

Supporting Information

Nitrated Confined Imidodiphosphates Enable a Catalytic Asymmetric Oxa-Pictet–Spengler Reaction

Sayantani Das,[#] Luping Liu,[#] Yiyang Zheng, M. Wasim Alachraf, Walter Thiel,* Chandra Kanta De,* and Benjamin List*

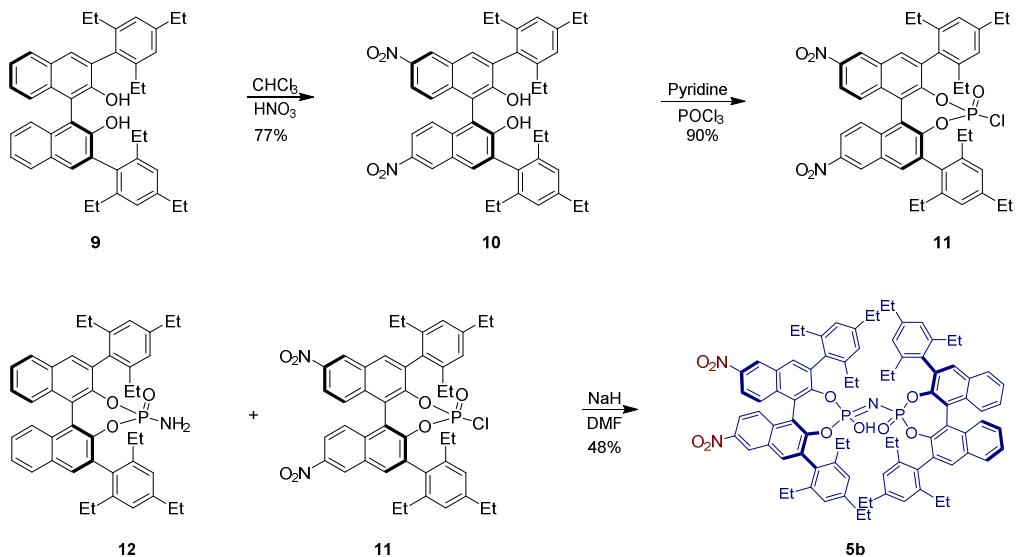
Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

General Information	S2
1. Catalyst Synthesis	S3
2. General Procedure for the Asymmetric Oxa-Pictet–Spengler Reaction	S6
3. Product Characterization	S6
4. Determination of the Absolute Configuration	S10
5. Experiment with low catalyst loading	S14
6. ESI–MS Study	S15
7. ¹ H and ¹³ C NMR Spectra	S17
8. HPLC Traces	S32
9. Computational Section	S43
10. References	S92

General information

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. All solvents used in the reactions were distilled from appropriate drying agents prior to use. Reactions were monitored by thin layer chromatography (TLC) on silica gel pre-coated plastic sheets (0.2 mm, Macherey-Nagel). Visualization was accomplished by irradiation with UV light at 254 nm and/or phosphomolybdic acid (PMA) stain. Column chromatography was performed on Merck silica gel (60, particle size 0.040-0.063 mm). Proton and carbon NMR spectra were recorded on a Bruker AV-500 spectrometer in deuterated solvents. Proton chemical shifts are reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard ($\text{CDCl}_3\delta$ 7.26 ppm, $\text{CD}_2\text{Cl}_2\delta$ 5.32 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, s = sextet, h = heptet, m = multiplet, br = broad), coupling constants (Hz) and integration. ^{13}C chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($\text{CDCl}_3\delta$ 77.16 ppm, $\text{CD}_2\text{Cl}_2\delta$ 53.84 ppm). High resolution mass spectra were determined on a Bruker APEX III FTMS (7 T magnet). Optical rotations were determined with an Autopol IV polarimeter (Rudolph Research Analytical) at 589 nm and 25 °C. Data are reported as follows: $[\alpha]_{\lambda}^{\text{temp}}$, concentration (c in g/100 mL), and solvent. Enantiomeric ratios (er) were determined by HPLC analysis employing a chiral stationary phase column specified in the individual experiment, by comparing the samples with the appropriate racemic mixtures.

1. Catalyst Synthesis



9 and **12** are synthesized according to literature.¹

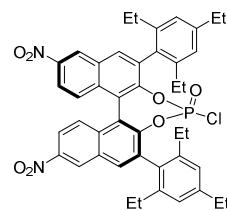
(1S,3'S)-6,6'-Dinitro-3,3'-bis(2,4,6-triethylphenyl)-[1,1'-binaphthalene]-2,2'-diol (**10**):

A solution of HNO₃ (94 μL, 2 mmol) in CHCl₃ (1.3 mL) was added dropwise to the solution of (*S*)-**9** (570mg, 0.94 mmol) in CHCl₃ (5.6 ml) at -40 °C under argon. After 20 min at 0 °C, the solution was warmed up to room temperature for further 20 min. The reaction was cooled to 0 °C, and then water (45 mL) was carefully added, and the mixture was extracted with CH₂Cl₂ (45×3 mL). The organic layer was collected, dried (MgSO₄), filtered, and the solvent was removed under reduced pressure. The residue was purified by column chromatography on silica gel using 50% CH₂Cl₂/i-hexanes as the eluent yielding the title compound as a yellow solid (504mg, 77%). ¹H NMR (500 MHz, CD₂Cl₂): δ 8.87 (d, *J* = 1.5 Hz, 2H), 8.09 (dd, *J* = 9.2 Hz, 1.7 Hz, 2H), 8.02 (br s, 2H), 7.34 (d, *J* = 9.2 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 4H), 5.43 (br s, 2H), 2.71 (q, *J* = 7.5 Hz, 4H), 2.54–2.31 (m, 8H), 1.30 (t, *J* = 7.5 Hz, 6H), 1.11 (t, *J* = 7.4 Hz, 6H), 1.02 (t, *J* = 7.4 Hz, 6H). ¹³C NMR (126 MHz, CD₂Cl₂): δ 154.1, 146.2, 144.4, 144.1, 144.0, 136.9, 133.3, 131.8, 129.7, 127.9, 126.8, 126.7, 126.0, 125.6, 120.5, 114.5, 29.2, 27.4, 27.3, 15.7, 15.6. HRMS *m/z* (ESI): calcd. for C₄₄H₄₃N₂O₆ [M-H]: 695.312662; found: 695.312750.

(2s,4R,11bS)-4-chloro-9,14-dinitro-2,6-bis(2,4,6-triethylphenyl)dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosph-epine 4-oxide (**11**):

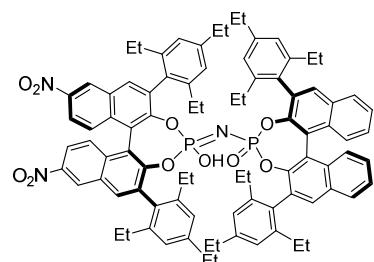
To a solution of (*S*)-**10** (350 mg, 0.50 mmol) in pyridine (1.6 mL) under argon was added POCl₃ (466 μl, 5.0 mmol) at room temperature. The mixture was stirred at room temperature for 5 h and then concentrated to dryness under vacuum. The residue was

passed through a short silica gel column using 40% $\text{CH}_2\text{Cl}_2/i$ -hexanes as the eluent yielding the title



compound as a colorless solid (350 mg, 90%). **$^1\text{H NMR}$** (600 MHz, CDCl_3): δ 8.94 (dd, $J = 6.1$ Hz, 2.3 Hz, 2H), 8.20 (d, $J = 17.4$ Hz, 2H), 8.15 (dq, $J = 9.4$ Hz, 0.9 Hz, 2H), 7.36 (dd, $J = 9.3$ Hz, 6.8 Hz, 2H), 7.13 (d, $J = 28.4$ Hz, 2H), 7.02 (d, $J = 7.9$ Hz, 2H), 2.74–2.69(m, 4H), 2.56–2.24(m, 8H), 1.36–1.31 (m, 6H), 1.27 (t, $J = 7.5$ Hz, 3H), 1.21 (t, $J = 7.6$ Hz, 3H), 7.36 (dt, $J = 7.6$ Hz, 4.0 Hz, 6H). **$^{13}\text{C NMR}$** (151 MHz, CDCl_3): δ 148.0, 147.9, 147.8, 145.9, 145.2, 144.9, 143.0, 142.5, 142.0, 141.7, 135.6, 135.5, 135.3, 135.1, 134.7, 134.6, 134.4, 134.3, 130.7, 130.4, 130.0, 129.8, 128.3, 128.2, 125.64, 125.62, 125.3, 125.1, 125.0, 124.7, 122.0, 121.9, 121.84, 121.82, 120.7, 120.6, 28.81, 28.80, 27.5, 27.0, 26.8, 16.1, 15.3, 15.2, 15.18, 14.7, 14.5. **$^{31}\text{P NMR}$** (202 MHz, CDCl_3): δ 6.52 (s). **HRMS** m/z (ESI): calcd. for $\text{C}_{44}\text{H}_{42}\text{N}_2\text{O}_7\text{P}_1\text{Na}_1[\text{M}+\text{Na}]$: 799.231039; found: 799.230700.

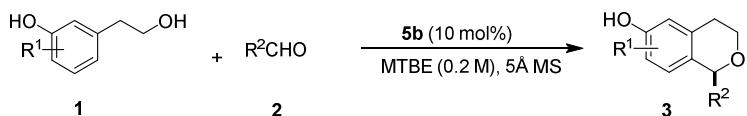
4-((4-hydroxy-9,14-dinitro-2,6-bis(2,4,6-triethylphenyl)-4*I*5-dinaphtho[2,1-d:1',2'-][1,3,2]dioxaphosphhepin-4-ylidene)amino)-2,6-bis(2,4,6-triethylphenyl)dinaphtho[2,1-d:1',2'-



f|1,3,2]dioxaphosphhepine 4-oxide (5b): Sodium hydride (60% dispersion in mineral oil, 48 mg, 1.2 mmol) was added to a solution of (*S*)-11 (250 mg, 0.32 mmol) and (*S*)-12 (203 mg, 0.30 mmol) in DMF (3 ml) under argon at room temperature. After 2.5 h at room temperature, 10% aqueous HCl solution (1 mL) was added. The organic layer was separated and the solvent was removed under reduced pressure. The residue was purified by column chromatography on silica gel using 5–15% ethyl acetate/*i*-hexanes as the eluents giving a colorless solid. The solid was dissolved in CH_2Cl_2 (5 mL) and stirred with 6N aqueous HCl (5 mL) for 1 h. The organic layer was separated, washed with 6N aqueous HCl (5 mL) and concentrated under reduced pressure to give the title compound as a pale yellow solid (206 mg, 48%). **$^1\text{H NMR}$** (500 MHz, CD_2Cl_2): δ 8.87 (d, $J = 2.3$ Hz, 1H), 8.84 (d, $J = 2.3$ Hz, 1H), 8.15 (dd, $J = 9.3$ Hz, 2.4 Hz, 1H), 8.05 (br s, 1H), 7.97 (dd, $J = 9.4$ Hz, 2.4 Hz, 1H), 7.90 (t, $J = 8.4$ Hz, 2H), 7.84 (d, $J = 14.5$ Hz, 2H), 7.61 (br s, 1H), 7.56–7.53(m, 1H), 7.48–7.42(m, 4H), 7.25–7.21(m, 1H), 7.06 (t, $J = 9.8$ Hz, 2H), 6.98 (d, $J = 4.9$ Hz, 2H), 6.87–6.86(m, 4H), 6.44 (br s, 1H), 6.33 (br s, 1H), 2.63–2.49(m, 8H), 2.29–2.09(m, 10H), 2.05–1.90(m, 3H), 1.78–1.71 (m, 1H), 1.22–1.15(m, 12H), 1.09 (q, $J = 7.7$ Hz, 6H), 0.98–0.92(m, 7H), 0.86–0.79(m, 7H), 0.08–0.01(m, 6H). **$^{13}\text{C NMR}$** (126 MHz, CD_2Cl_2): δ 150.4, 150.3, 149.5, 149.4, 146.1, 146.0, 145.8, 145.7, 145.67, 145.59, 145.0, 144.7, 144.6, 144.3, 144.1, 144.0, 143.71, 143.70, 143.4, 143.0, 142.9, 142.3, 136.3, 136.27, 135.8, 135.77, 135.7, 135.3, 135.2, 134.5, 133.3, 133.28, 133.0, 132.9, 132.7, 132.6, 132.0, 131.9, 131.88, 131.7, 130.6, 130.0, 128.9, 128.3, 127.8, 127.3, 127.0,

126.9, 126.4, 126.2, 126.0, 125.8, 125.7, 125.6, 125.4, 125.2, 125.1, 125.08, 124.9, 122.8, 122.7, 122.5, 122.2, 120.5, 120.3, 30.2, 29.2, 29.19, 29.18, 29.1, 27.5, 27.45, 27.4, 27.22, 27.2, 27.1, 24.1, 17.8, 17.77, 16.3, 16.0, 15.9, 15.8, 15.6, 15.5, 15.4, 15.3, 15.1. **³¹PNMR** (202 MHz, CD₂Cl₂): δ 5.90 (d, *J* = 86.0, 1P), 3.54 (d, *J* = 85.5, 1P). **HRMS** *m/z* (ESI): calcd. for C₈₈H₈₆N₃O₁₀P₂[M–H]: 1406.579400; found: 1406.579070.

2.General Procedure for the Asymmetric Oxa-Pictet–Spengler Reaction



A 2-mL GC vial was charged with starting material (0.1 mmol), catalyst (14.0 mg, 0.01 equiv., 10 mol%), molecular sieves 5 Å (50 mg) and a magnetic stirring bar at room temperature. Then 500 µL (0.2 M) of MTBE was added followed by aldehyde (2.5 equiv., 0.25 mmol). The vial was filled with argon and sealed. It was then introduced to the desired temperature for the reaction. The progress of the reaction was monitored by TLC. For aromatic aldehydes, the reactions were quenched with trimethylamine. Purification was performed by column chromatography or preparative thin layer chromatography on silica gel using EtOAc/*i*-hexanes as eluents.

Note: It was found that prolonged purification time on silica gel column chromatography deteriorates the enantio-purity of the products and with neutral Al₂O₃ column chromatography leads to complete racemization of the products.

3. Product Characterization

(S)-1-isobutylisochroman-6-ol (3d): Prepared according to the general procedure. 18.0 mg yellow oil, 87%. **¹H NMR** (500 MHz, CDCl₃): δ 6.92 (d, *J* = 8.5 Hz, 1H), 6.65 (dd, *J* = 8.4, 2.7 Hz, 1H), 6.57 (d, *J* = 2.7 Hz, 1H), 4.72 (d, *J* = 10.1 Hz, 1H), 4.09 (ddd, *J* = 11.5, 5.5, 1.8 Hz, 1H), 3.75 (ddd, *J* = 12.9, 8.8, 4.0 Hz, 1H), 2.90 (ddd, *J* = 16.3, 8.8, 5.3 Hz, 1H), 2.66 (td, *J* = 16.4, 4.2 Hz, 1H), 2.08–1.86 (m, 1H), 1.75 (ddd, *J* = 11.9, 10.2, 3.8 Hz, 1H), 1.59–1.51 (m, 1H), 1.01 (d, *J* = 6.6 Hz, 3H), 0.95 (d, *J* = 6.6 Hz, 3H). **¹³C NMR** (126 MHz, CDCl₃): δ 153.76, 135.45, 131.61, 126.21, 115.14, 113.48, 73.96, 62.74, 45.52, 29.37, 24.59, 24.12, 21.68. **HRMS m/z** (ESI): calcd. for C₁₃H₁₈O₂.H [M+H]: 207.138070; found: 207.137955. The enantiomeric ratio was measured by HPLC analysis using ChiralpakOJ-3, heptane/*i*-PrOH = 85:15, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 5.7 min (major) and t_R = 8.9 min (minor). er = 96.8:3.2. [α]_D²⁵ = -70.0 (*c* 0.50, CHCl₃).

(S)-1-butylisochroman-6-ol (3e): Prepared according to the general procedure. 17.0 mg colorless oil, 82%. **¹H NMR** (500 MHz, CDCl₃): δ 6.95 (d, *J* = 6.4 Hz, 1H), 6.67 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.57 (d, *J* = 2.6 Hz, 1H), 4.68 (dd, *J* = 7.9, 1.7 Hz, 1H), 4.1 (td, *J* = 5.6, 3.7 Hz, 1H), 3.74 (ddd, *J* = 12.6, 8.8, 3.7Hz, 1H), 2.93 (ddd, *J* = 16.3, 9.5, 4.9 Hz, 1H), 2.62 (td, *J* = 16.3, 3.6 Hz, 1H), 1.94–1.82 (m, 1H), 1.81–1.70 (m, 1H), 1.51–1.30 (m, 4H), 0.91 (t, *J* = 7.3 Hz, 3H). **¹³C NMR** (126 MHz, CDCl₃): δ 153.85, 135.61, 130.97, 126.22, 115.12, 113.58, 75.92, 63.14, 35.88, 29.41, 27.50, 22.95, 14.23. **HRMS m/z** (ESI): calcd. for C₁₃H₁₈O₂H [M+H]: 207.138000; found: 207.137955. The enantiomeric ratio was measured by HPLC analysis using ChiralpakOD-3, heptane/*i*-

i-PrOH = 95:5, flow rate = 0.5mL/min, λ = 279 nm, t_R = 12.7 min (major) and t_R = 14.4 min (minor). er = 97.3:2.7. $[\alpha]_D^{25} = -81.6$ (*c* 0.50, CHCl₃).

(S)-1-phenethylisochroman-6-ol (3f): Prepared according to the general procedure. 20.5 mg yellow oil, 80.6%. **¹H NMR** (500 MHz, CDCl₃): δ 7.28 (t, J = 7.7 Hz, 2H), 7.23 (d, J = 7.5 Hz, 2H), 7.18 (t, J = 7.4 Hz, 1H), 6.93 (d, J = 8.4 Hz, 1H), 6.65 (dd, J = 8.4, 2.6 Hz, 1H), 6.59 (d, J = 2.6 Hz, 1H), 4.78–4.63 (m, 1H), 4.23–4.09 (m, 1H), 3.85–3.71 (m, 1H), 2.97 (ddd, J = 16.4, 9.5, 5.4 Hz, 1H), 2.77 (t, J = 8.9 Hz, 2H), 2.65 (td, J = 16.4, 3.6 Hz, 1H), 2.63–2.13 (m, 1H), 2.13–1.97 (m, 1H), 1.62 (br s, 1H). **¹³C NMR** (126 MHz, CDCl₃): δ 153.88, 142.54, 135.74, 123.62, 128.66, 128.48, 126.13, 125.86, 11.20, 113.63, 75.11, 63.23, 37.90, 31.50, 29.41. **HRMS m/z** (ESI): calcd. for C₁₇H₁₈O₂Na [M+Na]: 277.120080; found: 277.119899. The enantiomeric ratio was measured by HPLC analysis using ChiralpakAD-3, heptane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 7.6 min (major) and t_R = 8.7 min (minor). er = 97.4:2.6. $[\alpha]_D^{25} = -27.6$ (*c* 0.55, CHCl₃).

(S)-1-phenylisochroman-6-ol (3g): Prepared according to the general procedure. 20.6 mg white solid, 91%. **¹H NMR** (500 MHz, CD₂Cl₂): δ 7.42–7.22 (m, 5H), 6.61 (d, J = 2.5 Hz, 1H), 6.58 (d, J = 8.4 Hz, 1H), 6.55 (dd, J = 8.4, 2.5 Hz, 1H), 5.65 (s, 1H), 5.12 (br s, 1H), 4.13 (ddd, J = 11.3, 5.6, 3.7 Hz, 1H), 3.87 (ddd, J = 13.6, 9.6, 4.0 Hz, 1H), 3.06 (ddd, J = 16.4, 9.5, 5.5 Hz, 1H), 2.73 (dd, J = 16.5, 3.8 Hz, 1H). **¹³C NMR** (126 MHz, CD₂Cl₂): δ 154.82, 143.26, 136.13, 123.32, 129, 30, 128.83, 128.63, 128.50, 79.87, 64.15, 29.48. **HRMS m/z** (ESI): calcd. for C₁₅H₁₃O₂ [M-H]: 225.092080; found: 225.092105. The enantiomeric ratio was measured by HPLC analysis using ChiralpakOD-3, heptan/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 7.1 min (major) and t_R = 12.7 min (minor). er = 96.7:3.3. $[\alpha]_D^{25} = -14.8$ (*c* 0.50, CHCl₃).

(S)-1-(3-bromophenyl)isochroman-6-ol (3h): Prepared according to the general procedure. 22.8 mg yellow solid, 75%. **¹H NMR** (500 MHz, CDCl₃): δ 7.49–7.41 (m, 2H), 7.26–7.17 (m, 2H), 6.65–6.52 (m, 3H), 5.64 (s, 1H), 4.99 (br s, 1H), 4.15 (ddd, J = 11.4, 5.6, 3.8 Hz, 1H), 3.89 (ddd, J = 13.5, 9.6, 4.1 Hz, 1H), 3.07 (ddd, J = 16.5, 9.5, 5.7 Hz, 1H), 2.74 (dd, J = 16.4, 3.9 Hz, 1H). **¹³C NMR** (126 MHz, CDCl₃): δ 154.41, 144.67, 135.49, 131.92, 131.37, 130.11, 128.90, 128.27, 12.61, 122.69, 115.07, 113.73, 78.86, 63.84, 28.90. **HRMS m/z** (ESI): calcd. for C₁₅H₁₃BrO₂Na [M+Na]: 326.999270; found: 326.999124. The enantiomeric ratio was measured by

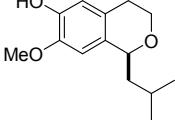
HPLC analysis using Chiralpak AS-3, heptane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 5.2 min (major) and t_R = 5.9 min (minor). er = 99.2:0.8. $[\alpha]_D^{25} = -5.6$ (*c* 0.50, CHCl₃).

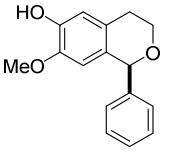
(S)-1-(3-methoxyphenyl)isochroman-6-ol (3i): Prepared according to the general procedure. 23.8 mg yellow oil, 93%. **¹H NMR** (500 MHz, CDCl₃): δ 7.34–7.17 (m, 1H), 6.90 (d, J = 7.6 Hz, 1H), 6.88–6.80 (m, 2H), 6.63 (d, J = 8.4 Hz, 1H), 6.59 (d, J = 2.6 Hz, 1H), 6.54 (dd, J = 8.4, 2.6 Hz, 1H), 5.65 (s, 1H), 5.08 (br s, 1H), 4.16 (ddd, J = 11.4, 5.5, 3.9 Hz, 1H), 3.90 (ddd, J = 13.6, 9.5, 4.1 Hz, 1H), 3.78 (s, 3H), 3.06 (ddd, J = 16.4, 9.4, 5.6 Hz), 2.74 (dd, J = 16.4, 4.0, 1H). **¹³C NMR** (126 MHz, CDCl₃): δ 159.76, 154.31, 143.87, 135.41, 129.52, 129.48, 128.32, 121.41, 114.91, 114.38, 113.84, 113.57, 79.48, 63.78, 55.37, 29.00. **HRMS m/z** (ESI): calcd. for C₁₆H₁₆O₃Na [M+Na]: 279.099350; found: 279.099164. The enantiomeric ratio was measured by HPLC analysis using Chiralpak AD-3, heptane/*i*-PrOH = 94:6, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 19.4 min (minor) and t_R = 20.6 min (major). er = 98.1:1.9. $[\alpha]_D^{25} = -14.4$ (*c* 0.50, CHCl₃).

(S)-1-(4-bromophenyl)isochroman-6-ol (3j): Prepared according to the general procedure. 26.4 mg yellow solid, 87%. **¹H NMR** (500 MHz, CDCl₃): δ 7.46 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 6.89–6.31 (m, 3H), 5.64 (s, 1H), 5.13 (br s, 1H), 4.14 (ddd, J = 11.4, 5.4, 3.9 Hz, 1H), 3.90 (ddd, J = 13.5, 9.6, 4.0 Hz, 1H), 3.06 (ddd, J = 16.5, 9.6, 5.5 Hz, 1H), 2.73 (td, J = 16.5, 4.0 Hz, 1H). **¹³C NMR** (126 MHz, CDCl₃): δ 154.42, 141.36, 135.45, 131.69, 130.66, 129.05, 128.23, 122.29, 115.02, 113.67, 78.88, 63.82, 28.95. **HRMS m/z** (ESI): calcd. for C₁₅H₁₃BrO₂Na [M+Na]: 326.999310; found: 326.999124. The enantiomeric ratio was measured by HPLC analysis using Chiralpak AD-3, heptane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 4.9 min (major) and t_R = 5.3 min (minor). er = 98.2:1.8. $[\alpha]_D^{25} = +4.0$ (*c* 0.50, CHCl₃).

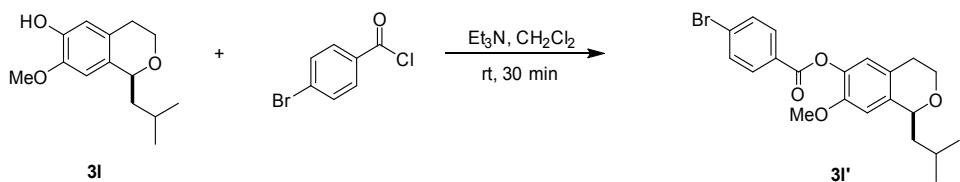
(S)-1-(naphthalen-1-yl)isochroman-6-ol (3k): Prepared according to the general procedure. 20.1 mg yellow solid, 73%. **¹H NMR** (500 MHz, CDCl₃): δ 7.90–7.79 (m, 3H), 7.76 (s, 1H), 7.55–7.44 (m, 2H), 7.40 (dd, J = 8.6, 1.7 Hz, 1H), 6.64 (d, J = 2.5 Hz, 1H), 6.62 (d, J = 3.50 Hz, 1H), 6.53 (dd, J = 8.50, 2.6 Hz, 1H), 5.84 (s, 1H), 4.20 (ddd, J = 11.4, 5.6, 3.8 Hz, 1H), 3.95 (ddd, J = 13.6, 9.6, 4.40 Hz, 1H), 3.12 (ddd, J = 16.5, 9.5, 5.5 Hz, 1H), 2.76 (dd, J = 16.5, 3.8, 1H). **¹³C NMR** (126 MHz, CDCl₃): δ 154.29, 139.72, 135.59, 133.37, 133.20, 129.67, 128.56, 128.50, 128.21, 128.16, 127.82, 126.53, 126.23, 114.98, 113.60, 79.74, 63.89, 29.07. **HRMS m/z** (ESI):

calcd. for $C_{19}H_{16}O_2Na$ [M+Na]: 299.104430; found: 299.104249. The enantiomeric ratio was measured by HPLC analysis using Chiralpak AD-3, heptane/*i*-PrOH = 94:6, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 12.3 min (major) and t_R = 13.5 min (minor). er 95.4:4.6. $[\alpha]_D^{25} = +25.4$ (*c* 0.27, CHCl₃).

(S)-1-isobutyl-7-methoxyisochroman-6-ol (3l): Prepared according to the general procedure. 21.7 mg  white solid, 92%. **¹H NMR** (500 MHz, CD₂Cl₂): δ 6.61 (s, 1H), 6.53 (s, 1H), 5.53 (br s, 1H), 4.67 (dd, J = 10.4, 2.0 Hz, 1H), 4.07–3.99 (m, 1H), 3.84 (s, 3H), 3.69 (ddd, J = 12.8, 8.7, 4.1 Hz, 1H), 2.79 (tddd, J = 16.2, 8.7, 5.3, 1.0 Hz, 1H), 2.58 (dd, J = 16.1, 4.4 Hz, 1H), 2.01–1.87 (m, 1H), 1.71 (ddd, J = 14.4, 10.4, 3.9 Hz, 1H), 1.54 (ddd, J = 14.2, 9.9, 2.9 Hz, 1H), 1.01 (d, J = 6.7 Hz, 3H), 0.95 (d, J = 6.7 Hz, 3H). **¹³C NMR** (126 MHz, CDCl₃): δ 145.64, 144.47, 131.27, 127.16, 124.68, 107.84, 74.14, 63.12, 56.63, 45.83, 28.99, 25.05, 24.30, 21.80. **HRMS m/z** (ESI): calcd. for $C_{14}H_{19}O_3$ [M-H]: 235.133940; found: 235.133970. The enantiomeric ratio was measured by HPLC analysis using OD-3, heptane/*i*-PrOH = 95:5, flow rate = 1 mL/min, λ = 279 nm t_R = 5.8 min (major) and t_R = 7.0 min (minor). er = 99.6:0.4 $[\alpha]_D^{25} = -116.4$ (*c* 0.50, CHCl₃).

(S)-7-methoxy-1-phenylisochroman-6-ol (3m): Prepared according to the general procedure. 25.0 mg  yellow solid, 98%. **¹H NMR** (500 MHz, CDCl₃): δ 7.43–7.28 (m, 5H), 6.73 (s, 1H), 6.21 (s, 1H), 5.67 (s, 1H), 5.56 (br s, 1H), 4.13 (ddd, J = 11.3, 5.3, 4.3 Hz, 1H), 3.88 (ddd, J = 13.3, 9.1, 4.1 Hz, 1H), 3.36 (s, 3H), 3.01 (ddd, J = 16.20, 9.1, 5.4 Hz, 1H), 2.71 (dd, J = 16.1, 4.2 Hz, 1H). **¹³C NMR** (126 MHz, CDCl₃): δ 159.76, 154.31, 143.87, 135.41, 129.52, 129.48, 128.32, 121.41, 114.91, 114.38, 113.84, 113.57, 79.48, 63.78, 55.37, 29.00. **HRMS m/z** (ESI): calcd. for $C_{16}H_{16}O_3Na$ [M+Na]: 279.099230; found: 279.099164. The enantiomeric ratio was measured by HPLC analysis using ChiralpakAD-3, heptane/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 11.8 min (major) and t_R = 16.2 min (minor). er = 98.8:1.2. $[\alpha]_D^{25} = -60.3$ (*c* 0.60, CHCl₃).

4.Determination of the Absolute Configuration



(S)-1-isobutyl-7-methoxyisochroman-6-yl 4-bromobenzoate (3I'): A 2-mL GC vial was charged with starting material **3I** (0.08 mmol), followed by triethylamine (1.2 equiv., 0.10 mmol), 4-bromobenzoylchloride (1.2 equiv., 0.10 mmol) and a magnetic stirring bar at room temperature. The vial was filled with argon and sealed. It was then stirred at room temperature for half an hour. The progress of the reaction was monitored by TLC. Purification was performed by column chromatography or preparative thin layer chromatography on silica gel using EtOAc/*i*-hexanes as the eluents. **¹H NMR** (500 MHz, CD₂Cl₂): δ 8.04 (dd, *J* = 8.7, 2.0 Hz, 2H), 7.68 (dd, *J* = 8.8, 2.0 Hz, 2H), 6.88 (s, 1H), 6.69 (s, 1H), 4.76 (dd, *J* = 10.4, 2.0 Hz, 1H), 4.13–4.03 (m, 1H), 3.77 (s, 3H), 3.76–3.69 (m, 1H), 2.93–2.79 (m, 1H), 2.66 (dd, *J* = 16.0, 4.4 Hz, 1H), 2.06–1.92 (m, 1H), 1.80 (ddd, *J* = 14.2, 10.5, 3.9 Hz, 1H), 1.60 (ddd, *J* = 12.0, 9.9, 2.9 Hz, 1H), 1.04 (d, *J* = 6.7 Hz, 3H), 0.98 (d, *J* = 6.7 Hz, 3H). **¹³C NMR** (126 MHz, CD₂Cl₂): δ 164.51, 149.77, 138.46, 138.41, 132.34, 132.04, 128.96, 128.89, 126.83, 123.12, 109.44, 74.09, 62.78, 56.42, 45.52, 28.59, 24.94, 24.11, 21.59. **HRMS m/z** (ESI): calcd. for C₂₁H₂₃O₄BrNa [M+Na]: 441.067410; found 441.067204. The enantiomeric ratio was measured by HPLC analysis using Chiralpak AD-3, heptane/*i*-PrOH = 70:30, flow rate = 1.0 mL/min, λ = 279 nm, t_R = 4.0 min (minor) and t_R = 5.2 min (major). er = 99.1:0.9.

Compound **3I'** was recrystallized from methanol. The absolute configuration of **3I'** was assigned by X-ray crystallography.

X-Ray structural analysis parameter for **3I'**:

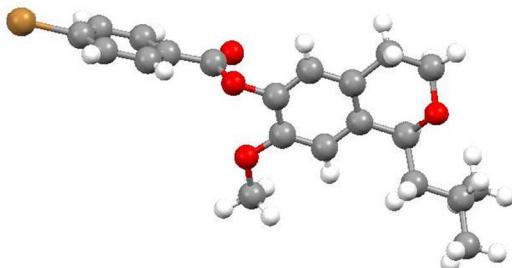


Table 1. Crystal data and structure refinement.

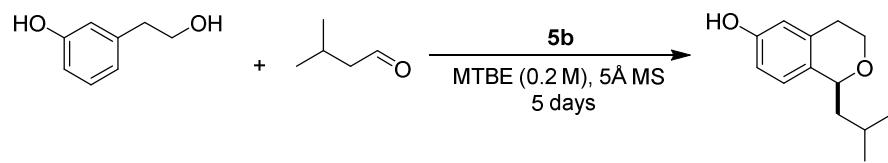
Identification code	9920	
Empirical formula	$C_{21}H_{23}BrO_4$	
Color	colorless	
Formula weight	$419.30 \text{ g} \cdot \text{mol}^{-1}$	
Temperature	100.15 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2₁2₁2₁, (no. 19)	
Unit cell dimensions	$a = 5.4738(5) \text{ Å}$	$\alpha = 90^\circ$.
	$b = 7.8392(11) \text{ Å}$	$\beta = 90^\circ$.
	$c = 45.290(3) \text{ Å}$	$\gamma = 90^\circ$.
Volume	$1943.4(4) \text{ Å}^3$	
Z	4	
Density (calculated)	$1.433 \text{ Mg} \cdot \text{m}^{-3}$	
Absorption coefficient	2.138 mm^{-1}	
F(000)	864 e	
Crystal size	$0.18 \times 0.12 \times 0.06 \text{ mm}^3$	
θ range for data collection	2.637 to 31.097°.	
Index ranges	$-7 \leq h \leq 7, -11 \leq k \leq 11, -65 \leq l \leq 65$	
Reflections collected	31126	
Independent reflections	6225 [$R_{\text{int}} = 0.0748$]	
Reflections with $I > 2\sigma(I)$	4759	
Completeness to $\theta = 25.242^\circ$	99.8 %	

Absorption correction	Gaussian	
Max. and min. transmission	0.89 and 0.75	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6225 / 0 / 238	
Goodness-of-fit on F^2	1.112	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0478$	$wR^2 = 0.1213$
R indices (all data)	$R_1 = 0.0759$	$wR^2 = 0.1534$
Absolute structure parameter	-0.031(7)	
Largest diff. peak and hole	0.7 and -1.2 e · Å ⁻³	

Table 2. Bond lengths [\AA] and angles [$^\circ$].

Br(1)-C(19)	1.903(4)	O(1)-C(5)	1.433(6)	O(1)-
C(6)	1.432(6)	O(2)-C(2)	1.350(6)	O(2)-
C(10)	1.428(6)	O(3)-C(1)	1.402(5)	O(3)-
C(15)	1.364(6)	O(4)-C(15)	1.196(6)	C(1)-
C(2)	1.401(7)	C(1)-C(9)	1.376(7)	C(2)-
C(3)	1.380(6)	C(3)-C(4)	1.405(7)	C(4)-
C(5)	1.527(6)	C(4)-C(8)	1.390(7)	C(5)-
C(11)	1.524(7)	C(6)-C(7)	1.517(7)	C(7)-
C(8)	1.511(7)	C(8)-C(9)	1.403(6)	C(11)-
C(12)	1.537(7)	C(12)-C(13)	1.521(8)	C(12)-
C(14)	1.548(8)	C(15)-C(16)	1.485(6)	C(16)-
C(17)	1.396(6)	C(16)-C(21)	1.385(6)	C(17)-
C(18)	1.388(6)	C(18)-C(19)	1.383(7)	C(19)-
C(20)	1.376(7)	C(20)-C(21)	1.383(6)	
C(6)-O(1)-C(5)	111.5(4)	C(2)-O(2)-C(10)	117.2(4)	C(15)-
O(3)-C(1)	114.3(3)	C(2)-C(1)-O(3)	118.5(4)	C(9)-
C(1)-O(3)	119.6(4)	C(9)-C(1)-C(2)	121.9(4)	O(2)-
C(2)-C(1)	115.9(4)	O(2)-C(2)-C(3)	126.2(4)	C(3)-
C(2)-C(1)	117.9(4)	C(2)-C(3)-C(4)	121.2(4)	C(3)-
C(4)-C(5)	120.3(4)	C(8)-C(4)-C(3)	119.9(4)	C(8)-
C(4)-C(5)	119.7(4)	O(1)-C(5)-C(4)	111.2(4)	O(1)-
C(5)-C(11)	105.5(4)	C(11)-C(5)-C(4)	113.8(4)	O(1)-
C(6)-C(7)	109.9(4)	C(8)-C(7)-C(6)	111.3(4)	C(4)-
C(8)-C(7)	121.4(4)	C(4)-C(8)-C(9)	119.1(4)	C(9)-
C(8)-C(7)	119.5(4)	C(1)-C(9)-C(8)	119.8(4)	C(5)-
C(11)-C(12)	114.4(4)	C(11)-C(12)-C(14)	112.5(5)	C(13)-
C(12)-C(11)	110.1(5)	C(13)-C(12)-C(14)	112.6(6)	O(3)-
C(15)-C(16)	112.9(4)	O(4)-C(15)-O(3)	122.5(4)	O(4)-
C(15)-C(16)	124.6(4)	C(17)-C(16)-C(15)	123.1(4)	C(21)-
C(16)-C(15)	117.1(4)	C(21)-C(16)-C(17)	119.8(4)	C(18)-
C(17)-C(16)	120.0(4)	C(19)-C(18)-C(17)	118.6(4)	C(18)-
C(19)-Br(1)	119.8(4)	C(20)-C(19)-Br(1)	118.0(3)	C(20)-
C(19)-C(18)	122.2(4)	C(19)-C(20)-C(21)	118.7(4)	C(20)-
C(21)-C(16)	120.6(4)			

5. Oxa-Pictet–Spengler reaction with low catalyst loading^a



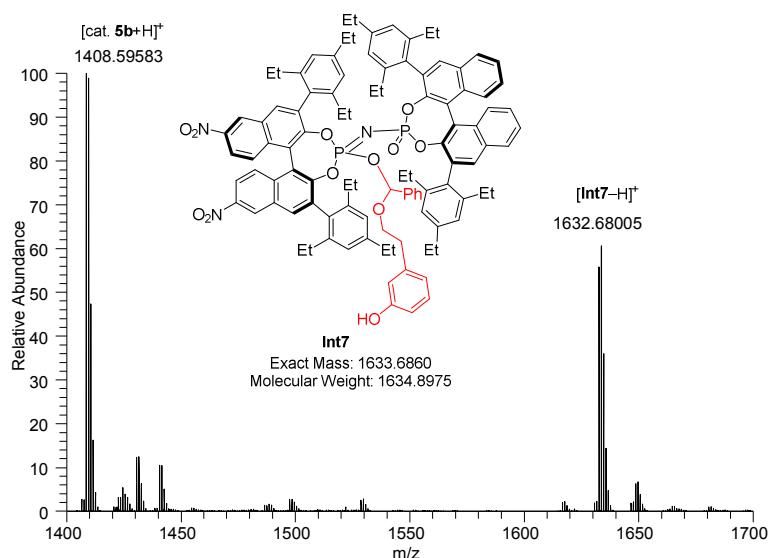
entry	catalyst loading (mol%, mg)	yield (%)	er
1.	5 (7 mg)	98.7	97.6:2.4
2.	2.5 (3.5mg)	55	97.8:2.2

^aReactions were run at 0.1 mmol scale and yields were determined from ¹H NMR using an internal standard.

6. ESI-MS Study

Electrospray Ionization Mass Spectrometry (ESI-MS) studies were performed to confirm the covalent catalyst intermediate as suggested by the DFT calculation. We have performed a reaction using substrate **1d**, catalyst **5b** under the optimized reaction conditions with benzaldehyde and the course of the reaction was studied with ESI-MS. New peaks at m/z 1632 (Figure 1a), matching the catalyst-substrate adduct (**Int7**), appeared within minutes and the intensity of the peak increased with time (Figure 2). A similar observation was observed in case of isovaleraldehyde (Figure 1b).

(a)



(b)

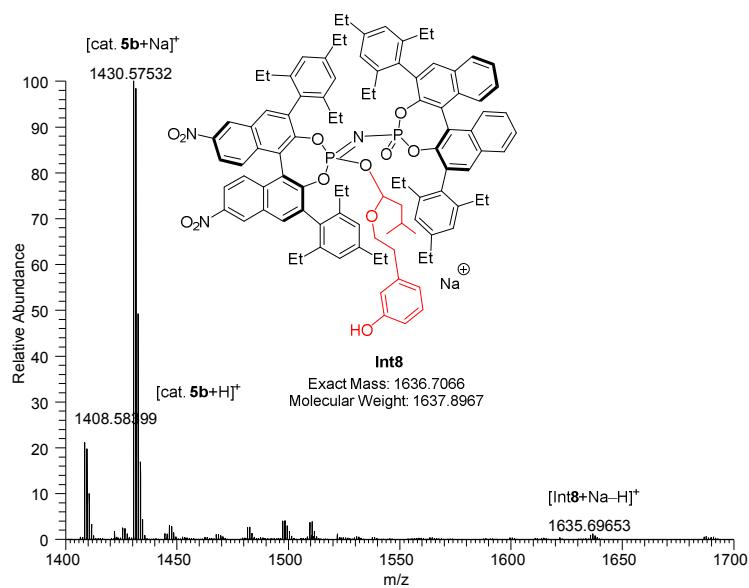


Figure 1. (a) ESI-MS of the covalent catalyst acetal intermediate with benzaldehyde and (b) isovaleraldehyde.

After three days the reaction was near to completion and was treated with trimethylamine (TEA). At this point, the intermediate peak disappeared and a peak matching the catalyst plus two molecules of TEA appeared (Figure 2). When MS/MS of the **Int7** peak was measured, a fragment appeared at m/z 968 (Figure 3) corresponding to **Int7'**.

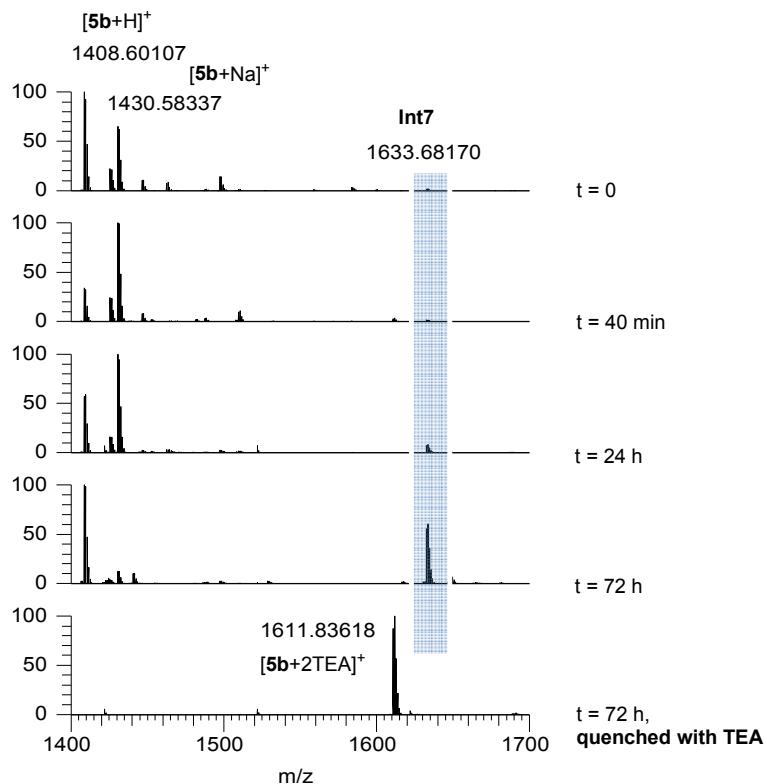


Figure 2. MS/MS of the peak m/z1633 and (c) ESI-MS study of the oxa-Pictet–Spengler reaction with time.

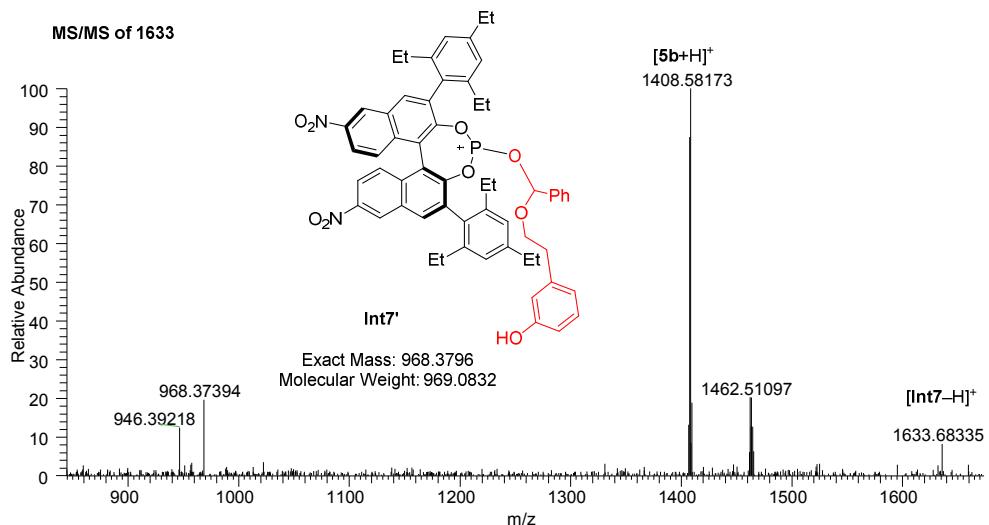
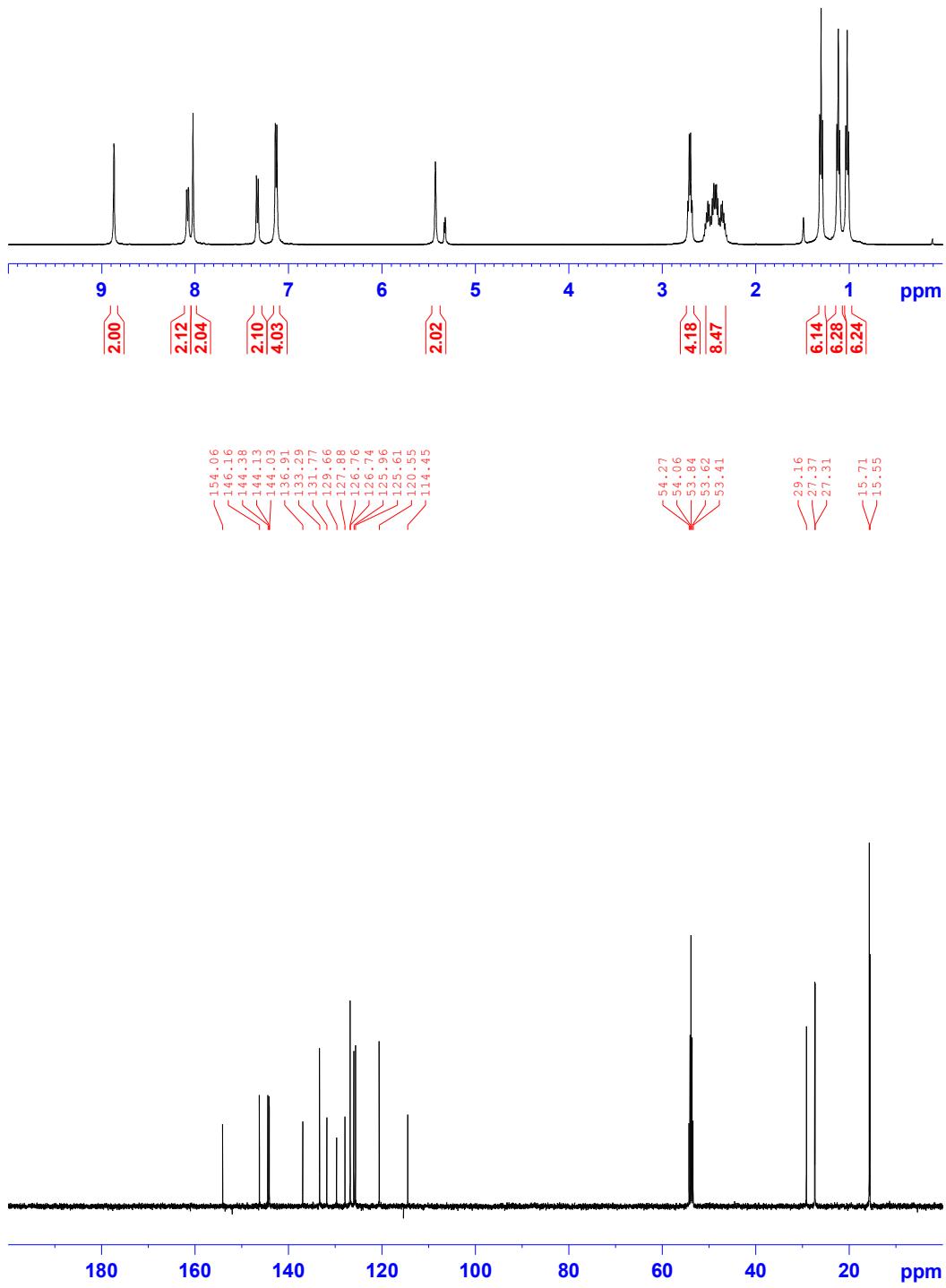
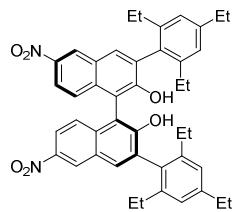
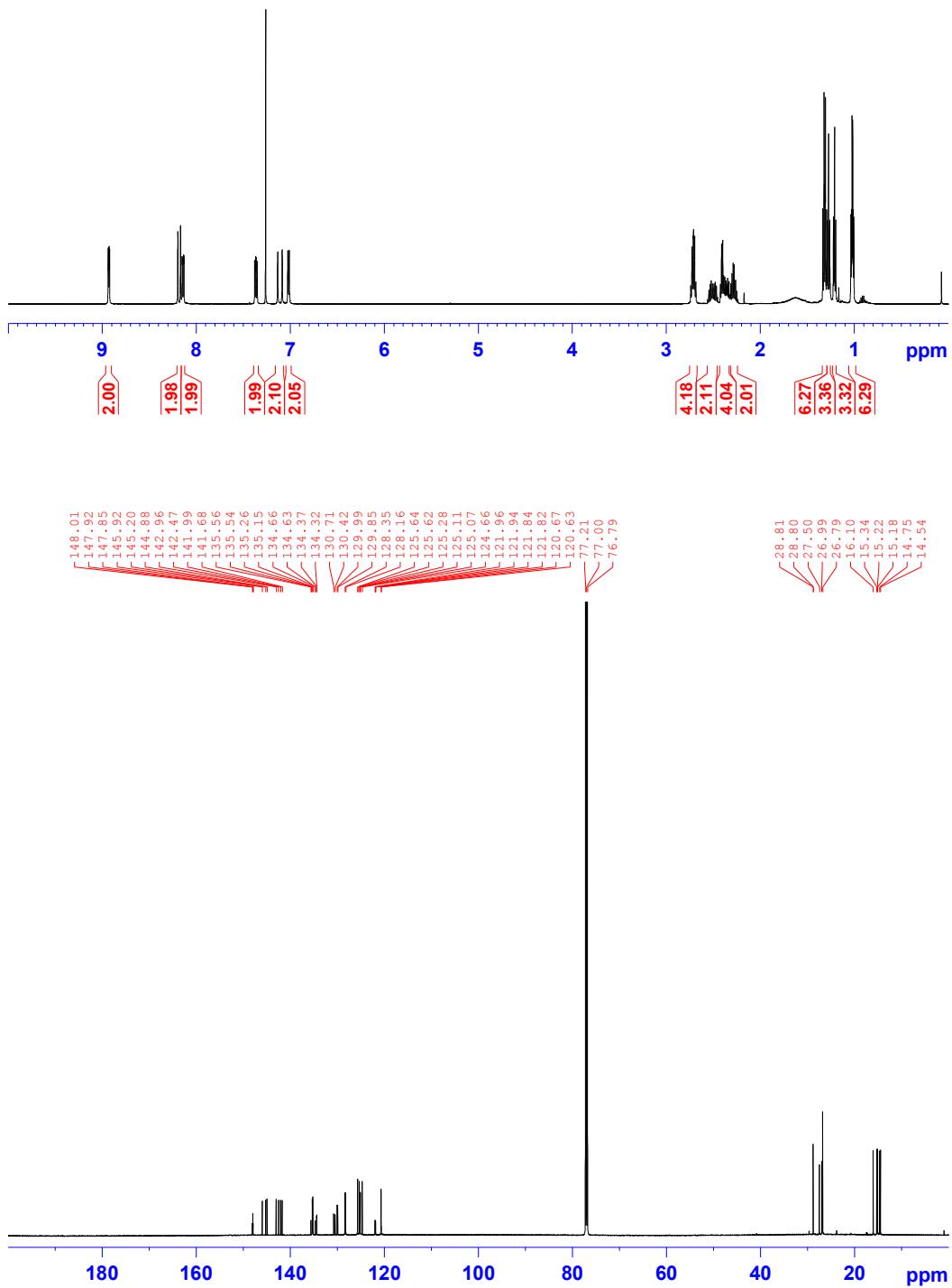
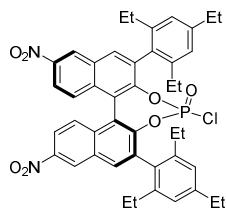


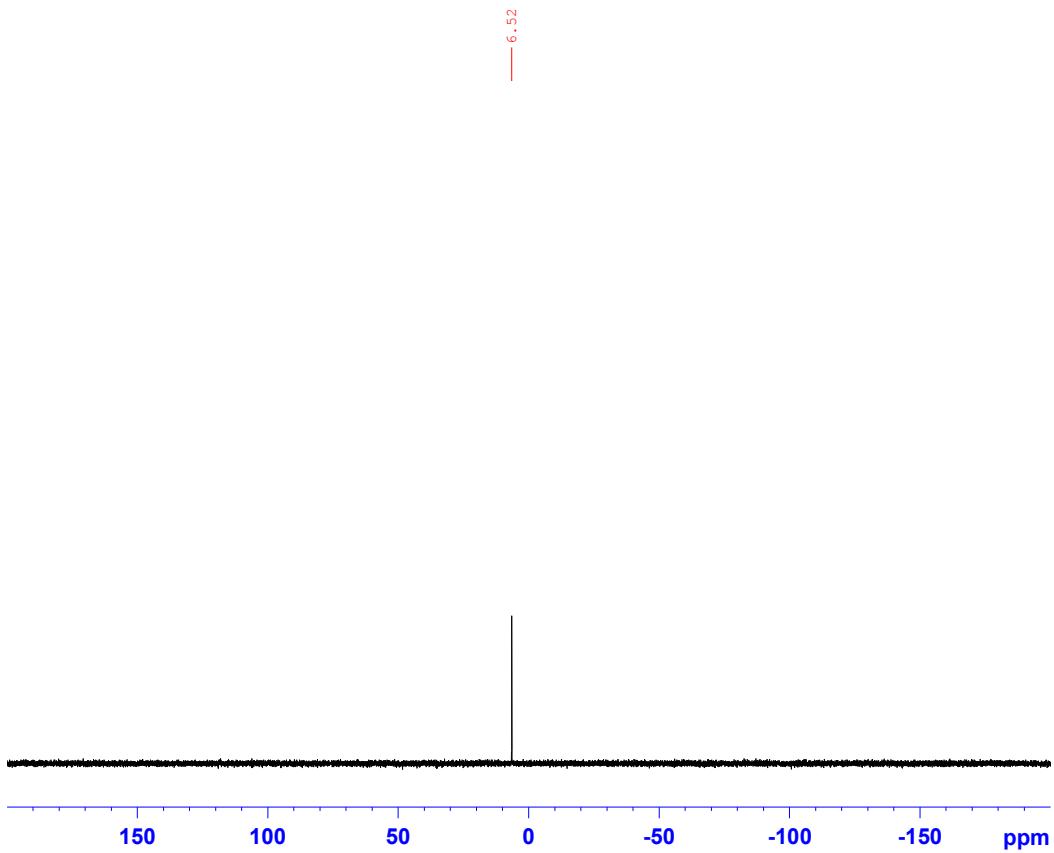
Figure 3. MS/MS of the **Int7** peak m/z1633.

¹H and ¹³C NMR Spectra 10

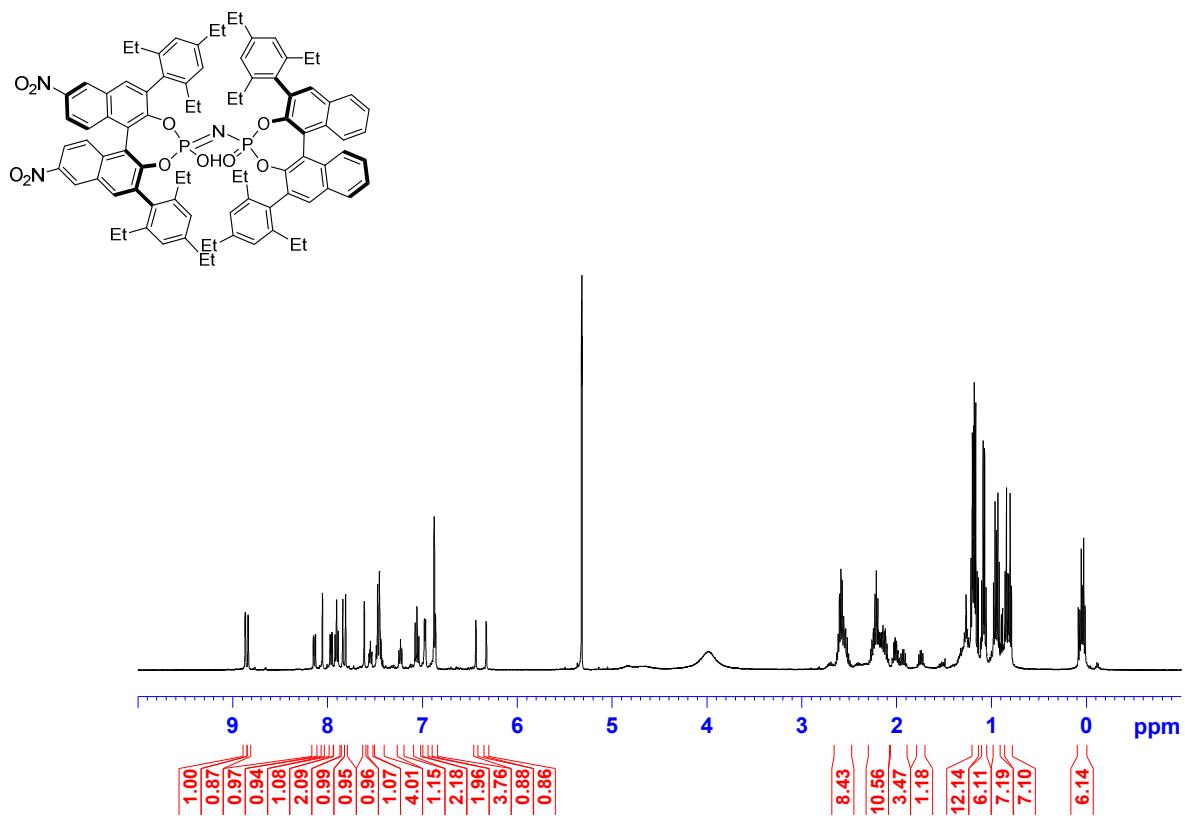


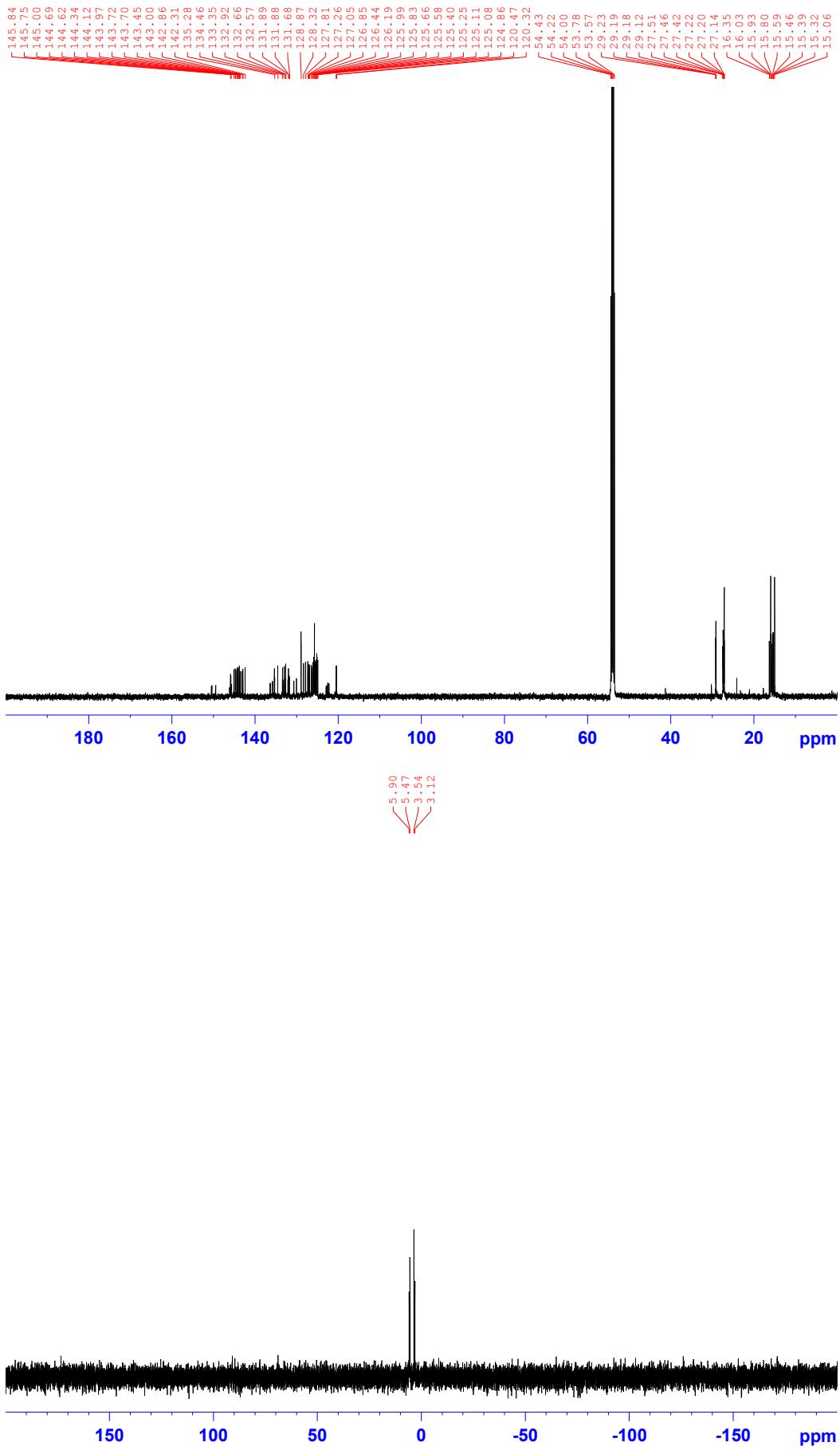
¹H, ¹³C and ³¹P NMR Spectra 11



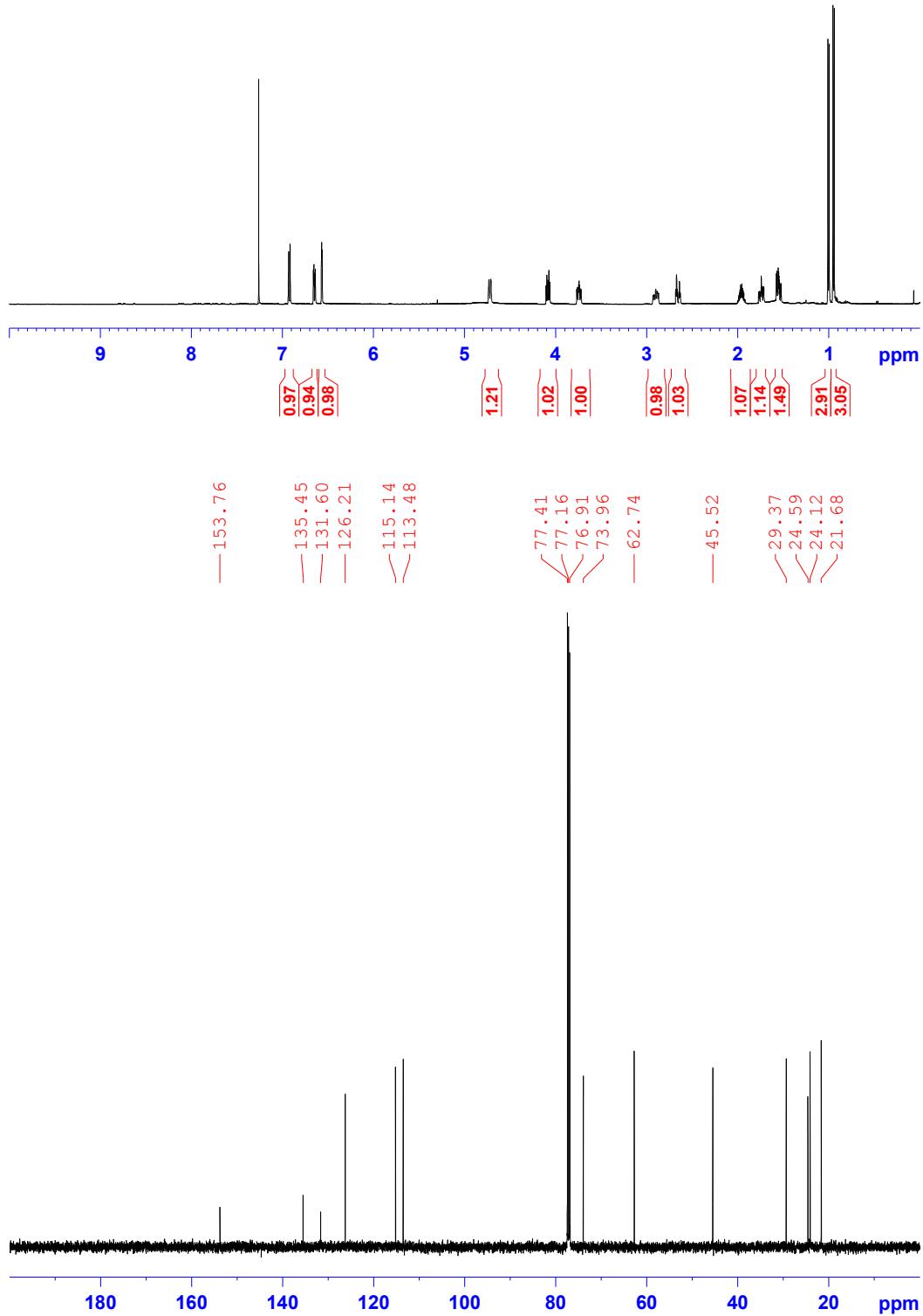
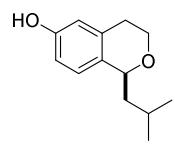


¹H, ¹³C and ³¹P NMR Spectra 5b

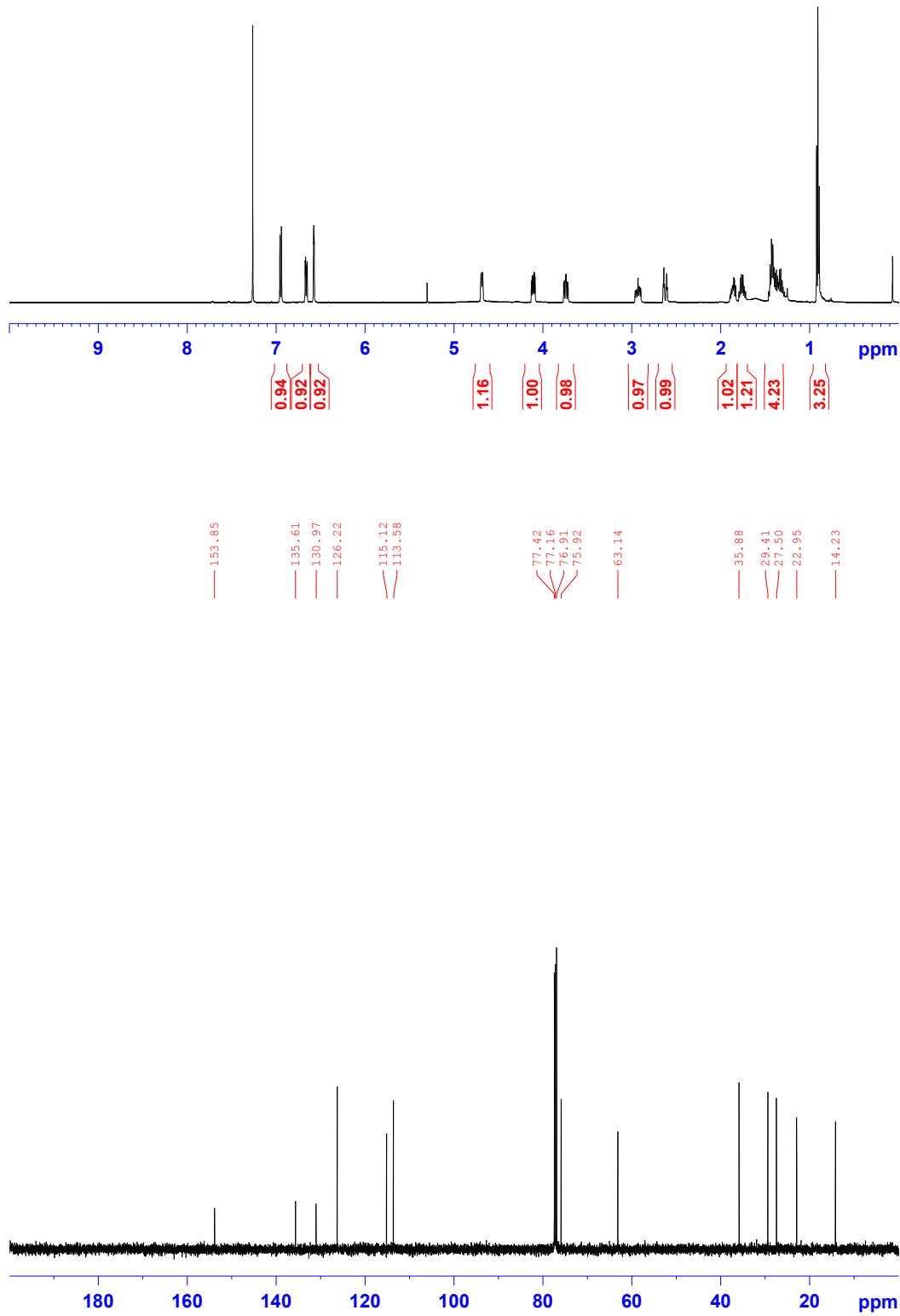
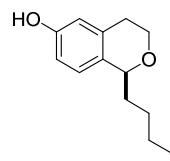




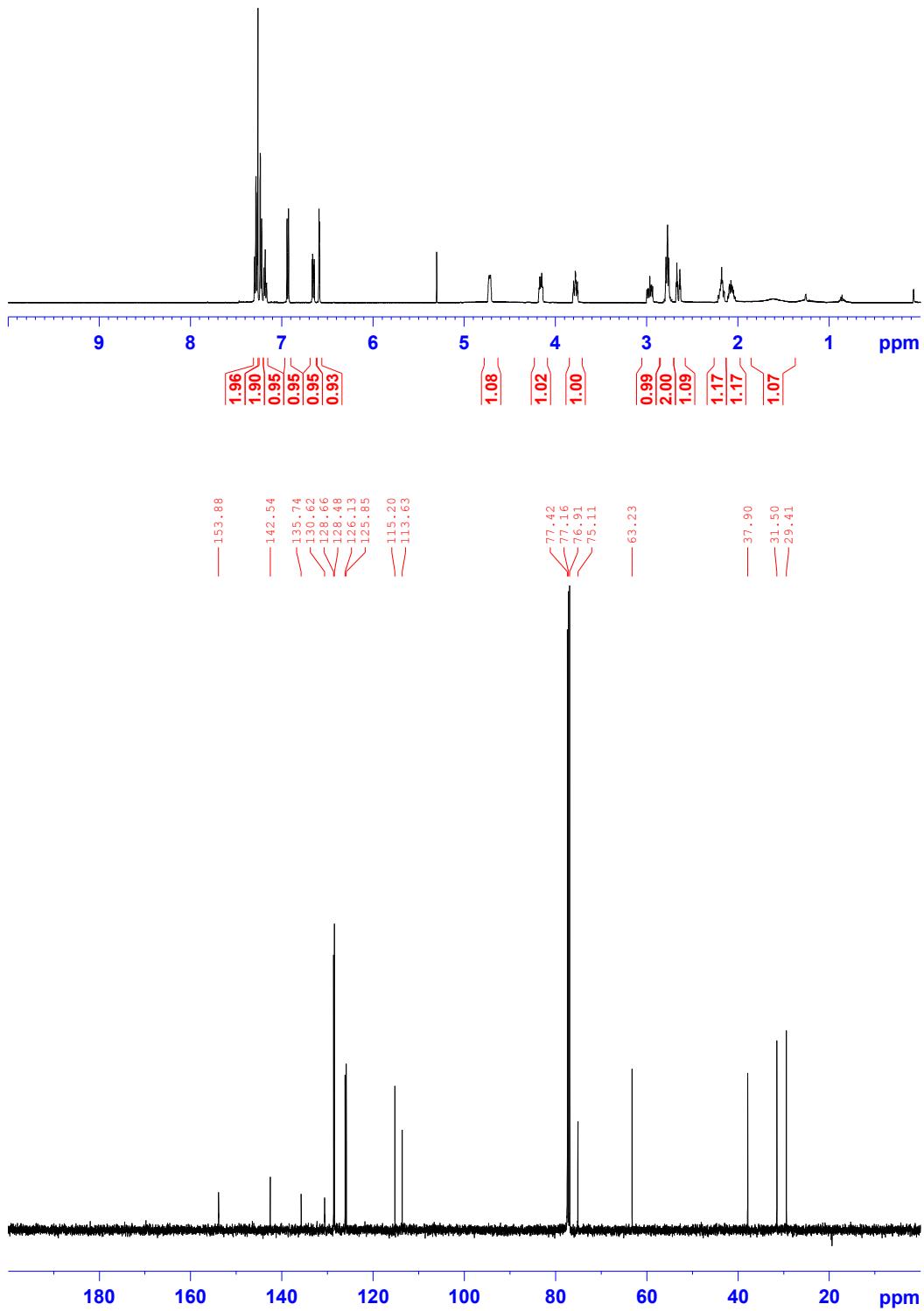
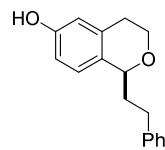
¹H and ¹³C NMR Spectra 3d



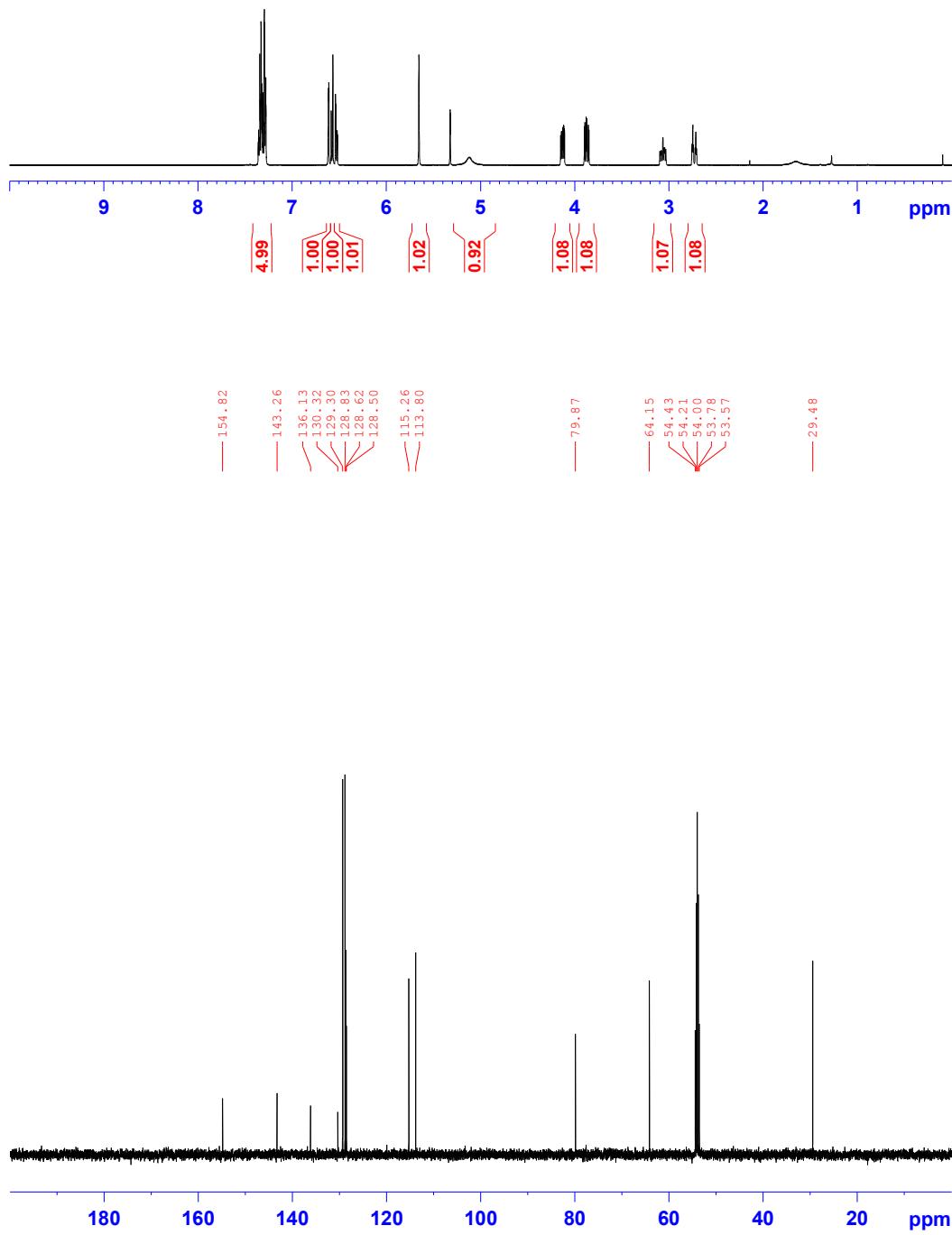
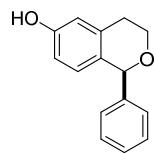
¹H and ¹³C NMR Spectra 3e



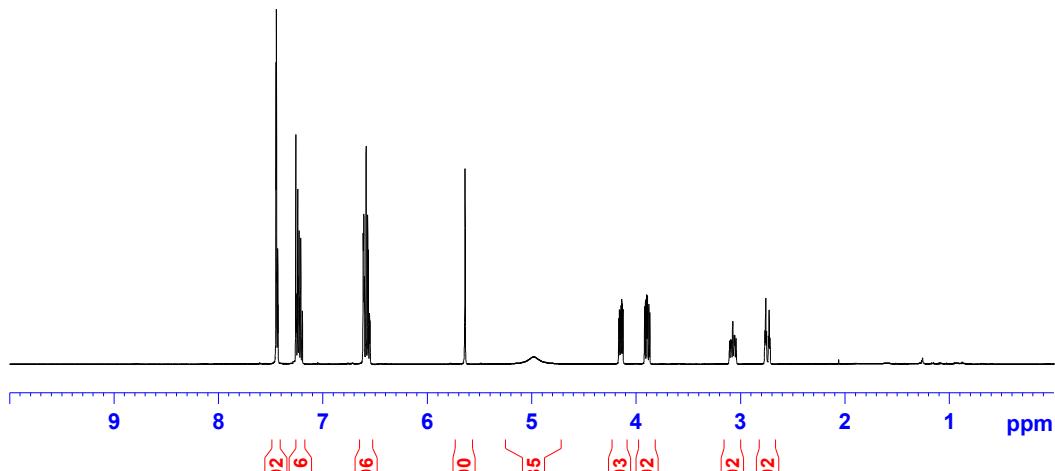
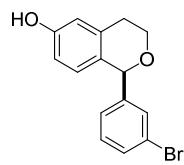
¹H and ¹³C NMR Spectra 3f



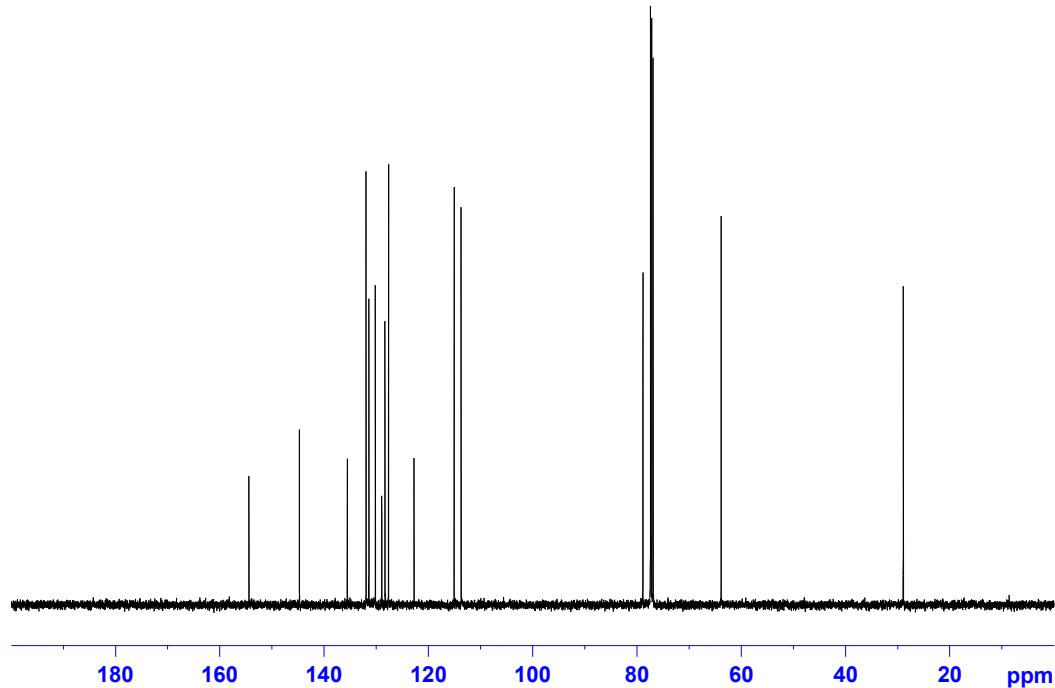
¹H and ¹³C NMR Spectra 3g



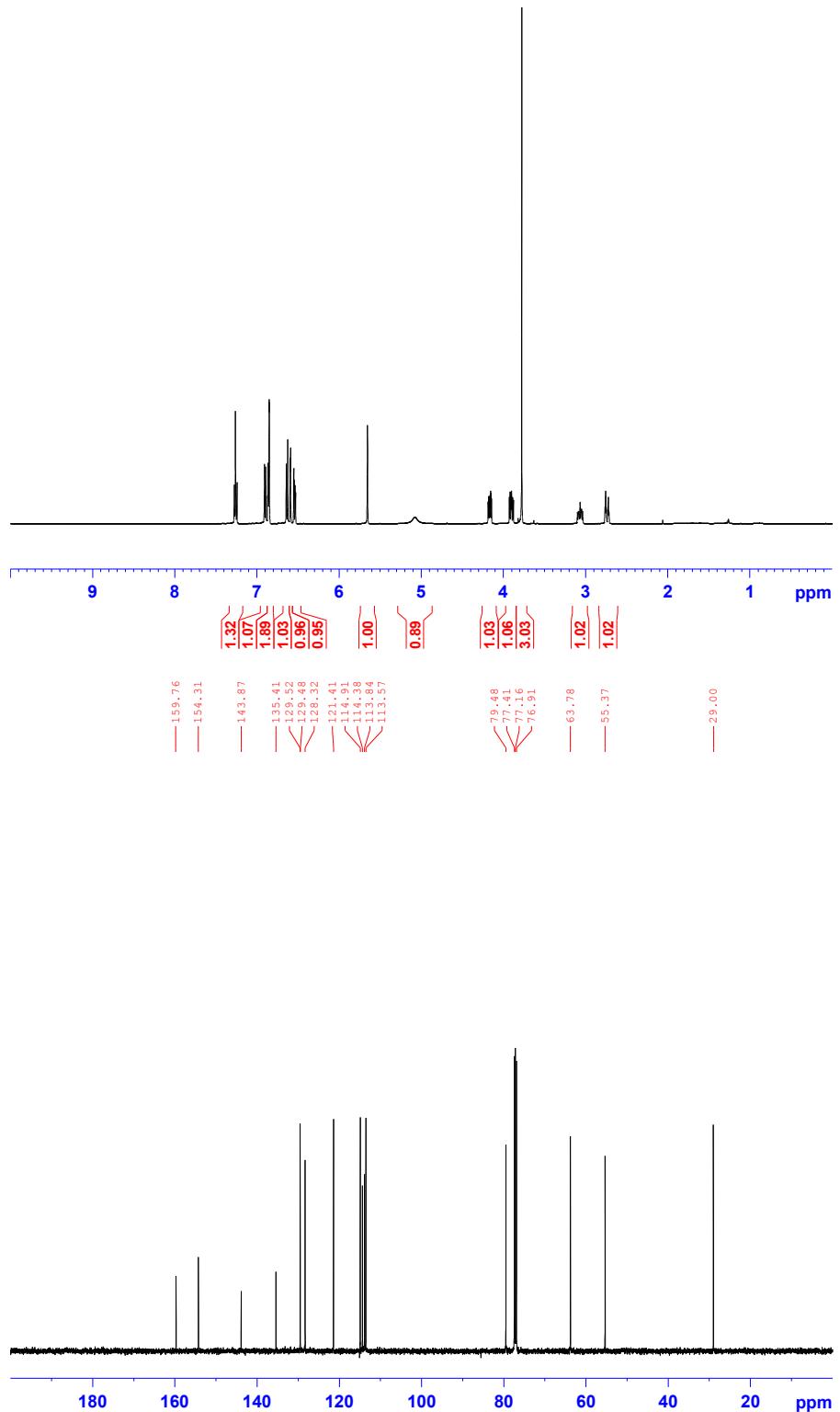
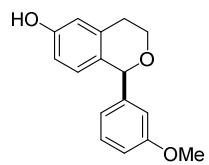
¹H and ¹³C NMR Spectra 3h



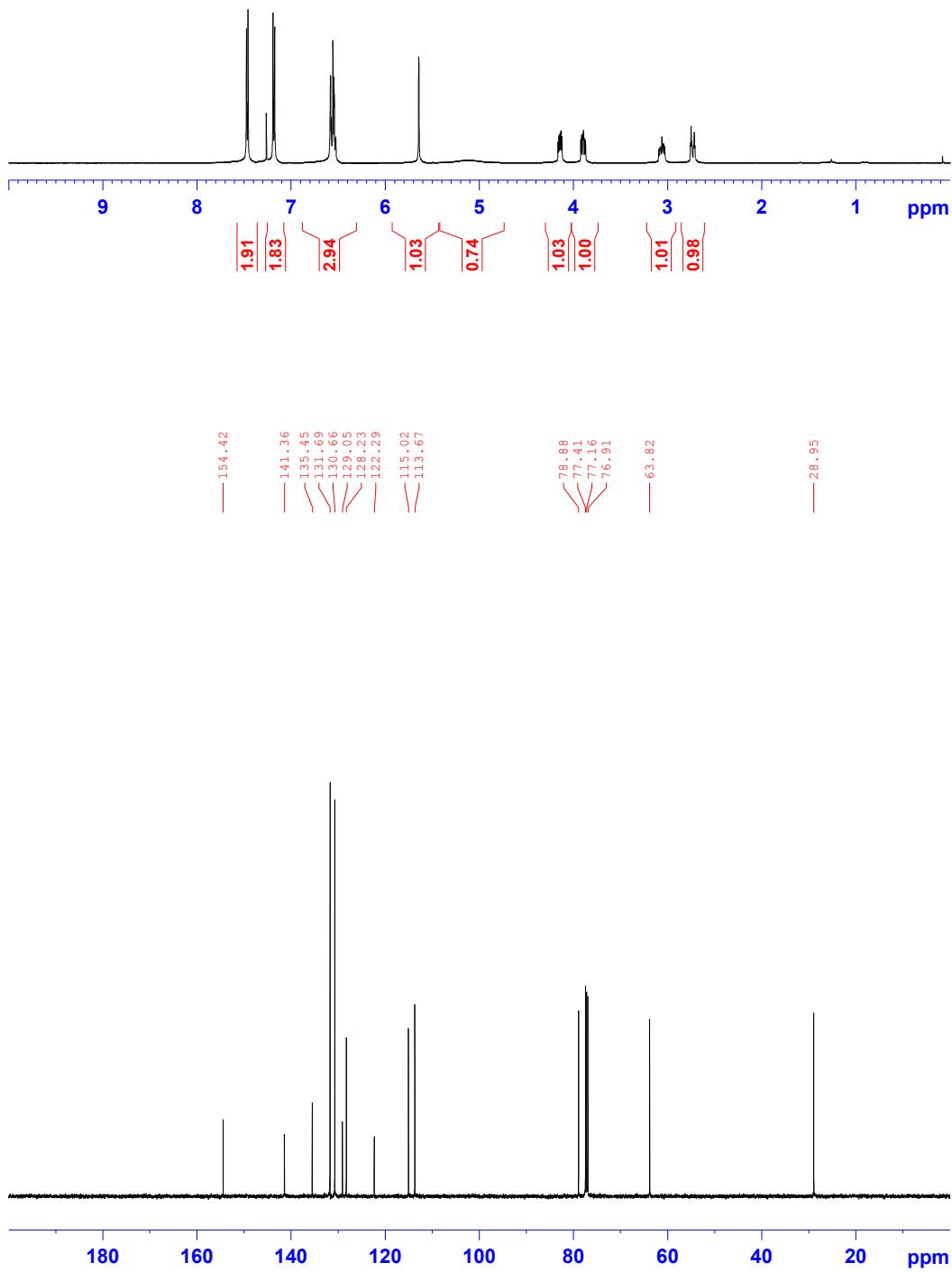
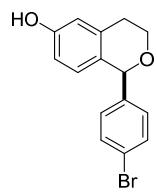
154.41
144.67
135.19
131.92
131.37
130.11
128.90
128.27
127.61
122.69
115.07
113.73
78.86
77.41
77.16
76.91
63.84
28.93



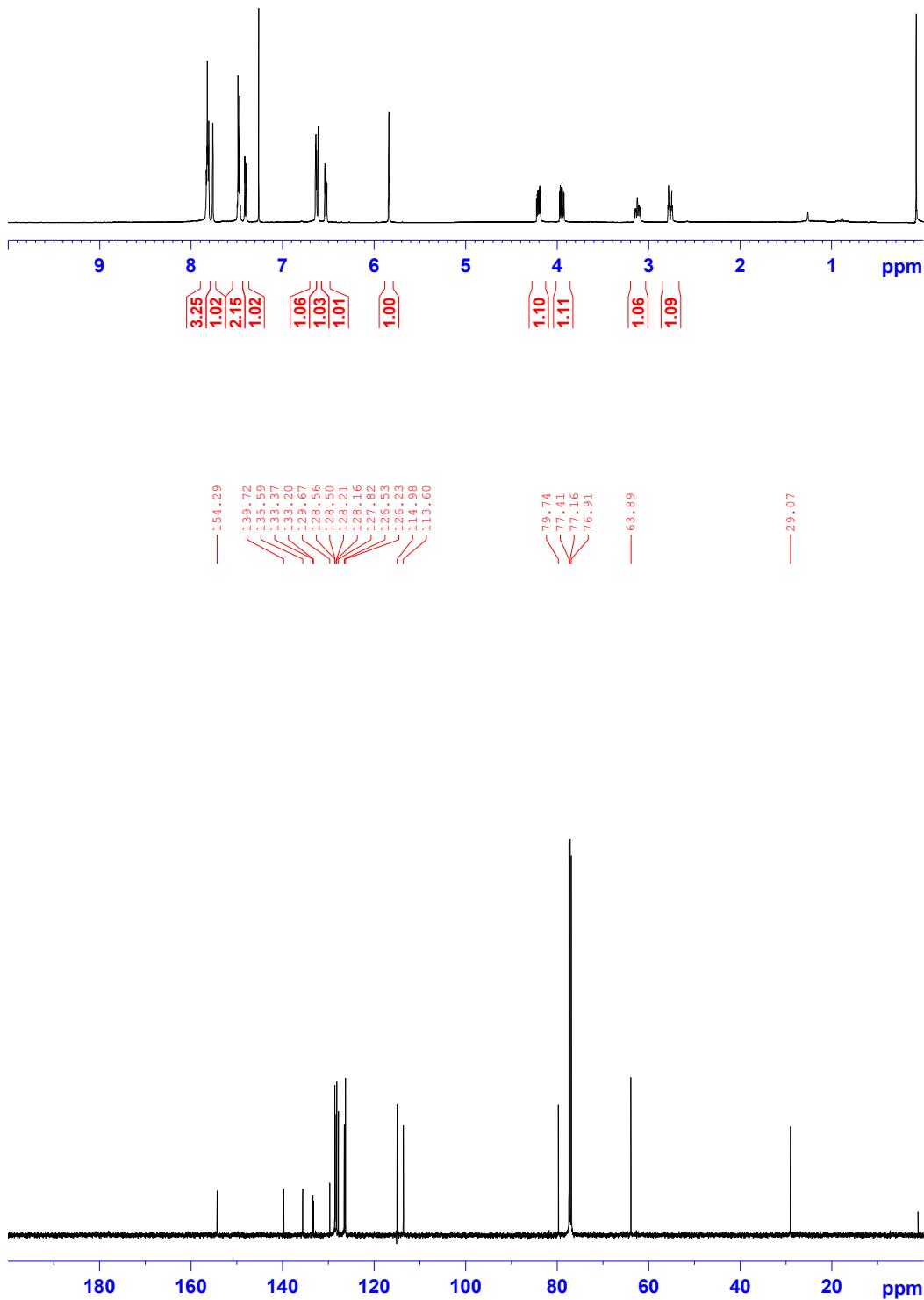
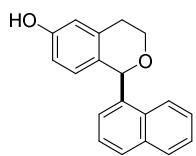
¹H and ¹³C NMR Spectra 3i



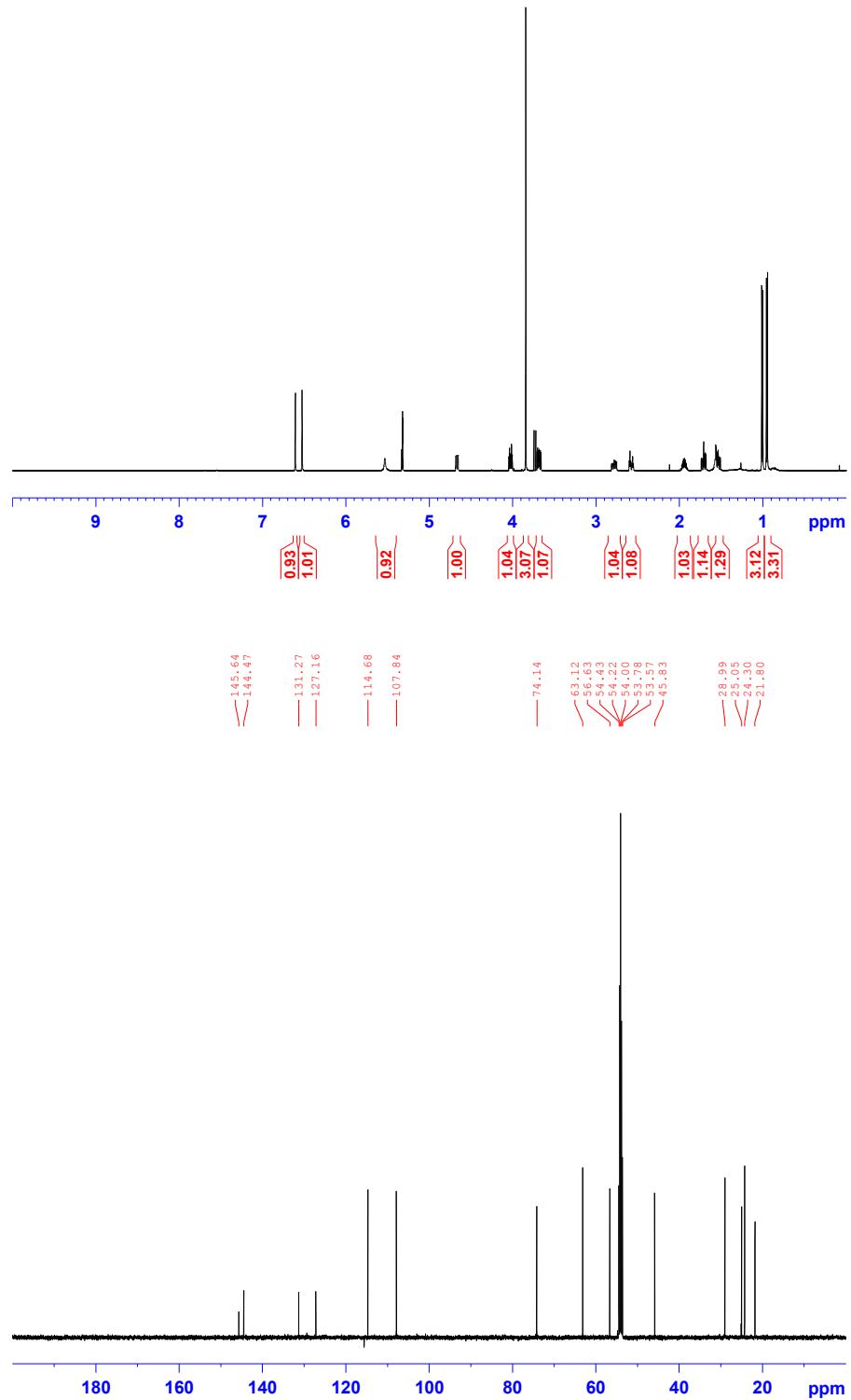
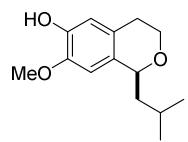
¹H and ¹³C NMR Spectra 3j



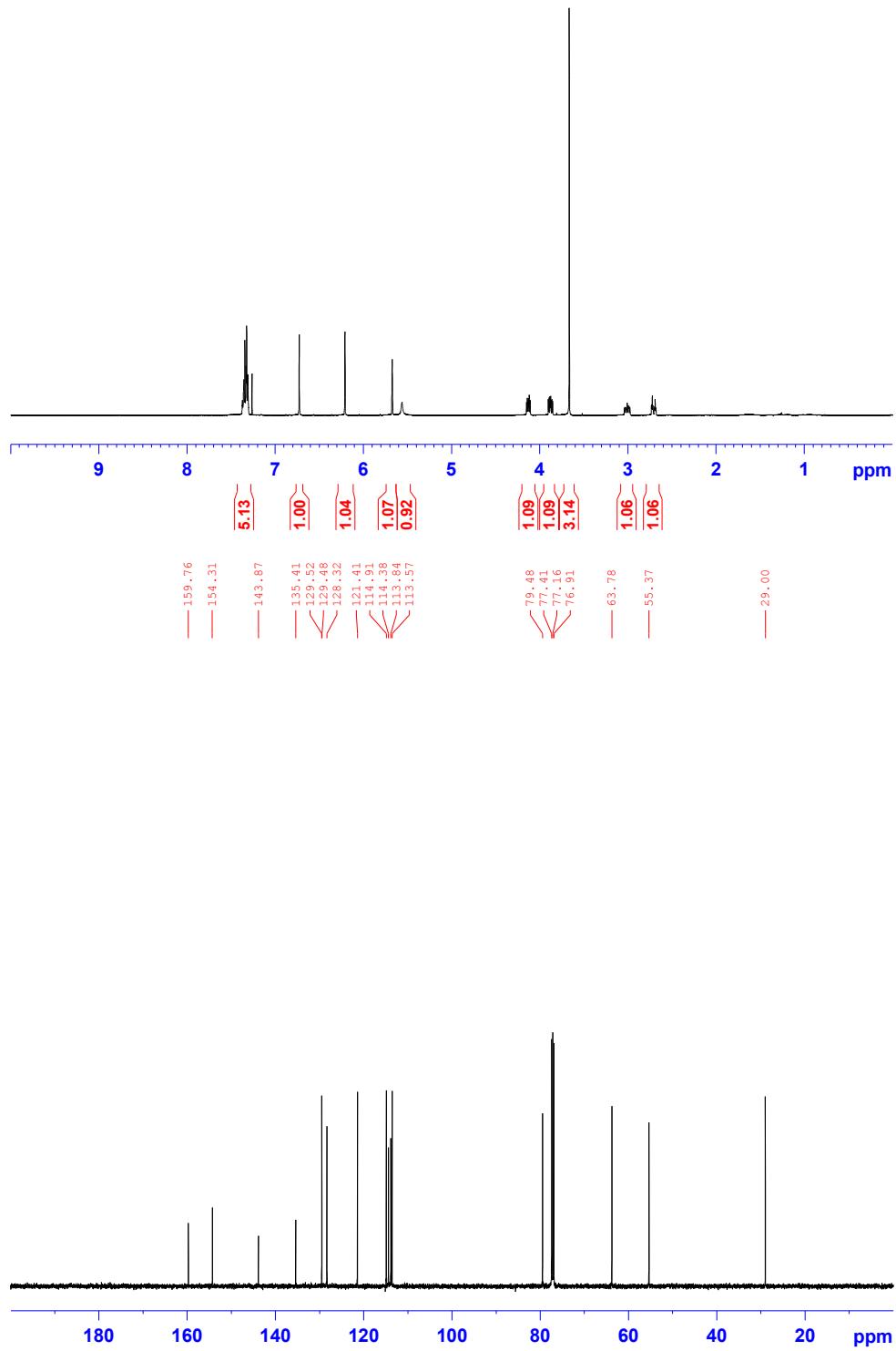
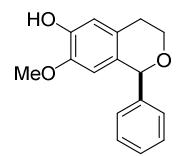
¹H and ¹³C NMR Spectra 3k



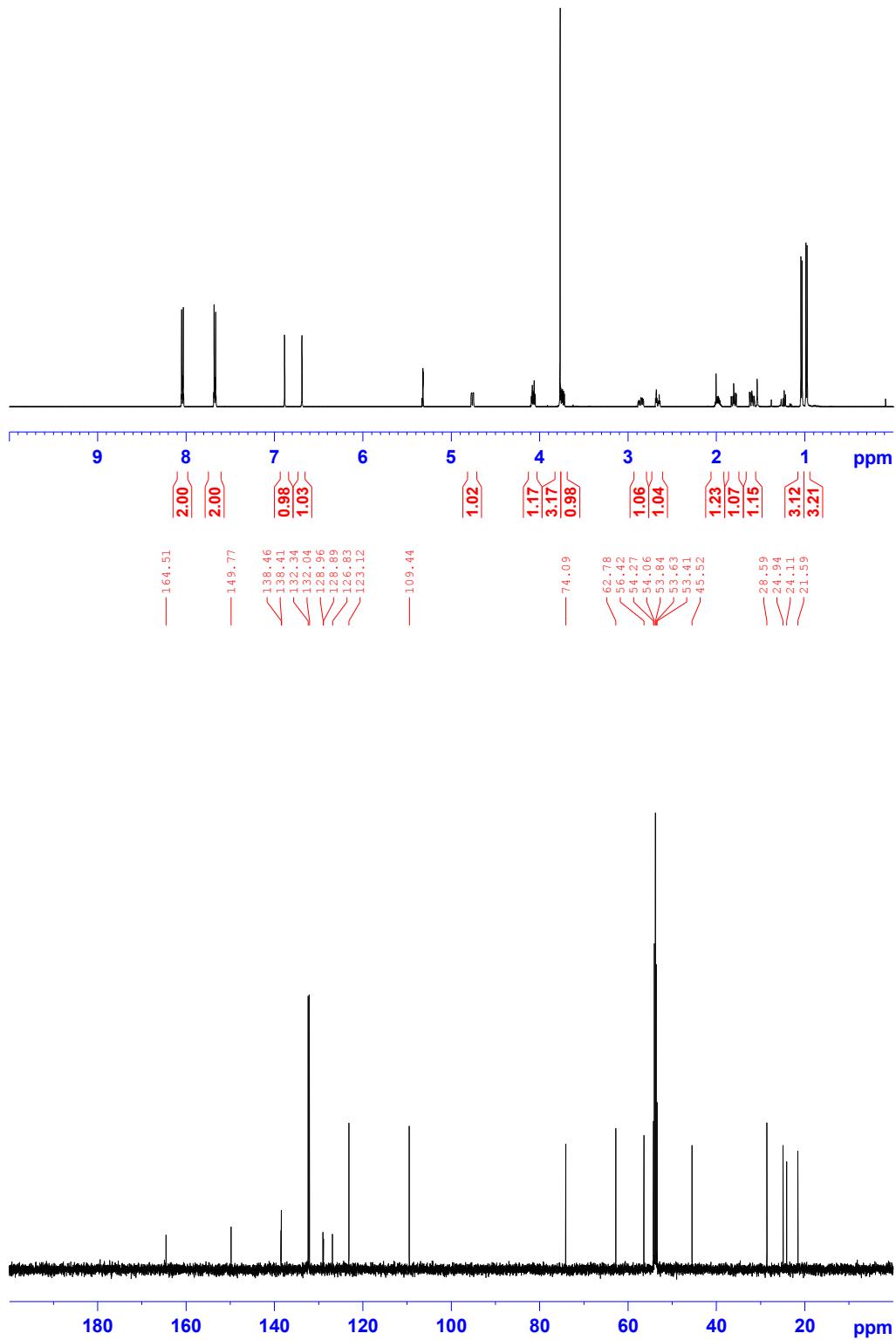
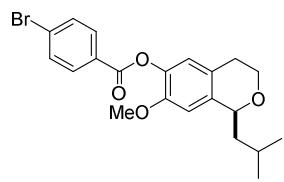
¹H and ¹³C NMR Spectra 3l



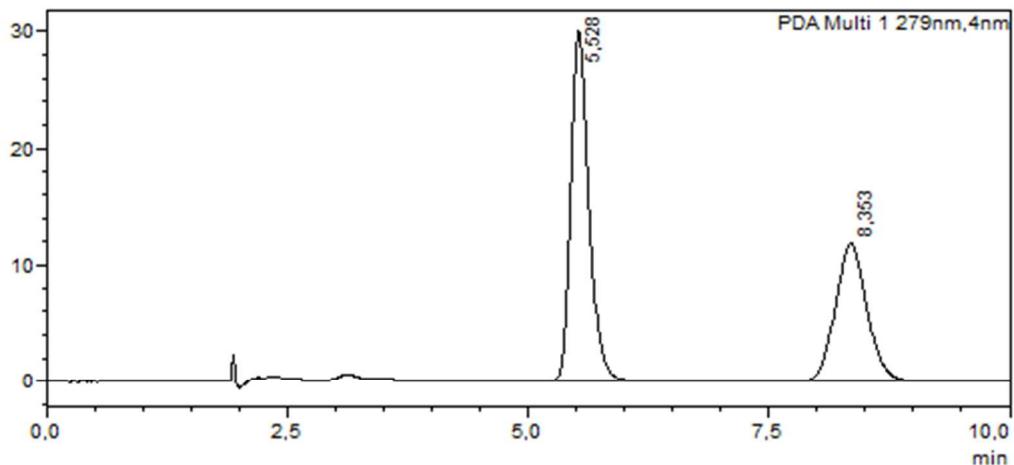
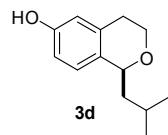
¹H and ¹³C NMR Spectra 3m



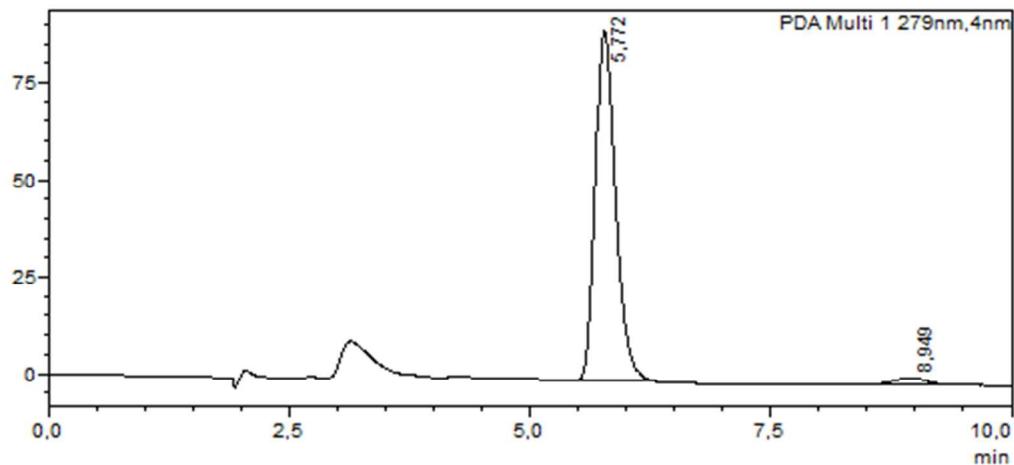
¹H and ¹³C NMR Spectra 3l'



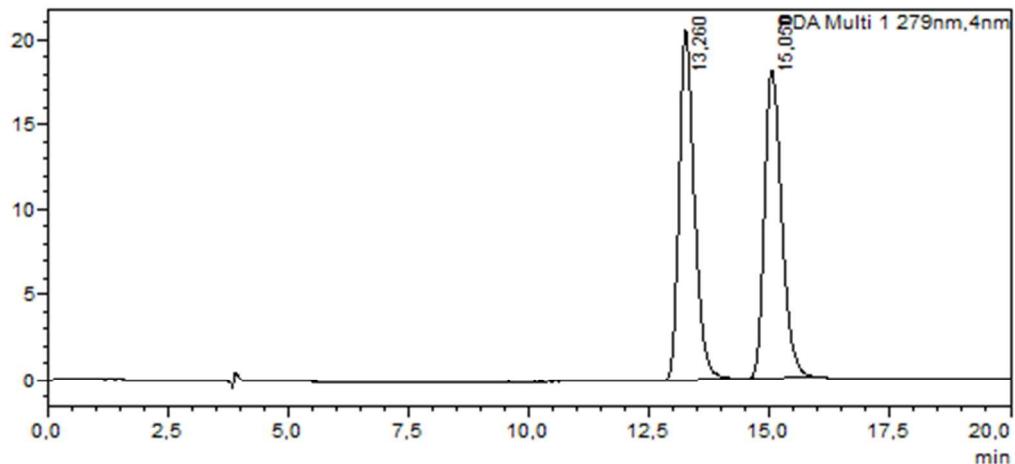
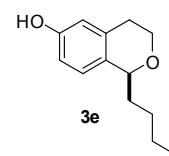
8. HPLC Traces



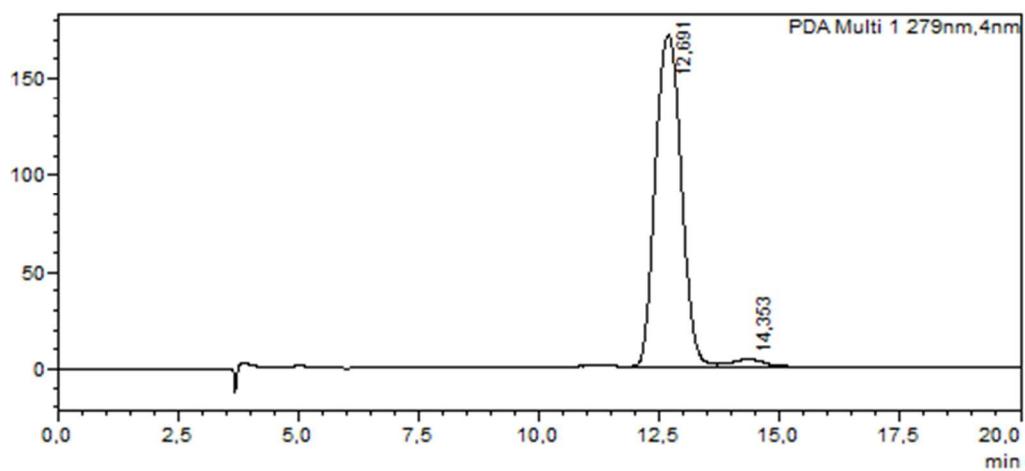
Peak	Retention time (min)	Area %
1	5.528	59.659
2	8.353	40.341
Total		100



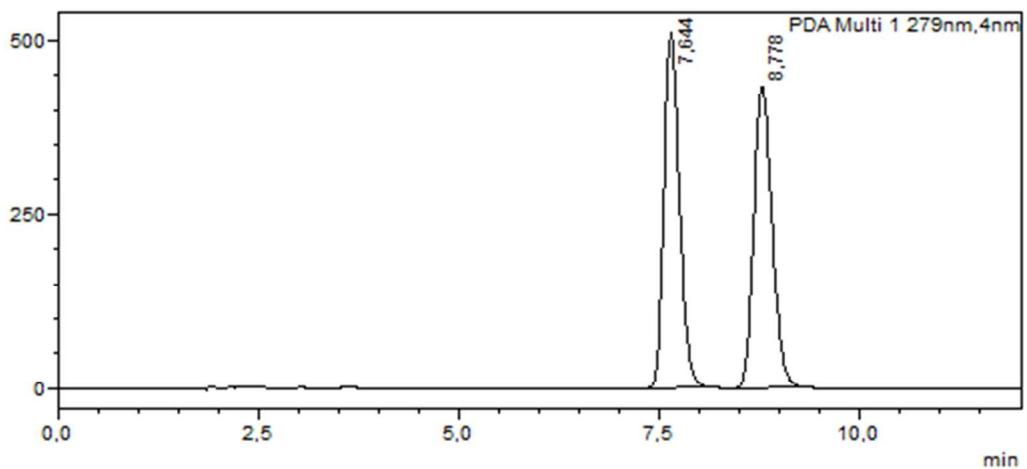
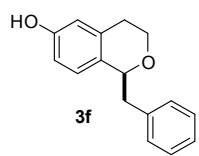
Peak	Retention time (min)	Area %
1	5.772	96.829
2	8.949	3.171
Total		100



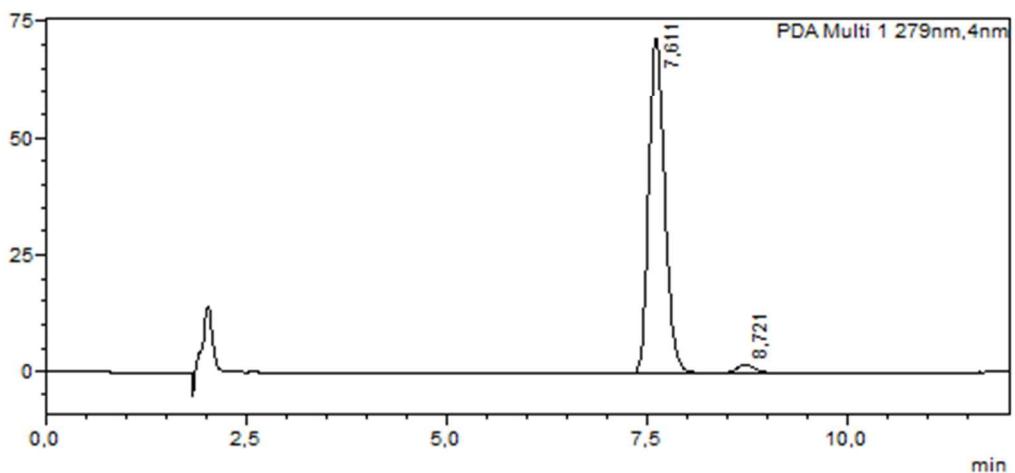
Peak	Retention time (min)	Area %
1	13.260	50.026
2	15.050	49.974
Total		100



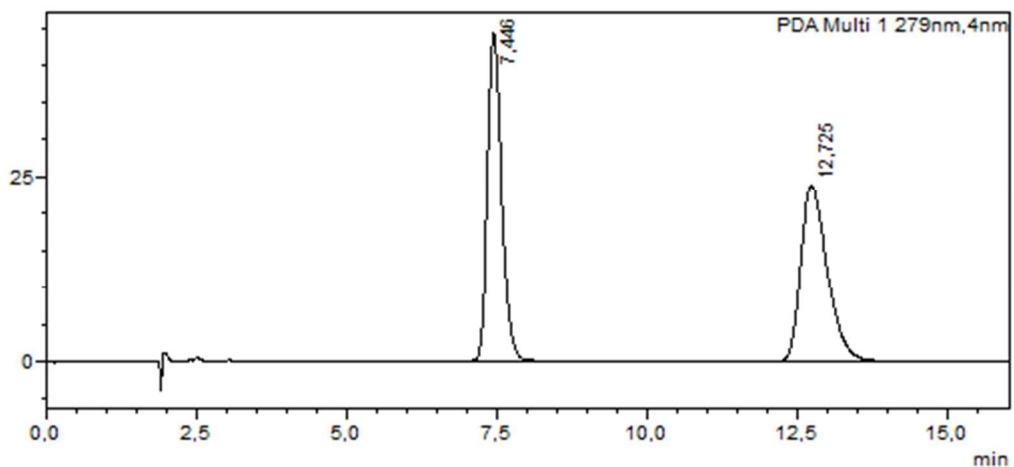
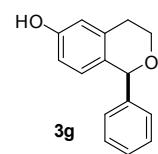
Peak	Retention time (min)	Area %
1	12.691	97.336
2	14.353	2.664
Total		100



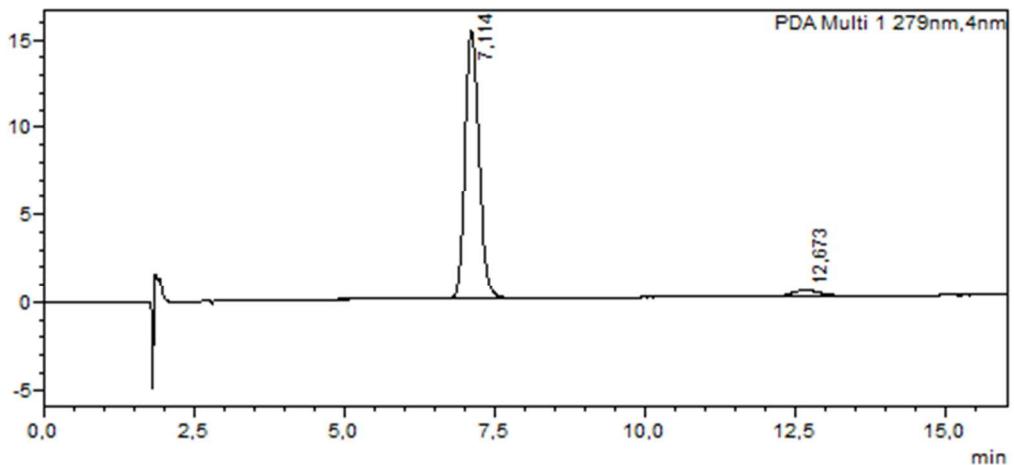
Peak	Retention time (min)	Area %
1	7.644	49.844
2	8.778	50.156
Total		100



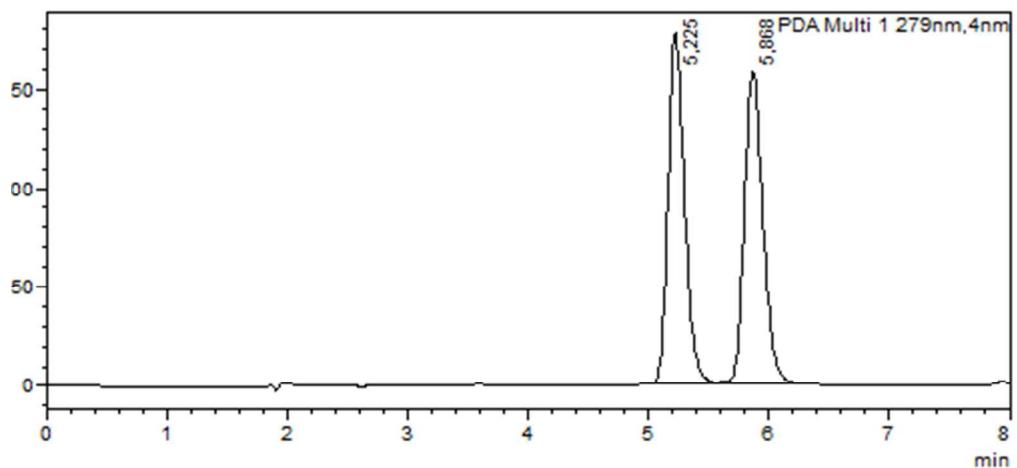
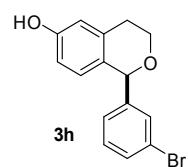
Peak	Retention time (min)	Area %
1	7.611	97.440
2	8.721	2.560
Total		100



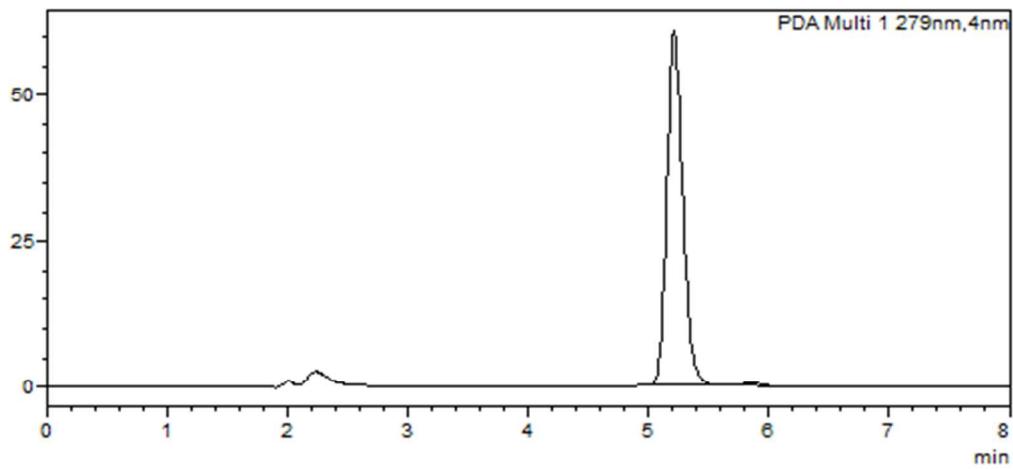
Peak	Retention time (min)	Area %
1	7.446	49.972
2	12.725	50.028
Total		100



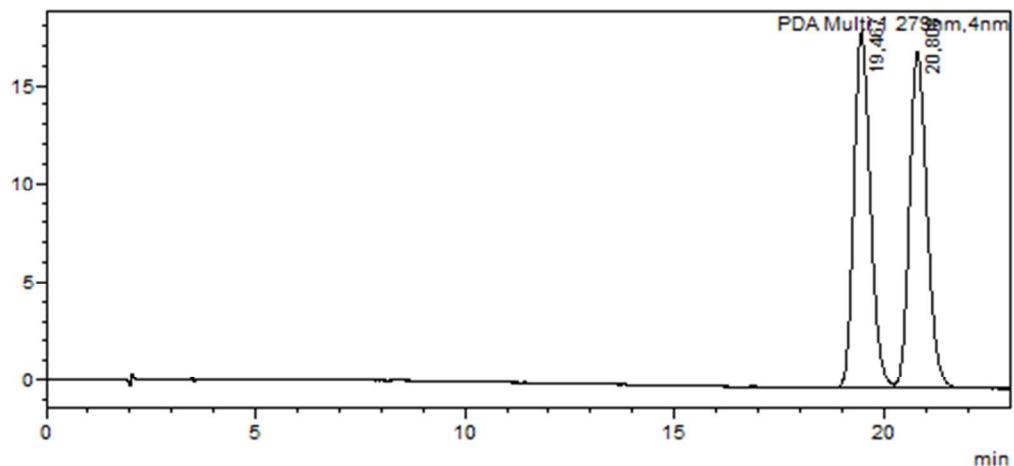
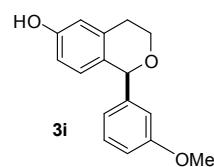
Peak	Retention time (min)	Area %
1	7.114	96.722
2	12.673	3.278
Total		100



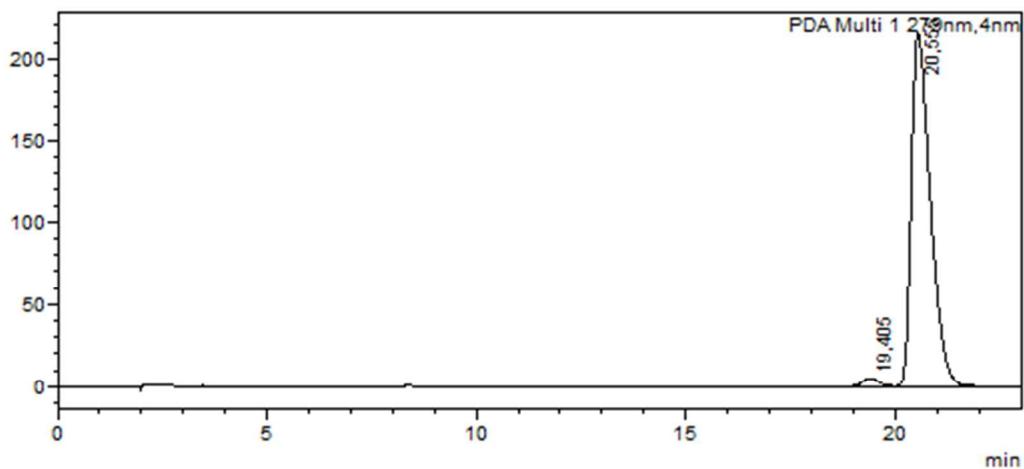
Peak	Retention time (min)	Area %
1	5.225	50.051
2	5.868	49.949
Total		100



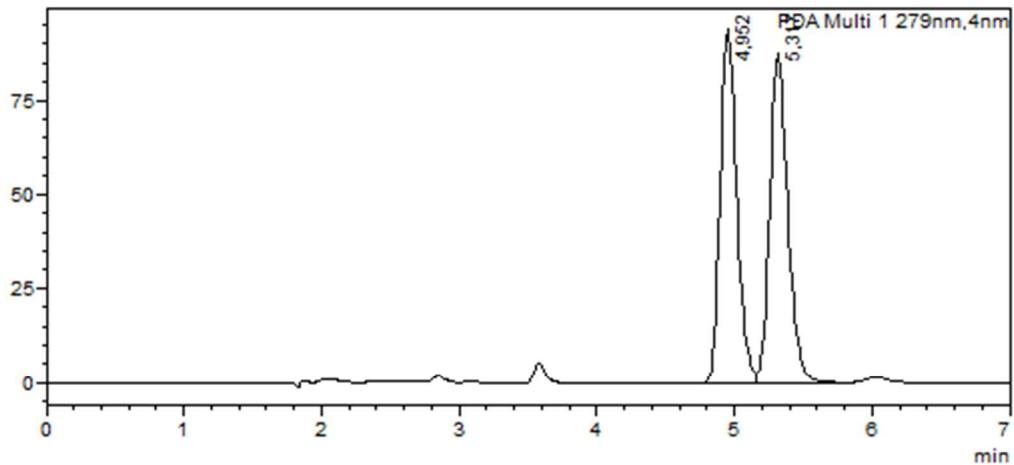
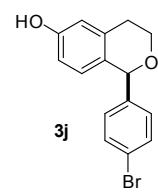
Peak	Retention time (min)	Area %
1	5.215	99.210
2	5.861	0.790
Total		100



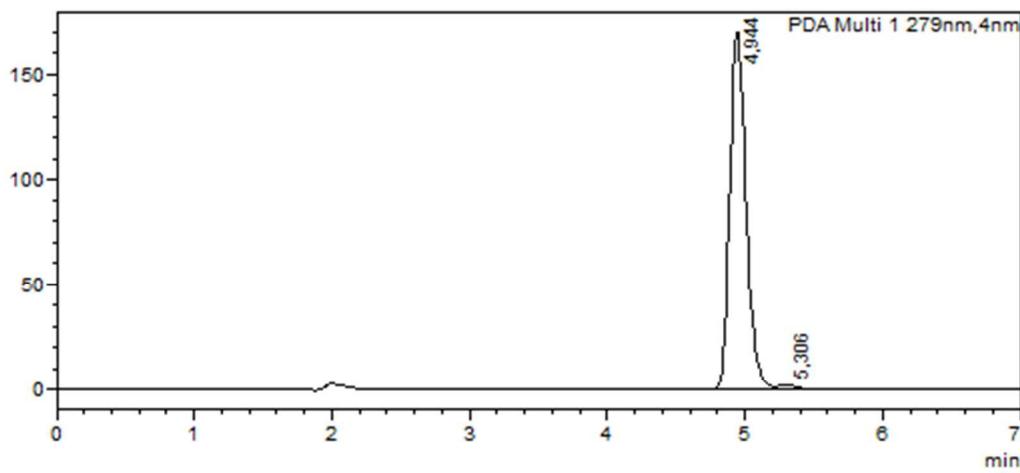
Peak	Retention time (min)	Area %
1	19.467	49.922
2	20.808	50.078
Total		100



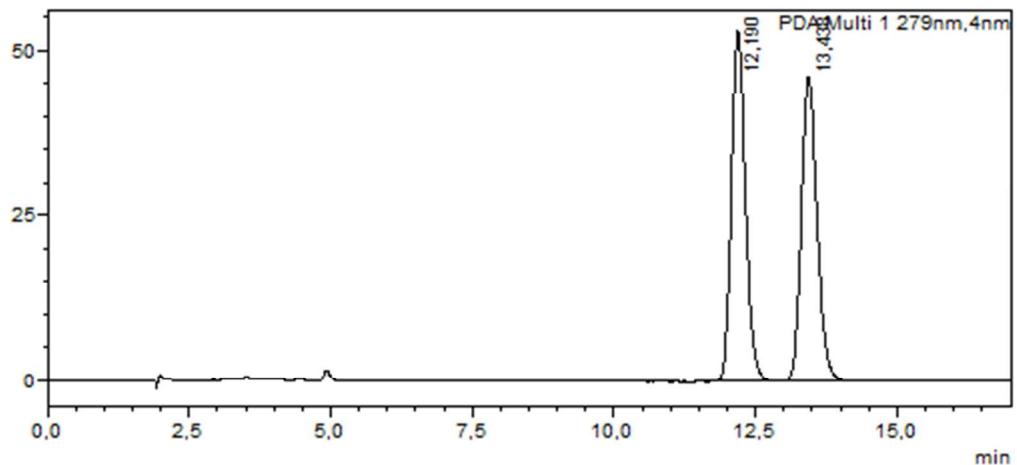
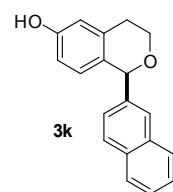
Peak	Retention time (min)	Area %
1	19.405	1.855
2	20.555	98.145
Total		100



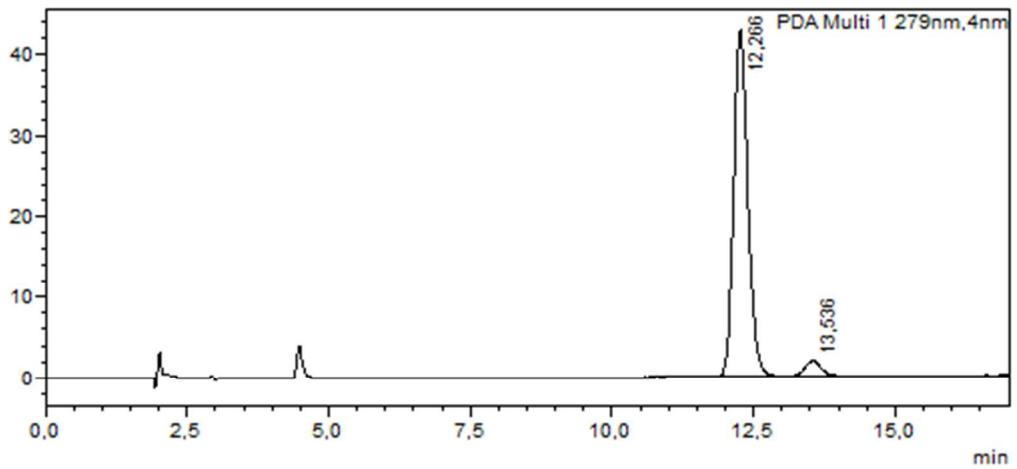
Peak	Retention time (min)	Area %
1	4.952	49.662
2	5.317	50.338
Total		100



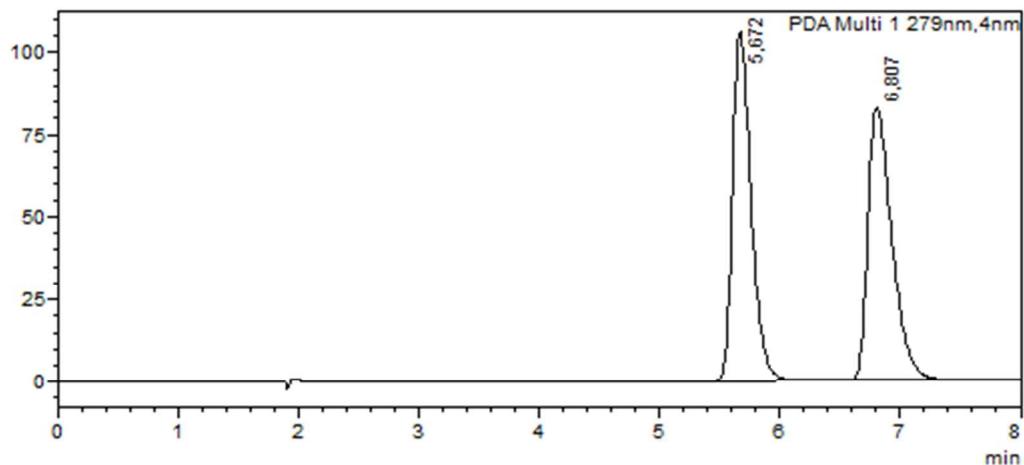
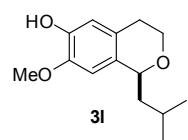
Peak	Retention time (min)	Area %
1	4.944	98.193
2	5.306	1.807
Total		100



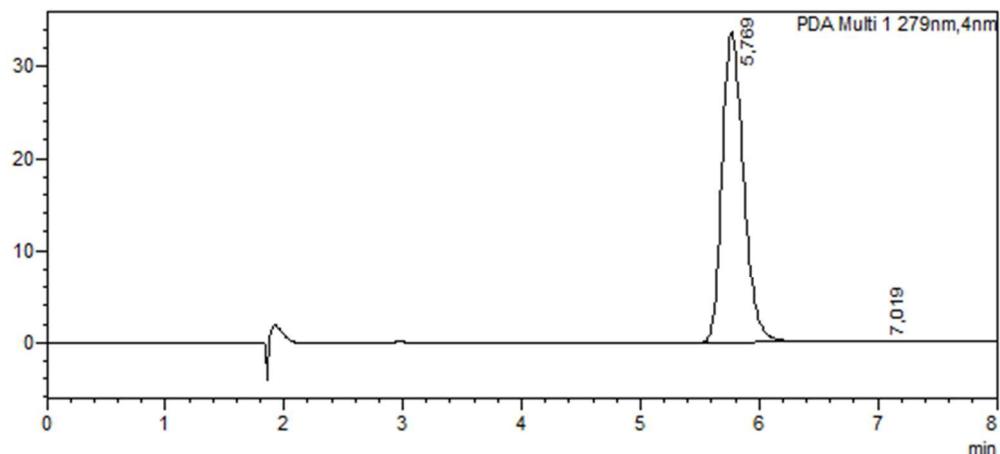
Peak	Retention time (min)	Area %
1	12.190	50.955
2	13.438	49.045
Total		100



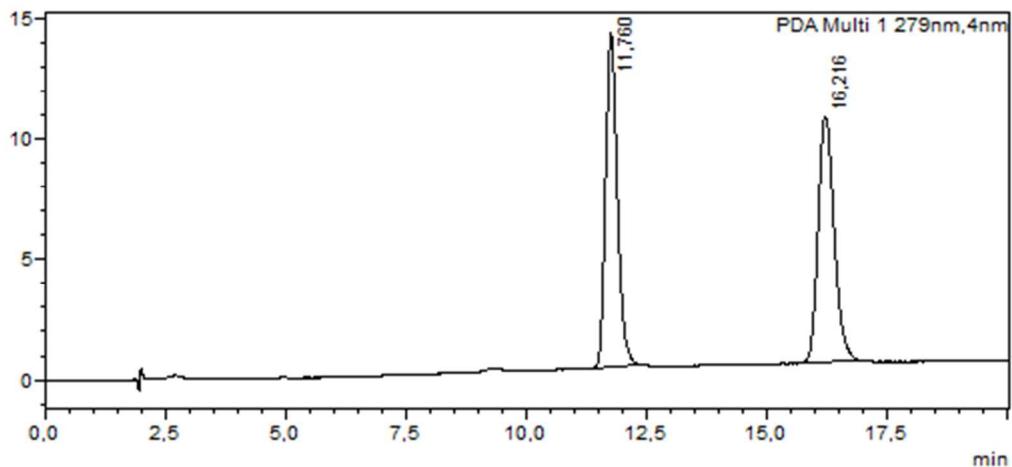
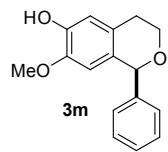
Peak	Retention time (min)	Area %
1	12.266	95.372
2	13.537	4.628
Total		100



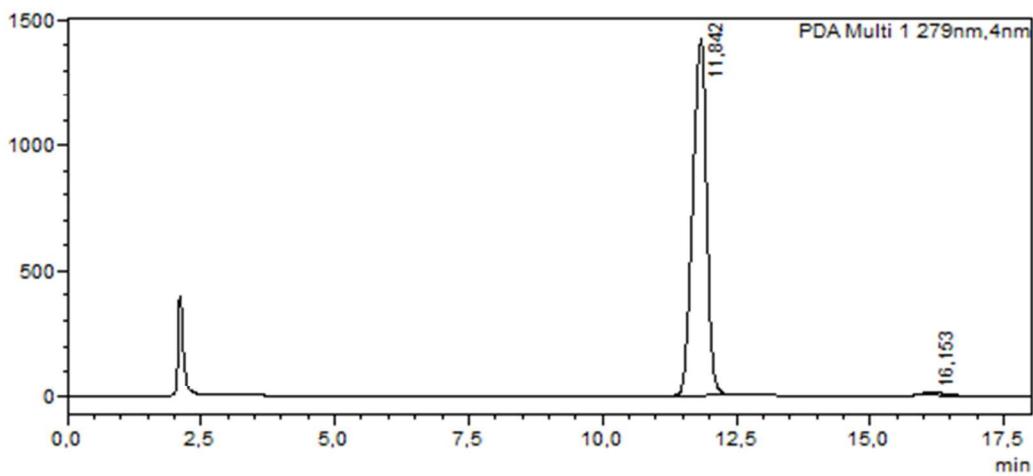
Peak	Retention time (min)	Area %
1	5.672	49.645
2	6.807	50.355
Total		100



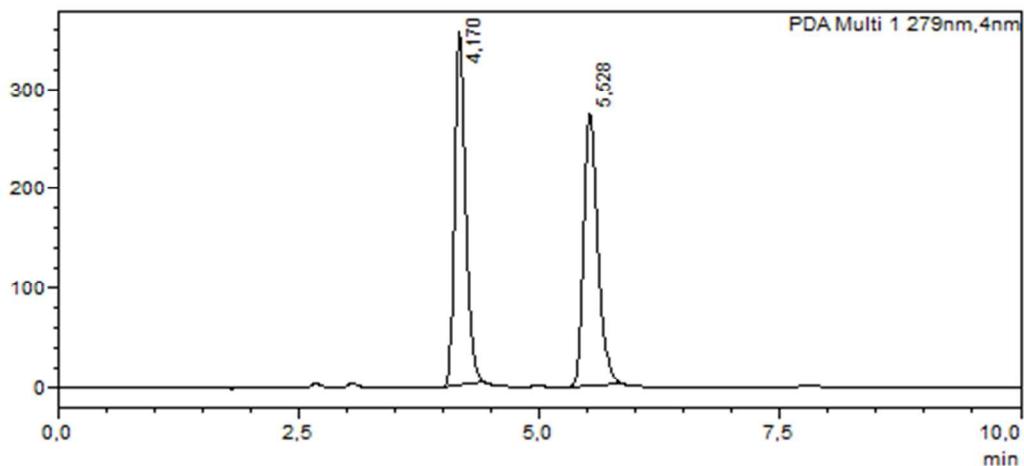
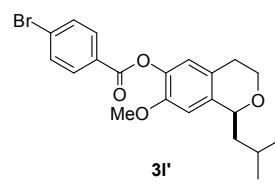
Peak	Retention time (min)	Area %
1	5.769	99.589
2	7.019	0.411
Total		100



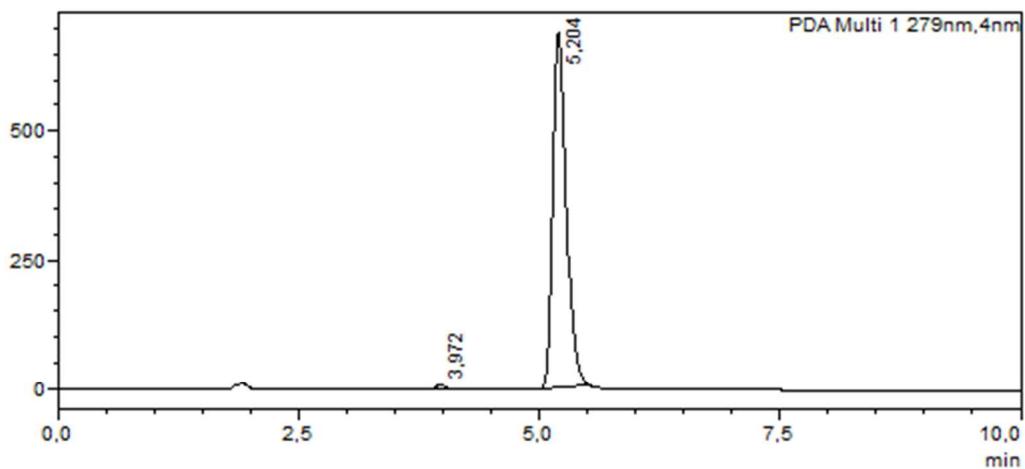
Peak	Retention time (min)	Area %
1	11.760	49.836
2	16.215	50.164
Total		100



Peak	Retention time (min)	Area %
1	11.842	98.754
2	16.153	1.246
Total		100



Peak	Retention time (min)	Area %
1	4.170	50.060
2	5.528	49.940
Total		100



Peak	Retention time (min)	Area %
1	3.972	0.870
2	5.204	99.130
Total		100

9. Computational Section

9.1. Methodology

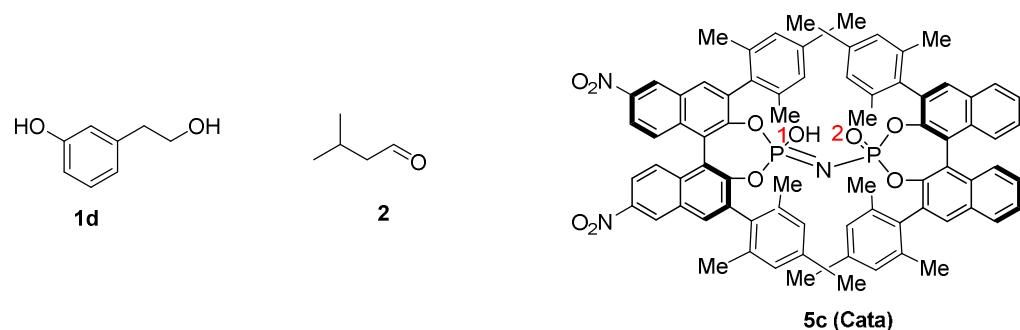
Density functional theory (DFT) was employed to study the catalytic asymmetric oxa-Pictet–Spengler reaction. All calculations were carried out using the Gaussian 09 program package.² Geometries were optimized at the TPSS-D3/SVP level,^{3,4} and the same level of theory was used for frequency calculations to confirm each stationary point to be either a minimum or transition state (TS) structure. Intrinsic reaction coordinate (IRC) calculations were also done at the same level to verify the identity of TS structures and to confirm the connection of each TS to the corresponding reactant and product. Relative enthalpies (ΔH) and free energies (ΔG) were determined at standard pressure (1 bar) and room temperature (298 K). Single-point calculations at the gas-phase optimized geometries were performed at the B3LYP-D3/TZVP level^{5,6} of theory with inclusion of continuum solvation using the polarizable continuum model (PCM) model⁷ with methyl *tert*-butyl ether (MTBE) as solvent (dielectric constant 2.6)⁸.

In the following subsections, we report structural data obtained from gas-phase TPSS-D3/SVP optimizations, relative energies (ΔE) from single-point B3LYP-D3/TZVP/CPCM calculations with zero-point vibrational corrections (ZPVE) from TPSS-D3/SVP, enthalpies (ΔH) derived from ΔE by including the thermal enthalpic corrections at 298 K from TPSS-D3/SVP (H_{corr}), and free energies (ΔG) derived from ΔH by including the entropic corrections at 298 K from TPSS-D3/SVP (G_{corr}). We also provide the total energies $E1$ and $E2$ computed at the TPSS-D3/SVP and B3LYP-D3/TZVP/CPCM levels, respectively.

9.2. Analysis of reaction pathways and selected geometries

We studied the oxa-Pictet–Spengler reaction between the substrates 3-(2-hydroxyethyl)phenol (**1d**) and isovaleraldehyde (**2**) in the presence of a slightly simplified catalyst **Cata** (**5c**) (Scheme 1). The substrates are the same as those used in the experimental work, while **Cata** contains methyl instead of ethyl groups in the Ar¹ substituents, i.e. Ar¹ = 2,4,6-(Me)₃-C₆H₂ (see Table 1 of the main article). The calculated free energy (enthalpy) profile is displayed in Figure 4, the corresponding reaction sequence is given in Figure 5, and the structural parameters of some selected species are shown in Figure 6.

Scheme 1. Substrates (**1d**, **2**) and simplified catalyst model **5c** (**Cata**).



The catalyst **Cata** contains an asymmetric hydrogen bond in the imidophosphate moiety (O1–H_{cata}: 1.04 Å, O2–H_{cata}: 1.59 Å, see Figure 6). In the initial step, **Cata** and substrate **2** form a hydrogen-bonded complex (**Com1**) involving H_{Cata} of **Cata** and the carbonyl oxygen of **2**, with concomitant lengthening of O1–H_{cata} by 0.10 Å. Compared with the separated species, **Com1** is lower in enthalpy (ΔH) by 23.9 kcal/mol, but higher in free energy (ΔG) by 11.9 kcal/mol, mainly because of the entropic penalty of complex formation. Thereafter, substrate **1d** coordinates to **Com1** by forming a hydrogen bond between the hydroxyl group of **1d** and O2 of **Cata** (O5–H5...O2: 1.80 Å) to yield **Com2**. In this complex, the two substrates are well positioned for nucleophilic attack of the carbonyl carbon C1 of **2** by the hydroxyl oxygen O5 of **1d**. This reaction is initiated by proton transfer of H_{Cata} from O1 (**Cata**) to O4 (**2**) and accompanied by a second proton transfer of H5 from O5 (**Cata**) to O2 (**1d**). The barrier for this transformation via **TS1** (Figure 6) is very small on the TPSS-D3/SVP potential energy surface (1.4 kcal/mol), and after applying the corresponding corrections, the free energy (ΔG) of **TS1** is below that of **Com2** by 2.1 kcal/mol. This indicates that the resulting intermediate **Int1** is actually formed spontaneously in a barrierless process upon coordination of **1d** to **Com1**; it contains a covalent C1–O5 bond (1.48 Å).

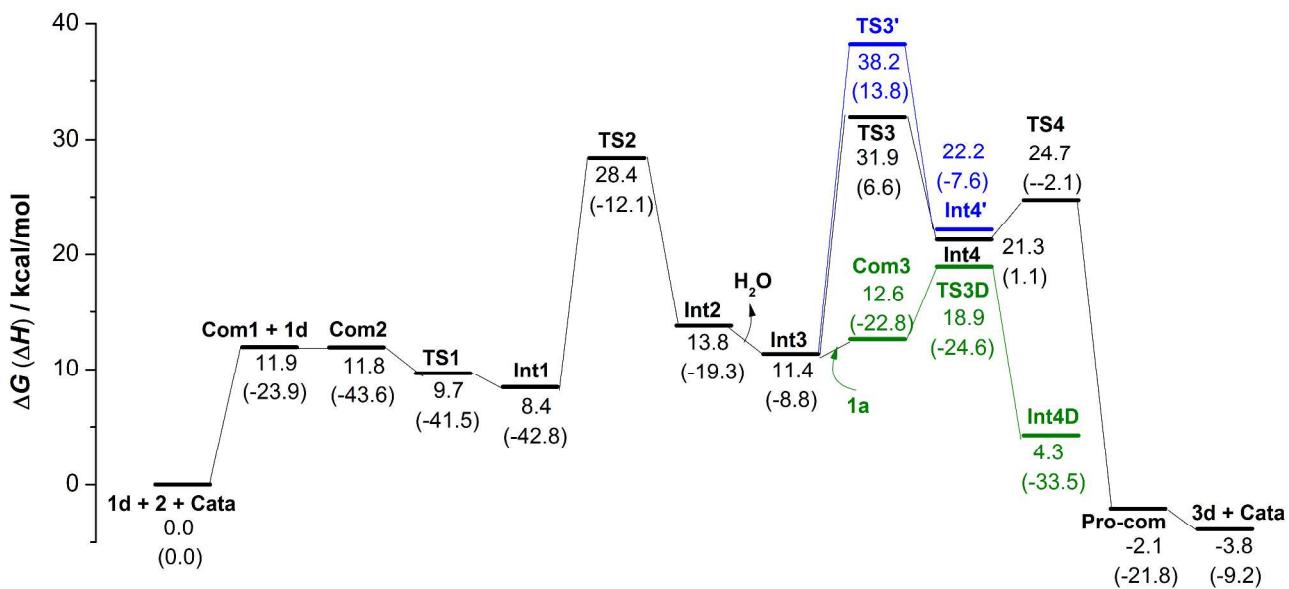


Figure 4. Computed free energy (enthalpy) profile for the **Cata**-catalyzed asymmetric oxa-Pictet–Spengler reaction between **1d** and **2** in MTBE at the B3LYP-D3/TZVP/PCM//TPSS-D3/SVP level. Energy values in kcal/mol. Black, full pathway with 6-endo-trig cyclization by *para*-nucleophilic attack; blue, cyclization by *ortho*-nucleophilic attack; green, acetal formation (see text and Figure 5).

In the computed mechanism, the next step involves a proton transfer (H5) from O2 (**1d**) to O4 (**2**), which triggers the release of water molecule (H5–O4–H_{Cata}) and the concomitant formation of a weak covalent bond C1–O1 (1.53 Å) between substrate **2** (C1) and the catalyst **Cata** (O1) via transition state **TS2**. The resulting acetal intermediate **Int3** also features a hydrogen bond between the phenolic hydroxyl group (O6-H6) of **1d** and the oxygen O3 of **Cata** (O6–H6...O3: 2.00 Å), which may direct the subsequent transformation. Thereafter, **Int3** may undergo a 6-endo-trig cyclization reaction with loss of aromaticity of the aryl ring, via transition states **TS3** or **TS3'**. This step is rate-limiting overall, and hence the nucleophilicity at the *ortho*- and *para*-positions will determine the regioselectivity. The computed free energy (ΔG) of **TS3** (31.9 kcal/mol, *para*) is lower than that of **TS3'** (38.2 kcal/mol, *ortho*). The regioselective preference for *para*-substitution in this reaction may be traced back to C–H... π interactions in **TS3** and **TS3'**. The computed electrostatic potential (ESP) charge on H1 is much higher in **TS3** (0.31e) than in **TS3'** (0.04e) indicating a much stronger C–H... π interaction between substrate **1d** and catalyst in **TS3**. Moreover, C_{para} is slightly more negatively charged (−0.18e) in **TS3** than C_{ortho} (−0.16e) in **TS3'** which should also facilitate the reaction. Consequently, **TS3** for *para*-substitution is earlier than **TS3'** for *ortho*-substitution, as indicated by the C1–C_{para} distance (1.98 Å) in **TS3** being larger than the C1–C_{ortho} distance (1.88 Å) in **TS3'**. Hence, the *para*-substitution is more favorable electronically and structurally for the 6-endo-trig cyclization.

The resulting intermediate **Int4** can easily rearrange via **TS4** by hydrogen transfer (H_{para}) from C_{para} to O1 of **Cata**, which restores the aromaticity and leads to a complex **Pro-com** that already contains the isochroman product **3d**. Catalyst releases then completes the reaction cycle.

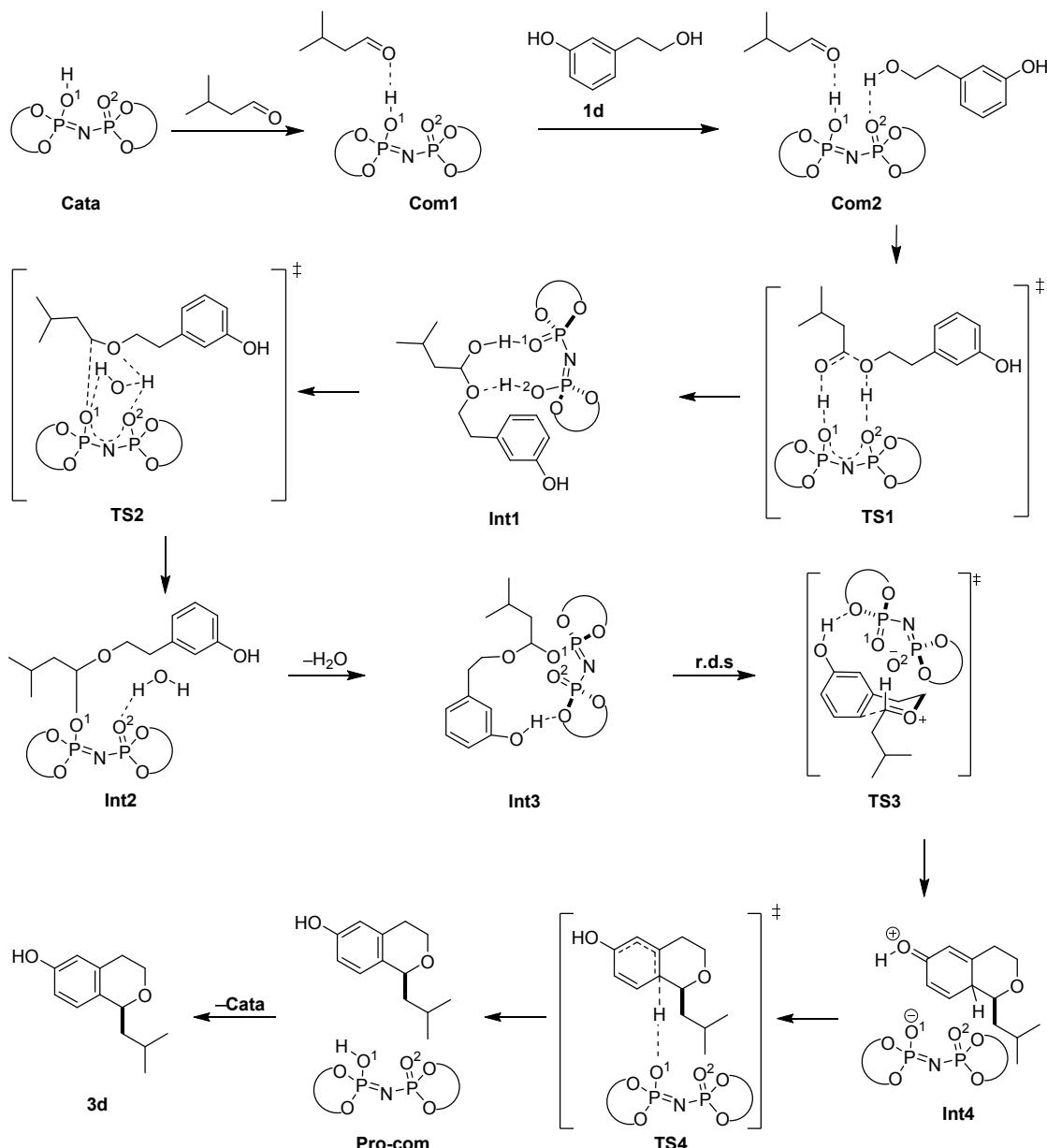
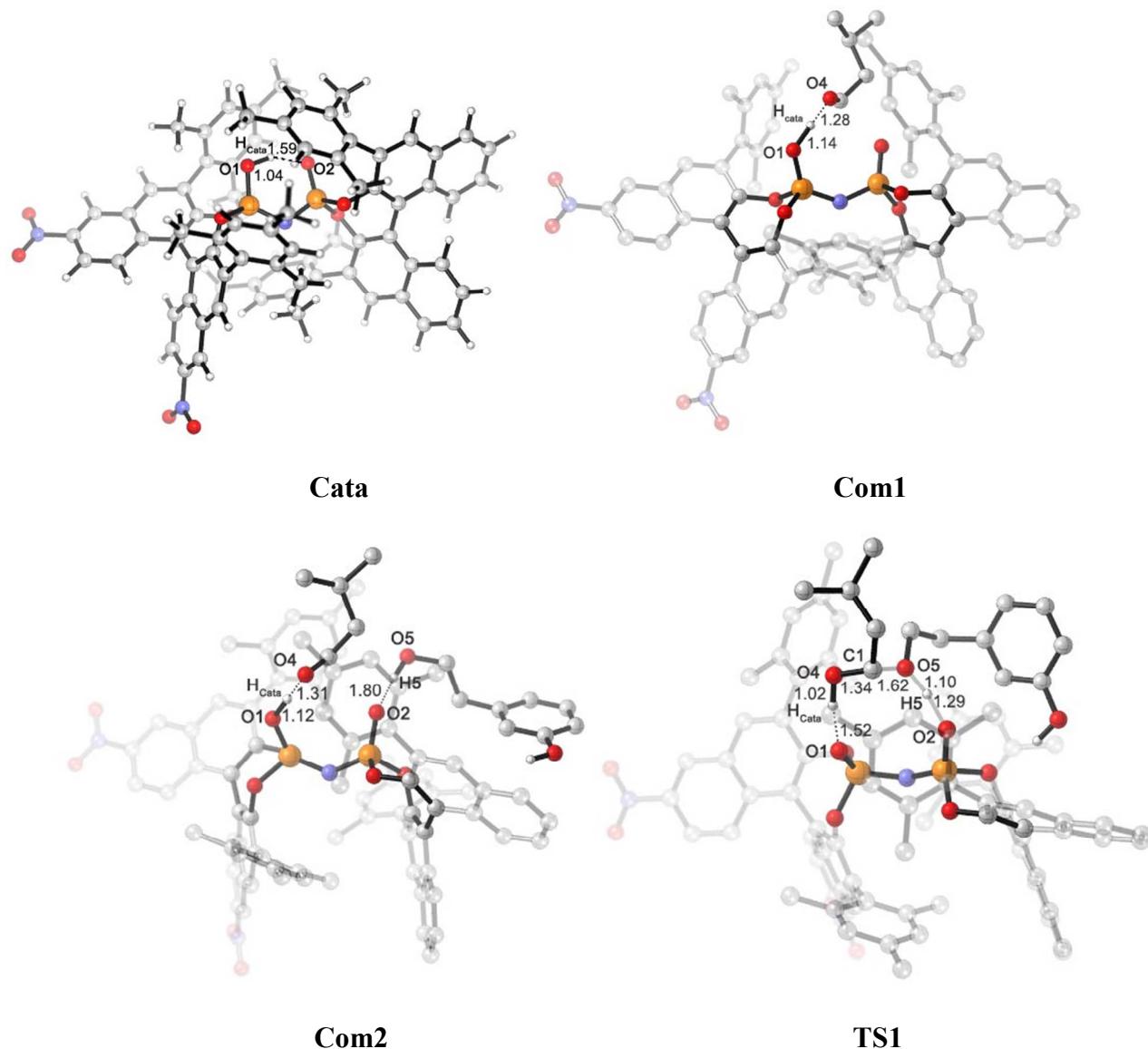
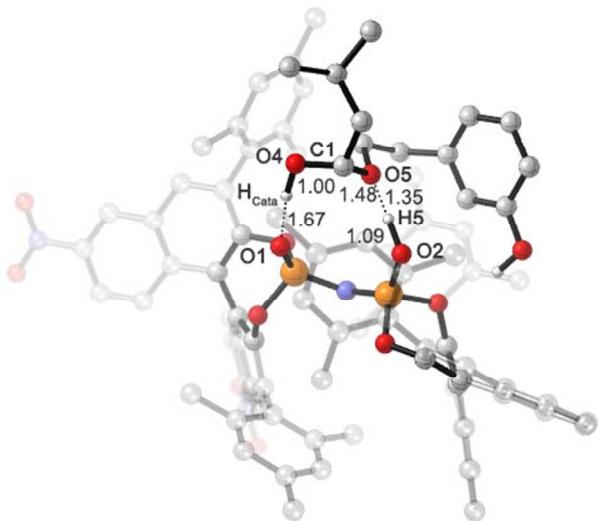


Figure 5. Reaction sequence considered for the **Cata**-catalyzed asymmetric oxa-Pictet–Spengler reaction between **1d** and **2** in MTBE (see Figure 4 for energy profiles).

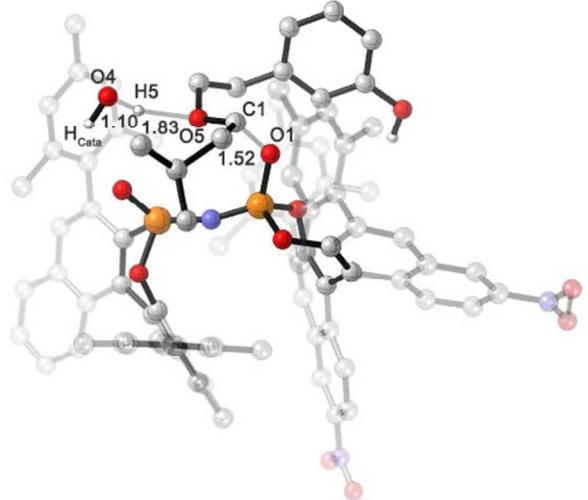
Alternatively, there is another pathway available to intermediate **Int3**, which may form a hydrogen bond between hydroxyl group O6–H6 (from **1d**) and O2 (from **Cata**) in a downhill process. In the resulting complex **Com3**, C1 (from **2**) and O7 (from **1d**) are positioned such that they can form a covalent C1–O7 bond via **TS3D**. This generates a stable acetal intermediate **Int4D**, with a computed

free energy of 4.3 kcal/mol. However, **Int4D** cannot rearrange directly to the final product **3d** and may thus convert via **TS3D** ($\Delta G = 18.9$ kcal/mol, computed free energy barrier of 14.6 kcal/mol) back to **Int3**, which can then react to the final product as described above.

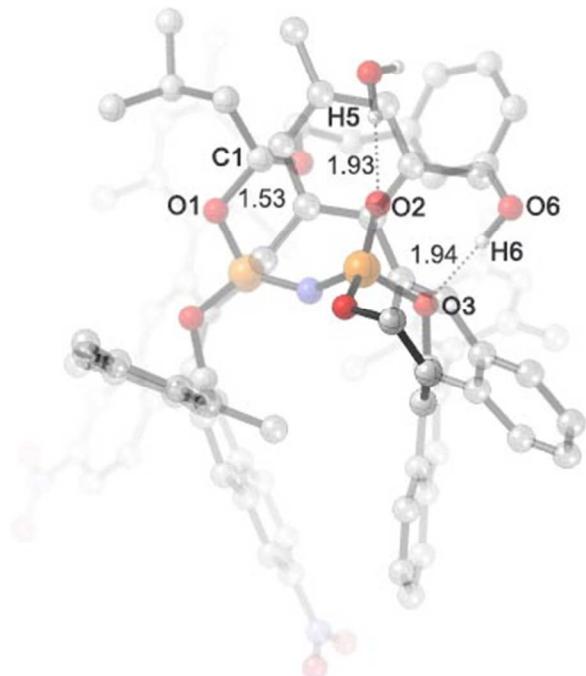




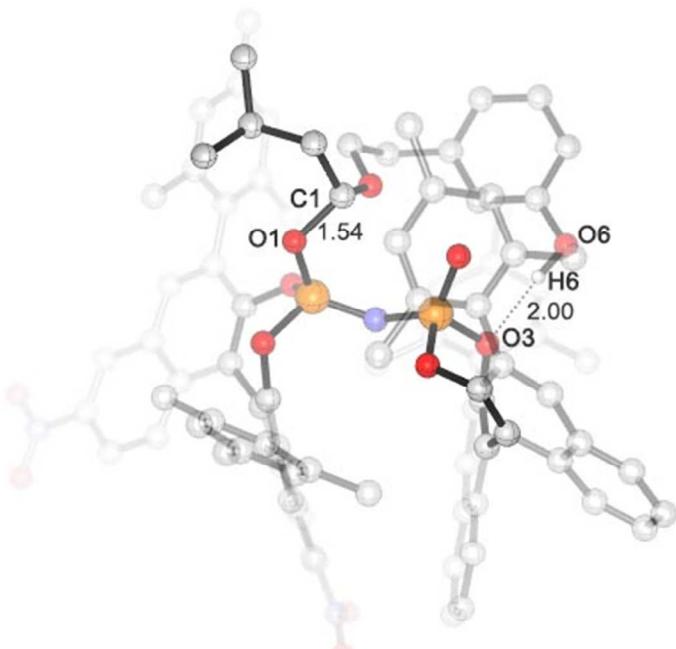
Int1



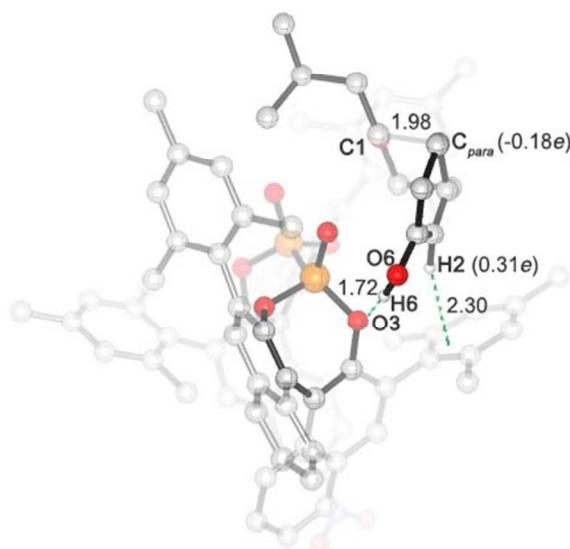
TS2



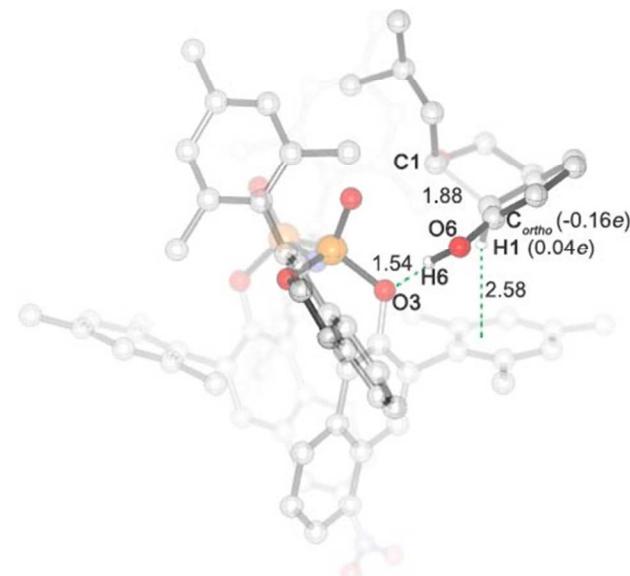
Int2



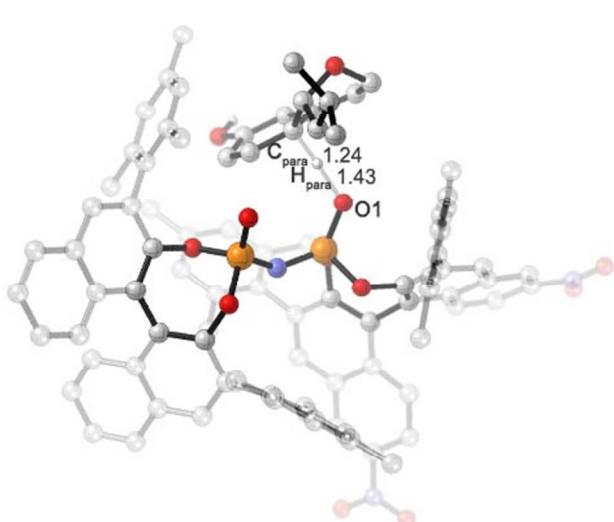
Int3



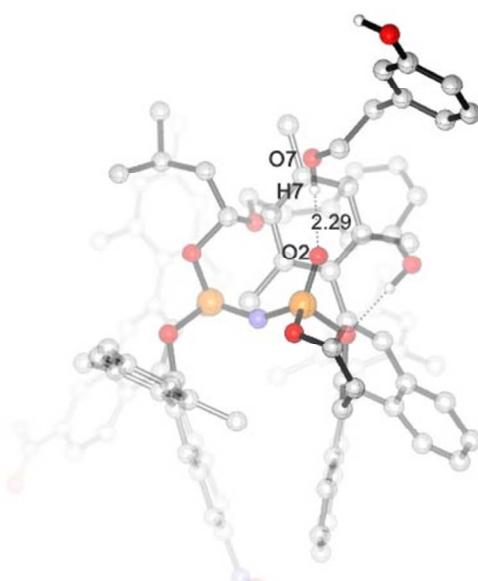
TS3



TS3'



Int4



Com3

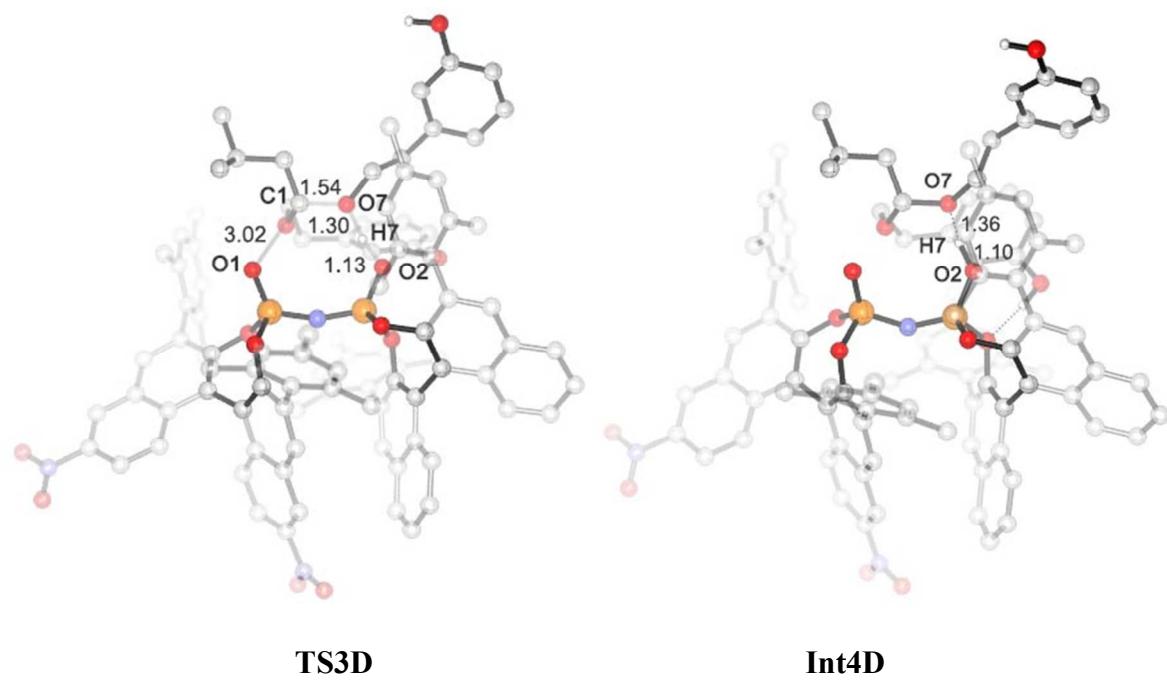


Figure 6. Selected TPSS/SVP optimized structures for the **Cata**-catalyzed asymmetric oxa-Pictet-Spengler reaction between **1d** and **2**. Selected distances in Å, ESP charges in parentheses.

9.3. Energy tables

Table 3. Absolute energies ($E1$), zero-point vibrational energy corrections ($ZPVE$), enthalpy corrections (H_{corr}), and Gibbs free energy corrections (G_{corr}) on the gas-phase geometries at the TPSS-D3/SVP level, and single-point solvent corrected SCF energies ($E2$) at the B3LYP-D3/TZVP/CPCM level. All energies are in atomic units.

Species	$E1$	$E2$	$ZPVE$	H_{corr}	G_{corr}
1a	-461.07479	-461.5167321	0.163291	0.173985	0.127261
2a	-271.633182	-271.8965045	0.138758	0.14743	0.106785
Cata	-4531.480407	-4535.042546	1.195188	1.278573	1.072521
H₂O (W)	-76.360989	-76.4656733	0.020779	0.024559	0.003092
Com1	-4803.142463	-4806.967344	1.338669	1.416160	1.226623
Com2	-5264.261875	-5268.516539	1.504956	1.591196	1.386326
TS1	-5264.264184	-5268.522235	1.506800	1.592206	1.388415
Int1	-5264.274059	-5268.522348	1.510000	1.598346	1.386595
TS2	-5264.224011	-5268.478615	1.505799	1.603564	1.374596
Int2	-5264.252799	-5268.495066	1.506531	1.608570	1.367846
Int3	-5187.861458	-5192.009821	1.481394	1.581139	1.341275
TS3	-5187.826207	-5191.979542	1.478651	1.575448	1.343808
TS3'	-5187.808616	-5191.963496	1.474990	1.570818	1.337776
Int4	-5187.834769	-5191.992528	1.479942	1.579539	1.339840
Int4'	-5187.837688	-5192.002635	1.481112	1.575811	1.351319
TS4	-5187.827632	-5191.988069	1.475215	1.570011	1.340859
Pro-com	-5187.863096	-5192.02766	1.478747	1.578165	1.337764
3d	-656.361656	-656.9632054	0.282237	0.297839	0.240479
Com3	-5648.970296	-5653.551554	1.647023	1.757744	1.495605
TS3D	-5648.962519	-5653.545000	1.643432	1.748411	1.499088
Int4D	-5648.986685	-5653.567056	1.646887	1.756322	1.497754

Table 4. Relative energies ($\Delta E1$ and $\Delta E2$) obtained from the corresponding absolute energies (see Table 3) and with inclusion of zero-point vibrational energy corrections ($ZPVE$), enthalpy corrections (H_{corr}), and Gibbs free energy corrections (G_{corr}): TPSS-D3/SVP results in the gas phase and B3LYP-D3/TZVP/PCM//TPSS-D3/SVP results in MTBE solution. All energies are in kcal/mol.

Species	TPSS-D3/SVP (gas phase)				B3LYP-D3/TZVP/PCM//TPSS-D3/SVP (MBTE: $\varepsilon=2.6$)			
	$\Delta E1$	$\Delta E1+ZPVE$	$\Delta E1+H_{corr}$	$\Delta E1+G_{corr}$	$\Delta E2$	$\Delta E2+ZPVE$	$\Delta E2+H_{corr}$	$\Delta E2+G_{corr}$
1a+2a+Cata	0	0	0	0	0	0	0	0
Com1+1a	-18.1	-15.2	-24.3	11.6	-17.8	-14.8	-23.9	11.9
Com2	-46.1	-41.3	-51.6	3.9	-38.1	-33.3	-43.6	11.9
TS1	-47.6	-41.6	-52.5	3.8	-41.7	-35.7	-46.6	9.7
Int1	-53.8	-45.8	-54.8	-3.5	-41.8	-33.8	-42.8	8.4
TS2	-22.4	-17.0	-20.1	20.3	-14.3	-9.0	-12.1	28.4
Int2	-40.4	-34.6	-35.0	-2.1	-24.7	-18.8	-19.3	13.8
Int3+W	-21.4	-18.3	-18.4	2.3	-12.4	-9.3	-8.8	11.4
TS3+W	0.7	2.1	0.8	26.1	6.6	8.0	6.6	31.9
TS3'+W	11.8	10.9	8.9	33.3	16.7	15.8	13.8	38.2
Int4+W	-4.6	-2.4	-2.1	18.2	-1.5	0.7	1.1	21.3
Int4'+W	-6.5	-3.5	-6.2	23.6	-7.9	-4.9	-7.6	22.2
TS4+W	-0.2	-0.9	-3.6	23.3	1.3	0.5	-2.1	24.7
Pro-com+W	-22.4	-21.0	-20.7	-0.9	-23.6	-22.1	-21.8	-2.0
3d+Cata+W	-9.2	-8.6	-8.6	-3.2	-9.8	-9.2	-9.2	-3.8
Com3+W-2a	-42.7	-38.2	-37.5	-2.0	-28.1	-23.5	-22.8	12.6
TS3D+W-2a	-37.9	-35.6	-38.5	5.0	-23.9	-21.6	-24.6	18.9
Int4D+W-2a	-53.0	-48.5	-48.7	-11.0	-37.8	-33.3	-33.5	4.3

9.4. Cartesian coordinates (Å) for all computed species and imaginary frequencies for transition states

1a			H	-0.84538100	-0.05771000	1.44302500	
C	1.97033000	-0.62010500	-0.03319700	H	-2.25329000	-1.71976600	0.21875300
C	2.44946700	0.68014800	-0.27571300	H	-3.07807500	-0.13596200	0.30303800
C	1.56856700	1.76170900	-0.17572300	H	-2.29240100	-0.65406400	-1.21429500
C	0.22025200	1.56565400	0.16014800	H	0.07751800	1.97233400	0.27572900
C	-0.26689800	0.26839400	0.40515800	H	-0.89791600	1.58930900	-1.16658700
C	0.61993800	-0.81921100	0.30321100	H	-1.70552000	2.03258600	0.36441500
H	3.50366500	0.81807700	-0.53261000				
H	1.94159200	2.77517300	-0.35944500	Cata			
H	-0.45753300	2.42247600	0.24034800	C	-5.12106500	0.40796100	-0.50447100
H	0.25569000	-1.83737500	0.49659100	C	-4.45253400	-0.47947300	0.33194000
O	2.85982800	-1.65322100	-0.13478000	C	-5.00185300	-1.69126300	0.84884900
H	2.39172200	-2.48387300	0.06420600	C	-6.31387500	-1.97961700	0.50551700
C	-1.72964600	0.03206100	0.71186300	H	-6.78826600	-2.88734900	0.89256300
H	-1.85491700	-0.84270900	1.37455200	C	-7.05658500	-1.13996600	-0.37641300
H	-2.16174100	0.90324000	1.23453100	C	-8.38440900	-1.48114400	-0.76853600
C	-2.54916000	-0.21485600	-0.55959000	H	-8.83816900	-2.38334500	-0.34376500
H	-2.44893400	0.66295000	-1.23422200	C	-9.08323800	-0.70467000	-1.67709300
H	-2.12874200	-1.09105100	-1.10029100	H	-10.10046700	-0.98280600	-1.97173400
O	-3.89912500	-0.43205200	-0.16827600	C	-8.47317500	0.44480100	-2.24318200
H	-4.42352600	-0.56749400	-0.97615300	H	-9.01856800	1.04145400	-2.98181900
			C	-7.18997600	0.81468900	-1.87343500	
2			H	-6.72356700	1.69725100	-2.31923700	
C	1.63590000	-0.27619600	0.36234900	C	-6.45433500	0.05454400	-0.91861200
O	2.57438900	0.15118000	-0.27840200	C	-4.41912900	1.65068700	-0.93543300
H	1.68397100	-0.32444200	1.48909200	C	-3.14338200	1.57881400	-1.50345200
C	0.32988900	-0.76847800	-0.22142600	C	-2.39251700	2.71951600	-1.91390100
H	0.38262200	-0.69330300	-1.32196000	C	-2.98490400	3.96530300	-1.75923300
H	0.23159300	-1.83920200	0.05026500	H	-2.43822900	4.85868500	-2.07922700
C	-0.89432200	-0.00040000	0.33627400	C	-4.26173900	4.12123700	-1.15255300
C	-2.20352000	-0.66729800	-0.11238200	C	-4.82406600	5.41459000	-0.94027800
C	-0.85098700	1.48250200	-0.06719100	H	-4.27183900	6.28910300	-1.30163800

C	-6.02893000	5.56709400	-0.27697900	C	3.07148400	2.15916200	-3.90277100
H	-6.44745800	6.56589800	-0.11533500	H	3.50544700	1.22400100	-3.49873800
C	-6.71297300	4.42492000	0.21541300	H	3.11445100	2.09272300	-5.00275900
H	-7.65018000	4.54952300	0.76785400	C	-1.91227800	1.54204500	-4.57743600
C	-6.20220600	3.15336600	0.01107300	H	-2.33322000	0.60676700	-4.16620300
H	-6.73279200	2.28360700	0.40587400	H	-1.57960100	1.34595100	-5.61000200
C	-4.98106800	2.95700300	-0.69948200	C	3.76702700	-0.41894700	-0.29116200
C	-4.08394800	-2.56404400	1.64133500	C	2.86255800	-1.13549800	-1.07120200
C	-3.57580400	-3.75725200	1.06744900	C	3.19682200	-2.26378800	-1.87734600
C	-2.50326000	-4.40591400	1.70067600	C	4.54139400	-2.58494200	-1.97857700
H	-2.08568400	-5.30624600	1.23305000	H	4.84938700	-3.43089300	-2.60112100
C	-1.92131700	-3.90816400	2.87937900	C	5.53338700	-1.87916000	-1.23608800
C	-2.49597200	-2.77220800	3.47051300	C	6.90050900	-2.25811700	-1.31799200
H	-2.07421500	-2.37982900	4.40190100	H	7.22459300	-3.04954600	-1.99811400
C	-3.56981200	-2.09282700	2.87357800	C	7.83227400	-1.63030600	-0.51350600
C	-4.11197800	-4.29016700	-0.24210600	C	7.47452900	-0.62602000	0.41632500
H	-4.03595800	-3.52079100	-1.02874500	H	8.25074000	-0.18988500	1.04808200
H	-5.17205200	-4.58882200	-0.16164500	C	6.15101200	-0.23491200	0.49961700
C	-0.67565100	-4.53878100	3.45688100	H	5.86363500	0.53068700	1.22372800
H	-0.55106900	-4.28711200	4.52343600	C	5.14908500	-0.81690900	-0.33487100
H	-0.68735800	-5.63765300	3.35334100	C	3.26545500	0.62807600	0.64374900
C	-4.13004900	-0.84756900	3.52277100	C	2.25628300	0.31535400	1.55922000
H	-3.67542900	0.05762000	3.08169400	C	1.85489200	1.15526500	2.63766300
H	-3.91497200	-0.83998100	4.60362500	C	2.42308000	2.42059600	2.69256000
C	-0.99894900	2.57716000	-2.43702100	H	2.15504900	3.09598600	3.51099100
C	0.08977200	3.02002800	-1.64603600	C	3.34292800	2.86914000	1.70159400
C	1.39576800	2.88282500	-2.14418900	C	3.83531500	4.20244000	1.71251700
H	2.23457100	3.21011200	-1.51967200	H	3.52606600	4.91144600	2.48413900
C	1.65285800	2.34124200	-3.41216900	C	4.70708100	4.61411300	0.72273700
C	0.55535000	1.93459800	-4.19054600	C	5.13734500	3.75531300	-0.31713000
H	0.73087300	1.52687100	-5.19317600	H	5.81013700	4.14707700	-1.08246300
C	-0.76493100	2.02571800	-3.72084200	C	4.68109500	2.45069000	-0.33385900
C	-0.11435300	3.63851400	-0.28229300	H	4.98680700	1.77961800	-1.14012600
H	0.75193200	3.43280200	0.36731900	C	3.78586900	1.96616400	0.66697200
H	-1.01903400	3.25146900	0.20761100	C	2.08095000	-3.10260300	-2.40928300

C	1.75848300	-4.29560700	-1.71669400	O	-2.55059600	0.33200300	-1.71523400
C	0.60098800	-4.99876300	-2.09017000	O	-2.01493500	-2.03184500	-0.91112700
H	0.33616100	-5.90818600	-1.53755400	O	1.53343100	-0.73244400	-1.06389000
C	-0.24288900	-4.54942400	-3.11804900	O	1.59486000	-0.91608400	1.45474500
C	0.12035200	-3.38181500	-3.81102800	O	0.19792400	-2.59560900	0.26063300
H	-0.51821800	-3.01739700	-4.62454300	P	-2.02626700	-0.58296400	-0.46054200
C	1.26694400	-2.64807900	-3.47372200	P	0.55874000	-1.05915300	0.20446800
C	2.58444600	-4.77077800	-0.54158500	H	-0.72701400	-2.66283800	-0.21367300
H	2.67447900	-3.97881700	0.22303100	H	-1.69842200	-5.33562000	-4.52784800
H	2.11613900	-5.64820800	-0.06712800	H	3.60961800	-5.05167900	-0.84140700
C	-1.53511200	-5.26292800	-3.43856900	H	0.21607700	-4.16409800	2.91865900
H	-1.55187500	-6.28060900	-3.01442900	H	-3.53427200	-5.17158200	-0.56512500
H	-2.38920400	-4.70402100	-3.01305100	H	-5.22157000	-0.77365200	3.38107800
C	1.60026900	-1.36922100	-4.20094000	H	-1.93224600	-1.80374200	6.75787500
H	1.00886500	-1.27333600	-5.12568400	H	3.55288500	-0.20243900	4.26684500
H	1.37059300	-0.49591500	-3.56613900	H	-0.31547000	3.09955500	2.82541800
C	0.93405600	0.64280300	3.69865100	H	-0.22354200	4.73719100	-0.35481700
C	-0.36502900	1.17986100	3.86299900	H	-2.73233800	2.28080800	-4.60797000
C	-1.15824500	0.71568300	4.92654000	H	3.72113000	2.98986200	-3.57770800
H	-2.15898700	1.14208300	5.05638300	N	9.25256600	-2.04182300	-0.61010900
C	-0.71356600	-0.27533100	5.81411100	N	5.20079800	6.01193000	0.74313100
C	0.56974800	-0.81290100	5.61243600	O	9.53876000	-2.92167200	-1.42454800
H	0.94162700	-1.58962500	6.29179800	O	10.05591500	-1.47415000	0.13309600
C	1.40346900	-0.37272100	4.57320100	O	5.97778600	6.34804100	-0.15280000
C	-0.93053500	2.18604400	2.88968700	O	4.80444300	6.74451700	1.65142200
H	-1.95168100	2.48048700	3.18027100	H	2.67138500	-1.31748000	-4.46345200
H	-0.97133900	1.74368500	1.87999900				
C	-1.59110100	-0.76764900	6.94261700	Com1			
H	-1.04441800	-0.77390900	7.90211700	C	4.71867300	-1.20473700	-0.20448700
H	-2.48678500	-0.13583100	7.05942300	C	4.23999500	-0.18180600	0.61295600
C	2.77962100	-0.97832900	4.40571800	C	5.07610600	0.70904600	1.34761200
H	3.05118700	-1.58296600	5.28609100	C	6.44649100	0.49842800	1.27609400
H	2.81406100	-1.63786100	3.51947300	H	7.11787700	1.14226100	1.85446500
N	-0.63192000	-0.02194400	0.16398500	C	7.01118300	-0.50040600	0.43445900
O	-3.13060700	-0.18287500	0.68271800	C	8.42439200	-0.65544500	0.32061200

H	9.07026300	-0.01937400	0.93606100	H	2.39492800	5.04625700	5.13253500
C	8.97211800	-1.57265000	-0.55929500	H	3.20425400	6.16248700	3.99041100
H	10.05900600	-1.67777200	-0.64105800	C	3.41442500	0.25677900	3.76137000
C	8.12153200	-2.36346600	-1.37521200	H	2.68466500	-0.27833500	3.12972700
H	8.55732700	-3.06561800	-2.09366000	H	3.01162500	0.29184400	4.78639300
C	6.74420600	-2.24980300	-1.27678600	C	0.87850400	-1.70771100	-3.44597000
H	6.10034500	-2.85724500	-1.91745300	C	-0.50604800	-1.88986800	-3.21246300
C	6.14575500	-1.34087200	-0.35521300	C	-1.42554700	-1.38080100	-4.14608600
C	3.76392100	-2.09122700	-0.92339100	H	-2.49673000	-1.52939500	-3.96252400
C	2.74476700	-1.54775300	-1.71203400	C	-1.01333700	-0.69352500	-5.29852600
C	1.88479700	-2.33441600	-2.53533300	C	0.36474400	-0.49832000	-5.49188400
C	2.04885700	-3.71301400	-2.50505600	H	0.71226400	0.04257100	-6.38090000
H	1.41982700	-4.33903900	-3.14683600	C	1.31933800	-0.99336600	-4.58910200
C	2.98834600	-4.33906100	-1.64158000	C	-1.01008500	-2.59254000	-1.97319300
C	3.06148400	-5.75888000	-1.53376500	H	-2.10871000	-2.54493600	-1.91996000
H	2.40966600	-6.36537000	-2.17209200	H	-0.59725900	-2.11931500	-1.06731300
C	3.91353200	-6.36043500	-0.62400500	C	-2.01500000	-0.20040300	-6.31834500
H	3.95093400	-7.45152000	-0.54079800	H	-3.04368800	-0.23761700	-5.92353200
C	4.72797400	-5.55844200	0.21865900	H	-1.79923500	0.83813700	-6.62654500
H	5.38055900	-6.03580800	0.95708700	C	2.79253700	-0.77397100	-4.84842400
C	4.69964500	-4.17656100	0.11937600	H	3.21137900	-0.05397100	-4.12299000
H	5.32162100	-3.56733300	0.77998700	H	2.96002900	-0.37991200	-5.86414900
C	3.84652100	-3.52541100	-0.81944200	C	-3.95184800	0.07967000	0.35143800
C	4.48009900	1.85841800	2.09128300	C	-3.22082500	1.07054600	-0.30111000
C	4.71261500	3.17407400	1.61596600	C	-3.73312100	2.35938300	-0.62914800
C	4.13094200	4.25417700	2.29856500	C	-5.04676700	2.62871100	-0.27166300
H	4.32292200	5.27218300	1.93739800	H	-5.48669100	3.59706800	-0.53010400
C	3.29539500	4.06858100	3.41216900	C	-5.83757800	1.68365400	0.44107900
C	3.08391700	2.75732100	3.86511300	C	-7.16387600	2.00190200	0.84019700
H	2.44730000	2.58821300	4.74228900	H	-7.61375700	2.96366700	0.58252500
C	3.66760100	1.64732300	3.23142700	C	-7.89126300	1.08603100	1.57576500
C	5.50766400	3.42210300	0.35204400	C	-7.35796400	-0.16485800	1.96768800
H	5.05455300	2.87121500	-0.49095400	H	-7.97174300	-0.83420600	2.57357500
H	6.55524700	3.08748100	0.43777600	C	-6.07416000	-0.49572600	1.57573900
C	2.60275500	5.24040000	4.06671500	H	-5.64761800	-1.45348000	1.88257800

C	-5.28560800	0.39576700	0.78616700	H	2.81826300	-3.71133400	2.91620900
C	-3.33006600	-1.24249500	0.63342300	C	1.79618600	-2.70470100	4.53851600
C	-2.12295400	-1.32129100	1.33640100	C	0.59422900	-2.08237800	4.91470000
C	-1.58378400	-2.54279000	1.84148700	H	0.50129000	-1.65780700	5.92171400
C	-2.24713700	-3.71613400	1.50634500	C	-0.50346800	-1.99520100	4.04351700
H	-1.87439500	-4.66951800	1.89399400	C	1.00544700	-3.71988900	0.94287100
C	-3.38923100	-3.71849800	0.65814100	H	1.83046000	-4.44708200	0.91913800
C	-3.98919600	-4.93631200	0.23881500	H	1.26281700	-2.89638600	0.25399600
H	-3.59672200	-5.90103000	0.56915900	C	2.94941600	-2.82677200	5.50784200
C	-5.07572200	-4.90054700	-0.61463600	H	2.92902900	-2.02320900	6.26288400
C	-5.62181300	-3.68673800	-1.09755700	H	2.90645400	-3.79153600	6.04853700
H	-6.46630000	-3.72580500	-1.78828600	C	-1.77714500	-1.32330400	4.50610800
C	-5.06176400	-2.49286000	-0.68327500	H	-1.77235500	-1.18427200	5.59942100
H	-5.46367100	-1.54760000	-1.05712700	H	-1.88903500	-0.33023600	4.03484800
C	-3.94667200	-2.46714000	0.20865100	N	0.51521200	0.19782400	-0.16306000
C	-2.89560100	3.36948600	-1.34245100	O	2.86451500	-0.03129600	0.74769700
C	-2.52176900	4.56861400	-0.68777600	O	2.58276900	-0.16908500	-1.77295700
C	-1.81596300	5.54567100	-1.41501400	O	2.35437500	2.12605000	-0.72633800
H	-1.54610300	6.48157600	-0.91097800	O	-1.91522000	0.78144000	-0.67450200
C	-1.46610800	5.36260300	-2.76326400	O	-1.44330500	-0.15577600	1.64937000
C	-1.81694100	4.14755200	-3.37651700	O	-0.80455200	2.17157900	1.23383000
H	-1.55159000	3.97909900	-4.42724600	P	2.01952800	0.68007700	-0.47631800
C	-2.52907400	3.14843500	-2.69514200	P	-0.76208800	0.80709200	0.50113300
C	-2.86027100	4.81338100	0.76712700	H	-0.03953100	3.00520500	1.10452700
H	-2.70493300	3.90270600	1.36774500	H	-0.68020600	7.37799000	-2.98544400
H	-2.22781900	5.61621700	1.18050500	H	-3.91428300	5.12119700	0.89512100
C	-0.74031200	6.43226000	-3.54847800	H	1.63491600	5.43360700	3.56667600
H	0.29017200	6.11737900	-3.79735700	H	5.51628600	4.49634300	0.10191100
H	-1.25428600	6.63577100	-4.50457200	H	4.33943300	-0.34544300	3.76930600
C	-2.90505300	1.87443300	-3.41123000	H	3.91916700	-2.78618100	4.98367200
H	-2.84624700	2.00851400	-4.50237600	H	-2.66936600	-1.91558900	4.23652100
H	-2.22039500	1.05367600	-3.13455400	H	0.10303100	-4.20446500	0.54183000
C	-0.39409100	-2.55613200	2.74452400	H	-0.71387500	-3.65556100	-1.94806000
C	0.81230300	-3.17796300	2.33760600	H	3.36403200	-1.71272900	-4.73992300
C	1.88553200	-3.23587800	3.24275700	H	-1.98438100	-0.82219900	-7.23285400

N	-9.27149000	1.43459100	1.98638200	C	7.15659100	-3.61030500	-0.40074600
N	-5.68100600	-6.17909600	-1.05318900	H	7.49761700	-4.39950300	-1.07777100
O	-9.71248300	2.53176000	1.63749800	C	5.81605600	-3.26243000	-0.37505200
O	-9.89004200	0.60078500	2.65141500	H	5.10766300	-3.77671200	-1.02833700
O	-6.64772200	-6.11400800	-1.81612300	C	5.34293500	-2.22457400	0.48210200
O	-5.18240200	-7.22402500	-0.62936900	C	2.90621700	-2.65374100	-0.12142600
H	-3.92868600	1.55142200	-3.15409300	C	2.00689000	-2.04417800	-0.99804700
O	0.82787100	3.93201800	0.92294100	C	1.16149200	-2.78048100	-1.88076300
C	1.11177300	4.03336000	-0.28870100	C	1.15235500	-4.16316900	-1.76201800
H	0.44832400	3.56999800	-1.04331700	H	0.52667200	-4.75053600	-2.44241500
C	2.21008800	4.92766000	-0.75429000	C	1.91591200	-4.83736900	-0.76981600
H	3.05573000	4.79809300	-0.06054700	C	1.80141500	-6.24412600	-0.57111000
H	2.52148400	4.59348400	-1.75615100	H	1.12858600	-6.81103500	-1.22371100
C	1.80295800	6.42892300	-0.79920800	C	2.50414600	-6.87902500	0.43853900
C	2.92657600	7.22972600	-1.47578200	H	2.39877400	-7.95827400	0.58953000
C	1.47096200	6.99467400	0.58876900	C	3.35150500	-6.12515300	1.29246900
H	0.90048000	6.51280700	-1.42934500	H	3.88515800	-6.62558500	2.10713600
H	3.12708700	6.85798700	-2.49597900	C	3.50344000	-4.75993000	1.10893100
H	2.65742900	8.29840700	-1.54633400	H	4.14757000	-4.18629600	1.78069300
H	3.86513000	7.15341800	-0.89648700	C	2.80477900	-4.07815000	0.06994100
H	0.65312800	6.43821200	1.07493000	C	4.12817800	1.20196700	2.89444100
H	2.34937000	6.94349000	1.25644800	C	4.60098800	2.48910500	2.53876100
H	1.16740800	8.05343000	0.50691100	C	4.24924300	3.58683100	3.34333100
				H	4.63537900	4.57972000	3.08062400
Com2				C	3.40643700	3.45249700	4.45804800
C	3.95066300	-1.86025800	0.57720600	C	2.94034400	2.16811400	4.78036900
C	3.61108700	-0.73781800	1.33021000	H	2.28885800	2.03706600	5.65306100
C	4.55197800	0.01833100	2.09029100	C	3.29248700	1.03658500	4.02750900
C	5.87612100	-0.39911700	2.06622200	C	5.41234000	2.70618900	1.27890300
H	6.61478800	0.13686900	2.67150700	H	4.88069400	2.28653300	0.40671200
C	6.30738000	-1.49823000	1.27151900	H	6.40185700	2.21932700	1.32034700
C	7.67933700	-1.89199600	1.23036000	C	2.97490700	4.65673300	5.26176800
H	8.39957200	-1.33877000	1.84263100	H	2.92818400	4.42872000	6.34058000
C	8.09572700	-2.93556800	0.42158400	H	3.66031500	5.50845500	5.11544800
H	9.15198300	-3.21992900	0.38941800	C	2.78064400	-0.32407500	4.43812000

H	1.93599600	-0.63906100	3.80062900	C	-2.81382800	-2.33452300	2.04597100
H	2.43071600	-0.30975600	5.48237000	C	-3.54396700	-3.43463100	1.61766600
C	0.38491500	-2.10065100	-2.96028800	H	-3.35939800	-4.41146700	2.07586500
C	-1.02210300	-2.00023500	-2.87996600	C	-4.51305900	-3.33265900	0.58052300
C	-1.72295800	-1.42122100	-3.95186400	C	-5.17527800	-4.48816600	0.08532700
H	-2.81463100	-1.34027000	-3.88427700	H	-4.97529100	-5.47595500	0.50734200
C	-1.06437400	-0.93481600	-5.09242000	C	-6.07134500	-4.36351000	-0.95925100
C	0.33650300	-1.04156500	-5.14454400	C	-6.35711700	-3.11804800	-1.56821900
H	0.87264700	-0.67255200	-6.02753300	H	-7.05349500	-3.08847700	-2.40840300
C	1.07515000	-1.62778600	-4.10429600	C	-5.73805500	-1.98129100	-1.08320900
C	-1.76637500	-2.49589700	-1.66404500	H	-5.93841600	-1.01539100	-1.55353100
H	-2.83416300	-2.24206800	-1.73269300	C	-4.81710900	-2.04505700	0.00669900
H	-1.35772100	-2.04571100	-0.74463200	C	-2.65034500	3.54663200	-1.38204400
C	-1.83807800	-0.33773200	-6.24628000	C	-2.36484500	4.73433700	-0.66073200
H	-2.85759800	-0.04873200	-5.94138800	C	-1.35466100	5.59044600	-1.13602600
H	-1.33090800	0.55547600	-6.65114400	H	-1.15092200	6.51629600	-0.58383600
C	2.57043800	-1.80732300	-4.23208100	C	-0.60282800	5.29299800	-2.28523200
H	3.11339100	-1.39806200	-3.36533800	C	-0.88218700	4.09270700	-2.95956100
H	2.95821000	-1.30867100	-5.13421900	H	-0.28966500	3.82604800	-3.84114400
C	-4.49681300	0.48831600	0.05667900	C	-1.89678700	3.21919000	-2.53922600
C	-3.51543600	1.34179000	-0.44875700	C	-3.09392400	5.07949500	0.62114800
C	-3.76276400	2.66469900	-0.91975300	H	-3.19532300	4.19241200	1.26820300
C	-5.07970100	3.10401300	-0.89521400	H	-2.54389100	5.85584100	1.17883400
H	-5.32029100	4.10016600	-1.27941100	C	0.49672900	6.20105600	-2.78152700
C	-6.12668500	2.30895000	-0.35019700	H	1.46743300	5.68089300	-2.69447700
C	-7.45461100	2.81045800	-0.27568000	H	0.35045200	6.45041500	-3.84760000
H	-7.70710500	3.79667400	-0.67243900	C	-2.15459300	1.95818000	-3.32708100
C	-8.43795800	2.04663900	0.32302800	H	-1.81810500	2.07446200	-4.36931000
C	-8.17166200	0.77608100	0.88675000	H	-1.60623200	1.10438500	-2.89419200
H	-8.98382200	0.23359500	1.37453600	C	-1.79080000	-2.43990800	3.12973700
C	-6.88895300	0.26662600	0.80761000	C	-0.58449300	-3.14892200	2.91320100
H	-6.66860900	-0.70728800	1.25081600	C	0.33511400	-3.26105200	3.97062400
C	-5.83836900	0.99437500	0.16997000	H	1.26999700	-3.80667800	3.79423300
C	-4.13730100	-0.88338800	0.50982800	C	0.09140400	-2.69816400	5.23249500
C	-3.10979200	-1.07884200	1.43767400	C	-1.10848300	-1.99058000	5.41908300

H	-1.32195300	-1.54247400	6.39724400	O	-10.66818100	1.88463700	0.94557100
C	-2.05553700	-1.84986500	4.39273100	O	-7.52600800	-5.43764100	-2.41434000
C	-0.22796000	-3.73084500	1.56754000	O	-6.47387100	-6.65414200	-0.93057700
H	0.55141300	-4.50033200	1.67072300	H	-3.22450600	1.68805500	-3.33494200
H	0.16482200	-2.93710900	0.90759900	O	0.70033700	3.50705600	1.96416800
C	1.06958600	-2.88334300	6.36997500	C	1.05831000	3.94460900	0.85502700
H	0.78808900	-3.75588800	6.98997000	H	0.39884600	3.79176200	-0.02199200
H	2.09211000	-3.05826500	5.99635900	C	2.28365500	4.75441800	0.66668900
C	-3.33764400	-1.08909300	4.64758900	H	2.99749500	4.50624600	1.46647100
H	-3.47076900	-0.89352400	5.72397800	H	2.69122200	4.48544500	-0.32261000
H	-3.32876600	-0.11721500	4.12231400	C	1.97872400	6.28386700	0.68113200
N	-0.05032200	-0.05144600	0.53600700	C	3.23349800	7.04573700	0.23021500
O	2.27484400	-0.37574100	1.42185600	C	1.48674100	6.75756000	2.05594000
O	1.97955600	-0.65525200	-1.10198900	H	1.18177900	6.47331200	-0.05958900
O	1.88785100	1.70828100	-0.18418000	H	3.54362600	6.73601200	-0.78255200
O	-2.20891100	0.87206500	-0.51648200	H	3.04551800	8.13386900	0.21648200
O	-2.36794000	0.01285100	1.86590800	H	4.07652000	6.85515300	0.91976500
O	-1.29513900	2.19767300	1.52298000	H	0.57639200	6.22078700	2.37425500
P	1.47352200	0.29694900	0.15176200	H	2.25926100	6.59126600	2.82794400
P	-1.32868800	0.79400000	0.86528500	H	1.25545700	7.83705800	2.03281600
H	-0.36358100	2.76816700	1.78208800	O	2.29643400	3.41580700	-2.31333700
H	0.53605400	7.14461300	-2.21239400	C	3.55026400	2.91255900	-2.75290800
H	-4.11076100	5.46808100	0.43111800	C	3.41350400	1.52404000	-3.40491800
H	1.96430800	4.98212500	4.95016800	H	4.27323900	2.84606400	-1.91248700
H	5.57273000	3.78195400	1.09865000	H	3.95740900	3.63987400	-3.47715900
H	3.56365900	-1.09669500	4.34371200	C	4.76026900	0.91361100	-3.71095700
H	1.08800400	-2.00266000	7.03453400	H	2.80101000	1.61329900	-4.31905300
H	-4.21848900	-1.64849600	4.28590600	H	2.86232400	0.87819700	-2.70107200
H	-1.09197900	-4.17854200	1.05366300	C	5.33421400	1.01003400	-4.99150000
H	-1.68396100	-3.59145300	-1.55147100	C	5.48935400	0.28991000	-2.67888000
H	2.82953100	-2.88063200	-4.29265200	C	6.61524000	0.48862800	-5.23081700
H	-1.93083000	-1.06336200	-7.07653100	H	4.77344100	1.49094000	-5.80054800
N	-9.81525000	2.58736500	0.39884100	C	6.77872100	-0.21684200	-2.91853400
N	-6.74173900	-5.58018600	-1.47363200	H	5.04586900	0.19596500	-1.67912200
O	-10.02026800	3.70125900	-0.08803900	C	7.34348700	-0.12077300	-4.20518000

H	7.05469900	0.55981200	-6.23197100	H	-4.86599400	-4.39753100	-0.99878900
O	7.53327500	-0.80519400	-1.94763200	C	-3.61156500	-4.05402200	0.74151000
H	8.34456500	-0.52830900	-4.37379300	C	-3.82369200	0.90070100	-2.94259900
H	7.02169900	-0.85085500	-1.11737400	C	-4.16149800	2.23975500	-2.64219900
H	1.97857900	2.77220900	-1.63449200	C	-3.49410500	3.26892100	-3.31654600
				H	-3.76012500	4.30364700	-3.08490900
TS1				C	-2.47474000	3.01391800	-4.24255200
C	-4.36656900	-1.86854400	-0.36464000	C	-2.16134000	1.68074900	-4.52172800
C	-3.77613500	-0.96392100	-1.23735500	H	-1.37079000	1.45517400	-5.24287400
C	-4.50005600	-0.18950900	-2.18390000	C	-2.82442500	0.61802000	-3.89655800
C	-5.85799100	-0.41886600	-2.28227500	C	-5.16554800	2.58181200	-1.56681700
H	-6.43822400	0.13666600	-3.02219900	H	-4.92864100	2.05821600	-0.62841200
C	-6.53765800	-1.30129500	-1.40455400	H	-6.19287200	2.29810100	-1.84249000
C	-7.95019600	-1.45785700	-1.46980800	C	-1.67735300	4.13800400	-4.85385300
H	-8.49646300	-0.93271300	-2.25729400	H	-1.34200800	3.89211300	-5.87264600
C	-8.61967900	-2.23258600	-0.54888100	H	-2.25677700	5.07267800	-4.89732200
H	-9.70540200	-2.33943700	-0.60387200	C	-2.43491400	-0.79683500	-4.22637100
C	-7.89933200	-2.87072600	0.48977700	H	-1.75483500	-1.20456700	-3.46501600
H	-8.43570300	-3.45324600	1.24226300	H	-1.91694300	-0.85068400	-5.19340200
C	-6.52756100	-2.75630700	0.56679400	C	-1.05597400	-1.72053300	3.38129200
H	-5.99171700	-3.24429500	1.37944300	C	0.34243000	-1.68691300	3.22051100
C	-5.79926600	-1.99829000	-0.39215200	C	1.10040900	-0.86418200	4.06650400
C	-3.53879000	-2.62563900	0.61366300	H	2.18618000	-0.84221500	3.94009000
C	-2.65413700	-1.94707200	1.43983500	C	0.50847000	-0.07792500	5.05932200
C	-1.90880300	-2.55698300	2.48497300	C	-0.88373400	-0.13452700	5.20313100
C	-2.05031400	-3.91975500	2.64944800	H	-1.36858500	0.46507800	5.97891700
H	-1.50445000	-4.41969000	3.45286500	C	-1.67562300	-0.95124400	4.39151800
C	-2.86685600	-4.69671400	1.78489700	C	1.02791300	-2.50148100	2.15672400
C	-2.92009000	-6.11304500	1.90354400	H	2.11635500	-2.37322400	2.20641900
H	-2.35787200	-6.58970900	2.71032100	H	0.69653700	-2.18489900	1.15904800
C	-3.64213300	-6.87306900	1.00989300	C	1.33145700	0.79224900	5.97497700
H	-3.66476600	-7.96094900	1.10488400	H	2.40404400	0.71904600	5.74710700
C	-4.34396600	-6.24220900	-0.04626500	H	1.03776000	1.85153300	5.89070100
H	-4.89346500	-6.84877000	-0.76970600	C	-3.16178600	-1.03332600	4.63126500
C	-4.33293100	-4.86928800	-0.17424300	H	-3.75256400	-0.84343700	3.72559400

H	-3.47894700	-0.30202500	5.38744900	H	2.06927600	4.80534400	3.66863100
C	4.13648000	-0.15228100	-0.27238800	C	2.88813800	3.53157600	2.14145800
C	3.42413400	0.96708800	0.14070400	C	3.41804700	4.44168900	-1.54766500
C	4.02429800	2.24998100	0.29592500	H	2.99389100	3.52336400	-1.98060000
C	5.36598300	2.37114400	-0.00949100	H	3.00609300	5.29955500	-2.09547900
H	5.85532600	3.33754100	0.12729800	C	1.60586100	7.13166000	2.32051700
C	6.12340300	1.28902000	-0.52334500	H	0.55462500	6.98645700	2.62481700
C	7.47794700	1.46348900	-0.90370600	H	2.14940900	7.48577800	3.21111000
H	7.97295500	2.42602600	-0.77852400	C	3.03078200	2.35549900	3.07039600
C	8.16932000	0.40863700	-1.45217800	H	3.00678600	2.67650100	4.12018000
C	7.56903100	-0.85306300	-1.66113100	H	2.21330600	1.63306200	2.91576100
H	8.15353400	-1.64561900	-2.12545900	C	0.82652800	-3.17875500	-2.51970500
C	6.26106600	-1.04228400	-1.27907300	C	-0.37409000	-3.83847500	-2.18020000
H	5.79206600	-2.00949100	-1.45095400	C	-1.30379400	-4.11977800	-3.18804500
C	5.50193300	0.00698500	-0.68286800	H	-2.23983500	-4.61340700	-2.91279400
C	3.49066400	-1.48764700	-0.34399600	C	-1.06815500	-3.78771000	-4.52534200
C	2.35516300	-1.68147100	-1.12366200	C	0.12833700	-3.13440500	-4.83889200
C	1.88719400	-2.97763800	-1.49042300	H	0.33026500	-2.85856200	-5.87795100
C	2.51571400	-4.06728500	-0.91881800	C	1.07803600	-2.81383600	-3.86228500
H	2.20347200	-5.07296900	-1.20597900	C	-0.69488800	-4.21787700	-0.75914800
C	3.55203800	-3.92231700	0.03820700	H	-1.65478700	-4.73986400	-0.71356600
C	4.10266500	-5.04706000	0.70124200	H	-0.76062800	-3.32664800	-0.11803400
H	3.74231000	-6.05304700	0.48818800	C	-2.06660200	-4.13167800	-5.60026800
C	5.09409300	-4.86442500	1.63782900	H	-2.11333300	-3.34804000	-6.37175200
C	5.59143500	-3.58299600	1.96582400	H	-1.79448100	-5.07339400	-6.10792000
H	6.36421000	-3.49561200	2.72772100	C	2.34554000	-2.10110700	-4.26179500
C	5.08047800	-2.48334100	1.31560600	H	2.49266500	-2.13916000	-5.35041400
H	5.45140800	-1.49006300	1.56744700	H	2.30929300	-1.04305100	-3.95746900
C	4.05672900	-2.61393400	0.33348800	N	-0.23482400	-0.07289200	0.10707300
C	3.28449300	3.44768600	0.78822700	O	-2.40003900	-0.77589100	-1.17833600
C	3.08923900	4.54109100	-0.07876400	O	-2.54126800	-0.56887800	1.31036800
C	2.55549900	5.72822200	0.43881100	O	-2.34279800	1.54530900	-0.01823900
H	2.40506500	6.57252000	-0.23711400	O	2.09134300	0.82142100	0.45646000
C	2.19970700	5.85354000	1.78367600	O	1.70305900	-0.59273900	-1.64321600
C	2.35673800	4.73563200	2.61519300	O	0.77522400	1.73067000	-1.63351400

P	-1.79019900	0.13394400	0.02153100	H	-0.55651100	7.69054700	-2.78724300
P	0.96812300	0.55854400	-0.72104800	H	0.72306600	8.09029000	-1.61692200
H	0.55889300	3.23510400	-1.56528000	O	-1.22647900	3.61307500	0.32780700
H	1.62387700	7.93285100	1.56791400	C	-1.00752900	4.43449800	1.49435300
H	4.50373200	4.41157200	-1.72991100	C	-1.17918700	3.63726800	2.78577600
H	-0.77183200	4.33534800	-4.25329700	H	-1.73669400	5.25631800	1.46774700
H	-5.16299000	3.66246700	-1.36292000	H	0.01102800	4.82591700	1.41058600
H	-3.30779900	-1.46586800	-4.26395100	C	-2.63965200	3.37224100	3.07165100
H	-3.07659700	-4.26233500	-5.18388500	H	-0.71651100	4.24802000	3.57928300
H	3.23183600	-2.54390100	-3.78167800	H	-0.60485400	2.69877900	2.73478300
H	0.06245500	-4.87538200	-0.31059000	C	-3.51488100	4.39271100	3.47568800
H	0.80459000	-3.57485900	2.25041700	C	-3.16006500	2.12106100	2.75233700
H	-3.44673300	-2.03767600	4.98615800	C	-4.89173400	4.14709800	3.51007700
H	1.18904100	0.50279600	7.02924100	H	-3.12638900	5.37804200	3.74767500
N	9.57493900	0.60564200	-1.85193100	C	-4.54045700	1.89832800	2.70674700
N	5.64671900	-6.04194400	2.33158600	H	-2.48404700	1.31660200	2.48664500
O	10.06980100	1.70590600	-1.66519500	C	-5.41573600	2.91532600	3.10746400
O	10.15612400	-0.34760400	-2.34563900	H	-5.57430100	4.93800100	3.83132500
O	6.52574300	-5.84584700	3.15583900	O	-5.04631900	0.72566500	2.24611700
O	5.19298300	-7.13763500	2.04121900	H	-6.49131600	2.73123300	3.08314400
H	3.97176600	1.81130100	2.89934800	H	-4.31551100	0.21009500	1.86525200
O	0.27775600	4.20321500	-1.42929900	H	-1.78242000	2.66779300	0.28126700
C	-1.03336300	4.18871100	-1.17028300				
H	-1.58361600	3.45206600	-1.77621500	Int1			
C	-1.67784100	5.55957100	-1.29781500	C	4.46951600	-1.83840400	0.26364100
H	-1.92074200	5.68348500	-2.36438000	C	3.85558800	-0.97964600	1.17463600
H	-2.64828500	5.52605300	-0.77772200	C	4.55107800	-0.20121400	2.14477700
C	-0.82337900	6.75871600	-0.83120700	C	5.92324500	-0.39719000	2.23548700
C	-1.70501400	7.86629700	-0.24983200	H	6.49067500	0.15456600	2.99175100
C	0.06015200	7.28266600	-1.96788800	C	6.62679800	-1.24413600	1.33549200
H	-0.14625900	6.41257300	-0.03724800	C	8.04594600	-1.36980100	1.40126200
H	-2.28240600	7.51088900	0.61961400	H	8.57904600	-0.84889900	2.20399700
H	-1.09973800	8.72621500	0.07897100	C	8.73922500	-2.11141700	0.46098900
H	-2.42669500	8.23510000	-0.99866000	H	9.82946300	-2.19397100	0.51827100
H	0.68307500	6.47499200	-2.37570000	C	8.03698300	-2.74508500	-0.59706600

H	8.59106600	-3.30082000	-1.36054400	H	2.05332900	-0.99348800	5.13778000
C	6.65663700	-2.65931200	-0.67884200	C	1.15492400	-1.52383600	-3.46901500
H	6.12957500	-3.14250800	-1.50497000	C	-0.25009100	-1.49351300	-3.30913100
C	5.90769000	-1.93756700	0.29607400	C	-0.99667000	-0.58278800	-4.07801200
C	3.65376100	-2.55623700	-0.75400600	H	-2.08557100	-0.55996000	-3.95153500
C	2.75496600	-1.84970600	-1.55273300	C	-0.39036000	0.28736700	-4.99833600
C	2.00242300	-2.41630100	-2.62039100	C	1.00336100	0.21172600	-5.16200000
C	2.14107100	-3.77960800	-2.83739100	H	1.49716200	0.86597900	-5.89017600
H	1.58894600	-4.25075500	-3.65722500	C	1.78821900	-0.68306000	-4.41823000
C	2.96866800	-4.58807800	-2.00702500	C	-0.94748800	-2.40569300	-2.32870000
C	3.02360100	-6.00246900	-2.17898500	H	-2.03554700	-2.24208800	-2.35233600
H	2.44616900	-6.45203700	-2.99401800	H	-0.59515600	-2.21346600	-1.30227700
C	3.76815100	-6.79595300	-1.32367300	C	-1.20281600	1.28759500	-5.78913500
H	3.79188700	-7.88192500	-1.46011600	H	-1.10948600	2.29987500	-5.35263200
C	4.48907100	-6.20204000	-0.25466900	H	-0.85359900	1.35081200	-6.83418900
H	5.05604200	-6.83503900	0.43568900	C	3.28204900	-0.74827700	-4.64216100
C	4.47457000	-4.82875100	-0.07210300	H	3.84399200	-0.29500300	-3.80728900
H	5.02024600	-4.38221900	0.76289600	H	3.56504500	-0.20113900	-5.55566900
C	3.73164100	-3.98122400	-0.94517800	C	-4.08735700	-0.28144900	0.34908200
C	3.84418400	0.85962400	2.92115000	C	-3.42035200	0.88383000	-0.03524000
C	4.20788700	2.21466900	2.69119400	C	-4.07736400	2.14636800	-0.14321900
C	3.51752700	3.22447100	3.37937600	C	-5.42159200	2.20641700	0.20148700
H	3.80220400	4.26892700	3.20192600	H	-5.94929200	3.16100000	0.10707400
C	2.45279600	2.94327200	4.25397300	C	-6.12923800	1.07670700	0.69238400
C	2.11191900	1.59884700	4.45952000	C	-7.48614600	1.18160000	1.10153200
H	1.28705200	1.35176900	5.13855900	H	-8.02633400	2.12838100	1.02653300
C	2.79200900	0.54990100	3.81646800	C	-8.12685700	0.07022700	1.61443600
C	5.26295400	2.60350400	1.67582400	C	-7.47447300	-1.17717500	1.76408600
H	5.15669200	2.02471300	0.74352700	H	-8.02444200	-2.01085100	2.20490800
H	6.28834100	2.43441800	2.05113400	C	-6.15973100	-1.29754600	1.35517900
C	1.65648000	4.05902800	4.89018700	H	-5.64388800	-2.25211500	1.48090600
H	1.21939300	3.74644200	5.85339200	C	-5.45364000	-0.19121900	0.78949000
H	2.27873200	4.95410600	5.06145900	C	-3.39941900	-1.59708000	0.35240200
C	2.36705800	-0.87290100	4.08756900	C	-2.24420500	-1.78841600	1.11486300
H	1.51001200	-1.15770300	3.45326700	C	-1.73021100	-3.08539700	1.42415200

C	-2.33277300	-4.17351600	0.80360300	C	-0.91993000	-3.00205100	3.80500200
H	-1.98503200	-5.18274400	1.04514700	C	0.87080900	-4.27060200	0.63618200
C	-3.38448000	-4.02044600	-0.13998200	H	1.77773500	-4.88813100	0.57678900
C	-3.90477400	-5.13329100	-0.85321000	H	1.05151900	-3.34109200	0.06963700
H	-3.50769200	-6.13924900	-0.69767600	C	2.25646400	-4.35064600	5.49143100
C	-4.91946700	-4.93643800	-1.77094000	H	1.77144800	-4.63402000	6.44112900
C	-5.47164000	-3.65819500	-2.02965600	H	2.90445700	-5.18288600	5.16889800
H	-6.26020500	-3.56641400	-2.77899100	C	-2.20288700	-2.32731600	4.23513100
C	-4.98849700	-2.56878500	-1.32935400	H	-2.33635000	-2.39972400	5.32662400
H	-5.39702500	-1.57375000	-1.52501000	H	-2.19325600	-1.25820100	3.95843300
C	-3.94209200	-2.71223700	-0.36800800	N	0.26374900	-0.12757300	-0.10822400
C	-3.42268400	3.39404700	-0.64066300	O	2.45790600	-0.85180800	1.13272100
C	-3.14282000	4.44058000	0.26839900	O	2.61474700	-0.46739000	-1.35000800
C	-2.69544800	5.67293600	-0.23939100	O	2.40959700	1.52759600	0.12839400
H	-2.47667500	6.48222000	0.46546700	O	-2.08094000	0.79215300	-0.39152000
C	-2.51947100	5.88941100	-1.61497600	O	-1.63043100	-0.68854300	1.68362500
C	-2.79091000	4.82625600	-2.49641500	O	-0.69981200	1.66161100	1.70830500
H	-2.65950000	4.97388300	-3.57541100	P	1.81777500	0.09902000	-0.01925000
C	-3.23454500	3.57742700	-2.03341200	P	-0.92905800	0.51027200	0.77347700
C	-3.31325400	4.24168100	1.75728000	H	-0.37946100	3.29836800	1.74098800
H	-2.90019500	3.26901400	2.07222900	H	-2.08322200	8.00325900	-1.37320200
H	-2.79311000	5.03507700	2.31527800	H	-4.37988600	4.25529800	2.04804400
C	-2.00347900	7.21166200	-2.13613100	H	0.82334900	4.35432200	4.22443300
H	-0.93672600	7.13458500	-2.42232000	H	5.17406100	3.67359400	1.42541000
H	-2.55734600	7.53508800	-3.03457500	H	3.17620300	-1.59179600	3.88115100
C	-3.50867000	2.44801700	-2.99824800	H	2.91116700	-3.48390000	5.70302500
H	-3.43969200	2.79280100	-4.04187600	H	-3.08383500	-2.78164400	3.74809300
H	-2.77811100	1.63139100	-2.85656800	H	0.05997400	-4.80529900	0.11805600
C	-0.66299800	-3.30988900	2.44323600	H	-0.75467200	-3.46998800	-2.54976000
C	0.54409700	-3.95530100	2.07611000	H	3.62861600	-1.79203700	-4.73618200
C	1.47374900	-4.28131600	3.07748500	H	-2.27320100	1.02392900	-5.79558900
H	2.40697000	-4.77689700	2.78402500	N	-9.53950600	0.19325400	2.04210500
C	1.23595900	-4.00295800	4.43271000	N	-5.43951900	-6.10283200	-2.52013000
C	0.03334600	-3.36135700	4.77179300	O	-10.08478700	1.29086500	1.90794200
H	-0.17853000	-3.13984800	5.82489800	O	-10.07924500	-0.81420900	2.50500100

O	-6.34862400	-5.89643000	-3.32748900	O	4.93331800	1.34232400	-2.26559700
O	-4.93223500	-7.20334400	-2.29132000	H	5.92798900	3.71981200	-2.77425800
H	-4.51345800	2.01762500	-2.83979000	H	4.31082100	0.66530800	-1.92614800
O	-0.10571500	4.25057900	1.62007200	H	1.79613600	2.39053900	-0.14418800
C	1.15363400	4.24349800	1.06298200				
H	1.85147600	3.58448600	1.60780400	TS2			
C	1.74737500	5.65136300	0.94823400	C	-3.34743100	0.83524700	0.06851500
H	2.32030800	5.84319000	1.87530200	C	-3.09609200	-0.31675400	0.81226500
H	2.49031700	5.60468000	0.13225100	C	-4.12235300	-1.21106600	1.23743700
C	0.76511800	6.82654700	0.72359100	C	-5.43627600	-0.85740300	0.95802200
C	1.47806100	7.97998800	0.00014400	H	-6.24151600	-1.52037600	1.29180000
C	0.13472300	7.30154100	2.04242800	C	-5.76841600	0.29828000	0.20347300
H	-0.05691900	6.47483000	0.07622700	C	-7.12434000	0.59734600	-0.12273500
H	1.87095000	7.65576200	-0.98084000	H	-7.91226200	-0.04328500	0.28793600
H	0.79129700	8.82886700	-0.16849000	C	-7.43753600	1.65464200	-0.95740300
H	2.33208400	8.35197600	0.59663900	C	-6.39549900	2.43827000	-1.51688500
H	-0.38681300	6.47149200	2.54357300	H	-6.63837400	3.24916700	-2.21133500
H	0.91278700	7.68814400	2.72788700	C	-5.07030700	2.18533300	-1.20212200
H	-0.58868700	8.11773900	1.86299900	H	-4.28764000	2.79424400	-1.65704100
O	1.14693200	3.56935400	-0.25822700	C	-4.71232100	1.13540600	-0.30329500
C	0.19197800	4.01085900	-1.25045100	C	-2.24287800	1.63719600	-0.52394200
C	0.53109000	3.39803700	-2.61541700	C	-1.31787100	0.99700300	-1.35278700
H	0.26624700	5.10707600	-1.30997400	C	-0.58392100	1.68240000	-2.36690600
H	-0.82106500	3.73974600	-0.91971700	C	-0.62542700	3.07157200	-2.35457600
C	2.01544100	3.51364800	-2.88503200	H	-0.09639400	3.62726900	-3.13492000
H	-0.08077800	3.93372900	-3.36294500	C	-1.37939200	3.79623400	-1.39049600
H	0.22481200	2.33753900	-2.64275800	C	-1.39456000	5.22134000	-1.37192700
C	2.65838500	4.74609500	-3.10651900	H	-0.77525800	5.76051700	-2.09639100
C	2.79336800	2.36578900	-2.70211400	C	-2.17260400	5.91337900	-0.45888800
C	4.06134000	4.80479200	-3.10424600	C	-2.96615300	5.20000100	0.47765400
H	2.07031000	5.65840100	-3.25911200	H	-3.56523100	5.75114300	1.20988800
C	4.19120600	2.44025600	-2.60730100	C	-2.99622400	3.81439300	0.46755600
H	2.29826400	1.40171100	-2.57278500	H	-3.62219700	3.26948900	1.17938000
C	4.83686700	3.66760400	-2.83287700	C	-2.21440600	3.07538600	-0.46573500
H	4.56382200	5.76166400	-3.28446600	C	-3.86701500	-2.53646900	1.88230900

C	-3.95017600	-3.70155800	1.08054600	C	5.35675000	-0.09902500	-0.82252000
C	-3.76867100	-4.95562600	1.69219800	C	6.53427900	0.63116500	-0.89296400
H	-3.81046700	-5.85639200	1.06806900	H	7.44950600	0.13673900	-1.23465100
C	-3.51781800	-5.08238800	3.06695400	C	6.60772200	1.98211000	-0.45243000
C	-3.46735000	-3.91002900	3.84319300	C	7.84355700	2.68316800	-0.47424500
H	-3.27686500	-3.98394900	4.92065600	H	8.73920800	2.22952200	-0.90549800
C	-3.64307400	-2.63943000	3.27479200	C	7.91960500	3.94775600	0.07753100
C	-4.21483100	-3.60806100	-0.40450300	C	6.80770700	4.56781700	0.69520400
H	-4.06125300	-4.58225400	-0.89578000	H	6.93709100	5.55059600	1.15253100
H	-3.54246200	-2.87990400	-0.88438300	C	5.59463000	3.90532200	0.70823700
C	-3.28497500	-6.43175200	3.70638100	H	4.73891100	4.37287400	1.19874400
H	-3.38658500	-7.24846900	2.97353200	C	5.43878400	2.61824300	0.10636700
H	-2.27158400	-6.48820200	4.14521000	C	2.95488300	2.50539600	0.66450300
C	-3.59050700	-1.39172000	4.12151800	C	2.27732400	1.82304700	1.68639500
H	-2.81097200	-0.70665900	3.75100400	C	1.33055900	2.45373400	2.55619000
H	-3.36231800	-1.63033100	5.17281100	C	0.95485200	3.75502200	2.25298100
C	0.00733200	0.92765100	-3.50938400	H	0.25123700	4.28000100	2.90487700
C	1.37880900	1.02403300	-3.83384800	C	1.46726200	4.43652100	1.11495000
C	1.86776100	0.30404400	-4.93973300	C	1.00730400	5.73492800	0.77613800
H	2.93217000	0.38014000	-5.18720500	H	0.24177800	6.23233700	1.37476300
C	1.04292700	-0.51895400	-5.71926600	C	1.50680300	6.36199600	-0.35026100
C	-0.32730100	-0.56380200	-5.40504400	C	2.48440300	5.76189900	-1.18069700
H	-1.00065000	-1.17170500	-6.02128800	H	2.82587300	6.29721500	-2.06873200
C	-0.86388600	0.16167500	-4.33210900	C	2.97148800	4.51435600	-0.84038400
C	2.31005800	1.89906400	-3.02895700	H	3.73290300	4.04081500	-1.46467500
H	3.35207400	1.55260800	-3.11361400	C	2.48459000	3.81359000	0.30518500
H	2.03105500	1.90450300	-1.96475700	C	5.36628000	-1.58364000	-0.99710600
C	1.59498700	-1.31248300	-6.88141000	C	5.90845600	-2.36622000	0.05637600
H	1.30559400	-0.85517800	-7.84625300	C	5.91130800	-3.76055200	-0.07478900
H	2.69628200	-1.35718700	-6.84935300	H	6.29725000	-4.36809300	0.75189400
C	-2.36236100	0.16573800	-4.11389600	C	5.39926400	-4.40539200	-1.21408300
H	-2.64852400	-0.35311900	-3.17944900	C	4.88641000	-3.60827800	-2.24721500
H	-2.87295000	-0.31562600	-4.96530600	H	4.48927300	-4.08758900	-3.15107100
C	4.18465100	1.91098900	0.06830700	C	4.84806000	-2.20549600	-2.15166500
C	4.17875600	0.59727000	-0.41128500	C	6.40667900	-1.72517300	1.33270800

H	7.26941100	-1.05848500	1.15640600	H	6.32720000	-6.36405500	-1.08297500
H	5.60681400	-1.12032000	1.79440500	H	6.71395600	-2.49647000	2.05716900
C	5.33714000	-5.91155800	-1.27125600	H	-4.00380900	-6.61366400	4.52614600
H	4.64900500	-6.26709300	-0.48269500	H	-5.24844300	-3.27840000	-0.61095400
H	4.97334400	-6.27025100	-2.24906300	H	-4.55051900	-0.84568700	4.08659100
C	4.22303000	-1.38389300	-3.25008000	H	-0.77378900	-1.33460300	7.09171600
H	4.86957100	-0.53872000	-3.54633800	H	3.48853200	2.48104600	4.10727300
H	4.01673400	-1.99480000	-4.14376300	H	-1.79124100	3.15814800	3.13558400
C	0.83845800	1.75751300	3.78123700	H	2.27816300	2.94437700	-3.38760600
C	-0.55339700	1.59494300	4.00770700	H	-2.75377300	1.19388700	-4.02319300
C	-0.98530600	0.96690600	5.18544200	H	1.20454400	-2.34531200	-6.88060400
H	-2.06137300	0.84979000	5.35432700	H	3.26494700	-0.95879900	-2.90628500
C	-0.08442400	0.47873800	6.14486200	O	3.18367800	-4.82139300	1.35618000
C	1.28514300	0.67898100	5.91766900	C	-0.29450000	-3.81242100	0.35237800
H	2.00834600	0.33784900	6.66831300	H	-0.81554400	-4.59524000	-0.22014500
C	1.76780400	1.31653100	4.76183000	C	-0.52599400	-3.95933500	1.86127400
C	-1.57993300	2.08066200	3.01199600	H	-1.53406000	-3.57653100	2.07065900
H	-2.53392100	1.54419900	3.14068300	H	-0.58964300	-5.05073000	2.02261900
H	-1.23685700	1.93249400	1.97743500	C	0.52073000	-3.35823600	2.84411200
C	-0.58030300	-0.27655900	7.35539800	C	1.07613200	-4.45311100	3.77327200
H	0.16100600	-0.26935200	8.17160600	C	-0.01481900	-2.18953300	3.69019700
H	-1.52661700	0.14358700	7.73768400	H	1.37215500	-2.97962600	2.25980300
C	3.25861800	1.53273400	4.62232100	H	1.61959200	-5.22127300	3.19855900
H	3.73865800	1.55370600	5.61449100	H	1.78572800	-4.01604400	4.49849500
H	3.72089200	0.72067400	4.03411600	H	0.25966500	-4.93292400	4.34756800
N	0.75803000	-0.72102500	0.50894800	H	-0.53247000	-1.42603300	3.08978400
O	-1.76738500	-0.59575300	1.17743100	H	-0.72517600	-2.55170600	4.45797100
O	-1.20834300	-0.40298000	-1.30933800	H	0.81638900	-1.68623200	4.21315800
O	-1.01135100	-2.61129200	-0.25077700	O	1.03251500	-3.71100200	0.01096200
O	2.96116800	-0.05424400	-0.49802200	C	1.49207900	-4.27533700	-1.24114200
O	2.59292200	0.51392100	1.95898900	C	0.89171000	-3.65830700	-2.50284000
O	3.08200800	-1.89967100	1.38250500	H	1.33311800	-5.36857800	-1.20357600
P	-0.66648900	-1.10472600	0.07934700	H	2.57283800	-4.08474200	-1.20953200
P	2.31225000	-0.72451100	0.88173700	C	-0.50671700	-4.12740100	-2.86788300
H	3.69053500	-4.08874900	1.74618200	H	1.58112100	-3.92242900	-3.32915500

H	0.92598900	-2.55839000	-2.42006200	C	-5.71736500	3.37770300	-1.35936300
C	-0.81019100	-5.50096900	-2.96187200	H	-4.93437800	3.74000500	-2.02869500
C	-1.50936200	-3.19193800	-3.16312300	C	-5.39462400	2.39836600	-0.37424700
C	-2.09576100	-5.91355500	-3.34268000	C	-2.91480100	2.30659300	-1.03098800
H	-0.04122800	-6.25315500	-2.75466300	C	-2.20830600	1.34966000	-1.76638500
C	-2.79588600	-3.60785300	-3.54703400	C	-1.31944700	1.66684300	-2.83579600
H	-1.28502200	-2.12589500	-3.07400900	C	-1.03303000	3.00487200	-3.06005100
C	-3.09511500	-4.97852400	-3.63708000	H	-0.37175100	3.28526600	-3.88647000
H	-2.32262500	-6.98274600	-3.41655900	C	-1.59214100	4.03055900	-2.24541000
O	-3.79581600	-2.71716500	-3.82251600	C	-1.25427500	5.40040500	-2.44858300
H	-4.10220000	-5.28617600	-3.93298500	H	-0.54628700	5.64975600	-3.24661500
H	-3.44893300	-1.81318200	-3.70710200	C	-1.79902300	6.39658500	-1.65574400
H	2.39311100	-4.32015400	1.07006900	H	-1.51637600	7.44100800	-1.81657700
O	-9.11008300	2.89171400	-2.03539400	C	-2.70233000	6.05385200	-0.61560500
O	-9.74196000	1.25148500	-0.82731900	H	-3.11684400	6.84058500	0.02347000
O	-2.84613000	7.99843200	0.37101700	C	-3.06979500	4.73382200	-0.40589600
O	-1.44646800	8.00024700	-1.23833400	H	-3.77544200	4.47912500	0.38909500
N	-8.84186100	1.94910900	-1.29212300	C	-2.54254400	3.68677600	-1.21717500
N	-2.15402600	7.38654400	-0.44107000	C	-4.74066900	-1.15973400	2.02975300
H	8.84960000	4.47531400	0.03639000	C	-5.18296600	-2.29572300	1.29827400
H	1.14172900	7.33537000	-0.60356800	C	-4.86183200	-3.57364000	1.77405600
				H	-5.15786300	-4.44571100	1.18172300
Int2				C	-4.10027800	-3.76599900	2.93937100
C	-4.06254400	1.87717600	-0.18042300	C	-3.68770700	-2.63035300	3.65245400
C	-3.90112600	0.83139400	0.72668400	H	-3.10158200	-2.75472000	4.57202300
C	-4.97046800	0.18452500	1.41375900	C	-3.99682400	-1.32844500	3.21761200
C	-6.22632200	0.76307700	1.29754000	C	-5.88417600	-2.15700200	-0.03474200
H	-7.07301400	0.31385700	1.82760500	H	-6.80361000	-1.55123100	0.02995500
C	-6.46629500	1.87315000	0.43802500	H	-6.14924900	-3.14920000	-0.43390200
C	-7.77775400	2.41448300	0.29401800	C	-3.71862800	-5.16301000	3.36951800
H	-8.57780700	2.01501100	0.92700000	H	-4.61161200	-5.75794100	3.63663600
C	-8.04489500	3.40152600	-0.63862900	H	-3.21279900	-5.67793900	2.53388900
H	-9.05779200	3.80436300	-0.74183400	C	-3.49374300	-0.13478200	3.98882700
C	-7.00685000	3.86960900	-1.48473500	H	-2.59775900	0.28982300	3.50534400
H	-7.22642800	4.62164600	-2.24977300	H	-3.21704100	-0.40744200	5.02058900

C	-0.84035700	0.55505700	-3.71180900	H	0.09376200	4.56792000	2.12777500
C	0.49494900	0.09930200	-3.65232800	C	1.38196400	4.07806000	0.45798800
C	0.87080500	-1.00697800	-4.43352800	C	1.24619200	5.34552200	-0.16697700
H	1.90374000	-1.36689700	-4.37918600	H	0.57475300	6.10362700	0.24087000
C	-0.04239200	-1.67191100	-5.26686800	C	1.95148500	5.60611900	-1.32588200
C	-1.35083500	-1.16620300	-5.34921500	C	2.82627500	4.65944300	-1.91238500
H	-2.07671500	-1.65722000	-6.00734600	H	3.33786100	4.91703900	-2.84171900
C	-1.76715200	-0.06096600	-4.59159000	C	3.00290500	3.43837400	-1.28911200
C	1.49639600	0.80009800	-2.76942400	H	3.68170800	2.70032000	-1.72308600
H	2.44557200	0.24315000	-2.72091600	C	2.28680700	3.10725300	-0.10026400
H	1.10423100	0.91643300	-1.74635700	C	4.35450300	-2.79670500	-0.41112300
C	0.34815100	-2.92728300	-6.00974100	C	4.44269200	-3.61350600	0.74218800
H	1.44336900	-3.01432200	-6.11036600	C	4.41738100	-5.00909600	0.58511300
H	-0.01413400	-3.81699700	-5.45991000	H	4.48677600	-5.64269800	1.47670700
C	-3.17579700	0.47331600	-4.73248900	C	4.30495400	-5.61144200	-0.68056300
H	-3.72654700	0.45153700	-3.77655500	C	4.23633900	-4.77644900	-1.80851600
H	-3.74864800	-0.12190700	-5.46019200	H	4.15944200	-5.22501900	-2.80598700
C	3.55101000	0.91746200	0.26761200	C	4.26142200	-3.37580400	-1.69610800
C	3.39873400	-0.44710900	0.00062800	C	4.56648000	-2.99101300	2.11412700
C	4.50450000	-1.31844700	-0.24416300	H	3.68376600	-2.37063800	2.34870200
C	5.77762000	-0.77130300	-0.25658400	H	4.65439800	-3.76456600	2.89231500
H	6.63307200	-1.42223000	-0.46420900	C	4.21530600	-7.11404200	-0.81505200
C	6.00942300	0.59369200	0.06064300	H	4.54617600	-7.45176500	-1.81121100
C	7.33172800	1.11047900	0.11830100	H	4.82640600	-7.62419900	-0.05138500
H	8.19106700	0.48763900	-0.14140000	C	4.21275600	-2.49839500	-2.92411700
C	7.53301500	2.41379300	0.52790500	H	3.96710100	-3.08346900	-3.82475800
C	6.46313000	3.25175100	0.91996600	H	3.45714400	-1.70393700	-2.80885600
H	6.68395400	4.25944200	1.27724200	C	0.02617700	2.26372900	3.53651200
C	5.17048500	2.76707200	0.84803700	C	-1.32938000	2.65072700	3.71777400
H	4.34758300	3.40904200	1.16635800	C	-1.90926500	2.52798600	4.99022000
C	4.89207600	1.44281800	0.38529200	H	-2.95822000	2.82041000	5.11707500
C	2.41103500	1.83325000	0.55078600	C	-1.20295400	2.01764000	6.08901400
C	1.51442100	1.53263100	1.57922400	C	0.13720700	1.65052900	5.89142800
C	0.70839100	2.51196200	2.23555600	H	0.71987000	1.27643300	6.74193300
C	0.67560000	3.77469800	1.65209100	C	0.77274800	1.77143900	4.64478800

C	-2.18319000	3.18154000	2.58807900	O	1.14820900	7.78509300	-1.38067000
H	-3.23417000	2.88267100	2.73215600	H	5.18250000	-1.99593400	-3.09461400
H	-1.85213700	2.80447200	1.61019300	O	-2.44788700	-4.97120500	0.14927000
C	-1.87487600	1.84241500	7.43079200	C	-0.12626900	-3.25861000	1.34119300
H	-2.45884600	0.90241800	7.45295200	H	-1.12436200	-2.81323400	1.43925200
H	-1.13750500	1.79500400	8.24938900	C	0.00271500	-4.47017300	2.24293800
C	2.24268900	1.42192900	4.55230400	H	-0.59655000	-4.25694600	3.14535800
H	2.71253800	1.47793100	5.54776100	H	-0.55654400	-5.25327700	1.69958200
H	2.38864300	0.39884900	4.16406200	C	1.42384100	-4.92035500	2.65552300
N	-0.35900200	-0.40183800	0.09175700	C	1.53209100	-6.45265200	2.65657800
O	-2.60258200	0.38092800	0.96634600	C	1.79890400	-4.33132900	4.02535700
O	-2.42327900	-0.01096800	-1.52895100	H	2.14400900	-4.53452000	1.91334300
O	-2.51448700	-2.06861300	-0.05397500	H	1.32754900	-6.86644100	1.65291000
O	2.14275600	-1.02244500	-0.12559800	H	2.54164500	-6.78186700	2.96173300
O	1.44024100	0.20619100	2.01572900	H	0.80532100	-6.90049200	3.35926800
O	0.82962100	-2.16703000	1.83427000	H	1.72873700	-3.23094200	4.01372900
P	-1.93933200	-0.69114300	-0.08498300	H	1.11386200	-4.70908900	4.80739800
P	0.87903700	-0.87477900	0.90544700	H	2.82689400	-4.61151100	4.31631800
H	-2.30523600	-5.26965700	-0.76890000	O	0.10083800	-3.38937000	-0.01109500
H	3.17089700	-7.45439300	-0.67849600	C	0.90646600	-4.43762700	-0.56226700
H	5.45039500	-2.33223700	2.17725300	C	0.82051000	-4.29560000	-2.08573400
H	-3.04599500	-5.14858300	4.24395900	H	0.49951700	-5.41359900	-0.24124900
H	-5.21864500	-1.67246800	-0.77070200	H	1.95290000	-4.34489900	-0.22723800
H	-4.24909600	0.66882500	4.03066100	C	-0.59812100	-4.39041100	-2.60183300
H	-2.57765800	2.66700600	7.64014800	H	1.44938200	-5.08783500	-2.52702700
H	2.78669600	2.10636200	3.87861900	H	1.26201800	-3.32460400	-2.36710600
H	-2.16257100	4.28626200	2.54733600	C	-1.16387700	-5.63589700	-2.94450500
H	1.71650000	1.81278300	-3.14937100	C	-1.39240400	-3.23580600	-2.65888300
H	-3.16308100	1.52642100	-5.06735000	C	-2.51137100	-5.70763600	-3.33523000
H	-0.09892600	-2.95807000	-7.01827700	H	-0.55167100	-6.54393400	-2.90509100
N	8.91643300	2.94008400	0.58750600	C	-2.75137600	-3.31367900	-3.01687400
N	1.75333100	6.90465800	-1.99784700	H	-0.95276700	-2.26593300	-2.41111800
O	9.82975600	2.18484100	0.24833100	C	-3.30994400	-4.55756600	-3.36792500
O	9.06188900	4.10206000	0.97264700	H	-2.94940100	-6.67428000	-3.60680700
O	2.19374400	7.02145400	-3.14530400	O	-3.56020400	-2.22382100	-3.03470400

H	-4.36663000	-4.60188700	-3.64704500	C	-4.48919400	-1.72565600	2.14797700
H	-3.09545100	-1.46849000	-2.61217800	C	-4.80703300	-2.95383400	1.50795900
H	-2.52419800	-3.99601800	0.04503500	C	-4.35226100	-4.15125200	2.07953700
				H	-4.58363600	-5.09398500	1.56930400
Int3				C	-3.58472100	-4.17477600	3.25623700
C	-4.28769000	1.30235900	-0.18820800	C	-3.27968900	-2.94922600	3.86745500
C	-3.95719500	0.30850000	0.73245700	H	-2.68310800	-2.93793300	4.78842000
C	-4.90712400	-0.45513300	1.47288300	C	-3.71936000	-1.72513100	3.33205800
C	-6.23320900	-0.05363200	1.38584300	C	-5.52798400	-2.99199500	0.17980100
H	-6.99417800	-0.59432300	1.95894500	H	-6.48667600	-2.44761400	0.20104300
C	-6.64792700	0.98922300	0.50887200	H	-5.72479700	-4.03284100	-0.12356300
C	-8.02444900	1.34416700	0.39488800	C	-3.10915900	-5.48636100	3.84051400
H	-8.74474300	0.85575200	1.06049800	H	-3.95854100	-6.08673500	4.21643500
C	-8.44920600	2.26298700	-0.54885000	H	-2.59364200	-6.09894400	3.07888500
H	-9.51005300	2.52199800	-0.62903900	C	-3.33212100	-0.43065600	3.99727200
C	-7.50853500	2.84798400	-1.43566700	H	-2.53311400	0.06968200	3.42493600
H	-7.85024800	3.54489600	-2.20808700	H	-2.95706000	-0.59634600	5.02015400
C	-6.16112000	2.53870700	-1.34072300	C	-0.96473900	0.35769800	-3.75937300
H	-5.45219600	2.98696000	-2.04046400	C	0.41809000	0.07460700	-3.70042800
C	-5.68151300	1.63477400	-0.34732700	C	0.92922900	-0.98334000	-4.47173400
C	-3.22953300	1.86657400	-1.07788400	H	1.99916300	-1.21245900	-4.41149700
C	-2.42681100	0.99486100	-1.82057200	C	0.10716300	-1.76500000	-5.29823500
C	-1.57973100	1.40784800	-2.89141100	C	-1.25432700	-1.42794200	-5.38200600
C	-1.45265000	2.76961700	-3.12064000	H	-1.91448800	-2.01473900	-6.03070700
H	-0.82651100	3.12200100	-3.94706000	C	-1.80694500	-0.38052100	-4.63002600
C	-2.12999600	3.72671100	-2.31241900	C	1.32869500	0.89836100	-2.82520900
C	-1.95525300	5.12532700	-2.52481700	H	2.34064900	0.46425400	-2.78483200
H	-1.28388000	5.44964300	-3.32763600	H	0.93389100	0.96547000	-1.79866300
C	-2.61086400	6.05659600	-1.73709400	C	0.65026700	-2.96926800	-6.02924300
H	-2.45058800	7.12551500	-1.90499500	H	1.74962100	-2.92879500	-6.11385000
C	-3.46871500	5.61701900	-0.69501600	H	0.38557500	-3.89213200	-5.47872100
H	-3.97387500	6.35367100	-0.06139300	C	-3.27650000	-0.04419600	-4.75842700
C	-3.67832600	4.26429100	-0.47584600	H	-3.81831800	-0.19460400	-3.80849400
H	-4.34837700	3.93493600	0.32243000	H	-3.75718900	-0.68059500	-5.51755000
C	-3.03067500	3.27999000	-1.27828200	C	3.36854300	1.22208900	0.25637900

C	3.39208200	-0.15200000	0.00147900	C	4.84511400	-2.50244500	2.17748200
C	4.60399600	-0.88123500	-0.20154200	H	3.90419400	-1.96479700	2.38848900
C	5.79989000	-0.18214700	-0.18473000	H	4.99548500	-3.25193000	2.96976000
H	6.73464300	-0.72427700	-0.36065000	C	5.00694500	-6.67446600	-0.70130200
C	5.85357700	1.20222900	0.12902300	H	5.43159500	-6.98207300	-1.67143000
C	7.10035600	1.87640000	0.22742200	H	5.62148700	-7.11046000	0.10426400
H	8.03723200	1.36287000	-0.00136200	C	4.50257000	-2.11551200	-2.87111400
C	7.12768100	3.19418200	0.63927800	H	4.35367500	-2.73714700	-3.76844700
C	5.95131600	3.89511200	0.99308000	H	3.64645900	-1.42619100	-2.78148200
H	6.03599800	4.92156900	1.35511700	C	-0.31584400	2.24740400	3.45157800
C	4.73032100	3.25688800	0.87987500	C	-1.69409600	2.53758600	3.64481600
H	3.82550500	3.79287400	1.17110600	C	-2.23982100	2.43643900	4.93387200
C	4.63085400	1.90859500	0.41353600	H	-3.30543700	2.65701000	5.06857300
C	2.11961300	1.99732800	0.49002500	C	-1.47853700	2.03142500	6.03949000
C	1.23598400	1.61056600	1.50186700	C	-0.11976700	1.75078700	5.82894100
C	0.32797300	2.51431400	2.13456000	H	0.50368800	1.45802100	6.68240400
C	0.16712300	3.75464800	1.52322500	C	0.48405700	1.86191900	4.56533000
H	-0.49710600	4.49158300	1.98088400	C	-2.61150400	2.93261700	2.50921400
C	0.85131000	4.11121900	0.33157200	H	-3.62461200	2.53477800	2.68413600
C	0.58376100	5.34119600	-0.32529900	H	-2.25822500	2.54936600	1.54151400
H	-0.18085500	6.02430300	0.04959800	C	-2.11162600	1.87321600	7.40209500
C	1.28478300	5.66017500	-1.47212200	H	-2.65620300	0.91184000	7.46838000
C	2.28244200	4.81340100	-2.01357300	H	-1.35457500	1.88323000	8.20378600
H	2.78803000	5.11272700	-2.93361300	C	1.97507800	1.62213000	4.46171900
C	2.58140200	3.63212400	-1.36064300	H	2.44913300	1.73187600	5.45057000
H	3.35201500	2.97002200	-1.76277100	H	2.19533900	0.60680500	4.08857500
C	1.87269300	3.23989700	-0.18603900	N	-0.33648200	-0.55270000	-0.05689100
C	4.64187900	-2.36745400	-0.35209500	O	-2.60337400	0.03623300	0.92364200
C	4.80789500	-3.15395800	0.81382000	O	-2.48913000	-0.37799100	-1.57751900
C	4.94413700	-4.54508100	0.67605800	O	-2.33171000	-2.41703800	-0.07142900
H	5.07023000	-5.15630600	1.57705000	O	2.22133800	-0.88029400	-0.15011400
C	4.92539800	-5.17013500	-0.58333700	O	1.29153800	0.28552200	1.94885900
C	4.78594100	-4.36127000	-1.72384500	O	0.98203100	-2.15425500	1.75126900
H	4.78462600	-4.82733800	-2.71629600	P	-1.89515200	-0.99515300	-0.14992800
C	4.64087700	-2.96671100	-1.63102800	P	0.90456000	-0.86250200	0.82546200

H	3.99802500	-7.12363900	-0.62428400	C	1.40329400	-4.15988700	-2.06006800
H	5.66023600	-1.76044400	2.24332700	H	1.32322700	-5.40190500	-0.25782600
H	-2.41388000	-5.32489900	4.68158600	H	2.40312000	-3.96605500	-0.13372200
H	-4.89723800	-2.53186900	-0.60074400	C	0.04952400	-4.47466600	-2.65960100
H	-4.18210000	0.27173800	4.04559000	H	2.18381300	-4.80800600	-2.49241600
H	-2.84295900	2.67518700	7.60195700	H	1.67682400	-3.11470800	-2.28387000
H	2.45896000	2.33383400	3.77038300	C	-0.25715200	-5.75909700	-3.14859900
H	-2.70513000	4.03077100	2.42249700	C	-0.93747200	-3.47830000	-2.67592800
H	1.41804000	1.93020400	-3.20661900	C	-1.54427400	-6.02799200	-3.63990300
H	-3.41634300	1.01441900	-5.04267100	H	0.50919600	-6.54302200	-3.14772600
H	0.22459600	-3.05460300	-7.04405100	C	-2.23744000	-3.75922500	-3.12932600
N	8.43368800	3.88522500	0.74574300	H	-0.69043000	-2.47257000	-2.32659500
N	0.95115200	6.91304300	-2.17748500	C	-2.53745700	-5.04109300	-3.62805300
O	9.44422900	3.24634400	0.44534100	H	-1.78139100	-7.02366900	-4.03130800
O	8.42194000	5.05701600	1.12842200	O	-3.22821300	-2.82724600	-3.11678800
O	1.42453300	7.07122100	-3.30637900	H	-3.54921200	-5.24301700	-3.99256200
O	0.20868700	7.71469600	-1.60398100	H	-2.91100800	-2.02869100	-2.64387700
H	5.40132600	-1.49185400	-3.02944400				
C	0.14819800	-3.37607100	1.32209600	TS3			
H	-0.89848000	-3.05520300	1.40975800	C	3.66483700	-2.36712700	-0.45952300
C	0.46030500	-4.50909500	2.29187600	C	3.63050100	-1.39332300	0.54364600
H	-0.20966300	-4.38494300	3.16042100	C	4.77654400	-0.99296800	1.29520800
H	0.11314600	-5.42167800	1.77325400	C	5.96299800	-1.67463300	1.05207100
C	1.91791400	-4.66775100	2.78696600	H	6.85248200	-1.41536700	1.63628600
C	2.28361600	-6.15210500	2.93735800	C	6.07605000	-2.66370900	0.03789700
C	2.12363000	-3.90629200	4.10714700	C	7.32143600	-3.30421400	-0.23302800
H	2.59243100	-4.23075100	2.03066000	H	8.18238600	-3.05917200	0.39873900
H	2.21408400	-6.68071100	1.96954200	C	7.44868200	-4.19939800	-1.28058400
H	3.31478900	-6.27105900	3.31509500	C	6.33246000	-4.47505500	-2.11301800
H	1.60559500	-6.65783000	3.64981900	H	6.44363300	-5.15752900	-2.96210500
H	1.86828800	-2.84008900	3.99276600	C	5.10483500	-3.88236900	-1.86620800
H	1.47926200	-4.33008300	4.90027300	H	4.25756700	-4.09493400	-2.52247400
H	3.17018400	-3.97864500	4.45130800	C	4.92718700	-2.98731000	-0.76943600
O	0.34477300	-3.57866300	-0.01623000	C	2.44840300	-2.65477200	-1.27509100
C	1.44634900	-4.33781800	-0.53676900	C	1.80912500	-1.59507500	-1.92226500

C	0.80724100	-1.76708400	-2.91901200	H	1.59042700	1.24693500	-6.39574000
C	0.30999200	-3.04771200	-3.11131700	C	1.28920400	-0.16818500	-4.79557300
H	-0.46830600	-3.21649100	-3.86283100	C	-1.82811300	-0.53462900	-2.59538800
C	0.79801200	-4.15788800	-2.36500400	H	-2.72183500	0.10461900	-2.51920600
C	0.21289700	-5.45039800	-2.50290200	H	-1.34336700	-0.57618200	-1.60724900
H	-0.65046800	-5.57304600	-3.16460800	C	-0.72067400	2.71406400	-6.34003700
C	0.70963400	-6.53314200	-1.79721700	H	-0.09579100	3.59673800	-6.10572400
C	1.82534600	-6.36515800	-0.93587800	H	-0.56436100	2.48499400	-7.40902700
H	2.21758000	-7.22418400	-0.38149100	C	2.64015700	-0.81884200	-4.99430500
C	2.41514300	-5.12078700	-0.77890300	H	2.56433100	-1.91947100	-4.98861500
H	3.26031700	-4.99843200	-0.09671900	H	3.34117900	-0.53672400	-4.18802300
C	1.91592800	-3.97927000	-1.47166500	C	-3.89958600	-0.00924900	0.61747000
C	4.75108100	0.14216700	2.26994700	C	-3.36935200	1.24912100	0.31899300
C	5.51810600	1.29908000	1.97192100	C	-4.18972300	2.41939800	0.20845200
C	5.61757300	2.31856800	2.93222000	C	-5.54141100	2.30186400	0.48756400
H	6.22285400	3.20382300	2.69970000	H	-6.18493300	3.18342300	0.39879700
C	4.96229800	2.24004300	4.17134200	C	-6.11879000	1.06636400	0.89297500
C	4.16261600	1.11430200	4.41934900	C	-7.49607800	0.97786300	1.22505500
H	3.62000300	1.03769500	5.36960000	H	-8.14649100	1.85401700	1.16690300
C	4.04769600	0.06178500	3.49553800	C	-8.02135500	-0.23301600	1.63614100
C	6.19906000	1.47012800	0.63143400	C	-7.22646700	-1.39839400	1.75226400
H	5.50377000	1.25617400	-0.19585800	H	-7.69077100	-2.32080900	2.10648900
H	7.06335300	0.79331800	0.50940400	C	-5.88597900	-1.33024100	1.42189400
C	5.11761700	3.32625300	5.21249400	H	-5.26385100	-2.22238100	1.52106000
H	4.15304700	3.56391000	5.69336900	C	-5.29089200	-0.11211400	0.96727300
H	5.81096000	3.00871900	6.01464000	C	-3.03714800	-1.22040500	0.66246500
C	3.17730800	-1.12134900	3.82773800	C	-1.95600200	-1.26879300	1.54716500
H	3.61592400	-2.06449400	3.46057100	C	-1.38396200	-2.50646600	1.98820400
H	2.18595700	-1.02077300	3.35353500	C	-1.67248400	-3.63254200	1.22873300
C	0.40091900	-0.61821400	-3.78489700	H	-1.23670700	-4.59669600	1.50430100
C	-0.86673700	-0.01315600	-3.63038100	C	-2.54835800	-3.57900600	0.10911600
C	-1.21525200	1.05937100	-4.47128500	C	-2.70714700	-4.69266900	-0.75454000
H	-2.20102600	1.52371900	-4.35092800	H	-2.11190900	-5.59774600	-0.61667600
C	-0.34566000	1.53815700	-5.46574600	C	-3.61261400	-4.61939400	-1.79851700
C	0.89931600	0.90226100	-5.61713700	C	-4.42492900	-3.47963500	-2.01761300

H	-5.13101300	-3.48625000	-2.85020500	C	-2.63101100	-1.48610700	4.47454800
C	-4.27514000	-2.38440100	-1.18677900	H	-3.05962700	-1.48479000	5.48978800
H	-4.86629100	-1.48219800	-1.36436200	H	-2.55460600	-0.43904200	4.13194200
C	-3.31853600	-2.38432200	-0.12717700	N	0.22175800	0.25505700	-0.00181700
C	-3.62509700	3.71009400	-0.29272100	O	2.40739500	-0.80865400	0.83969300
C	-3.00820400	4.63001300	0.58842800	O	2.23312300	-0.29407200	-1.64831300
C	-2.44270000	5.79970800	0.04966800	O	2.57830300	1.67238200	-0.07462100
H	-1.94287700	6.50011800	0.72952600	O	-2.03912000	1.36725000	0.01470900
C	-2.48020300	6.08253000	-1.32740000	O	-1.47045700	-0.09125700	2.07243500
C	-3.14229500	5.17641700	-2.17325500	O	-0.29911800	2.18340600	1.85838900
H	-3.19760400	5.38376100	-3.24914200	P	1.81073700	0.38390900	-0.13942000
C	-3.72553000	3.99635200	-1.67727900	P	-0.74409200	1.01815700	1.03412300
C	-2.92531100	4.35067100	2.06877500	H	-2.41327000	8.23614100	-1.60563700
H	-2.15163000	3.58777000	2.27213200	H	-3.88664100	3.97657800	2.46030800
H	-2.65135300	5.26378800	2.62286000	H	5.52131200	4.25393400	4.77178100
C	-1.83133500	7.33455900	-1.87311400	H	6.56782800	2.50389300	0.51996100
H	-0.81691400	7.46636000	-1.45730500	H	3.02185500	-1.20953800	4.91453500
H	-1.75254700	7.30133800	-2.97277500	H	2.07932700	-4.00148100	7.06823200
C	-4.44204400	3.04899000	-2.61333600	H	-3.34203700	-1.99739100	3.80246600
H	-4.27888200	3.33377500	-3.66569500	H	1.04047100	-4.79367000	1.84401900
H	-4.10126100	2.00881300	-2.47252500	H	-2.16376100	-1.55555300	-2.84478500
C	-0.64709600	-2.61238700	3.27872100	H	3.09102800	-0.50135100	-5.94853700
C	0.59929800	-3.28244000	3.35001200	H	-1.77670100	2.99950000	-6.20036600
C	1.19089000	-3.49857100	4.60615500	H	-5.53117100	3.05081000	-2.42609300
H	2.15775500	-4.01373700	4.64928800	C	1.81726322	4.61646273	-0.32843167
C	0.59954600	-3.04998600	5.79460100	H	2.19168601	3.58458065	-0.27026715
C	-0.63409000	-2.38297700	5.70222300	C	2.21613501	5.69072965	0.67091385
H	-1.12618600	-2.03687600	6.61944600	H	3.30838401	5.81827165	0.59423885
C	-1.27630200	-2.16070900	4.47477900	H	1.71440801	6.61870765	0.34522585
C	1.31756200	-3.75750000	2.10941300	C	1.83814401	5.39367365	2.16389785
H	2.40815700	-3.74615400	2.26772000	C	2.43162301	6.49783065	3.05080585
H	1.09050000	-3.12042000	1.24216400	C	2.30048801	4.00188565	2.61519485
C	1.27741300	-3.24718000	7.13097000	H	0.73600701	5.44693665	2.22039685
H	1.73398400	-2.30202100	7.48228600	H	2.11544401	7.50505265	2.72495185
H	0.55821500	-3.56756600	7.90507800	H	2.10843701	6.35876165	4.09731485

H	3.53687201	6.46100265	3.03376185	C	4.86207900	-0.07585500	1.44615500
H	1.75832701	3.18598765	2.10875385	C	6.15926600	-0.55169300	1.30160900
H	3.38033501	3.86672265	2.42756885	H	6.96486800	-0.07923600	1.87396800
H	2.13494801	3.88357565	3.69964785	C	6.48784300	-1.59196600	0.38915600
O	0.40426900	4.61161800	-0.40918100	C	7.83796800	-2.01556100	0.21056600
C	-0.07591100	3.57976000	-1.30658700	H	8.61236100	-1.56850700	0.84376800
C	0.38993000	3.97852900	-2.71807400	C	8.17006000	-2.95275100	-0.75204600
H	-1.16091900	3.58854500	-1.19368900	H	9.21121700	-3.26591000	-0.88208300
H	0.35839100	2.61606200	-1.01713100	C	7.15903900	-3.49117800	-1.59033200
C	1.88197800	3.84093800	-2.69102500	H	7.42754300	-4.20773600	-2.37370900
H	0.01895800	4.98709300	-2.95918800	C	5.83513500	-3.11430300	-1.43128800
H	-0.06044900	3.24648800	-3.41035500	H	5.06929500	-3.53013000	-2.09041900
C	2.58186068	4.95057071	-2.12662904	C	5.45156900	-2.18263200	-0.42121800
C	2.49266500	2.59231200	-2.74619200	C	2.96913900	-2.32289900	-1.02273300
C	4.06161100	4.84078700	-2.10761200	C	2.17758700	-1.44603900	-1.76720600
H	2.11833168	5.94252871	-2.10402104	C	1.26566500	-1.87567200	-2.77587700
C	3.85596500	2.44488800	-2.40708200	C	1.02045600	-3.23544700	-2.88949300
H	1.90032400	1.70088600	-2.97796400	H	0.32240400	-3.59602700	-3.65237100
C	4.65450700	3.58944700	-2.14427600	C	1.67218400	-4.18146700	-2.04855300
H	4.67122300	5.72438800	-1.89254700	C	1.35820100	-5.56962300	-2.12081400
O	4.41862400	1.22938600	-2.31106200	H	0.57433100	-5.90189700	-2.80796700
H	5.71637900	3.44742200	-1.92980900	C	2.01179100	-6.48892000	-1.31814200
H	3.67095700	0.59079100	-2.14590700	H	1.74633200	-7.54928300	-1.37539500
O	-10.12739800	0.72271200	1.87886800	C	3.01801600	-6.05154500	-0.41795300
O	-9.89656400	-1.40197800	2.34516400	H	3.53203500	-6.77946100	0.21853800
O	-4.61156600	-5.71791800	-3.58144500	C	3.35013000	-4.70903300	-0.32859900
O	-2.92956900	-6.69975000	-2.58668000	H	4.11557900	-4.38148400	0.37881900
N	-3.72811900	-5.76488300	-2.72177700	C	2.68871900	-3.73333400	-1.12972300
N	-9.45771900	-0.30854800	1.97971500	C	4.58225900	1.15475600	2.24974300
H	8.41148900	-4.67952900	-1.48241000	C	5.07890100	2.39486600	1.77356000
H	0.24003000	-7.51588700	-1.90302700	C	4.86197400	3.55366000	2.53637900
				H	5.24417200	4.51122400	2.16066700
Int4				C	4.16892600	3.52276400	3.75711100
C	4.08735700	-1.77281600	-0.20440700	C	3.66007500	2.28901400	4.19196900
C	3.83977600	-0.74868900	0.71280200	H	3.09788600	2.23908900	5.13241200

C	3.84929600	1.10580700	3.45951900	C	-7.67179700	-1.76437500	1.48301200
C	5.79885400	2.49803300	0.44668500	C	-6.63397400	-2.71200600	1.65069600
H	5.23048900	1.98398800	-0.34548400	H	-6.88291900	-3.70793300	2.02209400
H	6.80496800	2.04296100	0.47919900	C	-5.33591000	-2.34574400	1.34828100
C	3.99337000	4.76998700	4.59354000	H	-4.53237000	-3.07071600	1.49101000
H	4.67757400	4.75996800	5.46327700	C	-5.01962200	-1.03448300	0.87110800
H	4.20953500	5.68071600	4.01007200	C	-2.59531300	-1.64332700	0.61259400
C	3.25568700	-0.18564400	3.95856400	C	-1.55402000	-1.46254700	1.52809500
H	2.31189400	-0.40646300	3.43119600	C	-0.79361600	-2.56234400	2.04638800
H	3.03124500	-0.13495500	5.03597600	C	-0.87452700	-3.76222900	1.34967100
C	0.73328100	-0.88876200	-3.76619200	H	-0.30122000	-4.62641200	1.69596600
C	-0.59034300	-0.40065800	-3.68709000	C	-1.71850500	-3.91923900	0.21391100
C	-1.03104000	0.52547100	-4.65055700	C	-1.69680700	-5.10661400	-0.56293300
H	-2.06021600	0.89951000	-4.58732100	H	-0.98460300	-5.90524500	-0.34518600
C	-0.19532200	0.98209500	-5.68231700	C	-2.58196800	-5.24528000	-1.61864700
C	1.11022300	0.46340000	-5.75471500	C	-3.53995100	-4.25145900	-1.93964200
H	1.77600100	0.78920400	-6.56317900	H	-4.21681900	-4.42250200	-2.77871000
C	1.58783300	-0.46981300	-4.81942000	C	-3.57087700	-3.08957400	-1.19205800
C	-1.50317000	-0.87459600	-2.59002500	H	-4.28435000	-2.30078700	-1.44490600
H	-2.47564300	-0.35766500	-2.62252900	C	-2.65445700	-2.87428500	-0.11849000
H	-1.04255700	-0.69497500	-1.60455400	C	-4.28176000	3.10203100	-0.26677400
C	-0.67302900	2.01607200	-6.67652400	C	-3.86695400	4.06900100	0.68287200
H	-1.75724000	2.19284800	-6.58200400	C	-3.79334300	5.41422200	0.28215800
H	-0.15719600	2.98235100	-6.51878800	H	-3.47190600	6.16185900	1.01740200
C	2.98556100	-1.03400800	-4.95172700	C	-4.12808100	5.82805300	-1.01871600
H	3.60359100	-0.83398000	-4.05882700	C	-4.53486100	4.85031300	-1.94144700
H	3.50288400	-0.60694500	-5.82581400	H	-4.79083300	5.14817100	-2.96561800
C	-3.67803700	-0.62536400	0.53923900	C	-4.61286700	3.49066600	-1.58902800
C	-3.43116300	0.72608100	0.25917100	C	-3.49715300	3.67277000	2.09058000
C	-4.49620200	1.67811600	0.13743400	H	-2.47134200	3.25780500	2.11824000
C	-5.79489800	1.25361000	0.37010800	H	-3.53178500	4.54433400	2.76501800
H	-6.61457900	1.97339500	0.27422100	C	-4.03308100	7.28620700	-1.40840200
C	-6.09241700	-0.07920500	0.76055500	H	-4.69867800	7.90992000	-0.78445000
C	-7.42339400	-0.47235000	1.05936900	H	-3.00586800	7.67015200	-1.26437300
H	-8.25241400	0.23355000	0.96819700	C	-5.01706000	2.45949300	-2.62096700

H	-5.09389600	2.91448000	-3.62225700	H	1.99632300	-4.46823600	2.15446500
H	-4.28192100	1.63589700	-2.66636000	H	-1.68722600	-1.95784100	-2.67676300
C	-0.08648000	-2.47432600	3.35673900	H	2.95619000	-2.13247400	-5.06333600
C	1.24784200	-2.93386200	3.50322000	H	-0.46346500	1.70443900	-7.71503700
C	1.82947400	-2.96349600	4.78052800	N	-9.06204700	-2.16078700	1.79193500
H	2.86465500	-3.31293100	4.87659700	N	-2.52193300	-6.46489300	-2.44520100
C	1.14164200	-2.53184200	5.92336400	O	-9.94791600	-1.31613200	1.63606000
C	-0.17933100	-2.08599300	5.76055200	O	-9.24834500	-3.31506700	2.18601000
H	-0.74797300	-1.76467500	6.64161500	O	-3.38136500	-6.60515400	-3.31927400
C	-0.81409000	-2.05631500	4.50819200	O	-1.61038400	-7.27140700	-2.22184700
C	2.07298600	-3.37854200	2.32101700	H	-5.99129300	1.99815000	-2.38052500
H	3.13862600	-3.15083100	2.48869100	C	0.84518500	4.71816200	-0.54785300
H	1.75667900	-2.87803500	1.39501400	H	1.54832400	4.05577500	-0.02101400
C	1.81446700	-2.51431400	7.27634800	C	0.73139400	6.09708600	0.10104200
H	2.44416600	-1.61041400	7.38715600	H	1.73440400	6.56693400	0.12235000
H	1.07570300	-2.50574300	8.09518900	H	0.08505200	6.74636600	-0.52226300
C	-2.26266000	-1.62295500	4.44690500	C	0.15860100	6.02609300	1.53385400
H	-2.71688400	-1.65970900	5.45040300	C	0.00723200	7.44565700	2.10176500
H	-2.35309400	-0.59194100	4.06410500	C	1.00382900	5.12913300	2.45115700
N	0.26215500	0.44286500	-0.03307600	H	-0.84585500	5.57244500	1.45130700
O	2.52050100	-0.37004300	0.91815900	H	-0.61657200	8.08173900	1.44654700
O	2.33937300	-0.06897600	-1.60294900	H	-0.46586300	7.41899200	3.09926100
O	2.50306200	2.03548200	-0.17777000	H	0.99218900	7.93778700	2.21156100
O	-2.16315200	1.17168400	-0.01255800	H	0.94499000	4.06989100	2.15431900
O	-1.32321900	-0.20687400	2.02528700	H	2.06321800	5.44540600	2.44713300
O	-0.60077800	2.22381000	1.87114800	H	0.63641000	5.19398900	3.49041500
P	1.82680200	0.69530200	-0.14181100	O	-0.38835500	4.04055800	-0.54851000
P	-0.82184900	1.03713300	0.99609700	C	-1.21100800	4.26210500	-1.67908800
H	-4.31186800	7.44167300	-2.46380500	C	-0.57909200	3.52546400	-2.88204100
H	-4.17965900	2.89916200	2.48267200	H	-1.34244800	5.34347100	-1.87987000
H	2.96508400	4.84849300	4.98643400	H	-2.19056600	3.83598900	-1.43873600
H	5.92003600	3.55658700	0.16061200	C	0.90777800	3.61900000	-2.75404400
H	3.93169000	-1.03932400	3.78188900	H	-0.91611800	3.99597500	-3.82694400
H	2.47427700	-3.38890900	7.41047600	H	-0.88201000	2.46837900	-2.90306000
H	-2.85543200	-2.27066600	3.77773600	C	1.40980900	4.84809000	-2.09388500

C	1.74890800	2.56335500	-2.97368400	C	3.51762400	6.74123200	-1.29185200
C	2.87732400	5.00879800	-2.06827600	H	3.56812600	7.70855900	-1.80247300
H	0.91246900	5.75259800	-2.48789800	C	4.55690200	5.79065900	-1.47581700
C	3.13975500	2.69445100	-2.67871000	H	5.39884700	6.02883700	-2.13434600
H	1.36942700	1.59764700	-3.31618700	C	4.51258200	4.56425400	-0.83251000
C	3.71238700	3.97200300	-2.35299000	H	5.31319700	3.83414500	-0.98309000
H	3.28713800	5.96924300	-1.73710500	C	3.41971000	4.22668800	0.01870000
O	3.94601000	1.65848000	-2.71048800	C	5.20335400	-1.53076400	-0.65697900
H	4.79786000	4.04190700	-2.25193100	C	5.13059300	-2.74073900	0.08043700
H	3.39666400	0.83434700	-2.50118000	C	5.06504300	-3.95581000	-0.62084500
				H	4.99972000	-4.89132900	-0.05489800
TS4				C	5.08318900	-4.00536100	-2.02660400
C	4.44417000	1.99229000	0.66973000	C	5.19062200	-2.79603100	-2.72840600
C	4.26683400	0.71767200	0.13967500	H	5.21479000	-2.81401200	-3.82361300
C	5.32888300	-0.23172700	0.06846200	C	5.24238700	-1.55444000	-2.06925200
C	6.55052500	0.11563000	0.63196600	C	5.10006800	-2.71564300	1.59159300
H	7.37923000	-0.59847400	0.57475700	H	4.41840700	-1.92565200	1.94687600
C	6.76521400	1.36903200	1.26749200	H	6.10516800	-2.52499900	2.01049900
C	8.00837600	1.69145100	1.88652600	C	4.94548400	-5.32797600	-2.74716000
H	8.81386700	0.94913700	1.86125800	H	4.93980800	-5.19217300	-3.84127800
C	8.19294900	2.91137200	2.51420600	H	5.77176300	-6.01636300	-2.49036200
H	9.15048900	3.14742200	2.99014000	C	5.31627700	-0.27371200	-2.86884300
C	7.13297400	3.85516300	2.55338300	H	4.30368700	0.09134200	-3.12415400
H	7.27658800	4.81076700	3.06852600	H	5.86202200	-0.42680100	-3.81466600
C	5.91603500	3.57583700	1.95295200	C	0.02499400	3.38606700	2.60538100
H	5.10272900	4.30450000	1.99830300	C	-1.32470100	3.56077900	2.21930000
C	5.69923000	2.33568800	1.28274100	C	-2.31191800	3.64674100	3.21605000
C	3.31375300	2.95224800	0.66905000	H	-3.35157500	3.80909200	2.91215500
C	2.13818600	2.62245900	1.34479900	C	-2.00367400	3.54337300	4.58046500
C	1.12388300	3.58983600	1.61599300	C	-0.66449300	3.30790800	4.93626800
C	1.26153900	4.84465200	1.02961500	H	-0.39937100	3.20983300	5.99638300
H	0.50503100	5.60775100	1.24080900	C	0.35862200	3.23218800	3.97812700
C	2.35644800	5.18085300	0.18815300	C	-1.72343300	3.65447900	0.76269000
C	2.44044600	6.43986700	-0.47522200	H	-2.79335400	3.42089200	0.64302300
H	1.62931000	7.16242900	-0.33213300	H	-1.14275000	2.95158100	0.14344900

C	-3.07415200	3.66715500	5.64184700	C	-2.71510300	-3.54166200	3.12744800
H	-4.04289000	3.96004600	5.20451700	C	-2.16155800	-3.96336800	4.34751300
H	-3.22154400	2.71082100	6.17789400	H	-1.90259800	-5.02266200	4.46809600
C	1.79076300	3.04305900	4.42459100	C	-1.92899300	-3.07321200	5.40936600
H	2.16751800	2.04767600	4.12982400	C	-2.24379900	-1.72032600	5.21001900
H	1.87436100	3.13659400	5.51963500	H	-2.06337500	-1.00083500	6.01736900
C	-3.95241600	-0.26626300	-0.27374300	C	-2.79753500	-1.25460100	4.00562600
C	-3.23336100	-0.78669800	0.80304500	C	-2.84732700	-4.54169200	2.00440900
C	-3.78794100	-1.71016400	1.74650700	H	-2.01555100	-4.38828300	1.30295100
C	-5.08630500	-2.14860300	1.51426000	H	-2.77026600	-5.56871800	2.39903000
H	-5.55087400	-2.83514800	2.22970700	C	-1.33123600	-3.56031700	6.70942600
C	-5.82697400	-1.74602100	0.36702100	H	-1.81826100	-4.49073200	7.05063800
C	-7.11819500	-2.27665900	0.10338300	H	-0.25443200	-3.78223300	6.58632000
H	-7.58360000	-2.99203100	0.78557000	C	-3.15854500	0.20226600	3.85643600
C	-7.79151300	-1.89157400	-1.04132500	H	-2.75229600	0.78563400	4.69418300
C	-7.24136500	-0.98040100	-1.97560600	H	-2.74886100	0.63081100	2.92940400
H	-7.81475200	-0.73203100	-2.87073000	C	-0.36627300	1.19271300	-3.48771100
C	-5.99272300	-0.44284200	-1.72563900	C	0.87660900	1.82557800	-3.26213200
H	-5.54979400	0.25602300	-2.44021000	C	1.95024600	1.53345700	-4.12235200
C	-5.25643100	-0.79303600	-0.55284400	H	2.91574400	2.01935200	-3.93882400
C	-3.34995500	0.81583900	-1.09909200	C	1.81624500	0.64853600	-5.20456600
C	-2.12152200	0.60816000	-1.73666100	C	0.56510800	0.04131600	-5.41029100
C	-1.55361100	1.54299800	-2.65318300	H	0.43550400	-0.64747200	-6.25517700
C	-2.20055900	2.75854100	-2.81938200	C	-0.52634600	0.28345400	-4.56205000
H	-1.78824600	3.49283800	-3.51874900	C	1.04529100	2.79634200	-2.12125500
C	-3.39013100	3.07803200	-2.10715400	H	2.08937600	3.12318600	-2.03999500
C	-3.99667500	4.35555100	-2.23281300	H	0.75502100	2.32325500	-1.16966500
H	-3.56987600	5.11994500	-2.88638700	C	2.98552600	0.32765100	-6.10698400
C	-5.13655400	4.64224900	-1.50492600	H	3.41208200	-0.65925400	-5.84950800
C	-5.72904000	3.70505900	-0.62482900	H	2.67528100	0.28424500	-7.16605800
H	-6.61704700	3.99787800	-0.06136900	C	-1.84177800	-0.42684900	-4.79385700
C	-5.15754300	2.45242500	-0.50102100	H	-1.90444000	-0.81926900	-5.82280300
H	-5.59518800	1.72571900	0.18761400	H	-1.95329800	-1.27671500	-4.09363000
C	-3.98719900	2.09410700	-1.23790600	N	0.47617900	0.04815200	0.15654800
C	-3.04503800	-2.17449500	2.95817200	O	2.99382300	0.37293600	-0.32141600

O	1.99751600	1.34431200	1.85746100	H	-0.48326400	-6.32824000	-2.74911300
O	2.33907500	-1.20372300	1.68366800	C	1.70275300	-3.00063800	-3.77478100
O	-1.94037700	-0.31873900	0.98049300	H	0.27980000	-4.50776800	-4.43468600
O	-1.45105800	-0.58279700	-1.53569000	H	2.91212100	-1.44679300	-2.87736700
O	-0.75498600	-2.42239200	0.06998400	O	0.95642200	-6.15166400	-0.21582500
P	1.90478700	-0.00761700	0.89312500	H	-0.94056800	-5.38466900	0.13356500
P	-0.76389800	-0.89630200	-0.04029300	H	-0.84146700	-7.06214100	-0.48949500
H	-1.42931400	-2.80457000	7.50603000	O	2.08633500	-2.62564200	-5.00460700
H	-3.78523800	-4.45454100	1.43412700	C	1.55445300	-4.87299500	0.01183700
H	4.00456300	-5.83620900	-2.46312400	H	1.63629700	-3.16992100	-5.67837000
H	4.74913400	-3.67987200	1.99268000	H	2.63302600	-5.05940400	-0.11405300
H	5.81157300	0.53048700	-2.30171400	C	1.27033200	-4.31986900	1.40742100
H	3.78700500	1.07921000	-6.01280400	H	1.78870500	-3.34795200	1.51141700
H	-2.70320000	0.24157500	-4.62571800	H	0.19705600	-4.07526100	1.48506400
H	0.42130600	3.70112600	-2.25057400	C	1.62740400	-5.26466800	2.57527200
H	-1.56067200	4.66625000	0.34872500	C	1.51250900	-4.48543800	3.89550100
H	2.45893100	3.79037400	3.96066900	C	2.99700100	-5.94602600	2.44597400
H	-2.79727600	4.42177500	6.39983100	H	0.86661500	-6.06967600	2.58495100
N	-9.12761600	-2.46811100	-1.30947000	H	0.51049100	-4.03320400	3.99957500
N	-5.74954900	5.98207200	-1.63936900	H	1.68834400	-5.14461700	4.76487400
O	-9.58643300	-3.26154000	-0.48423600	H	2.24801500	-3.66155300	3.92865600
O	-9.69716300	-2.11849000	-2.34638500	H	3.04677000	-6.60478000	1.56146100
O	-6.77043700	6.20534400	-0.98410000	H	3.80716600	-5.19934300	2.37415800
O	-5.20364000	6.78922800	-2.39542000	H	3.19874800	-6.56935000	3.33519300
H	-4.25596400	0.34477300	3.84127200				
H	0.22376100	-3.21264700	-0.60784000	Pro-com			
C	1.14001700	-3.86728100	-1.13542600	C	5.52728500	-0.39795500	0.01951600
C	0.48405900	-4.46997300	-2.28447200	C	4.63305300	-1.45951500	-0.09113300
C	2.06715100	-2.78535200	-1.41018500	C	5.01226000	-2.83187300	-0.05713800
C	-0.55444100	-5.51690500	-2.00340100	C	6.36490900	-3.11669100	0.05763600
C	0.77081800	-4.04271300	-3.57054100	H	6.69460500	-4.16122900	0.06778700
C	2.27861900	-2.31006000	-2.68294700	C	7.33778100	-2.08574900	0.19853000
H	2.56747800	-2.30783400	-0.56090800	C	8.71972700	-2.39606500	0.36320100
C	-0.41502000	-6.05034400	-0.57284600	H	9.02409200	-3.44833200	0.33893500
H	-1.55097100	-5.04903200	-2.12966200	C	9.65686100	-1.39744200	0.56449200

H	10.71432100	-1.65095900	0.69308300	C	3.67458500	-3.44201300	-2.59339900
C	9.24193100	-0.04173600	0.62547000	H	3.31208900	-2.39839700	-2.55149900
H	9.98047300	0.74462200	0.81365200	H	3.22619100	-3.92311000	-3.47677400
C	7.90854000	0.29600400	0.45705400	C	2.67732800	3.13709400	2.18812600
H	7.59974300	1.34269300	0.51659400	C	1.41667100	3.71621400	1.89860300
C	6.92195100	-0.70449900	0.21381200	C	0.61338700	4.17301700	2.95580100
C	5.01571900	1.00005000	0.00434300	H	-0.36225000	4.61642200	2.71992300
C	4.01279700	1.38537200	0.89919900	C	1.01906400	4.07081300	4.29657400
C	3.60790700	2.74222300	1.08594600	C	2.25969300	3.47071100	4.56230500
C	4.17756100	3.70074400	0.25719400	H	2.59610900	3.37176300	5.60165300
H	3.90779700	4.75335900	0.39453800	C	3.09931200	3.00439300	3.53580300
C	5.09515700	3.35632800	-0.77339000	C	0.90254300	3.81813500	0.48223300
C	5.59014800	4.33398000	-1.68560600	H	-0.13212600	4.19371700	0.47383900
H	5.26685400	5.37370800	-1.56342200	H	0.92153700	2.82981100	-0.00329500
C	6.44455200	3.97897900	-2.71541300	C	0.15561000	4.61252100	5.41280800
H	6.80969500	4.73778600	-3.41527600	H	-0.91709200	4.52940600	5.16802900
C	6.83758700	2.62366300	-2.87371500	H	0.33787300	4.07772100	6.36029500
H	7.49566400	2.34265000	-3.70262700	C	4.43487300	2.38696000	3.88313100
C	6.39192000	1.65288000	-1.99097300	H	4.41244300	1.29454100	3.72237000
H	6.69336800	0.61006800	-2.12260300	H	4.69217900	2.57607000	4.93809400
C	5.52262500	1.98744000	-0.91119400	C	-3.09893400	1.53180100	0.44436000
C	3.95271000	-3.88350500	-0.10571000	C	-2.42911300	0.77880500	1.40522000
C	3.57354300	-4.54415200	1.08774900	C	-3.04735200	0.00903200	2.43792500
C	2.53831000	-5.49162500	1.03381300	C	-4.43338600	0.00667700	2.46287600
H	2.23455500	-5.99242300	1.96124900	H	-4.96181900	-0.55866500	3.23639700
C	1.87644000	-5.80249800	-0.16520900	C	-5.19618100	0.70077300	1.47716400
C	2.27980000	-5.14035300	-1.33683300	C	-6.61471600	0.61503000	1.47518000
H	1.78638200	-5.36810300	-2.28762700	H	-7.14524500	0.05446900	2.24854100
C	3.29977200	-4.17547800	-1.32588900	C	-7.33502700	1.22817900	0.46792000
C	4.23503700	-4.20818300	2.40489800	C	-6.71225200	1.94225400	-0.58241300
H	4.12693900	-3.13155800	2.61864300	H	-7.33408200	2.38149000	-1.36489000
H	5.31425900	-4.44220100	2.39473300	C	-5.33356100	2.05367100	-0.58596700
C	0.73249800	-6.79177800	-0.18565000	H	-4.83911900	2.59175500	-1.39825100
H	0.81867800	-7.52593600	0.63338800	C	-4.53735900	1.46191200	0.44011600
H	-0.23725200	-6.27149900	-0.06597900	C	-2.33128300	2.29174900	-0.58711000

C	-1.37799400	1.64902900	-1.37900400	C	0.02037200	-0.46102100	-5.06361700
C	-0.73805800	2.22988100	-2.51522700	H	-0.54433600	-1.09819200	-5.75472100
C	-0.99032200	3.56788300	-2.76793700	C	-0.67231600	0.49775600	-4.30735200
H	-0.52932400	4.05414700	-3.63332600	C	2.26754900	2.06985600	-2.37488200
C	-1.84185000	4.33263400	-1.91565800	H	3.31594800	2.12408900	-2.70452100
C	-2.02428500	5.72439200	-2.13298700	H	2.25677100	1.63982000	-1.35797300
H	-1.52438200	6.23606300	-2.95883600	C	2.13646600	-1.66548800	-5.78152200
C	-2.83521100	6.44744700	-1.27876200	H	1.69818600	-2.66474900	-5.61186400
C	-3.49704200	5.85526300	-0.17755300	H	2.04984500	-1.44588000	-6.86124600
H	-4.10648900	6.48462800	0.47389100	C	-2.16896000	0.65526100	-4.46539000
C	-3.34250600	4.49867400	0.04113100	H	-2.57636300	-0.10895900	-5.14617900
H	-3.83583900	4.02842900	0.89564000	H	-2.69733500	0.56907200	-3.49998900
C	-2.52951700	3.69751600	-0.81594600	N	1.21199400	0.11647900	0.26476700
C	-2.14638100	-0.76624600	3.34083400	O	3.28590900	-1.16951900	-0.27322500
C	-2.05261200	-2.17439700	3.21163700	O	3.41275600	0.42846500	1.70584700
C	-1.01056400	-2.84447600	3.86985300	O	2.07600900	-1.73827500	2.06175200
H	-0.90913100	-3.92668700	3.72691600	O	-1.03768200	0.75547700	1.36410200
C	-0.06724400	-2.16544700	4.65692800	O	-1.07432200	0.31563700	-1.13451600
C	-0.23403900	-0.78328700	4.83892200	O	-0.87921000	-1.65298700	0.35855900
H	0.47220400	-0.23389700	5.47273000	P	2.40053500	-0.70316900	1.04363800
C	-1.25213900	-0.06897600	4.19119300	P	-0.30977200	-0.16805200	0.24057300
C	-3.01024600	-2.95609600	2.34445600	H	1.50261000	-2.40631200	6.14076100
H	-3.14345700	-2.47688200	1.36096100	H	-4.01077600	-3.03722300	2.80892500
H	-2.63586700	-3.97816500	2.17592900	H	0.69230200	-7.34297800	-1.14132400
C	1.13458000	-2.88378100	5.21694300	H	3.76727400	-4.76942900	3.23021600
H	0.91509600	-3.94394300	5.42948900	H	4.76973900	-3.40056600	-2.72839600
H	1.94463200	-2.84579200	4.46529600	H	3.20673200	-1.71118600	-5.52467800
C	-1.350555000	1.42734300	4.37297800	H	-2.41919600	1.65187200	-4.87181100
H	-0.90121100	1.73152500	5.33178900	H	1.86693700	3.09316200	-2.30835000
H	-0.80047200	1.95759200	3.57536500	H	1.51444700	4.49462700	-0.13906300
C	0.05321200	1.32172500	-3.40641500	H	5.24287000	2.79226700	3.24909800
C	1.45831300	1.20744700	-3.30804300	H	0.37011700	5.68351100	5.59158300
C	2.11232900	0.23135200	-4.08514100	N	-8.81313800	1.11052900	0.47389400
H	3.20061500	0.13697500	-3.99557800	N	-3.00542500	7.90093800	-1.51689400
C	1.41806800	-0.61908600	-4.95939400	O	-9.33119600	0.47506100	1.39366000

O	-9.42518300	1.65842700	-0.44494800	H	-7.42251400	-5.69251800	-1.48344200
O	-3.72959900	8.51903900	-0.73424100	H	-6.78711000	-7.09823000	-0.57515700
O	-2.41427700	8.39465800	-2.47895800	H	-8.30776400	-6.31164500	-0.06916700
H	-2.39742500	1.77590300	4.35294800				
H	-1.19505700	-2.03114600	-0.51304400	3			
C	-3.55885200	-3.94339500	-1.85170100	C	-0.88917200	0.22214700	-0.40726200
C	-3.11967200	-2.61397200	-1.99601600	C	-1.81044800	-0.75149900	0.34111600
C	-2.65115700	-4.98599700	-2.13418400	H	-1.66674200	-1.76560500	-0.07741300
C	-4.06695500	-1.46543200	-1.72120300	H	-1.47670200	-0.78944600	1.39444000
C	-1.80039500	-2.35832900	-2.43475100	C	-3.30727700	-0.38494400	0.29164900
C	-1.35156900	-4.74068400	-2.57983600	C	-4.11947000	-1.38601300	1.12833300
H	-2.98053700	-6.02599300	-2.02491700	C	-3.84464900	-0.29846800	-1.14512400
C	-5.27032200	-1.93961500	-0.90852400	H	-3.40693900	0.61553900	0.75099500
H	-3.53508100	-0.65238600	-1.19737400	H	-3.75249300	-1.42897700	2.16953700
H	-4.42295500	-1.04995900	-2.68290900	H	-5.18824700	-1.10777200	1.15533000
C	-0.92324000	-3.41036500	-2.75690700	H	-4.04822500	-2.40586600	0.70467700
H	-1.48056600	-1.32897900	-2.61894800	H	-3.34083800	0.49887000	-1.71817300
H	-0.67231300	-5.56116200	-2.82225400	H	-3.69970000	-1.25454900	-1.68382900
O	-5.83703800	-3.09781300	-1.51183700	H	-4.92643700	-0.07481900	-1.14529400
H	-4.97342900	-2.13882600	0.14138600	O	-1.21071900	1.52642600	0.08133400
H	-6.06656400	-1.17917000	-0.89246100	C	-0.27382200	2.52262500	-0.30189600
O	0.32677400	-3.18970000	-3.24057600	C	1.04856400	2.28025100	0.42391100
C	-4.99306100	-4.25364600	-1.44269500	H	-0.71916600	3.49194500	-0.02383300
H	0.46314600	-2.22959000	-3.38593600	H	-0.11938100	2.51202700	-1.40317300
H	-5.42247700	-4.93735500	-2.19625000	C	1.51896700	0.86282300	0.16678900
C	-5.07511600	-4.92884000	-0.05647900	H	0.89122300	2.43840300	1.50824300
H	-4.51870500	-5.88533100	-0.10273200	H	1.81712300	3.00512700	0.09753500
H	-4.53631000	-4.30167000	0.67355100	C	0.58992000	-0.11719200	-0.24259400
C	-6.50852900	-5.18046400	0.44821000	C	2.87602800	0.52098000	0.30877200
C	-6.47202700	-5.71275500	1.88947700	C	1.06187500	-1.41359100	-0.52976200
C	-7.29817400	-6.12172200	-0.47441400	C	3.32569800	-0.78090800	0.04254000
H	-7.02453900	-4.20169500	0.44985300	H	3.59443500	1.28943300	0.62481900
H	-5.93190100	-5.01915700	2.55912500	C	2.40740000	-1.75596100	-0.38834600
H	-7.49181900	-5.84902800	2.29103100	H	0.35902700	-2.18060300	-0.87350900
H	-5.95767200	-6.69112400	1.93630000	O	4.63528700	-1.15209600	0.17101400

H	2.76622000	-2.76592700	-0.60651300	C	4.80189700	2.38030500	3.70253300
H	5.14631000	-0.38040100	0.47417900	H	5.20259000	3.38230500	3.50414100
H	-1.12770300	0.18648400	-1.49556300	C	4.05873700	2.16152600	4.87043500
				C	3.53417400	0.87520800	5.08694900
TS3'				H	2.94630700	0.67860300	5.99193800
C	3.69614800	-2.33028100	0.11339800	C	3.72424700	-0.16688700	4.16876700
C	3.57640700	-1.44018600	1.17842500	C	5.80439700	1.70060600	1.50244700
C	4.67187700	-0.99596800	1.97448700	H	5.63382400	0.97110000	0.69801700
C	5.91780400	-1.54167400	1.69592000	H	6.89157100	1.73739000	1.70728900
H	6.78011600	-1.22827100	2.29435200	C	3.81732500	3.27087900	5.86860000
C	6.11942400	-2.45250900	0.62006600	H	4.18632400	4.23852700	5.48995700
C	7.41966200	-2.94941200	0.31007000	H	2.74022800	3.37672200	6.08972000
H	8.25540100	-2.65555700	0.95491500	C	3.09725000	-1.51607800	4.42483400
C	7.62953300	-3.77015300	-0.78470000	H	3.72981700	-2.33915400	4.05141200
C	6.53963700	-4.11533500	-1.62586800	H	2.12376600	-1.59180600	3.91011500
H	6.70973900	-4.74445500	-2.50607200	C	0.81964700	-0.60821000	-3.49551600
C	5.26052900	-3.66031000	-1.34767400	C	-0.25067600	0.30877800	-3.51605500
H	4.43200300	-3.92755500	-2.00776000	C	-0.45590900	1.09763800	-4.66773200
C	5.00437000	-2.83804800	-0.21103500	H	-1.33415500	1.75486600	-4.69939700
C	2.50952900	-2.59634000	-0.74771300	C	0.38037800	1.00630400	-5.78858300
C	1.86782900	-1.52570100	-1.36710800	C	1.51039600	0.16963500	-5.69713000
C	0.96179700	-1.68057900	-2.45194900	H	2.19990900	0.10687800	-6.54774700
C	0.49193100	-2.96025200	-2.71738600	C	1.74875500	-0.64117400	-4.57602700
H	-0.20694400	-3.11425800	-3.54663400	C	-1.17692900	0.44207000	-2.33732700
C	0.96557200	-4.09253500	-1.99420200	H	-2.19217500	0.08738500	-2.58510800
C	0.47285200	-5.40314800	-2.26395500	H	-1.25107700	1.49812500	-2.03565600
H	-0.31429000	-5.53029800	-3.01426300	C	0.08210500	1.76340700	-7.06420700
C	0.98891900	-6.50332400	-1.59959300	H	0.63087300	2.72226600	-7.12302600
C	2.03591400	-6.33732700	-0.65546600	H	0.38007400	1.17263400	-7.94741500
H	2.44059600	-7.21122700	-0.13421000	C	2.96446400	-1.54320300	-4.55008500
C	2.55245200	-5.07986500	-0.38806300	H	3.67572600	-1.23017700	-3.76404000
H	3.35674700	-4.95859700	0.34231000	H	3.49030400	-1.51482600	-5.51800600
C	2.03094300	-3.92321900	-1.03624500	C	-3.93065200	0.08101800	0.30296700
C	4.47926800	0.07894600	2.99332700	C	-3.36471300	1.35442600	0.43148000
C	5.02386600	1.36425400	2.75538000	C	-4.14288400	2.54520400	0.55299900

C	-5.52195900	2.43500200	0.49520200	H	-2.66744300	3.49956100	3.88975500
H	-6.13710100	3.33766100	0.56911400	C	-1.64365300	7.78128700	1.15714900
C	-6.16237800	1.16906700	0.37767000	H	-2.05940000	8.52137900	0.45055900
C	-7.57891500	1.07524700	0.35369100	H	-1.75547300	8.17860000	2.17954400
H	-8.20207400	1.97254300	0.36948800	C	-3.28879600	4.01463100	-1.80200900
C	-8.18045500	-0.16901500	0.32213300	H	-3.02397100	4.74163900	-2.58817000
C	-7.42902600	-1.36783100	0.34020400	H	-2.64543300	3.12468200	-1.91710400
H	-7.95757300	-2.32280400	0.35560800	C	-1.20294200	-2.91058100	3.13293200
C	-6.04894200	-1.29149900	0.34612100	C	0.07031600	-3.51171300	3.30445500
H	-5.46755300	-2.21465900	0.37778400	C	0.52914100	-3.78423500	4.60186000
C	-5.36654600	-0.03490600	0.32718700	H	1.52121300	-4.23610500	4.72112400
C	-3.08330600	-1.14179500	0.31814400	C	-0.23444500	-3.48331600	5.74154600
C	-2.20364600	-1.35236700	1.38925700	C	-1.49718300	-2.90458500	5.54886900
C	-1.76098400	-2.66399700	1.76937000	H	-2.11824600	-2.67105800	6.42212100
C	-2.00239000	-3.70284100	0.88081700	C	-2.00170500	-2.61394600	4.26923600
H	-1.69576100	-4.72011100	1.14142100	C	0.94980300	-3.83406500	2.12180100
C	-2.65196500	-3.48392400	-0.36746800	H	1.95690300	-4.13240800	2.45520400
C	-2.77589700	-4.52307200	-1.32649200	H	1.04815300	-2.96172200	1.45789100
H	-2.36654900	-5.51671000	-1.13068900	C	0.29295800	-3.78790200	7.12516100
C	-3.40681700	-4.26459500	-2.53216500	H	1.30107200	-3.35792000	7.26863100
C	-3.97919100	-3.00398400	-2.83394900	H	-0.36859500	-3.38071000	7.90746700
H	-4.47360300	-2.86506600	-3.79723400	C	-3.38472400	-2.01427600	4.14481500
C	-3.89650700	-1.99485300	-1.89402900	H	-3.92650900	-2.08860900	5.10166000
H	-4.33732900	-1.01669300	-2.10588200	H	-3.32678100	-0.94849500	3.86435300
C	-3.22786100	-2.19200800	-0.64790200	N	0.22490200	0.38916900	0.69289800
C	-3.48105300	3.87397400	0.72661300	O	2.31022500	-0.93322700	1.45465400
C	-3.24348100	4.39117000	2.01693900	O	2.17909800	-0.21649900	-0.99983800
C	-2.67706700	5.67643300	2.13142900	O	2.69749800	1.56793100	0.68886700
H	-2.48371700	6.07747300	3.13390400	O	-2.00332600	1.49265000	0.37540300
C	-2.31592300	6.43516000	1.01044600	O	-1.84872800	-0.30508000	2.19673600
C	-2.53867800	5.88201600	-0.26538600	O	-0.78077800	1.97350600	2.69465700
H	-2.25464200	6.45378100	-1.15827900	P	1.79137500	0.37434900	0.59793300
C	-3.11027400	4.61344600	-0.42628500	P	-0.95986700	0.99550700	1.58860800
C	-3.57253200	3.61332200	3.27142100	H	-0.56009600	7.69938900	0.94699700
H	-3.94500300	2.60321400	3.04450500	H	-4.34113400	4.13682900	3.87027300

H	4.32846800	3.06344700	6.82739400	C	4.63528100	3.97386400	-4.17060900
H	5.50370100	2.69389800	1.12865100	H	3.24325100	5.47204300	-4.92691900
H	2.91594700	-1.67277600	5.50116200	C	3.74158300	2.20059900	-2.78933800
H	0.37991200	-4.87851900	7.28733800	H	1.65881100	2.06745100	-3.03461400
H	-3.98119600	-2.52599900	3.36887900	C	4.83771500	2.81131500	-3.44433900
H	0.54512100	-4.66005300	1.51361300	H	5.49287600	4.44415900	-4.66530900
H	-0.81436200	-0.11832900	-1.46309600	O	3.95168200	1.07109900	-2.18421000
H	2.69266600	-2.58960400	-4.33098000	H	5.81595200	2.32790500	-3.38280900
H	-0.99383400	1.99056000	-7.15051400	H	3.13788400	0.63246100	-1.69678600
H	-4.32821400	3.68428000	-1.97405600	O	-10.28919700	0.81061300	0.29661700
C	1.79665300	3.59162800	-1.17722700	O	-10.16213300	-1.37405100	0.26528900
H	1.60256100	2.78615700	-0.46584300	O	-2.79962100	-6.34824500	-3.36675700
C	2.86846500	4.45878500	-0.50776300	O	-4.23704700	-5.15272900	-4.50471500
H	3.53409700	3.74261700	0.00664700	N	-9.65650500	-0.24877200	0.29319500
H	3.47941600	4.99587800	-1.26292800	N	-3.48910800	-5.33482600	-3.54065800
C	2.32475100	5.46744700	0.52451800	H	8.63391700	-4.14460000	-1.01039100
C	3.51572600	6.17379100	1.19602300	H	0.59602400	-7.50421300	-1.80733100
C	1.39936600	4.81841400	1.56880200				
H	1.75124400	6.24477400	-0.01934700	Int4'			
H	4.15537100	6.69104500	0.45743700	C	4.38525600	-1.73084300	0.46894200
H	3.16668100	6.92136800	1.92940000	C	3.70372100	-1.11249400	1.51322400
H	4.14439100	5.44113100	1.73534900	C	4.33586700	-0.45071300	2.61224300
H	0.44471900	4.49365600	1.12427900	C	5.72036900	-0.53086100	2.67261400
H	1.87007600	3.93635900	2.03541500	H	6.24802700	-0.06634900	3.51194200
H	1.16201900	5.54434500	2.36549700	C	6.48791200	-1.14579100	1.64197200
O	0.52586700	4.13120500	-1.38257700	C	7.91301800	-1.15347200	1.69260700
C	0.37397300	5.09198100	-2.41468000	H	8.40490400	-0.73135000	2.57603000
C	0.89674000	4.60484700	-3.81022000	C	8.66328500	-1.66344700	0.64652800
H	0.84952300	6.05554100	-2.14417400	C	8.01195500	-2.17635200	-0.50509500
H	-0.70958400	5.24908500	-2.50396800	H	8.60686400	-2.55477600	-1.34313800
C	2.24958400	3.99163700	-3.72725900	C	6.62793200	-2.20065400	-0.57955400
H	0.90514900	5.47277600	-4.48833000	H	6.13791100	-2.59422000	-1.47394500
H	0.18150300	3.84619400	-4.17223700	C	5.82571500	-1.71568000	0.49409700
C	3.35180200	4.56879700	-4.31837500	C	3.61212700	-2.30229000	-0.66903300
C	2.40366700	2.85203700	-2.79535700	C	2.67675400	-1.52216500	-1.35482700

C	2.04397000	-1.93878900	-2.56292800	H	1.83947100	1.48541800	-5.71237700
C	2.27367400	-3.23186400	-3.00701800	C	1.98858500	-0.09643500	-4.24714800
H	1.80612600	-3.57193200	-3.93733300	C	-0.91975000	-1.73971200	-2.34955000
C	3.10011900	-4.13205400	-2.27627500	H	-1.99696000	-1.67414400	-2.56275500
C	3.25555100	-5.48993900	-2.68055500	H	-0.75586700	-1.44426200	-1.29805500
H	2.73415400	-5.82996600	-3.58201800	C	-0.85385000	2.05879500	-5.68502500
C	4.03070300	-6.36795000	-1.94252300	H	-0.20230800	2.53699800	-6.43586200
C	4.68144500	-5.91881900	-0.76375900	H	-1.72175900	1.62605200	-6.21280300
H	5.27412400	-6.62188200	-0.16936000	C	3.48895300	-0.23221600	-4.40061000
C	4.56599300	-4.60046500	-0.35371000	H	4.01008900	-0.16692800	-3.42919500
H	5.05872700	-4.26536600	0.56269800	H	3.89156300	0.55060600	-5.06506300
C	3.78715500	-3.66638900	-1.09831800	C	-4.23823200	-0.07228900	0.31759700
C	3.50242800	0.40331000	3.50826800	C	-3.46017800	1.09000800	0.27807600
C	3.67993300	1.81195900	3.45684700	C	-4.02373500	2.39695900	0.38403200
C	2.75008800	2.63629100	4.10729800	C	-5.39967100	2.49951800	0.54146700
H	2.86958200	3.72396700	4.03386000	H	-5.85476900	3.49345300	0.60549900
C	1.63566300	2.11519200	4.78350000	C	-6.23436900	1.35393300	0.65086500
C	1.51358900	0.72105400	4.87066400	C	-7.63194000	1.48392600	0.86904600
H	0.65919500	0.28897400	5.40503600	H	-8.10383600	2.46768200	0.92867800
C	2.42742200	-0.14469200	4.25055000	C	-8.40517000	0.34809700	1.02130300
C	4.77762000	2.45128000	2.63364100	C	-7.85000700	-0.95432300	0.98396900
H	4.79104700	2.03170800	1.61365200	H	-8.50634000	-1.81249500	1.14047300
H	5.78024400	2.29577200	3.07090900	C	-6.49384800	-1.09643900	0.75973700
C	0.55316300	3.01867200	5.32150600	H	-6.05377000	-2.09626500	0.74438400
H	0.90771800	4.05705500	5.43620900	C	-5.64856300	0.03958600	0.56320500
H	-0.29663100	3.01828000	4.61377200	C	-3.59796200	-1.40363500	0.16389500
C	2.20476700	-1.63436200	4.35362800	C	-2.55999600	-1.77693200	1.02579000
H	3.11898800	-2.20672800	4.12550800	C	-2.05272900	-3.11299200	1.09046800
H	1.42510400	-1.96205800	3.64597300	C	-2.54267800	-4.02925500	0.16840300
C	1.27069100	-0.94036200	-3.36561100	H	-2.19065600	-5.06474000	0.20683000
C	-0.13654900	-0.83462300	-3.26355000	C	-3.48238100	-3.66403700	-0.83440600
C	-0.79810700	0.14716700	-4.02116300	C	-3.88654600	-4.58567600	-1.83630200
H	-1.88731000	0.23248900	-3.92828300	H	-3.49630500	-5.60610400	-1.85414300
C	-0.11013600	1.00627300	-4.89367800	C	-4.77386000	-4.18049900	-2.81673200
C	1.28302100	0.85775400	-5.00433800	C	-5.30579000	-2.86840500	-2.86197700

H	-5.98757200	-2.60299500	-3.67213200	C	-2.81600600	-3.01202100	3.94323800
C	-4.93713300	-1.96620700	-1.88199500	H	-3.03334500	-3.30015800	4.98460200
H	-5.32863400	-0.94595100	-1.90851300	H	-2.82827100	-1.90979500	3.87693300
C	-4.02897300	-2.33035900	-0.84100400	N	0.09414200	-0.23453100	0.49638400
C	-3.21428900	3.65204300	0.32548200	O	2.31527600	-1.11150000	1.45564000
C	-3.03460300	4.41051900	1.51008300	O	2.38784600	-0.22682800	-0.92323300
C	-2.45155500	5.68317700	1.41449400	O	2.21404800	1.47625500	0.88692100
H	-2.31424600	6.26950700	2.33119200	O	-2.10391800	0.96877800	0.07588900
C	-2.03447100	6.21909400	0.18398300	O	-2.05444600	-0.84132400	1.89623000
C	-2.16827700	5.42122200	-0.96194100	O	-0.96103600	1.41535500	2.43831000
H	-1.83466100	5.81613600	-1.92895800	P	1.63318200	0.12176900	0.60230300
C	-2.74141800	4.13801900	-0.91427500	P	-1.11856200	0.43202300	1.32793000
C	-3.40049200	3.83224100	2.85839100	H	-0.72277500	7.79539700	0.90419800
H	-4.47615300	3.59536500	2.93245400	H	-3.14634200	4.53645800	3.66751800
H	-2.83968100	2.89377000	3.02056000	H	0.17429200	2.66683900	6.29698100
C	-1.46261100	7.61681400	0.10432900	H	4.61180000	3.53935900	2.56060700
H	-0.96979500	7.79652700	-0.86631500	H	1.86719700	-1.90640100	5.36826500
H	-2.25728900	8.37763200	0.22118700	H	2.21621300	-6.01268300	4.72416300
C	-2.82710800	3.29061500	-2.16229300	H	-3.63476600	-3.38537600	3.30250700
H	-2.67876600	3.90243100	-3.06823700	H	0.11848800	-4.78845300	-0.30375400
H	-2.04782300	2.50720000	-2.14003100	H	-0.60368700	-2.79070000	-2.45330900
C	-1.08615100	-3.55277000	2.13931900	H	3.75760200	-1.21577900	-4.82597200
C	0.17546200	-4.07441700	1.75916000	H	-1.24620800	2.84777700	-5.01643400
C	1.01626900	-4.61288400	2.74626000	H	-3.80352800	2.78254500	-2.24553000
H	1.99434200	-5.00686900	2.44460100	C	1.88910100	3.44204800	-1.33526400
C	0.64277400	-4.65317100	4.09924600	H	1.66232600	2.56589500	-0.71364600
C	-0.60292000	-4.11075400	4.45480300	C	2.47788900	4.54510200	-0.46132200
H	-0.91514000	-4.12695000	5.50624300	H	3.25363600	4.05592400	0.15504900
C	-1.47638500	-3.55778100	3.50315700	H	2.98580300	5.31995300	-1.06643800
C	0.63872200	-4.04201400	0.32270400	C	1.44443400	5.20833300	0.47897300
H	1.71482400	-4.25492900	0.26516500	C	2.17859400	6.19175400	1.40443100
H	0.45467000	-3.05258400	-0.12323900	C	0.62444300	4.18616000	1.27929700
C	1.57439800	-5.22029900	5.14558000	H	0.74408200	5.79019700	-0.15029400
H	2.24170300	-4.43324600	5.54463600	H	2.76688200	6.93483300	0.83442800
H	1.01518200	-5.64241800	5.99780900	H	1.46023200	6.73843000	2.04002800

H	2.87217100	5.65029400	2.07411400	C	4.27071300	2.47557900	-1.81912300
H	-0.09011900	3.65056000	0.63447400	H	2.45068700	2.00779000	-2.86395900
H	1.26589800	3.43431500	1.76396900	C	5.42851800	3.27625600	-1.95548000
H	0.03242500	4.69748100	2.05480600	H	6.32595500	4.95808400	-2.93215700
O	0.72668200	3.74664800	-2.04471600	O	4.37967400	1.39563400	-1.09916400
C	0.82765500	4.80144200	-2.98028400	H	6.32937100	2.97873800	-1.41276300
C	1.81894300	4.37933000	-4.10288400	H	3.52920100	0.82778400	-1.01664000
H	1.16440400	5.73945300	-2.50152100	O	-10.31827800	1.64358000	1.28729700
H	-0.18010900	4.94830000	-3.39456700	O	-10.52011300	-0.53248800	1.39156400
C	3.10195600	3.98632600	-3.45494800	O	-4.68774600	-6.28118600	-3.81170700
H	1.96102000	5.21025700	-4.81322900	O	-5.94985500	-4.75090900	-4.73452200
H	1.37024600	3.51990100	-4.62678500	N	-9.85806500	0.49930600	1.25109000
C	4.26256000	4.71702500	-3.57648800	N	-5.16656000	-5.14526700	-3.86609600
C	3.00251100	2.87954200	-2.46919800	H	9.75710200	-1.65926500	0.69885800
C	5.41407500	4.36137100	-2.81786700	H	4.13271900	-7.41147900	-2.25777000
H	4.30599500	5.57326800	-4.25665300				

10. References

1. I. Coric and B. List, *Nature* **2012**, *483*, 315.
2. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.
3. (a) J. M. Tao, J. P. Perdew, V. N. Staroverov, and G. E. Scuseria, *Phys. Rev. Lett.* **2003**, *91*, 146401. (b) A. Schäfer, H. Horn, and R. Ahlrichs, *J. Chem. Phys.* **1992**, *97*, 2571. (c) A. Schäfer, C. Huber, and R. Ahlrichs, *J. Chem. Phys.* **1994**, *100*, 5829.
4. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.
5. (a) Becke, A. D. *J. Chem. Phys.*, **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.
6. (a) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297. (b) Weigend, F. *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057.
7. (a) J. B. Foresman, T. A. Keith, K. B. Wiberg, J. Snoonian, and M. J. Frisch, *J. Phys. Chem.* **1996**, *100*, 16098. (b) V. Barone and M. Cossi, *J. Phys. Chem. A* **1998**, *102*, 1995. (c) M. Cossi, N. Rega, G. Scalmani, and V. Barone, *J. Comput. Chem.* **2003**, *24*, 669.
8. Staginus, J.; Aerts, I. M.; Chang, Z.; Meijer, C. M.; Smet, L. C. P. M. de; Sudhölter, E. J. R. *Sensors and Actuators B*, **2013**, *184*, 130-142.