	0.409343000	-1.054549000	-2.461536000
C	-0.852845000	-0.517012000	-2.192141000
H	-1.238590000	0.296591000	-2.798397000
C	-1.646927000	-1.007152000	-1.103395000
H	-2.608085000	-0.544735000	-0.909477000
C	-1.227349000	-2.075671000	-0.291015000
C	0.100270000	-2.578776000	-0.516516000
H	0.491612000	-3.376508000	0.103985000
C	0.899505000	-2.064853000	-1.562768000
H	1.894474000	-2.471670000	-1.718726000
C	1.247239000	-0.600544000	-3.629349000
H	1.216810000	-1.342258000	-4.438676000
H	2.296835000	-0.474317000	-3.342182000
H	0.885312000	0.349175000	-4.035033000
C	-2.170865000	-2.672140000	0.742947000
H	-2.858047000	-1.869295000	1.035435000
C	-1.474108000	-3.178078000	2.014935000
H	-0.850713000	-2.397252000	2.461152000
H	-0.840576000	-4.051256000	1.814473000
H	-2.224372000	-3.487402000	2.751264000
C	-3.004987000	-3.796878000	0.091764000
H	-3.561230000	-3.429876000	-0.777821000
H	-3.725662000	-4.204963000	0.810045000
H	-2.362405000	-4.620686000	-0.243711000
H	0.653110000	-0.638845000	1.445056000

1,4-TS^{IJ}

Ru	-1.057836000	0.323651000	0.704185000
O	1.017107000	-3.451883000	0.540677000
O	-3.101567000	-3.214197000	-0.965937000
N	-0.304590000	-1.591466000	0.209132000
N	1.493699000	-0.321885000	2.160853000
N	1.363469000	1.794386000	1.994504000
N	2.540182000	1.554646000	2.665353000
C	0.682340000	0.663664000	1.667541000
C	2.589245000	0.256493000	2.742514000
H	3.394315000	-0.303586000	3.195185000
C	0.953497000	3.186339000	1.766930000
H	0.247062000	3.471930000	2.555286000
H	0.422535000	3.204250000	0.814133000

C	2.131629000	4.154605000	1.761846000
H	1.757406000	5.156239000	1.526097000
H	2.869096000	3.877591000	1.004656000
H	2.631976000	4.183192000	2.732142000
C	1.190664000	-1.750946000	2.159658000
H	0.486519000	-1.958448000	2.975650000
H	2.117969000	-2.289090000	2.357559000
C	0.618543000	-2.314950000	0.852984000
C	-0.832719000	-2.273290000	-0.992730000
H	0.018504000	-2.617881000	-1.589285000
H	-1.369028000	-1.533410000	-1.589881000
C	-1.757393000	-3.426438000	-0.723462000
C	-1.582390000	-4.713053000	-0.300124000
H	-0.630721000	-5.144878000	-0.033039000
C	-2.877105000	-5.328862000	-0.274212000
H	-3.113078000	-6.346277000	0.007405000
C	-3.759797000	-4.380335000	-0.687324000
H	-4.827497000	-4.366598000	-0.847366000
C	-2.363712000	1.166683000	2.465146000
C	-2.819177000	-0.150556000	2.208889000
H	-2.807670000	-0.893644000	2.998986000
C	-3.279366000	-0.503210000	0.914745000
H	-3.589435000	-1.525947000	0.729459000
C	-3.338817000	0.424287000	-0.151178000
C	-2.798274000	1.723301000	0.102354000
H	-2.763628000	2.459724000	-0.692402000
C	-2.370479000	2.109660000	1.395458000
H	-2.034715000	3.126032000	1.566864000
C	-1.949018000	1.569874000	3.858416000
H	-2.823867000	1.916241000	4.423911000
H	-1.220058000	2.384718000	3.849854000
H	-1.513866000	0.726194000	4.402625000
C	-4.064449000	0.045929000	-1.435310000
H	-4.008693000	-1.044332000	-1.516267000
C	-3.469673000	0.634839000	-2.720721000
H	-2.419476000	0.351973000	-2.842673000
H	-3.541531000	1.729178000	-2.744694000
H	-4.020042000	0.258324000	-3.590046000
C	-5.555042000	0.432190000	-1.305236000
H	-6.013071000	-0.029330000	-0.423378000
H	-6.113795000	0.103894000	-2.189466000
H	-5.674678000	1.519357000	-1.215830000
C	2.518708000	-0.848081000	-1.739072000
O	1.787374000	-1.559919000	-2.445602000
C	3.819298000	-1.411447000	-1.226500000
C	4.949811000	-0.618858000	-0.973136000

C	3.898686000	-2.796969000	-1.013447000
C	6.135989000	-1.197773000	-0.519376000
H	4.917044000	0.450803000	-1.160841000
C	5.077722000	-3.371006000	-0.541138000
H	3.015000000	-3.398289000	-1.193711000
C	6.200795000	-2.575132000	-0.296675000
H	7.009655000	-0.574644000	-0.344515000
H	5.121253000	-4.442609000	-0.363913000
H	7.122651000	-3.026065000	0.062571000
C	2.170788000	0.512709000	-1.377853000
C	0.922047000	1.044618000	-1.693282000
C	0.723850000	2.516897000	-1.903300000
C	-0.500480000	2.990984000	-2.401803000
C	1.751742000	3.453441000	-1.704866000
C	-0.705240000	4.345458000	-2.664309000
H	-1.292769000	2.279068000	-2.603275000
C	1.550003000	4.811302000	-1.957586000
H	2.730431000	3.115060000	-1.382181000
C	0.318531000	5.266822000	-2.432728000
H	-1.659975000	4.679815000	-3.062980000
H	2.366279000	5.511969000	-1.801382000
H	0.166118000	6.322448000	-2.640698000
H	0.354266000	0.418492000	-2.383618000
H	2.868580000	1.079926000	-0.770674000
H	0.008541000	0.791065000	-0.613115000

(**J**)

Ru	0.821998000	0.844612000	0.452601000
O	2.081704000	-0.726682000	-3.360385000
O	2.814276000	-3.162262000	0.320243000
N	1.262507000	-0.383503000	-1.234705000
N	0.825873000	2.402371000	-2.110495000
N	-0.389272000	3.465065000	-0.728566000
N	-0.357333000	4.248011000	-1.858183000
C	0.318225000	2.309990000	-0.840211000
C	0.389399000	3.570492000	-2.676999000
H	0.644177000	3.881240000	-3.679860000
C	-1.237954000	3.924859000	0.368931000
H	-0.789549000	4.834197000	0.788318000
H	-1.201091000	3.143018000	1.125340000
C	-2.669857000	4.195028000	-0.092203000
H	-3.291803000	4.454395000	0.771717000
H	-3.079671000	3.307100000	-0.580431000
H	-2.695893000	5.024225000	-0.803646000
C	1.806439000	1.512418000	-2.724279000
H	2.811442000	1.832949000	-2.418085000

H	1.734274000	1.631737000	-3.806170000
C	1.684778000	0.013037000	-2.440952000
C	1.295658000	-1.851183000	-1.082486000
H	0.876830000	-2.302463000	-1.988276000
H	0.656567000	-2.132483000	-0.244286000
C	2.659641000	-2.436051000	-0.842283000
C	3.836958000	-2.445384000	-1.535133000
H	3.987554000	-1.970954000	-2.492692000
C	4.772214000	-3.208120000	-0.759791000
H	5.801901000	-3.428639000	-1.007294000
C	4.102193000	-3.622252000	0.349835000
H	4.364834000	-4.228353000	1.203709000
C	2.278607000	2.364718000	1.555575000
C	3.066389000	1.257326000	1.177842000
H	3.923905000	1.395090000	0.527797000
C	2.729113000	-0.048705000	1.624427000
H	3.343604000	-0.881289000	1.299302000
C	1.645268000	-0.296344000	2.492799000
C	0.817444000	0.824730000	2.805443000
H	-0.055016000	0.683259000	3.433004000
C	1.140285000	2.132978000	2.389699000
H	0.528253000	2.968354000	2.712279000
C	2.660260000	3.765939000	1.149982000
H	3.211741000	4.256533000	1.962522000
H	1.779670000	4.376827000	0.931439000
H	3.302962000	3.762936000	0.264667000
C	1.464460000	-1.674315000	3.115555000
H	1.777075000	-2.405983000	2.362819000
C	0.024054000	-2.008275000	3.526926000
H	-0.674149000	-1.912166000	2.690422000
H	-0.328884000	-1.366198000	4.344099000
H	-0.025786000	-3.041354000	3.888185000
C	2.414046000	-1.816393000	4.326484000
H	3.457772000	-1.647125000	4.039790000
H	2.338583000	-2.822488000	4.755647000
H	2.159739000	-1.094671000	5.113031000
C	-1.732023000	0.016077000	-1.103645000
O	-2.113658000	1.058755000	-1.645046000
C	-1.838053000	-1.260937000	-1.895915000
C	-1.760806000	-1.184564000	-3.295779000
C	-2.096552000	-2.504409000	-1.300068000
C	-1.897875000	-2.327080000	-4.078840000
H	-1.585786000	-0.215887000	-3.751763000
C	-2.261044000	-3.646491000	-2.086160000
H	-2.201683000	-2.579246000	-0.222456000
C	-2.150220000	-3.563023000	-3.474928000

H	-1.810083000	-2.256982000	-5.159735000
H	-2.475093000	-4.600937000	-1.612260000
H	-2.263189000	-4.455214000	-4.085500000
C	-1.228183000	0.007299000	0.312659000
C	-2.283916000	0.651109000	1.250295000
C	-3.531148000	-0.197908000	1.454054000
C	-4.569989000	-0.200043000	0.508606000
C	-3.675244000	-1.004561000	2.592261000
C	-5.706806000	-0.987880000	0.693582000
H	-4.483118000	0.421099000	-0.378515000
C	-4.811535000	-1.794545000	2.781645000
H	-2.892020000	-1.004930000	3.347316000
C	-5.832549000	-1.790045000	1.830317000
H	-6.498489000	-0.971685000	-0.051284000
H	-4.900522000	-2.407628000	3.675285000
H	-6.719683000	-2.401083000	1.974993000
H	-1.845287000	0.855238000	2.232087000
H	-1.048339000	-1.020383000	0.640950000
H	-2.584731000	1.609972000	0.824777000

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Ru	0.690744000	-0.621405000	0.858211000
O	1.063950000	-3.305095000	-2.489419000
O	-2.831181000	-3.051444000	-0.351020000
N	0.376523000	-1.826980000	-0.860434000
N	3.252825000	-1.329675000	-0.547272000
N	3.515551000	0.605081000	0.292563000
N	4.713927000	0.304155000	-0.308760000
C	2.590285000	-0.377330000	0.180076000
C	4.516936000	-0.877422000	-0.816508000
H	5.247525000	-1.434501000	-1.384662000
C	3.377833000	1.881336000	1.009676000
H	3.616739000	1.698457000	2.064468000
H	2.329908000	2.180723000	0.929514000
C	4.289240000	2.968616000	0.449667000
H	4.094681000	3.897104000	0.997142000
H	4.080944000	3.142660000	-0.609072000
H	5.345219000	2.710837000	0.559070000
C	2.702214000	-2.627946000	-0.918533000
H	2.716774000	-3.282634000	-0.037648000
H	3.346977000	-3.064319000	-1.682060000
C	1.280452000	-2.584389000	-1.498809000
C	-0.969902000	-1.914124000	-1.462536000
H	-0.874400000	-1.819616000	-2.552292000
H	-1.562186000	-1.076237000	-1.093034000

C	-1.728943000	-3.177954000	-1.170724000
C	-1.601994000	-4.483027000	-1.553081000
H	-0.824817000	-4.860936000	-2.199403000
C	-2.674645000	-5.205468000	-0.933221000
H	-2.888303000	-6.262298000	-1.019380000
C	-3.388599000	-4.292523000	-0.219528000
H	-4.279397000	-4.344482000	0.388197000
C	0.006337000	-2.360089000	2.338363000
C	-1.124669000	-1.546382000	1.995634000
H	-1.975451000	-2.004983000	1.506239000
C	-1.119417000	-0.163163000	2.223953000
H	-1.973082000	0.424434000	1.904732000
C	-0.015602000	0.493842000	2.874194000
C	1.111432000	-0.302806000	3.150902000
H	1.991290000	0.147053000	3.595511000
C	1.126774000	-1.713087000	2.889799000
H	2.015209000	-2.286759000	3.137016000
C	-0.010600000	-3.849550000	2.092143000
H	-1.009093000	-4.191956000	1.809226000
H	0.298927000	-4.394683000	2.991309000
H	0.667096000	-4.125254000	1.278025000
C	-0.135947000	1.967482000	3.240771000
H	-0.242093000	2.514151000	2.293118000
C	1.085454000	2.533043000	3.977221000
H	2.001956000	2.448283000	3.387760000
H	1.247107000	2.032644000	4.941167000
H	0.928671000	3.597486000	4.181003000
C	-1.402315000	2.206807000	4.092630000
H	-2.317084000	1.888002000	3.583440000
H	-1.503914000	3.275397000	4.312603000
H	-1.344479000	1.670480000	5.048437000
C	0.061457000	2.088055000	-0.682038000
O	0.320192000	2.926341000	0.225288000
C	0.971811000	2.070141000	-1.915658000
C	1.715169000	3.229488000	-2.173830000
C	1.033951000	1.008171000	-2.827225000
C	2.502446000	3.327603000	-3.322452000
H	1.651046000	4.048497000	-1.465138000
C	1.827157000	1.102144000	-3.971563000
H	0.488131000	0.092463000	-2.629648000
C	2.562114000	2.263330000	-4.224716000
H	3.065223000	4.237737000	-3.515341000
H	1.870184000	0.265678000	-4.664453000
H	3.175336000	2.337813000	-5.119111000
H	0.392932000	0.776642000	-0.162776000
C	-1.382981000	1.771861000	-0.999154000

C	-2.383881000	2.448758000	-0.410186000
H	-1.567887000	1.031376000	-1.770846000
H	-2.090469000	3.209574000	0.312047000
C	-3.825403000	2.306636000	-0.645585000
C	-4.383718000	1.301759000	-1.460482000
C	-4.704648000	3.214285000	-0.025825000
C	-5.759946000	1.216823000	-1.649425000
H	-3.735780000	0.578545000	-1.947172000
C	-6.083340000	3.130826000	-0.214991000
H	-4.292623000	3.997027000	0.607044000
C	-6.617935000	2.130980000	-1.028992000
H	-6.167047000	0.432277000	-2.281955000
H	-6.739458000	3.846963000	0.272935000
H	-7.691983000	2.061341000	-1.178587000

(**1,2-J**)

Ru	-1.255802000	0.507921000	-0.741513000
O	-4.219278000	0.353286000	2.306162000
O	-1.836015000	-3.384658000	0.896051000
N	-2.289199000	0.115392000	1.054412000
N	-2.521637000	2.910883000	0.454108000
N	-0.599680000	3.477257000	-0.268083000
N	-1.120837000	4.613751000	0.305078000
C	-1.428694000	2.416172000	-0.194241000
C	-2.288524000	4.230384000	0.738767000
H	-2.993877000	4.866907000	1.252918000
C	0.751170000	3.531597000	-0.833178000
H	0.719340000	4.195035000	-1.705380000
H	0.979918000	2.513562000	-1.143072000
C	1.774358000	4.019951000	0.188383000
H	2.766205000	4.047168000	-0.275984000
H	1.805027000	3.329577000	1.034881000
H	1.529441000	5.023221000	0.547785000
C	-3.690838000	2.115734000	0.823386000
H	-4.310923000	1.966581000	-0.067803000
H	-4.272403000	2.688482000	1.547174000
C	-3.393429000	0.745767000	1.461644000
C	-1.991934000	-1.114610000	1.795163000
H	-2.286321000	-0.963676000	2.841036000
H	-0.915944000	-1.277958000	1.775587000
C	-2.662488000	-2.351084000	1.272423000
C	-3.962829000	-2.715371000	1.059945000
H	-4.820206000	-2.104006000	1.300001000
C	-3.940963000	-4.047214000	0.527704000
H	-4.790182000	-4.658007000	0.251382000
C	-2.628702000	-4.405558000	0.449781000

H	-2.112927000	-5.303899000	0.145659000
C	-2.497494000	0.792372000	-2.666033000
C	-2.920730000	-0.388635000	-2.017912000
H	-3.946684000	-0.484785000	-1.679618000
C	-2.041013000	-1.510282000	-1.874658000
H	-2.433994000	-2.419482000	-1.434473000
C	-0.700354000	-1.439289000	-2.257809000
C	-0.225959000	-0.175123000	-2.768289000
H	0.822150000	-0.048590000	-3.007622000
C	-1.109844000	0.885591000	-3.020444000
H	-0.734189000	1.803824000	-3.462884000
C	-3.457440000	1.898337000	-3.021095000
H	-3.722790000	1.839311000	-4.084926000
H	-3.020240000	2.887069000	-2.845142000
H	-4.385753000	1.822496000	-2.447085000
C	0.177296000	-2.689192000	-2.171891000
H	0.140482000	-3.038035000	-1.131480000
C	1.646577000	-2.459177000	-2.549470000
H	2.115501000	-1.682767000	-1.939916000
H	1.748360000	-2.176989000	-3.605094000
H	2.213898000	-3.384688000	-2.403369000
C	-0.414014000	-3.810074000	-3.055571000
H	-1.434445000	-4.069701000	-2.758128000
H	0.199523000	-4.714953000	-2.976147000
H	-0.433935000	-3.506967000	-4.109532000
C	1.336154000	-0.300772000	0.779005000
O	0.462461000	0.728185000	0.430407000
C	1.396796000	-0.502108000	2.298130000
C	1.219727000	0.587900000	3.159375000
C	1.655928000	-1.759645000	2.859470000
C	1.313903000	0.428940000	4.542276000
H	0.978288000	1.553508000	2.726437000
C	1.752614000	-1.924251000	4.243545000
H	1.775341000	-2.622698000	2.207142000
C	1.584499000	-0.827610000	5.090628000
H	1.168583000	1.286058000	5.195837000
H	1.949637000	-2.909745000	4.658786000
H	1.652559000	-0.952415000	6.168427000
C	2.745876000	0.070983000	0.226044000
H	3.016101000	1.052267000	0.635995000
C	3.892504000	-0.923517000	0.502591000
H	4.038108000	-1.013088000	1.584492000
H	3.608745000	-1.922454000	0.144304000
C	5.191216000	-0.504156000	-0.155152000
C	5.547389000	-0.979132000	-1.425325000
C	6.056684000	0.400742000	0.477447000

C	6.726064000	-0.563183000	-2.047717000
H	4.895432000	-1.690105000	-1.929405000
C	7.235591000	0.821134000	-0.139877000
H	5.802067000	0.775410000	1.466692000
C	7.575123000	0.340882000	-1.406927000
H	6.983508000	-0.949718000	-3.030969000
H	7.893176000	1.519887000	0.371473000
H	8.495334000	0.663558000	-1.887066000
H	1.049327000	-1.272730000	0.334101000
H	2.640850000	0.210534000	-0.858728000

(**K**)

Ru	-2.583429000	0.681104000	0.290695000
O	0.827426000	-1.769294000	-0.662790000
O	-3.308607000	-2.602670000	-2.429344000
N	-1.145048000	-0.568617000	-0.667238000
N	0.206191000	1.096636000	1.239378000
N	-0.660186000	3.022355000	1.015543000
N	0.643718000	3.253166000	1.398381000
C	-0.967986000	1.711630000	0.892994000
C	1.146005000	2.056156000	1.522983000
H	2.170692000	1.833047000	1.788367000
C	-1.501667000	4.168511000	0.686660000
H	-1.463285000	4.859151000	1.535403000
H	-2.516313000	3.779576000	0.589663000
C	-1.054571000	4.860398000	-0.600775000
H	-1.692396000	5.729510000	-0.796641000
H	-1.130586000	4.174261000	-1.450347000
H	-0.018948000	5.202145000	-0.515763000
C	0.375983000	-0.355040000	1.219737000
H	-0.258885000	-0.792103000	1.999270000
H	1.415453000	-0.584116000	1.448703000
C	0.018169000	-0.961537000	-0.149251000
C	-1.415957000	-1.095230000	-2.015041000
H	-0.475657000	-1.104072000	-2.579828000
H	-2.114483000	-0.418017000	-2.510213000
C	-1.993108000	-2.479949000	-2.040176000
C	-1.491112000	-3.716435000	-1.751219000
H	-0.481171000	-3.906999000	-1.420012000
C	-2.550765000	-4.657761000	-1.969106000
H	-2.510799000	-5.731568000	-1.844915000
C	-3.626145000	-3.932140000	-2.381064000
H	-4.631800000	-4.185479000	-2.681046000
C	-3.663430000	0.198994000	2.447038000
C	-3.751216000	-0.965747000	1.677264000
H	-3.389361000	-1.909705000	2.073830000

C	-4.307063000	-0.935172000	0.356101000
H	-4.329139000	-1.853163000	-0.220860000
C	-4.845415000	0.236355000	-0.207309000
C	-4.680868000	1.448331000	0.547320000
H	-5.039007000	2.390147000	0.148323000
C	-4.087056000	1.426359000	1.831314000
H	-3.995534000	2.353892000	2.388580000
C	-3.109452000	0.189575000	3.854264000
H	-3.508549000	-0.655016000	4.426186000
H	-3.371131000	1.109741000	4.385876000
H	-2.017140000	0.104547000	3.860208000
C	-5.589262000	0.181257000	-1.533323000
H	-5.174853000	-0.670336000	-2.086329000
C	-5.417972000	1.433480000	-2.406578000
H	-4.360172000	1.664794000	-2.564670000
H	-5.898145000	2.312753000	-1.959195000
H	-5.888437000	1.272479000	-3.383099000
C	-7.085029000	-0.103615000	-1.275524000
H	-7.224172000	-1.029549000	-0.706651000
H	-7.625659000	-0.201900000	-2.224099000
H	-7.548803000	0.712810000	-0.707763000
C	4.076092000	-0.406501000	0.612480000
O	4.100749000	0.694577000	1.158524000
C	4.178294000	-1.650477000	1.442299000
C	3.668820000	-2.885064000	1.007792000
C	4.784690000	-1.559715000	2.705936000
C	3.777790000	-4.010316000	1.825836000
H	3.141108000	-2.954099000	0.062744000
C	4.908363000	-2.688966000	3.510501000
H	5.159699000	-0.594823000	3.032422000
C	4.405539000	-3.917480000	3.069998000
H	3.368384000	-4.959771000	1.491836000
H	5.393988000	-2.614868000	4.479936000
H	4.498361000	-4.799209000	3.698929000
C	3.905708000	-0.550148000	-0.889937000
C	4.123479000	0.754511000	-1.679706000
H	2.878405000	-0.919012000	-1.045532000
H	3.578348000	1.562014000	-1.180668000
C	5.581327000	1.138242000	-1.848287000
C	6.222721000	1.993395000	-0.940665000
C	6.327458000	0.626683000	-2.920034000
C	7.569857000	2.324076000	-1.099708000
H	5.658912000	2.390397000	-0.101955000
C	7.674829000	0.953185000	-3.081324000
H	5.843528000	-0.030586000	-3.640236000
C	8.301648000	1.805127000	-2.169595000

H	8.047801000	2.991147000	-0.386381000
H	8.232592000	0.547522000	-3.921842000
H	9.349732000	2.064954000	-2.294356000
H	3.669769000	0.624937000	-2.669525000
H	4.570450000	-1.342413000	-1.256160000
H	-2.363394000	1.592861000	-0.997712000

TS^{KL}

Ru	1.382998000	-0.650222000	-0.174154000
O	2.037354000	2.190834000	2.995999000
O	2.989672000	3.346240000	-1.210487000
N	1.579128000	1.090559000	1.023779000
N	1.180892000	-1.232419000	2.767991000
N	-0.055944000	-2.635667000	1.758555000
N	-0.156036000	-2.956058000	3.090552000
C	0.763234000	-1.585235000	1.513651000
C	0.603909000	-2.077955000	3.677560000
H	0.760038000	-2.012079000	4.744359000
C	-0.770790000	-3.451802000	0.765107000
H	-0.050924000	-4.159244000	0.335836000
H	-1.108294000	-2.773336000	-0.023191000
C	-1.947809000	-4.211637000	1.367437000
H	-2.460082000	-4.747635000	0.561121000
H	-2.658622000	-3.524635000	1.833125000
H	-1.624210000	-4.935556000	2.119139000
C	2.139826000	-0.173236000	3.059262000
H	3.147260000	-0.535427000	2.816733000
H	2.099072000	0.037888000	4.128305000
C	1.884614000	1.152772000	2.327432000
C	1.403186000	2.423716000	0.412777000
H	0.794551000	3.039826000	1.087192000
H	0.859849000	2.301476000	-0.524485000
C	2.672926000	3.172317000	0.121114000
C	3.629474000	3.769711000	0.891321000
H	3.624971000	3.788721000	1.970388000
C	4.593395000	4.337713000	-0.006131000
H	5.484443000	4.892470000	0.255128000
C	4.157742000	4.055093000	-1.264082000
H	4.522999000	4.283231000	-2.254084000
C	3.672457000	-0.641776000	-0.832087000
C	2.908085000	0.135744000	-1.764308000
H	3.153795000	1.181250000	-1.906953000
C	1.819181000	-0.416128000	-2.451524000
H	1.258151000	0.212709000	-3.133892000
C	1.442002000	-1.796355000	-2.293862000
C	2.166167000	-2.539194000	-1.342967000

H	1.904238000	-3.573492000	-1.155304000
C	3.266342000	-1.971319000	-0.618561000
H	3.799325000	-2.588863000	0.098680000
C	4.851543000	-0.037469000	-0.106961000
H	5.715788000	-0.710522000	-0.137345000
H	4.614034000	0.163162000	0.942789000
H	5.142128000	0.915627000	-0.556693000
C	0.332611000	-2.369789000	-3.166948000
H	-0.582805000	-1.819509000	-2.906269000
C	0.056097000	-3.860678000	-2.933911000
H	-0.243018000	-4.068093000	-1.903749000
H	0.929666000	-4.480874000	-3.174605000
H	-0.765964000	-4.184372000	-3.580809000
C	0.648244000	-2.134690000	-4.660763000
H	0.786676000	-1.075749000	-4.900696000
H	-0.178640000	-2.505235000	-5.276504000
H	1.558364000	-2.668933000	-4.961830000
C	-1.710991000	-0.117474000	-0.686552000
O	-1.997388000	-1.148340000	-1.356521000
C	-2.302490000	0.001295000	0.718906000
C	-3.351367000	-0.861801000	1.062099000
C	-1.882616000	0.957105000	1.654087000
C	-3.968960000	-0.772631000	2.310182000
H	-3.679735000	-1.586533000	0.324971000
C	-2.491995000	1.041915000	2.906160000
H	-1.059263000	1.621422000	1.417433000
C	-3.538527000	0.177772000	3.238334000
H	-4.791871000	-1.439787000	2.555265000
H	-2.148706000	1.785416000	3.620976000
H	-4.018332000	0.249317000	4.211132000
H	-0.320228000	-0.238983000	-0.298833000
C	-1.566194000	1.211409000	-1.480857000
C	-2.780925000	1.465363000	-2.406301000
H	-1.413451000	2.060228000	-0.807835000
H	-2.509737000	2.293451000	-3.075354000
H	-2.909435000	0.575069000	-3.030265000
C	-4.087926000	1.798799000	-1.717564000
C	-4.301190000	3.066501000	-1.156525000
C	-5.122816000	0.857487000	-1.642387000
C	-5.508860000	3.383409000	-0.534570000
H	-3.513655000	3.815709000	-1.213532000
C	-6.334908000	1.170472000	-1.023774000
H	-4.969708000	-0.130261000	-2.070202000
C	-6.532171000	2.434824000	-0.466906000
H	-5.653772000	4.372899000	-0.108065000
H	-7.125636000	0.425608000	-0.978505000

H	-7.475674000	2.681285000	0.013174000
H	-0.681883000	1.131847000	-2.119331000

(**L**)

Ru	-1.148828000	-0.478283000	-0.806203000
O	-4.132258000	1.443992000	1.588076000
O	-1.761351000	-2.074512000	3.125675000
N	-2.222076000	0.448582000	0.766479000
N	-2.806688000	1.865809000	-1.696719000
N	-1.008532000	1.855760000	-2.830597000
N	-1.702489000	2.962212000	-3.262264000
C	-1.652532000	1.157030000	-1.869991000
C	-2.791508000	2.939097000	-2.548368000
H	-3.587031000	3.667174000	-2.612457000
C	0.307527000	1.595736000	-3.416979000
H	0.162308000	1.462520000	-4.495112000
H	0.651226000	0.661688000	-2.978267000
C	1.297409000	2.721839000	-3.132669000
H	2.254360000	2.495359000	-3.615951000
H	1.459149000	2.805931000	-2.055394000
H	0.930684000	3.676076000	-3.521703000
C	-3.860331000	1.509878000	-0.751318000
H	-4.455478000	0.691128000	-1.172082000
H	-4.513683000	2.374790000	-0.630382000
C	-3.375081000	1.122160000	0.655439000
C	-1.851178000	0.172727000	2.166827000
H	-2.057597000	1.072157000	2.756619000
H	-0.781182000	-0.019811000	2.214014000
C	-2.552939000	-0.995527000	2.794364000
C	-3.849590000	-1.269037000	3.128407000
H	-4.675705000	-0.588432000	2.987289000
C	-3.864681000	-2.587818000	3.692343000
H	-4.720465000	-3.127468000	4.075144000
C	-2.576054000	-3.027599000	3.669886000
H	-2.086445000	-3.931307000	4.000384000
C	-2.648162000	-2.225504000	-1.224890000
C	-1.881346000	-2.582692000	-0.077337000
H	-2.395950000	-2.771461000	0.857376000
C	-0.477751000	-2.665836000	-0.113959000
H	0.063306000	-2.916265000	0.791971000
C	0.242314000	-2.415646000	-1.326507000
C	-0.490258000	-2.037968000	-2.466218000
H	0.014949000	-1.824691000	-3.400403000
C	-1.912584000	-1.883972000	-2.388672000
H	-2.450524000	-1.556360000	-3.274424000
C	-4.154179000	-2.237171000	-1.185401000

H	-4.536789000	-3.260080000	-1.301209000
H	-4.579928000	-1.635057000	-1.995019000
H	-4.524878000	-1.852384000	-0.229856000
C	1.748076000	-2.619472000	-1.342471000
H	2.112862000	-2.349227000	-0.344422000
C	2.499087000	-1.740587000	-2.349642000
H	2.283212000	-0.685217000	-2.165293000
H	2.243894000	-1.990030000	-3.387326000
H	3.577773000	-1.890539000	-2.234607000
C	2.052578000	-4.117325000	-1.566488000
H	1.561390000	-4.748169000	-0.817135000
H	3.132228000	-4.294023000	-1.504716000
H	1.712107000	-4.443423000	-2.556827000
C	1.257949000	0.725534000	0.741490000
O	0.577452000	0.665104000	-0.475692000
C	0.952230000	1.992296000	1.562228000
C	0.257800000	3.065451000	0.997377000
C	1.397655000	2.103447000	2.887107000
C	0.009509000	4.223797000	1.738586000
H	-0.095237000	2.972244000	-0.023197000
C	1.147970000	3.255538000	3.632118000
H	1.948944000	1.280218000	3.337409000
C	0.452110000	4.323459000	3.058179000
H	-0.535002000	5.048763000	1.284821000
H	1.495188000	3.320836000	4.660482000
H	0.255288000	5.222457000	3.636707000
C	2.747788000	0.692664000	0.448751000
H	3.078500000	1.455535000	-0.255131000
C	3.616523000	-0.175547000	0.991638000
H	3.226152000	-0.909226000	1.699763000
C	5.067247000	-0.265610000	0.760439000
C	5.807708000	-1.239312000	1.455467000
C	5.764970000	0.575455000	-0.128252000
C	7.184128000	-1.371768000	1.275252000
H	5.290603000	-1.897799000	2.150353000
C	7.138825000	0.443783000	-0.310556000
H	5.227297000	1.341506000	-0.679405000
C	7.858151000	-0.530211000	0.389460000
H	7.729536000	-2.132180000	1.828501000
H	7.653554000	1.106611000	-1.001691000
H	8.930762000	-0.628673000	0.245891000
H	1.040517000	-0.149657000	1.381607000

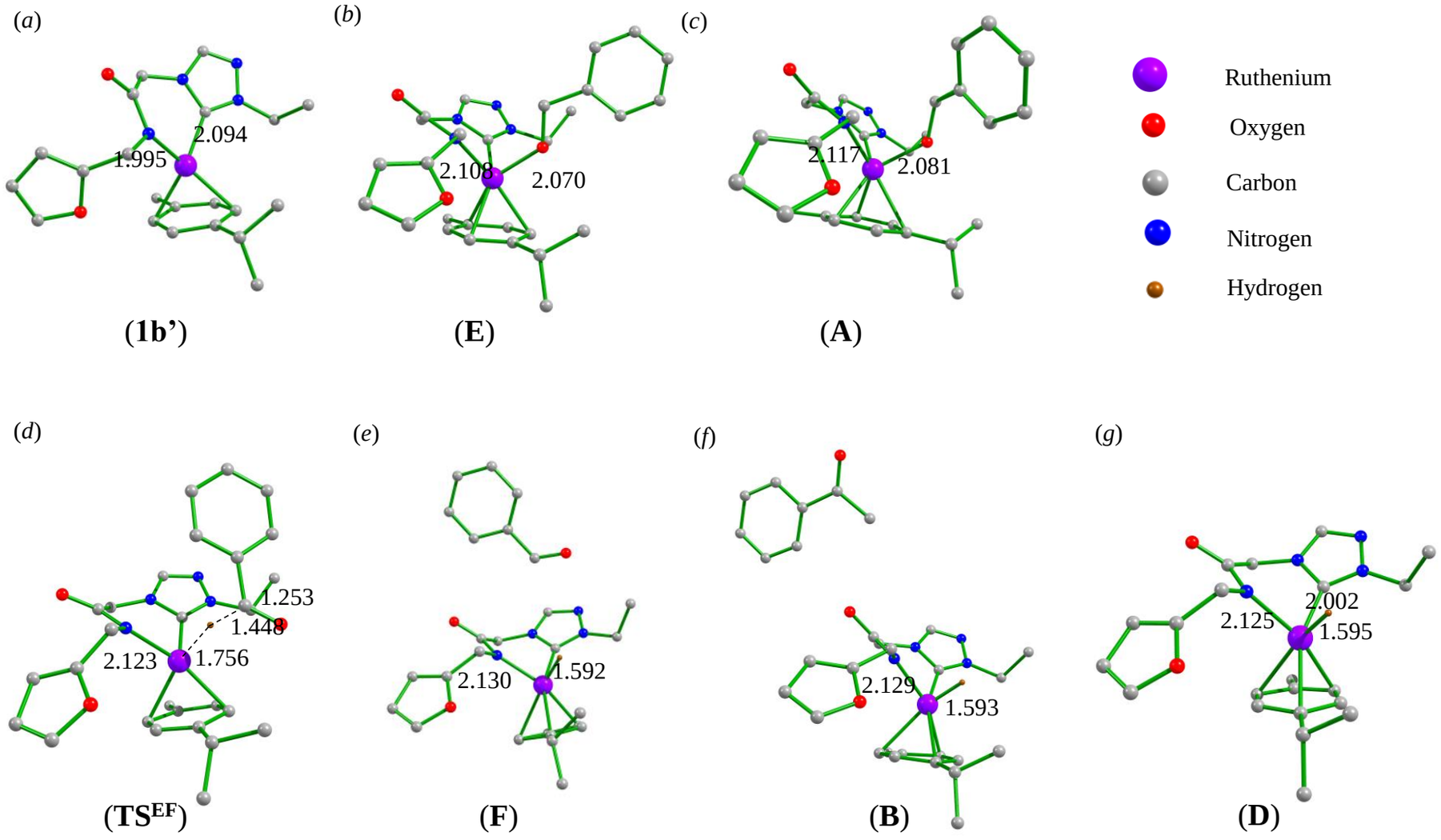

Figure S140. DFT Optimised geometries of species involved in the the substitution and dehydrogenation of alcohols :(*a*) (**1b'**), (*b*) (**E**), (*c*) (**A**), (d) **TS^{EF},** (*e*) (**F**), (*f*) (**B**), and (*g*) (**D**) (deprotonated alcohol pathway).

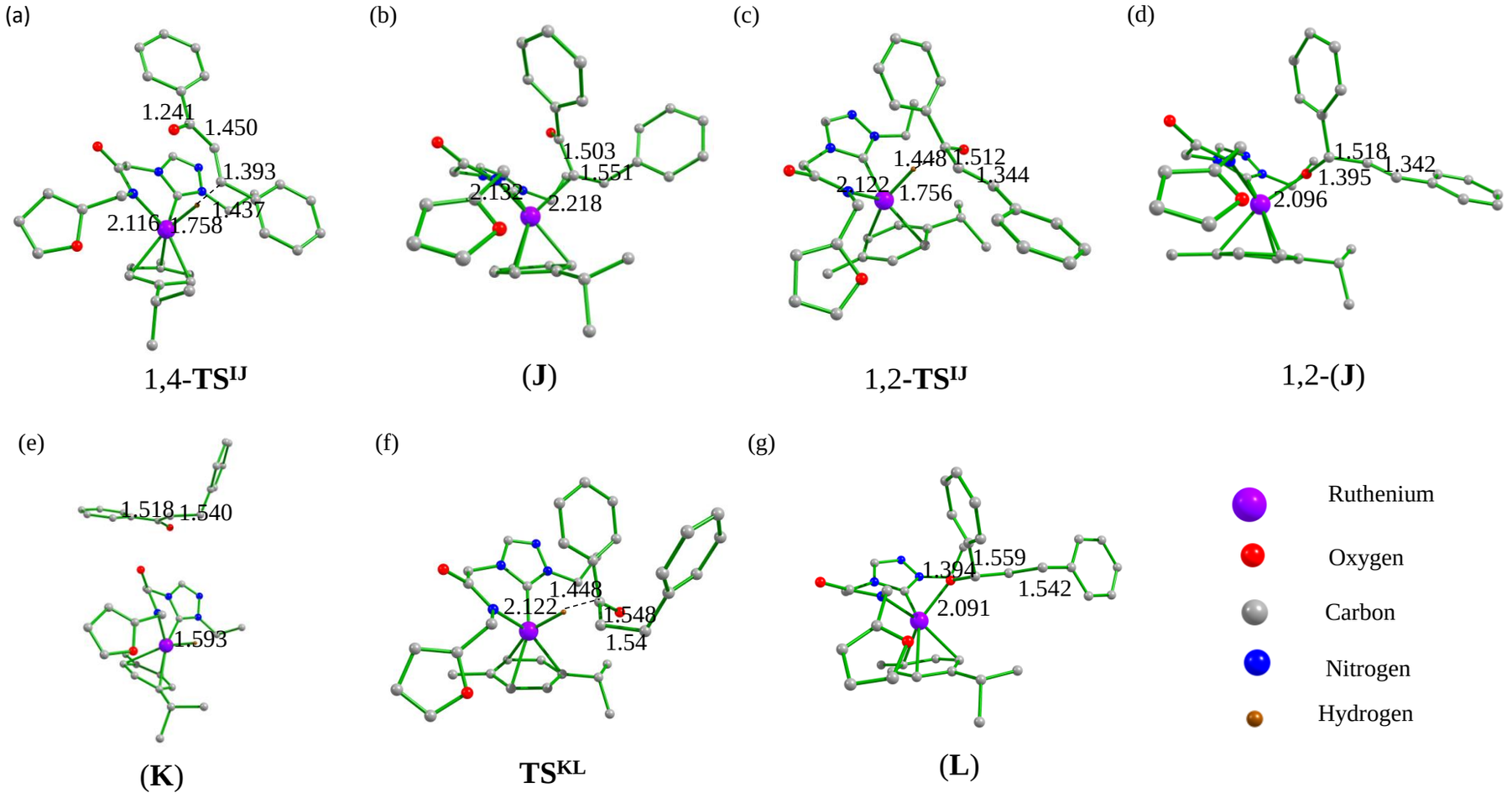

Figure S141. DFT Optimised geometries of species involved in the hydrogenation of olefin and ketone (*a*) **1,4-TS^{IJ}** (*b*) (**J**), (*c*) **1,2-TS^{IJ}**, (*d*) **1,2-(J)**, (*e*) (**K**), (*f*) **TS^{KL}**, and (*g*) (**L**) (deprotonated alcohol pathway).

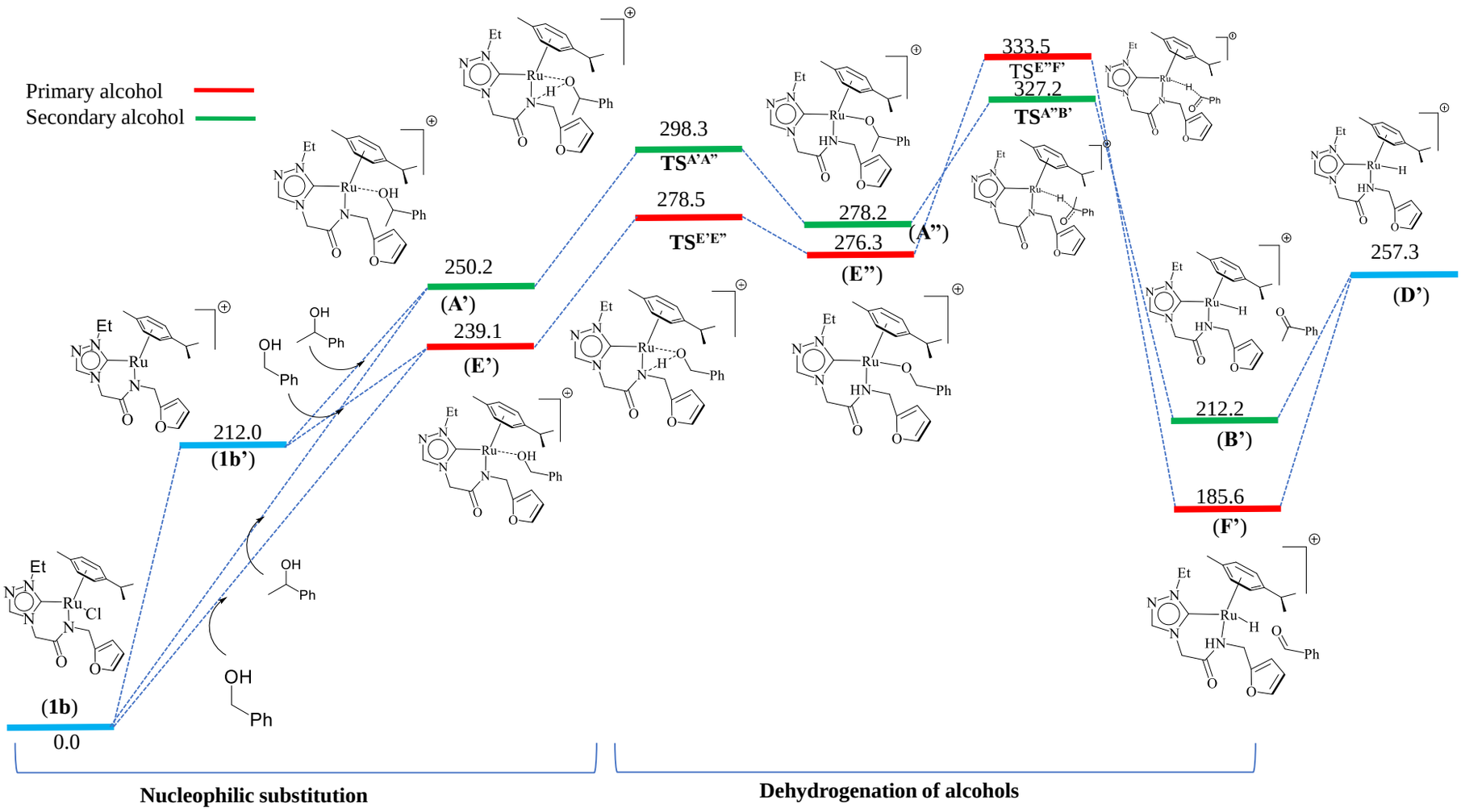

Figure S142. Energy profile diagram of nucleophilic substitution and dehydrogenation of alcohols by (**1b**) (alcohol pathway or the ionic pathway).

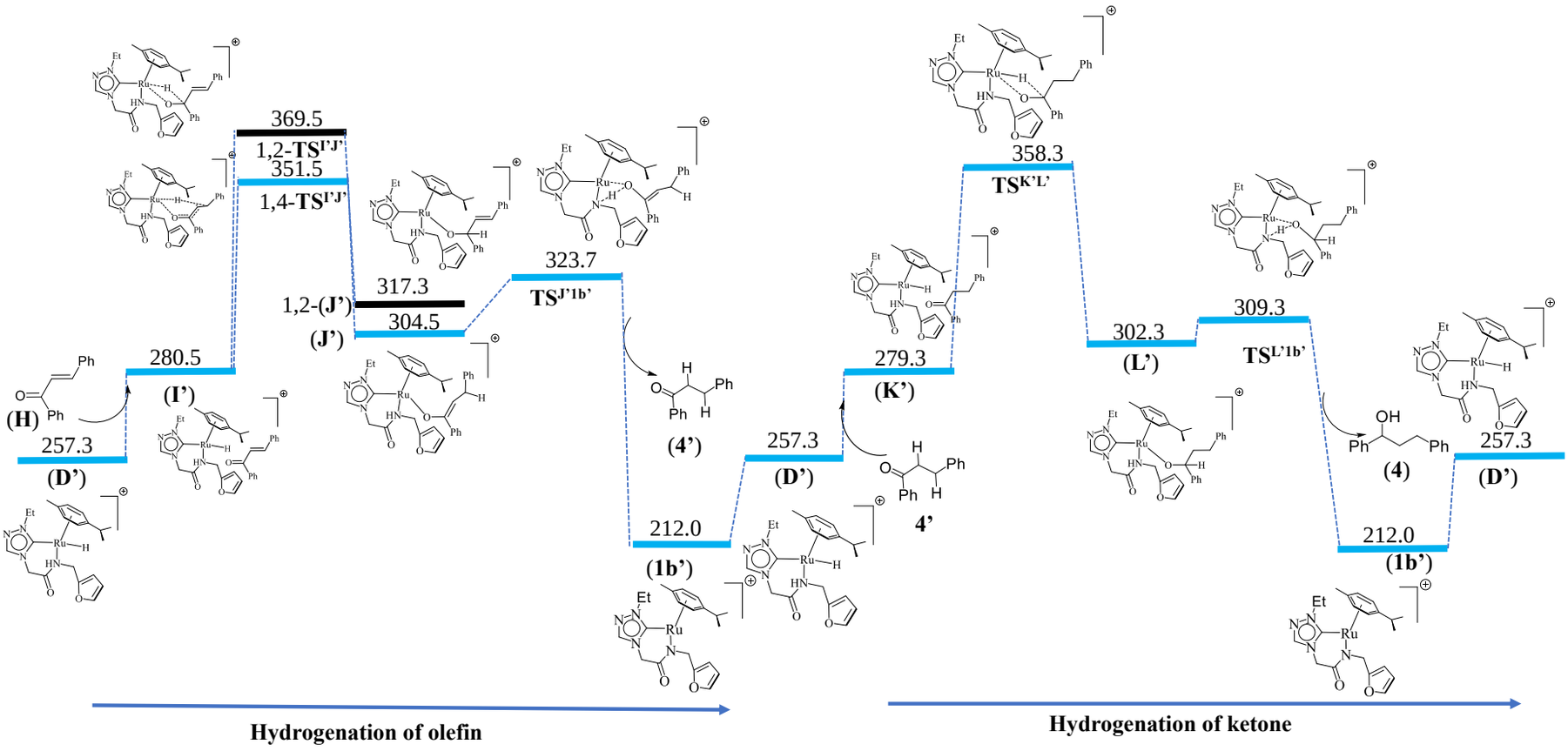

Figure S143. Energy profile diagram for hydrogenation of ketone and olefin by ruthenium hydride active species (**D'**) (alcohol pathway or the ionic pathway).

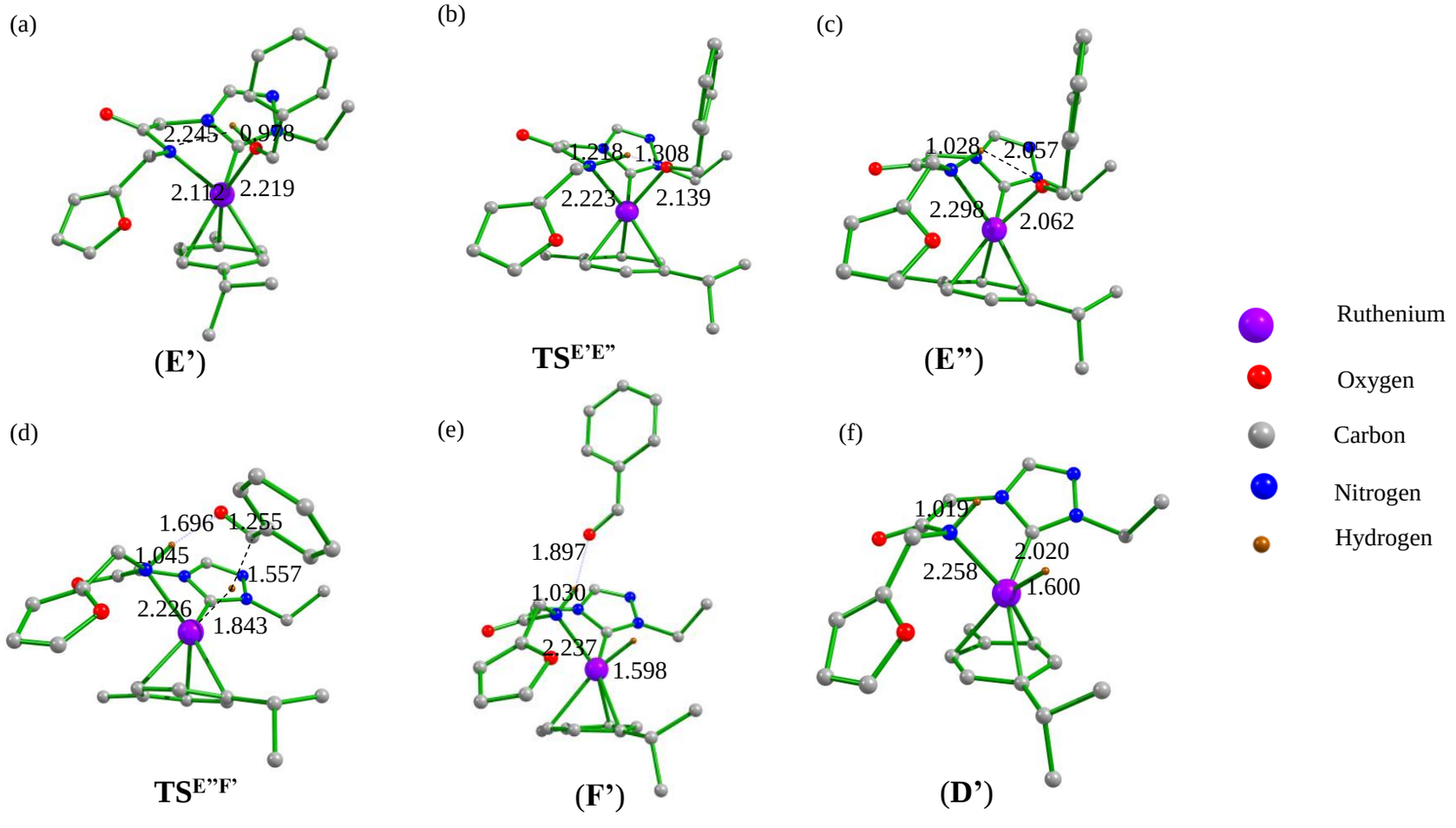

Figure S144. DFT optimized geometries involved in the dehydrogenation of primary alcohols (*a*) (**E'**), (*b*) **TS$^{E'E"}$**, (*c*) (**E''**), (*d*) **TS$^{E"F'}$** (*e*) (**F'**), and (*f*) (**D'**) (alcohol pathway or the ionic pathway).

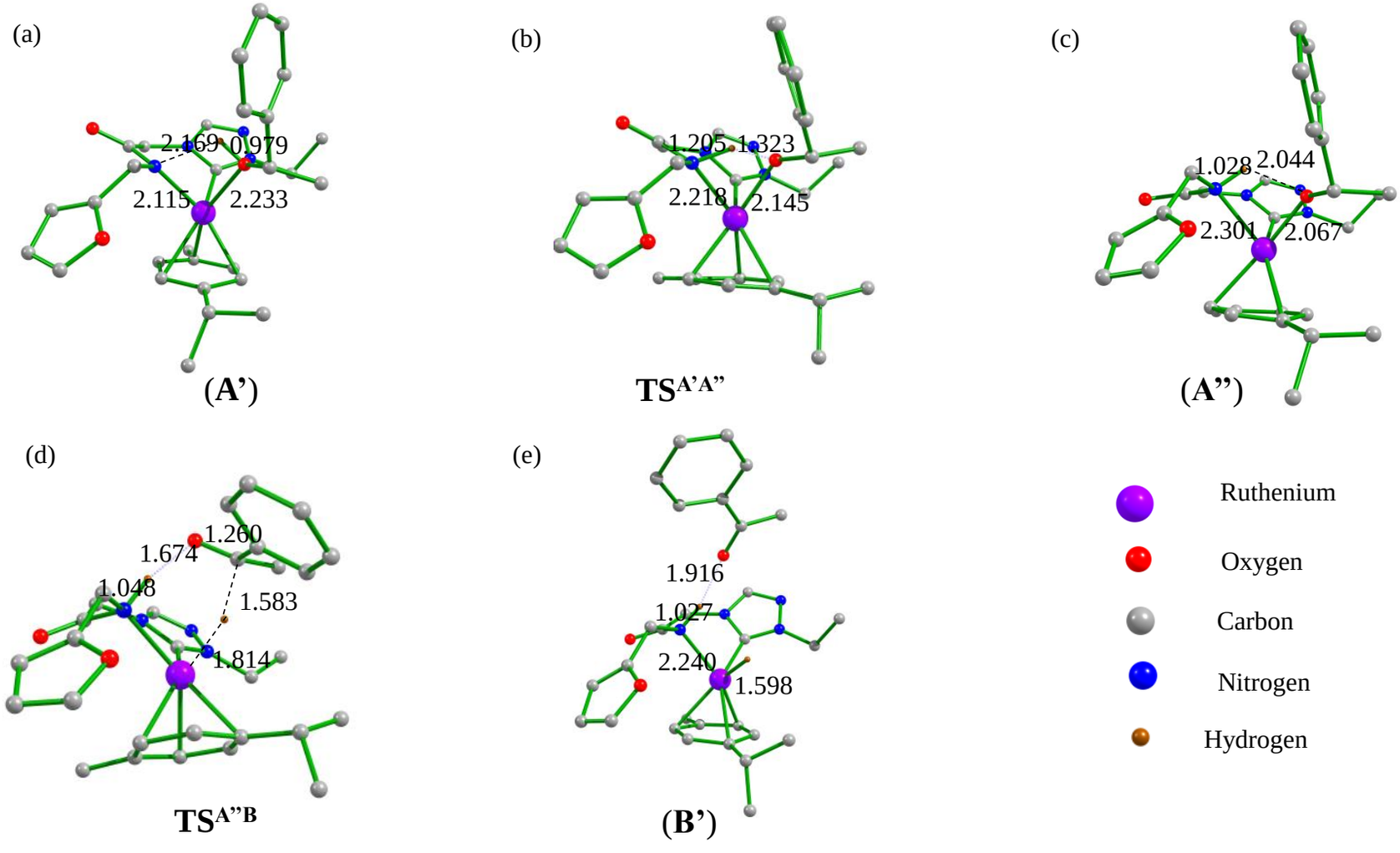

Figure S145. DFT optimized geometries involved in the dehydrogenation of secondary alcohols (*a*) (**A'**), (*b*) **TS$^{A'A"}$**(*c*) (**A''**) (*d*) **TS$^{A"B}$** and (*e*) (**B'**) (alcohol pathway or the ionic pathway).

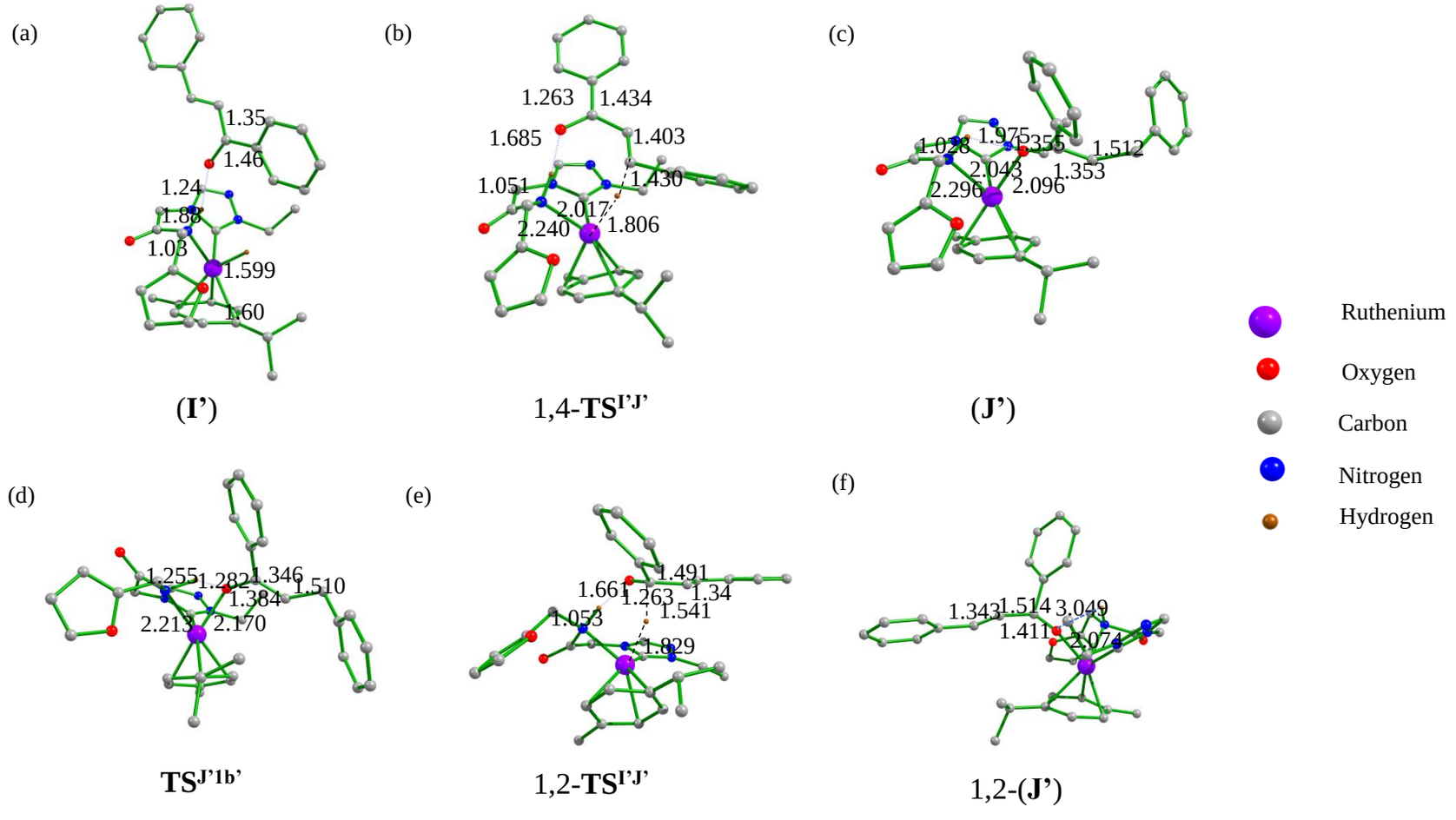

Figure S146. DFT optimized geometries of species involved in the (*a*) (**I'**), (*b*) **1,4-TS$^{I'J'}$**, (*c*) (**J'**), (*d*) **TS$^{J'1b'}$**, (*e*) **1,2-TS$^{I'J'}$**, and (*f*) **1,2-(J')** (alcohol pathway or the ionic pathway).

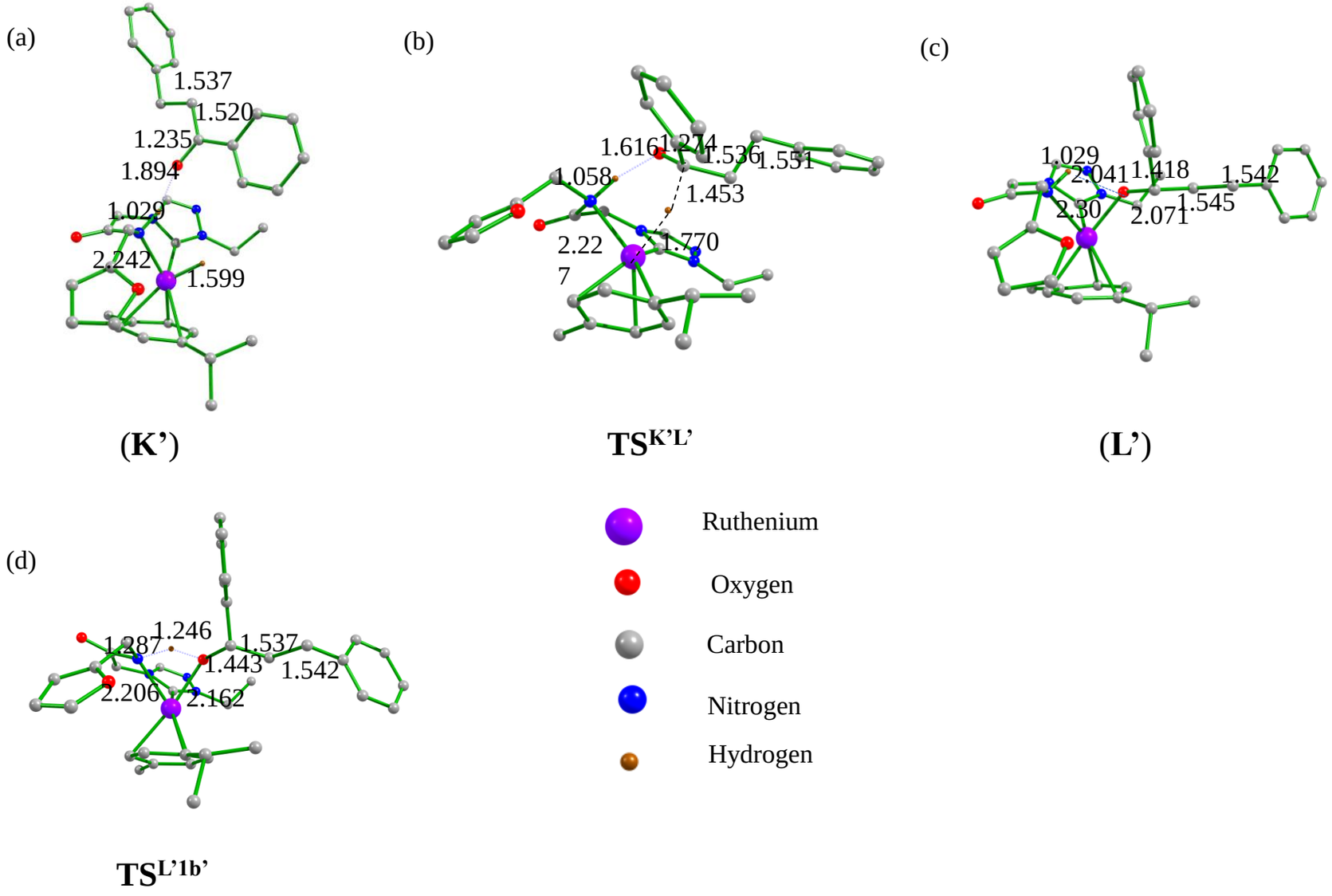

Figure S147. DFT optimized geometries involved in the dehydrogenation of secondary alcohols (*a*) (**K'**), (*b*) **TS$^{K'L'}$**, (*c*) (**L'**), and (*d*) **TS$^{L'1b'}$** (alcohol pathway or the ionic pathway).

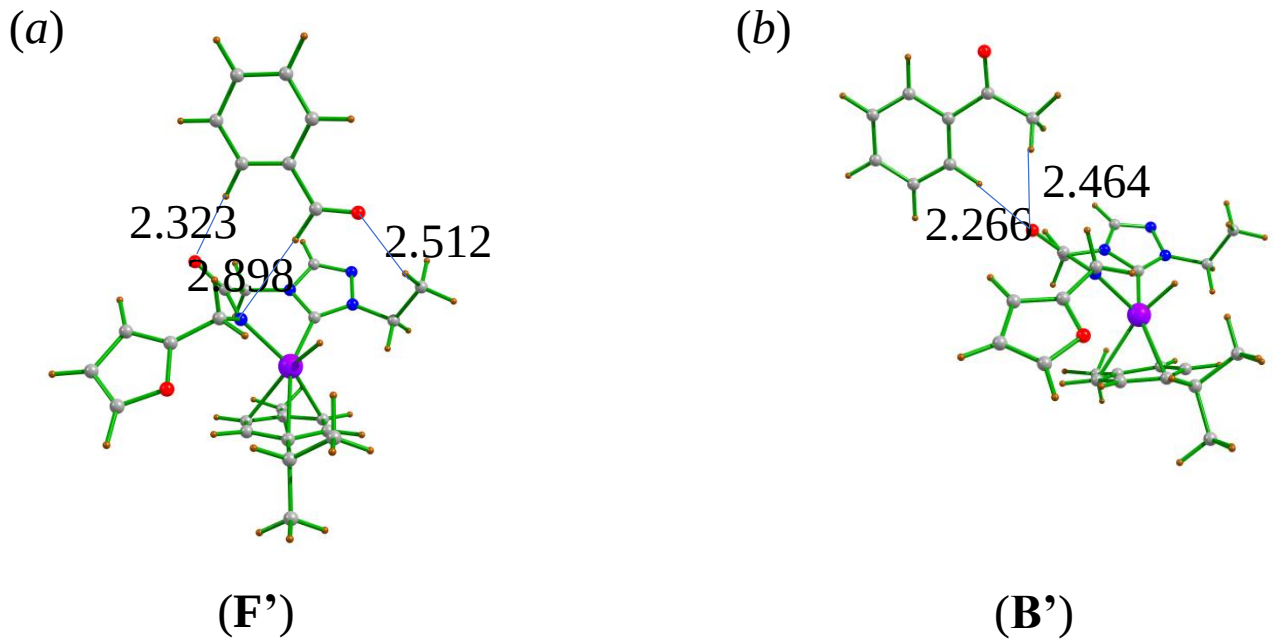

Figure S148. Non-covalent interactions present between ruthenium catalyst and aldehyde and ketone (*a*) (**F'**) and (*b*) (**B'**) (alcohol pathway or the ionic pathway).

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