Supporting Information

Consecutive borylcupration/C-C coupling of γ-alkenyl aldehydes towards diastereoselective 2-(borylmethyl)cycloalkanols

Ricardo J. Maza, Jordi Royes, Jorge J. Carbó,* Elena Fernández*

Dept. Química Física i Inorgànica, University Rovira i Virgili, 43007-Tarragona, (Spain).

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1. General Information

Solvents and reagents: Solvents and reagents were obtained from commercial suppliers and dried and/or purified (if needed) by standard procedures, as specified in "Purification of Laboratory Chemicals". Tetrahydrofuran was dried by distillation from sodium benzophenone ketyl. All reactions were conducted in oven and flame-dried glassware under an inert atmosphere of argon, using Schlenk-type techniques. *Flash chromatography* was performed on standard silica gel (Merck Kieselgel 60 F254 400-630 mesh). *Thin layer chromatography* was performed on Merck Kieselgel 60 F254 which was developed using standard visualizing agents: UV fluorescence (254 and 366 nm) or potassium permanganate/Δ.

*NMR spectr*a were recorded at a Varian Goku 400 or a Varian Mercury 400 spectrometer. ^{1}H NMR and ^{13}C{^{1}H} NMR chemical shifts (δ) are reported in ppm with the solvent resonance as the internal standard ($CHCl_3$: 7.26 ppm (^{1}H) and $CDCl_3$: 77.16 ppm (^{13}C)). ^{11}B{^{1}H} NMR chemical shifts (δ) are reported in ppm relative to $(CH_3)_2O\cdots BF_3$. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, hept = heptuplet, br = broad, m = multiplet), coupling constants (Hz) and integration.

High resolution mass spectra (HRMS) were recorded using a 6210 Time of Flight (TOF) mass spectrometer from Agilent Technologies (Waldbronn, Germany) with an ESI interface and it was performed at the Servei de Recursos Científics i Tècnics (Universitat Rovira i Virgili, Tarragona). GC-MS analyses were performed on a HP6890 gas chromatograph and an Agilent Technologies 5973 Mass selective detector (Waldbronn, Germany) equipped with an achiral capillary column HP-5 (30m, 0.25mm i. d., 0.25µm thickness) using He as the carrier gas.

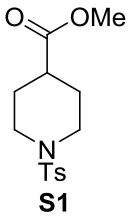
Reagents 3-bromoprop-1-ene, 4-bromobut-1-ene, prop-2-en-1-ol and 2-methylprop-2-en-1-ol were used as purchased from Sigma-Aldrich.

2. Experimental procedures and spectral data.

2.1.General procedure for the protection of amines with sulphonyl chloride derivatives[1]

N,*N*-diisopropyletilamina (DIPEA, 2 equiv, 20 mmol) and the tosyl chloride derivative (1 equiv, 10 mmol) were added to a solution of methyl piperidine-4-carboxylate (1 equiv, 10 mmol) in dry dichlorometane (0.14 M) at room temperature. The mixture was stirred for 4-16 h until complete consumption of the corresponding arenesulphonyl chloride. The organic phase was washed with 10% of $NaHCO_3$. The aqueous phase was extracted with ethyl acetate. The organic extracts were combined, washed with H_2O and NaCl sat. solution, dried ($MgSO_4$), filtered and the volatiles removed *in vacuo*. The crude product was purified by flash column chromatography.

Methyl 1-tosylpiperidine-4-carboxylate (S1)

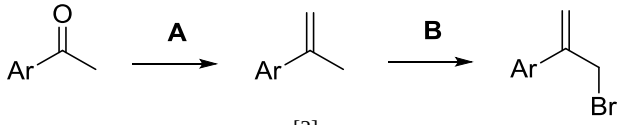


S1

Flash column chromatography (pentane: EtOAc 100:0 to 60:40) yielded the product **S1** (60% yield) as white solid. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 7.62 (d, *J* = 7.9 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 3.64 (s, 3H), 3.61 (m, 2H), 2.43 (td, J = 11.4, 2.9 Hz, 2H), 2.42 (s, 3H), 2.24 (dt, *J* = 10.7, 4.0 Hz, 1H), 1.95 (m, 2H), 1.79 (m, 2H). **^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz)** δ 174.2, 143.5, 132.9, 129.6, 127.6, 51.8, 45.3, 39.8, 27.4, 21.5. **HRMS (ESI) for $C_{28}H_{38}N_2NaO_8S_2$ [2M + Na]$^+$:** calculated: 617.1968, found: 617.1985.

2.2.General procedure for the preparation of alkyl bromides

This protocol covers two consecutive synthetic procedures:

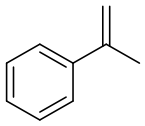


A)Wittig reaction on aryl methyl ketones:[2] a mixture of methyltriphenylphosphonium bromide (1.2 equiv) in dry THF (0.5 M) under argon atmosphere was cooled to 0 °C. Then, *n*-BuLi (2.5 M solution in hexane, 1.2 equiv) was added slowly under stirring. After, the resulting orange mixture was maintained at 0 °C for 1 h, a solution of the corresponding ketone (15 mmol, 1.0 equiv) in dry THF was added dropwise, at 0 °C. The reaction was allowed to warm up to rt, stirred overnight, and finally quenched with a saturated aqueous solution of NaCl. The resulting mixture was extracted with Et_2O. The combined organic phases were washed with brine, dried over Mg_2SO_4, and concentrated under reduced pressure. The resulting crude product was purified by flash column chromatography to give the corresponding alkene. **B)** Bromination of 1,1-disubstituted alkenes; **Method B1**:[3] The previously prepared alkene (1 eq.) was dissolved in a round bottom flask containing DCM (10 mL x 3 mmol alkene). NBS (2 eq.) was added to the solution which was then allowed to stir at 45 ºC for 18 h. Then the reaction mixture was concentrated and petroleum ether was added. The precipitate formed was filtered off and then the organic layer was dried over Mg_2SO_4 and concentrated under vacuum. The crude product was purified by flash column chromatography to give the corresponding brominated product. **Method B2**:[4] To a mixture of the α-methylstyrene derivative (1.0 equiv) and TMS-Cl (10 mol %) in dry CH_2Cl_2/THF (4:1, 3 mL x 1 mmol) under an argon atmosphere were added NBS (1.2 equiv) and $Yb(OTf)_3$ (10 mol %) in one portion. After stirring for 1 h, the mixture was concentrated under reduced pressure. The resulting residue was filtered three times with

pentane or diethyl ether, and the combined filtrates were concentrated under reduced pressure. The crude product mixture was then purified by silica gel chromatography

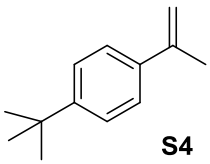
Products from Wittig Reaction (Method A)

Prop-1-en-2-ylbenzene (S2) was purchased from Sigma-Aldrich



S2

1-(tert-butyl)-4-(prop-1-en-2-yl)benzene (S4)



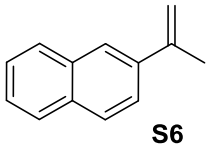
S4

The product **S4** was purified by flash column chromatography using pentane/diethyl ether (10:1) as eluent. The product was obtained as colourless oil (2385.5 mg, 91 %).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.49 (d, *J* = 8.3 Hz, 2H) – 7.35 (d, *J* = 8.2 Hz, 2H), 5.41 – 5.37 (m, 1H), 5.09 – 5.05 (m, 1H), 2.18 (s, 3H), 1.36 (s, 9H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 150.4, 142.9, 138.3, 125.1, 125.1, 111.6, 34.5, 31.3, 21.7.

2-(prop-1-en-2-yl)naphthalene (S6)



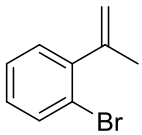
S6

The product **S6** was purified by flash column chromatography using pentane/diethyl ether (10:1) as eluent. The product was obtained as white solid (2132.2 mg, 85 %).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.82 – 7.68 (m, 4H), 7.60 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.46 – 7.30 (m, 2H), 5.46 (d, *J* = 1.5Hz, 1H), 5.12 (d, *J* = 1.5 Hz, 1H), 2.20 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 143.0, 138.3, 133.3, 132.8, 128.2, 127.6, 127.5, 126.1, 125.8, 124.2, 123.9, 113.0, 21.8.

1-bromo-2-(prop-1-en-2-yl)benzene (S8)



S8

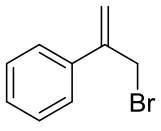
The product **S8** was purified by flash column chromatography using pentane/diethyl ether (10:1) as eluent. The product was obtained as white solid (2388.8 mg, 79 %).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.23 (d, *J* = 8.0 Hz, 1H), 7.12 (dd, *J* = 7.6, 1.9 Hz, 1H), 7,08 (d, *J* = 7.9 Hz, 1H), 7.04 (dd, *J* = 8.0, 1.9 Hz, 1H), 5.15 (d, *J* = 1.7 Hz, 1H), 4.86 (d, *J* = 2.0 Hz, 1H), 2.02 (s, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz) δ 145.8, 144.8, 132.7, 129.7, 128.3, 127.2, 121.5, 116.0, 23.5.

Products from Bromination Reaction (Method B)

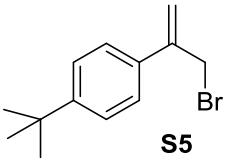
(3-bromoprop-1-en-2-yl)benzene (S3)



S3

The product **S3** was purified by flash column chromatography using pentane/diethyl ether (10:1) as eluent. The product was obtained as colourless oil (1434.8 mg, 52 %).
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.39 – 7.20 (m, 4H), 5.49 (d, *J* = 0.7 Hz, 1H), 5.42 (d, *J* = 0.8 Hz, 1H), 4.32 (s, 2H).
^{13}C NMR ($CDCl_3$, 100 MHz) δ 144.2, 137.6, 128.5, 128.3, 127.8, 126.1, 126.0, 117.2, 34.2.

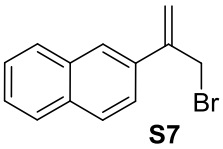
1-(3-bromoprop-1-en-2-yl)-4-(tert-butyl)benzene (S5)



S5

The product **S5** was purified by flash column chromatography using pentane/diethyl ether (10:1) as eluent. The product was obtained as a yellow oil (1556.9 mg, 45 %).
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42 (dd, *J* = 8.1, 1.7 Hz, 2H) 7.28 (dd, *J* = 8.4, 1.5 Hz, 2H)), 5.48 (d, *J* = 0.8 Hz, 1H), 5.38 (d, *J* = 0.8 Hz, 1H), 4.31 (s, 2H), 1.26 (s, 9H).
^{13}C NMR ($CDCl_3$, 100 MHz) δ 151.3, 143.8, 134.5, 125.7, 125.4, 116.5, 34.6, 34.2, 31.2.

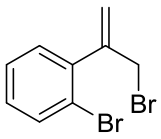
2-(3-bromoprop-1-en-2-yl)naphthalene (S7)



S7

The product **S7** was purified by flash column chromatography using pentane/ethyl acetate (10:1) as eluent. The product was obtained as a yellow oil (2536.5 mg, 81 %).
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.97 (d, *J* = 1.9 Hz, 1H), 7.94 – 7.81 (m, 3H), 7.65 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.57 – 7.46 (m, 2H), 5.73 (t, *J* = 0.8 Hz, 1H), 5.62 (t, *J* = 0.8 Hz, 1H), 4.53 (s, 2H).
^{13}C NMR ($CDCl_3$, 100 MHz) δ144.1, 134.7, 133.2, 133.1, 128.3, 128.20, 127.6, 126.3, 126.3, 125.2, 124.0, 117.6, 34.1.

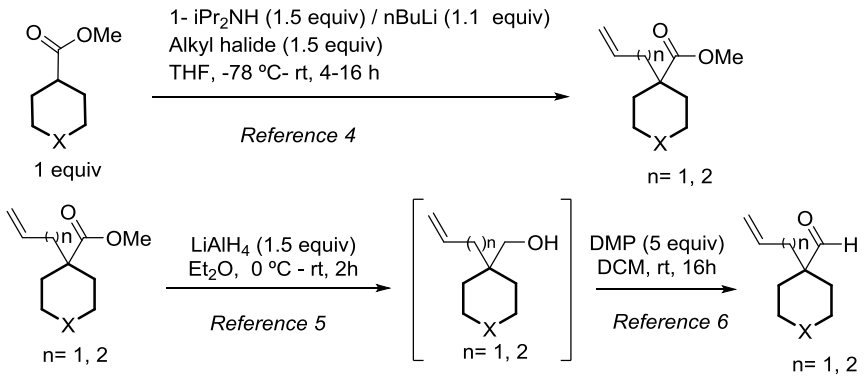
1-bromo-2-(3-bromoprop-1-en-2-yl)benzene (S9)



S9

The product **S9** was purified by flash column chromatography using pentane/ethyl acetate (10:1) as eluent. The product was obtained as colourless oil (795.1 mg, 20 %).
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.60 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.29 (m, 2H), 7.25 – 7.20 (m, 1H), 5.67 (d, *J* = 1.0 Hz, 1H), 5.24 (d, *J* = 1.0 Hz, 1H), 4.38 (d, *J* = 0.9 Hz, 2H).
^{13}C NMR ($CDCl_3$, 100 MHz) δ 145.6, 140.2, 136.2, 132.7, 131.6, 129.4, 127.2, 120.8, 35.4.

2.3.General procedure for the alkylation of ester substrates with alkyl bromides followed by reduction to alcohols and oxidation to aldehydes

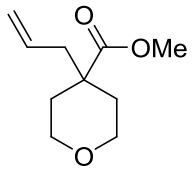


The initial step proceeded towards **the alkylation of ester substrates with alkyl bromides**:[5] To a 0 °C solution of $^{i}Pr_2NH$ (1.5 equiv, 15 mmol) in THF (15 mL), was added dropwise a solution of nBuLi 2.0 M (1.1 equiv, 11 mmol) in hexane. The reaction mixture was stirred for 20 minutes and then cooled to -78 °C. The substrate with the ester functionality (1 equiv, 10 mmol) was added dropwise and the reaction mixture was stirred for 1 h at -78 °C. The corresponding alkyl halide (1.5 equiv, 15 mmol, for n=1, allyl bromide; n=2, 4-bromobut-1-ene; n=3, 5-bromo-1-pentene) was then added dropwise into the reaction mixture. The reaction mixture was then warmed naturally to room temperature and stirred until consumption of the starting sulphonamide. The reaction mixture was quenched by addition of saturated NH_4Cl aq. and extracted with Et_2O three times. The combined organic layers were then dried ($MgSO_4$) filtered and concentrated under reduced pressure. The crude product of the alkylated ester was purified by flash column chromatography.

Next step proceeded towards **the reduction of the ester group to the corresponding alcohol**:[6] to a slurry of $LiAlH_4$ (1.5 equiv, 6 mmol) in anhydrous Et_2O (0.9 M) was added a solution of the alkenyl ester (1 equiv, 4 mmol) in Et_2O (1 M) dropwise at 0 °C. The mixture was stirred for 2 h (or until consumption of the substrate). The reaction was then quenched by addition of EtOH dropwise after no observation of bubbles. Then, water was added and the mixture was stirred until a white solid was formed. The mixture was then filtered and extracted with EtOAc. The organic layers were separated, dried ($MgSO_4$), filtered and concentrated under reduced pressure to obtain the alcohol without need of further purification for the next reaction step.

The last step involves a **general procedure for the oxidation of primary alcohols to aldehydes**:[7] to a solution of the alkenyl alcohol (2 mmol, 1 equiv) in DCM (2 mL) was added DMP (5 mmol, 2 equiv) and stirred at room temperature for 16 h. Then $NaHCO_3$ saturated solution was added and extracted few times with DCM. The organic layer was separated, dried ($MgSO_4$), filtered and the solvent removed in vacuum. The crude was purified by flash column chromatography.

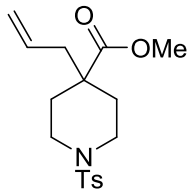
Methyl 4-allyltetrahydro-2*H*-pyran-4-carboxylate (S10)



S10

Flash column chromatography (20:1 Hexane:EtOAc) yielded the product **S10** (2485.5 mg, 90% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 5.63 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.08 – 4.94 (m, 2H), 3.74 (m, 2H), 3.67 (s, 3H), 3.40 (t, *J* = 10.4 Hz, 2H), 2.20 (dd, *J* = 7.4, 1.0 Hz, 2H), 2.02 - 1.94 (m, 2H), 1.52 (m, 2H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 175.5, 132.5, 118.2, 65.2, 51.6, 45.1, 44.7, 33.7. **HRMS (ESI) for $C_{10}H_{16}O_3$ $[M]^+$:** calculated: 184.1102, found: 184.1099.

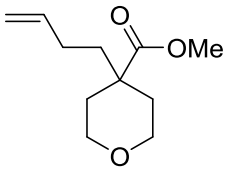
Methyl 4-allyl-1-tosylpiperidine-4-carboxylate (S11)



S11

Flash column chromatography (pentane: EtOAc 100:0 to 60:40) yielded the product **S11** (3135.4 mg, 62% yield) as white solid. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 5.58 (ddt, *J* = 14.9, 10.1, 7.5 Hz, 1H), 5.06 – 4.90 (m, 2H), 3.60 – 3.50 (m, 2H), 3.55 (s, 3H), 2.40 (s, 3H), 2.37 (dd, *J* = 12.0, 2.1 Hz, 2H), 2.19 (d, *J* = 7.5 Hz, 2H), 2.15 (m, 2H), 1.54 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 174.8, 143.3, 133.3, 132.1, 129.5, 127.5, 118.6, 51.7, 45.2, 44.2, 43.6, 32.4, 21.4. **HRMS (ESI) for $C_{17}H_{24}NO_4S$ $[M+H]^+$:** calculated: 338.1421, found: 338.1425.

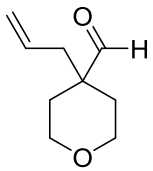
Methyl 4-(but-3-en-1-yl)tetrahydro-2*H*-pyran-4-carboxylate (S12)



S12

Flash column chromatography (hexane:ethyl acetate 20:1) yielded the product **S12** (2229.0 mg, 75% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 5.74 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 4.97 – 4.80 (m, 2H), 3.82 (m, 2H), 3.71 (s, 3H), 3.42 (t, *J* = 7.5 Hz, 2H), 2.15 (d, *J* = 6.5 Hz, , 2H), 1.98 – 1.90 (m, 2H), 1.67 – 1.57 (m, 2H), 1.50 (m, 2H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 176.0, 137.8, 114.8, 65.4, 51.8, 44.8, 39.9, 34.2, 28.0. **HRMS (ESI) for $C_{11}H_{18}O_3$ $[M]^+$:** calculated: 198.1255, found: 198.1256.

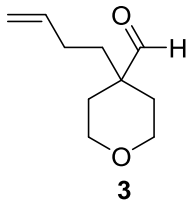
4-Allyltetrahydro-2*H*-pyran-4-carbaldehyde (1)



1

Flash column chromatography (pentane:Et_2O 100:0 to 60:40) yielded **1** (1081.8 mg, 52% yield) as a clear oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 9.50 (s, 1H), 5.66 (m, 1H), 5.10 (m, 2H), 3.81 (d, *J* = 12.0 Hz, 2H), 3.43 (dt, *J* = 12.0, 4.3 Hz, 2H), 2.25 (d, *J* = 7.5 Hz, 2H), 1.93 (d, *J* = 13.7 Hz, 2H), 1.60 (m, 2H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 204.6, 131.2, 118.5, 64.0, 46.9, 40.4, 30.2. **HRMS (ESI) for $C_9H_{15}O_2$ $[M+H]^+$:** calculated:155.1067, found: 155.1053.

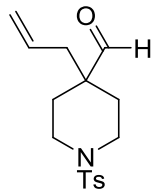
4-(But-3-en-1-yl)tetrahydro-2*H*-pyran-4-carbaldehyde (3)



3

Flash column chromatography (pentane:Et_2O 100:0 to 60:40) yielded **3** (1437.3 mg, 76% yield) as a clear oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 9.42 (s, 1H), 5.67 (ddt, *J* = 16.8, 10.1, 6.5 Hz, 1H), 4.92 (m, 2H), 3.76 (dt, *J* = 11.8, 4.0 Hz, 2H), 3.36 (td, *J* = 11.5, 2.6 Hz, 2H), 1.94 – 1.81 (m, 4H), 1.59 – 1.45 (m, 4H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 205.3, 137.4, 115.1, 64.5, 47.3, 35.9, 30.9, 27.3. **HRMS (ESI) for $C_{10}H_{17}O_2$ $[M+H]^+$:** calculated: 169.1223, found:169.1221.

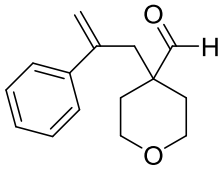
4-Allyl-1-tosylpiperidine-4-carbaldehyde (5)



5

Flash column chromatography (pentane:ethyl acetate 100:0 to 60:40) yielded **5** (2199.3 mg, 77% yield) as a clear oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 9.32 (s, 1H), 7.57 (d, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 5.56 (m, 1H), 5.05 (m, 2H), 3.54 (dt, *J* = 11.8, 3.2 Hz, 2H), 2.40 (s, 3H), 2.33 (td, *J* = 12.1, 2.8 Hz, 2H), 2.16 (d, *J* = 7.5 Hz, 2H), 2.05 (m, 2H), 1.64 (td, *J* = 12.0, 2.7 Hz, 2H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 204.7, 143.6, 132.8, 130.9, 129.6, 127.4, 119.5, 47.6, 43.2, 40.6, 29.6, 21.4. **HRMS (ESI) for $C_{16}H_{22}NO_3S$ $[M+H]^+$:** calculated: 308.1315, found: 308.1315.

4-(2-phenylallyl)tetrahydro-2H-pyran-4-carbaldehyde (16)

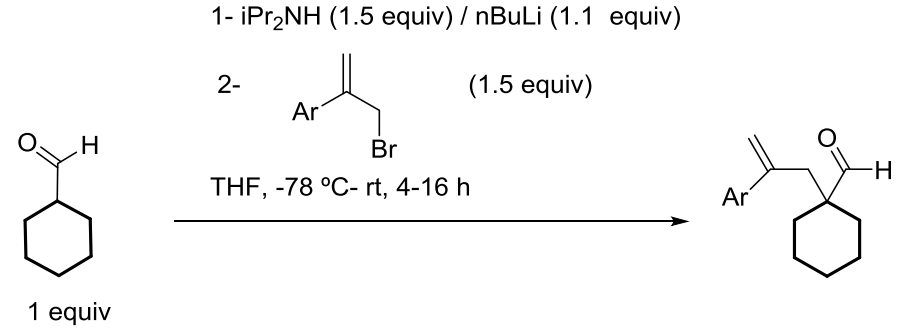


16

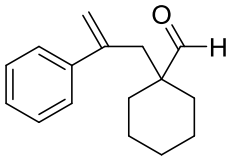
Flash column chromatography (pentane:ethylacetate:methanol 10:4:1) yielded **16** (280.5 mg, 88 %) as colourless oil.
^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.23 (s, 1H), 7.31 – 7.16 (m, 5H), 5.21 (d, *J* = 1.5 Hz, 1H), 5.01 (m, 1H), 3.67 (ddd, *J* = 12.0, 4.4, 3.2 Hz, 2H), 3.31 – 3.20 (m, 2H), 2.68 (d, *J* = 0.9 Hz, 2H), 1.81 – 1.71 (m, 2H), 1.55 – 1.43 (m, 2H).
^{13}C NMR ($CDCl_3$, 100 MHz) δ 204.9, 143.9, 141.6, 128.5, 127.8, 126.5, 117.8, 64.6, 48.0, 43.6, 31.5.
HRMS (ESI) for $C_{15}H_{18}O_2$ $[M]^+$: calculated: 230.1308, found: 230.1307.

2.4. General procedure for the alkylation of aldehyde substrates with alkyl bromides[5]

To a 0 °C solution of $^{i}Pr_2NH$ (1.5 equiv, 15 mmol) in THF (15 mL), was added dropwise a solution of nBuLi 2.0 M (1.1 equiv, 11 mmol) in hexane. The reaction mixture was stirred for 20 minutes and then cooled to -78 °C. The substrate with the aldehyde functionality (1 equiv, 10 mmol) was added dropwise and the reaction mixture was stirred for 1 h at -78 °C. The corresponding alkyl halide (1.5 equiv, 15 mmol) was then added dropwise into the reaction mixture. The reaction mixture was then warmed naturally to room temperature and stirred until consumption of the starting sulphonamide. The reaction mixture was quenched by addition of saturated NH_4Cl aq. and extracted with Et_2O three times. The combined organic layers were then dried ($MgSO_4$) filtered and concentrated under reduced pressure. The crude product of the alkylated aldehyde was purified by flash column chromatography.



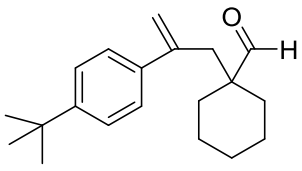
1-(2-phenylallyl)cyclohexane-1-carbaldehyde (14)



14

Flash column chromatography (pentane:ethyl acetate 10:1) yielded the product **14** as colourless oil (233.8 mg, 56 %). **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 9.18 (s, 1H), 7.28 – 7.18 (m, 5H), 5.17 (d, *J* = 1.5 Hz, 1H), 4.97 (dd, *J* = 1.6, 0.9 Hz, 1H), 2.61 (d, *J* = 0.9 Hz, 2H), 1.80 – 1.67 (m, 2H), 1.51 – 1.32 (m, 3H), 1.22 – 1.01 (m, 5H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 206.5, 144.7, 142.1, 128.3, 127.6, 126.6, 117.3, 50.2, 43.5, 31.5, 25.5, 22.6.

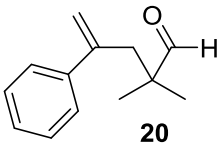
1-(2-(4-(tert-butyl)phenyl)allyl)cyclohexane-1-carbaldehyde (18)



18

Flash column chromatography (pentane:ethyl acetate 10:1) yielded the product **18** as yellow oil (1449.5 mg, 91 %). **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 9.18 (s, 1H), 7.23 (d, *J* = 8.5 Hz, 2H), 7.15 (d, *J* = 8.5 Hz, 2H), 5.16 (d, *J* = 1.6 Hz, 1H), 4.94 – 4.89 (m, 1H), 2.58 (d, *J* = 0.9 Hz, 2H), 1.81 – 1.69 (m, 2H), 1.50 – 1.37 (m, 3H), 1.23 (s, 9H), 1.20 – 1.04 (m, 5H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 206.6, 150.6, 144.3, 139.0, 126.1, 125.2, 116.6, 50.1, 43.4, 34.5, 31.6, 31.3, 31.3, 25.6, 22.7. **HRMS (ESI) for $C_{20}H_{29}O$ $[M+H]^+$:** calculated: 285.2199, found: 285.2218.

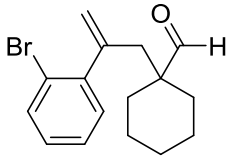
2,2-dimethyl-4-phenylpent-4-enal (20)



20

Flash column chromatography (pentane:diethyl ether 10:1) yielded the product **20** as colourless oil (520.4 mg, 64 %). **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 9.26 (s, 1H), 7.29 – 7.14 (m, 5H), 5.20 (d, *J* = 1.6 Hz, 1H), 5.03 – 4.97 (m, 1H), 2.67 (d, *J* = 0.9 Hz, 2H), 0.91 (s, 6H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 205.3, 145.3, 142.1, 128.3, 127.6, 126.5, 117.2, 46.4, 43.2, 21.8. **HRMS (ESI) for $C_{13}H_{16}O$ $[M]^+$:** calculated: 188.1201, found: 188.1200.

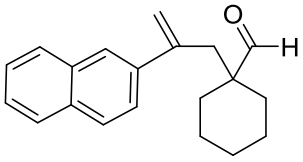
1-(2-(2-bromophenyl)allyl)cyclohexane-1-carbaldehyde (22)



22

Flash column chromatography (pentane:ethyl acetate 10:1) yielded the product **22** as colourless oil (198.2 mg, 25 %). **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 9.20 (s, 1H), 7.46 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.18 (td, *J* = 7.5, 1.3 Hz, 1H), 7.11 – 7.00 (m, 2H), 5.17 (d, *J* = 1.3 Hz, 1H), 5.04 (d, *J* = 1.5 Hz, 1H), 2.70 (d, *J* = 1.0 Hz, 2H), 1.81 – 1.73 (m, 2H), 1.47 – 1.38 (m, 3H), 1.26 – 1.13 (m, 5H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 206.2, 145.1, 143.2, 133.0, 130.9, 128.8, 127.3, 121.7, 120.6, 50.4, 31.3, 25.5, 22.4. **HRMS (ESI) for $C_{16}H_{20}BrO$ $[M+H]^+$:** calculated: 306.0622, found: 306.0619.

1-(2-(naphthalen-2-yl)allyl)cyclohexane-1-carbaldehyde (24)

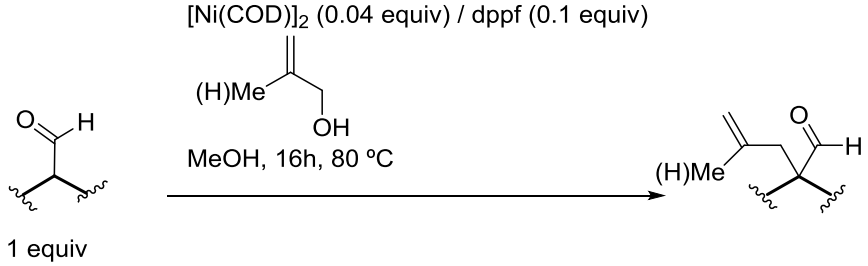


24

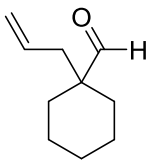
Flash column chromatography (pentane:ethyl acetate 10:1) yielded the product **24** as yellow oil (750 mg, 30 %). **^{1}H NMR ($CDCl_3$, 400 MHz)** δ 9.22 (s, 1H), 7.82 – 7.66 (m, 4H), 7.45 – 7.33 (m, 3H), 5.32 (d, *J* = 1.5 Hz, 1H), 5.07 (d, *J* = 1.4 Hz, 1H), 2.72 (d, *J* = 0.9 Hz, 2H), 1.84 – 1.75 (m, 2H), 1.50 – 1.34 (m, 3H), 1.16 (tdd, *J* = 19.4, 10.5, 5.0 Hz, 6H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 128.0, 127.6, 126.2, 125.9, 125.2, 125.0, 118.0, 50.3, 43.4, 31.6, 25.5, 22.6. **HRMS (ESI) for $C_{20}H_{22}O$ $[M]^+$:** calculated: 278.1677, found: 278.1671.

2.5. General procedure for the alkylation of aldehyde substrates with allyl alcohols[8]

To a dry reaction vessel equipped with a magnetic stirrer bar was introduced 1,1′-bis(diphenylphosphino)ferrocene (0.4 mmol, 0.1 equiv) and bis(1,5-cyclooctadiene)nickel (0.16 mmol, 0.04 equiv) in methanol (2 mL) into a glove box. The mixture was stirred and the corresponding allyl alcohol (4 mmol, 1 eq.) and aldehyde (4 mmol, 1 eq.) were added dropwise. Finally the Schlenk tube was sealed then warmed up to 80 ºC and stirred for 16 h. Once the reaction was finished, the solvent was removed, and the crude was purified by silica-gel column chromatography to give the desired allylated aldehyde.



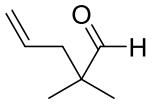
1-Allylcyclohexane-1-carbaldehyde (7)



7

Flash column chromatography (pentane:dichloromethane 80:20) yielded the product **7** (223.9 mg, 82% yield) as a colorless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 9.38 (s, 1H), 5.69 – 5.48 (m, 1H), 4.97 (dd, *J* = 10.8, 2.7 Hz, 2H), 2.11 (d, *J* = 7.5 Hz, 2H), 1.86 – 1.76 (m, 2H), 1.56 – 1.43 (m, 3H), 1.31 – 1.16 (m, 5H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 206.8, 132.6, 118.2, 49.6, 40.7, 30.7, 29.6, 25.6, 22.4.

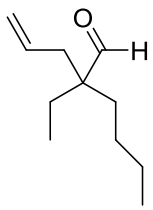
2,2-dimethylpent-4-enal (9)



9

Flash column chromatography (pentane:dichloromethane 4:1) yielded **9** (400.3 mg, 89% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 9.42 (s, 1H), 5.73 – 5.53 (m, 1H), 5.06 – 4.92 (m, 2H), 2.15 (d, *J* = 7.3 Hz, 2H), 0.99 (s, 6H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 205.5, 133.1, 118.4, 53.4, 53.1, 41.4, 21.1.

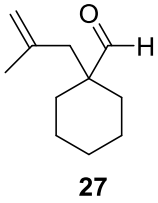
2-allyl-2-ethylhexanal (11)



11

Flash column chromatography (pentane:dichloromethane 4:1) yielded **11** (359.8 mg, 54% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 9.39 (s, 1H), 5.59 (ddt, *J* = 17.6, 10.2, 7.4 Hz, 1H), 5.06 – 4.95 (m, 2H), 2.19 (dd, *J* = 7.4, 1.0 Hz, 2H), 1.52 – 1.38 (m, 4H), 1.28 – 1.15 (m, 2H), 1.15 – 1.00 (m, 2H), 0.82 (t, *J* = 7.3 Hz, 3H), 0.73 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 206.8, 133.1, 118.2, 52.2, 35.4, 31.7, 25.6, 24.7, 23.2, 13.8, 7.8.

1-(2-methylallyl)cyclohexane-1-carbaldehyde (27)

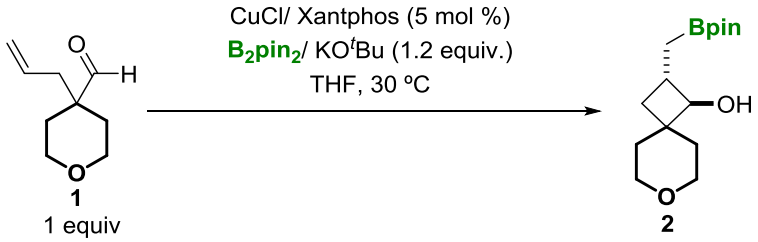


27

Flash column chromatography (pentane:dichloromethane 4:1) yielded **27** (359.8 mg, 54% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 9.45 (s, 1H), 4.76 (d, *J* = 1.2 Hz, 1H), 4.60 (d, *J* = 0.8 Hz, 1H), 2.14 (s, 2H), 1.87 – 1.72 (m, 2H), 1.57 (s, 3H), 1.56 – 1.41 (m, 3H), 1.33 – 1.13 (m, 5H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 207.1, 141.0, 115.0, 49.6, 45.2, 31.3, 25.6, 24.3, 22.5.

2.6.General procedure for the copper catalyzed borylative cyclization (exemplified for synthesis of product 2)

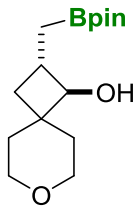
Copper chloride (0.98 mg, 5 mol%, 0.01 mmol) and bis(pinacolato)diboron (60.9 mg, 1.2 equiv, 0.24 mmol), Xantphos (138.8 mg, 5 mol%, 0.01 mmol) were placed in an oven-dried reaction vial. The vial was sealed with a screw cap containing a teflon-coated rubber septum. The vial was connected to a vacuum/nitrogen manifold through a needle, evacuated and backfilled with nitrogen and THF (0.24 ml, 1 M). KO^{t}Bu (26.9 mg, 1.2 equiv, 0.24 mmol) in THF (0.24 ml, 1 M) were added in the vial through the rubber septum. Then substrate 4-Allyltetrahydro-2*H*-pyran-4-carbaldehyde **(1)** (1 equiv, 0.2 mmol) in THF (0.2 ml, 1 M) was added dropwise at 30 °C. After the reaction was complete, the reaction mixture was filtered over Celite. The organic extracts were then concentrated in *vacuo*. The crude product was purified by flash chromatography.



1
1 equiv

2

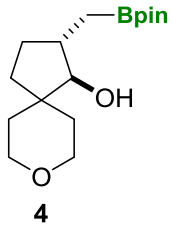
***anti*-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-7-oxaspiro[3.5]nonan-1-ol (2)**



2

Flash column chromatography (pentane:ethyl acetate 3:2) yielded **2** (100.2 mg, 71% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 3.87 (dt, *J* = 10.8, 4.4 Hz, 1H), 3.72 (dt, *J* = 10.9, 4.4 Hz, 1H), 3.59 (m, 1H), 3.46 (d, *J* = 8 Hz, 1H), 3.43 (dd, *J* = 11.5, 2.3 Hz, 1H), 2.14 (m, 1H), 1.93 (m, 2H), 1.76 (ddd, *J* = 13.3, 9.6, 3.9 Hz, 1H), 1.49 (m, 1H), 1.39 (m, 1H), 1.25 (s, 12H), 1.09 (dd, *J* = 16.4, 5.1 Hz, 1H), 0.95 (t, *J* = 10.2 Hz, 1H), 0.86 (dd, *J* = 16.4, 10.6 Hz, 1H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 83.3, 80.9, 64.9, 64.7, 39.4, 38.8, 36.3, 33.6, 30.5, 24.7, 24.7. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 33.8. **HRMS (ESI) for $C_{15}H_{26}BO_3$ $[M\text{-}H_2O+H]^+$:** calculated: 265.1975, found: 265.1964.

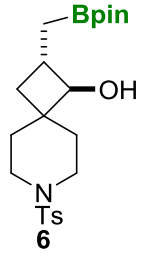
2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-7-oxaspiro[3.5]nonan-1-ol (4)



4

Flash column chromatography (pentane:ethyl acetate 1:1) yielded **4** (66.6 mg, 45% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 3.82 (m, 2H), 3.49 (m, 2H), 3.12 (d, *J* = 8.3 Hz, 1H), 1.84 (m, 4H), 1.72 (m, 1H), 1.40 (m, 2H), 1.24 (s, 12H), 1.13 (m, 2H), 1.06 – 0.93 (m, 2H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 87.0, 83.3, 65.3, 64.5, 42.2, 40.6, 36.9, 31.9, 30.2, 29.3, 24.7. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 33.8. **HRMS (ESI) for $C_{16}H_{30}BO_4$ $[M+H]^+$:** calculated: 297.2237, found: 297.2238.

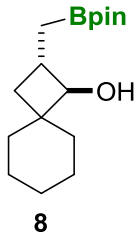
***anti*-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-7-tosyl-7-azaspiro [3.5] nonan-1-ol (6)**



6

Flash column chromatography (pentane:ethyl acetate 3:2) yielded **6** (145.8 mg, 67% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.63 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 3.43 (d, *J* = 7.8 Hz, 1H), 3.38 (m, 1H), 3.21 (m, 1H), 2.84 (s, 1H), 2.79 (m, 1H), 2.42 (s, 3H), 2.07 (m, 1H), 1.95 (m, 1H), 1.77 (m, 1H), 1.73 (t, *J* = 10.2 Hz, 1H), 1.63 (m, 1H), 1.52 (m, 1H), 1.22 (s, 12H), 1.04 (dd, *J* = 16.7, 4.9 Hz, 1H), 0.81 (t, *J* = 10.2 Hz, 1H), 0.76 (m, 1H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 143.1, 133.5, 129.4, 127.5, 83.4, 80.4, 43.4, 43.2, 39.4, 37.5, 36.2, 29.4, 24.7, 21.4. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 33.0. **HRMS (ESI) for $C_{22}H_{35}BNO_5S$ $[M-H_2O+H]^+$:** calculated: 436.2329, found: 436.2330.

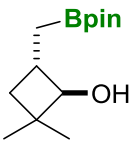
***anti*-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)spiro[3.5]nonan-1-ol (8)**



8

Flash column chromatography (pentane:ethyl acetate 3:2) yielded **8** (70.1 mg, 50% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 3.33 (d, *J* = 7.6 Hz, 1H), 2.09 – 1.95 (m, 1H), 1.84 – 1.76 (m, 1H), 1.64 – 1.24 (m, 10H), 1.18 (s, 12H), 0.99 (dd, *J* = 16.4, 5.6 Hz, 1H), 0.83 – 0.79 (m, 1H), 0.77 (d, *J* = 10.5 Hz, 1H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 83.3, 81.8, 42.1, 39.4, 36.6, 34.0, 29.9, 26.4, 24.8, 23.3, 23.0, 22.5. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 34.0. **HRMS (ESI) for $C_{16}H_{33}BNO_3$ $[M+NH_4]^+$:** calculated: 298.2557, found: 298.2553.

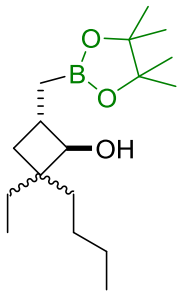
2,2-dimethyl-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)cyclobutan-1-ol (10)



10

Flash column chromatography (pentane:ethyl acetate 3:2) yielded **10** (78 mg, 59% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 3.34 (dd, *J* = 7.7, 3.1 Hz, 1H), 2.76 (d, *J* = 3.4 Hz, 1H), 2.10 – 1.93 (m, 1H), 1.65 (t, *J* = 9.9 Hz, 1H), 1.18 (s, 12H), 1.13 (dd, *J* = 4.7, 1.5 Hz, 1H), 1.00 (d, *J* = 2.5 Hz, 6H), 0.89 (t, *J* = 10.2 Hz, 1H), 0.78 (dd, *J* = 16.3, 10.5 Hz, 1H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 83.3, 81.0, 37.5, 36.7, 36.6, 28.8, 24.8, 21.0. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ 33.8. **HRMS (ESI) for $C_{13}H_{29}NBO_2$ $[M-NH_4]^+$:** calculated: 258.2240, found: 258.2242.

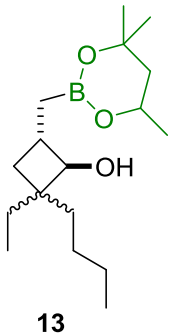
2-butyl-2-ethyl-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)cyclobutan-1-ol (12) *(as a mixture of two diastereoisomers)*



12

Flash column chromatography (pentane:diethyl ether 3:2) yielded **12** (50.9 mg, 34% yield) as a colourless oil *as a mixture of two diastereoisomers*. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 3.44 (d, *J* = 7.6 Hz, 1H), δ = 3.43 (d, *J* = 7.6 Hz, 1H), 2.08 – 1.92 (m, 2H), 1.79 – 1.68 (m, 2H), 1.62 – 1.48 (m, 4H), 1.43 – 1.25 (m, 8H), 1.18 (s, 24H), 0.98 (t, *J* = 16.3 Hz, 6H), 0.79 (t, *J* = 13.5, Hz, 6H), 0.75 (m, 10H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 83.3, 81.2, 81.0, 44.3, 44.2, 38.6, 36.6, 36.5, 33.6, 33.5, 31.7, 29.3, 26.2, 25.8, 24.8, 24.8, 23.7, 23.4, 22.5, 14.2, 14.1, 8.3, 7.9. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ 34.7. **HRMS (ESI) for $C_{17}H_{33}BO_3$ $[M]^+$:**calculated: 297.2611, found: 297.2601.

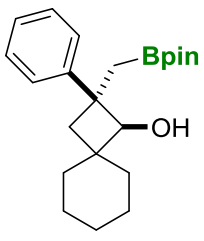
2-butyl-2-ethyl-4-((4,4,6-trimethyl-1,3,2-dioxaborinan-2-yl)methyl)cyclobutan-1-ol (13) *(as a mixture of two diastereoisomers)*



13

Flash column chromatography (pentane:diethyl ether 3:2) yielded **13** (75.9 mg, 51% yield) as a colourless oil *as a mixture of two diastereoisomers*. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 4.11 (m, 2H), 3.42 (t, *J* = 7.5 Hz, 1H), 3.41 (t, *J* = 7.5 Hz, 1H), 2.07 – 1.89 (m, 2H), 1.76 – 1.64 (m, 4H), 1.64 – 1.48 (m, 4H), 1.48 – 1.34 (m, 12H), 1.22 (s, 12H), 1.18 (d, *J* = 6.1 Hz, 6H), 0.94 – 0.63 (m, 20H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 81.4, 81.4, 81.1, 71.0, 65.8, 64.8, 64.8, 45.7, 44.0, 43.9, 38.6, 36.6, 36.5, 33.6, 33.4, 31.8, 31.2, 31.1, 29.4, 29.3, 28.1, 28.0, 26.2, 25.8, 25.8, 23.7, 23.4, 23.1, 23.0, 22.6, 22.6, 15.2, 14.2, 14.1, 8.3, 8.0, 7.9. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 30.2. **HRMS (ESI) for $C_{17}H_{32}BO_2$ $[M–H_2O]^+$:** calculated: 279.2498, found: 279.2495.

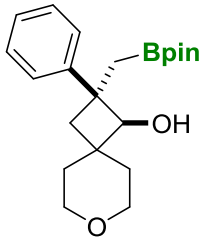
2-phenyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)spiro[3.5]nonan-1-ol (15)



15

Flash column chromatography (pentane:diethyl ether 3:2) yielded **15** (131.6 mg, 76% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.33 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.24 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.17 – 7.07 (m, 1H), 3.83 (s, 1H), 2.57 (d, *J* = 12.6 Hz, 1H), 1.54 (d, *J* = 12.7 Hz, 1H), 1.46 (d, *J* = 6.0 Hz, 6H), 1.25 (d, *J* = 15.0 Hz, 3H), 1.12 (s, 4H), 0.97 (s, 6H), 0.96 (s, 6H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 143.1, 128.5, 128.0, 125.8, 84.2, 82.7, 46.6, 41.4, 39.7, 37.6, 30.0, 26.1, 24.7, 24.6, 23.2, 21.9. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 33.2. **HRMS (ESI) for $C_{22}H_{34}O_3$ $[M+H]^+$:** calculated: 357.2601, found: 357.260.

2-phenyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-7-oxaspiro[3.5] nonan-1-ol (17)

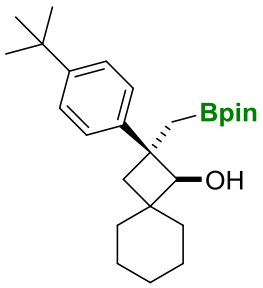


17

Flash column chromatography (pentane:diethyl ether 3:2) yielded **17** (131.6 mg, 24% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.36 – 7.29 (m, 2H), 7.29 (s, 2H), 7.19 – 7.07 (m, 1H), 3.93 (s, 1H), 3.67 (ddt, *J* = 13.5, 11.3, 4.4 Hz, 2H), 3.50 – 3.36 (m,

2H), 2.65 (d, *J* = 12.7 Hz, 1H), 1.78 (ddd, *J* = 13.4, 9.6, 4.0 Hz, 2H), 1.66 (d, *J* = 12.8 Hz, 1H), 1.47 (dd, *J* = 14.3, 5.0 Hz, 2H), 1.27 (d, *J* = 15.2 Hz, 2H), 0.97 (s, 6H), 0.96 (s, 6H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 142.9, 128.2, 128.2, 126.1, 83.4, 82.9, 65.0, 64.3, 46.6, 39.3, 38.9, 37.8, 30.9, 24.8, 24.7. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 33.6. **HRMS (ESI) for $C_{21}H_{32}BO_4$ $[M+H]^+$:**calculated: 359.2397, found: 359.2394**.**

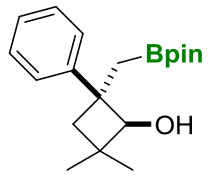
2-(4-(tert-butyl)phenyl)-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl) spiro[3.5]nonan-1-ol (19)



19

Flash column chromatography (pentane:ethyl acetate 10:1) yielded **19** (50.5 mg, 25% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.28 – 7.21 (m, 4H), 3.80 (s, 1H), 2.57 (dd, *J* = 12.7, 1.0 Hz, 2H), 1.57 – 1.37 (m, 6H), 1.24 (d, *J* = 4.1 Hz, 3H), 1.22 (s, 9H), 1.15 – 1.07 (m, 3H), 0.94 (s, 6H), 0.89 (s, 6H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 148.6, 139.5, 128.1, 124.9, 84.0, 82.6, 46.1, 41.3, 39.8, 37.5, 34.2, 31.4, 31.3, 30.1, 26.1, 24.6, 24.6, 23.2, 22.0. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 33.7. **HRMS (ESI) for $C_{26}H_{42}BO_3$ $[M+H]^+$:**calculated: 413.3235, found: 413.3227.

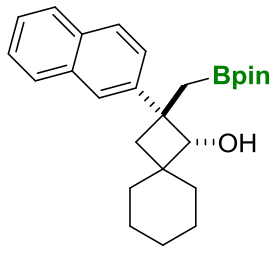
2,2-dimethyl-4-phenyl-4-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl) cyclobutan-1-ol (21)



21

Flash column chromatography (pentane:diethyl ether 3:2) yielded **21** (36.5 mg, 27% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.35 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.24 (dd, *J* = 8.6, 7.0 Hz, 2H), 7.15 – 7.04 (m, 1H), 3.90 (m, 1H), 2.46 (dd, *J* = 12.5, 1.0 Hz, 1H), 1.62 (d, *J* = 12.5 Hz, 1H), 1.44 (d, *J* = 15.1 Hz, 1H), 1.26 (7, *J* = 15.1 Hz, 1H), 1.11 (s, 3H), 0.99 (s, 6H), 0.97 (s, 6H), 0.68 (s, 3H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 143.2, 128.5, 128.0, 125.8, 83.8, 82.8, 47.0, 40.1, 37.3, 29.8, 24.7, 24.6, 21.3. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ = 33.4. **HRMS (ESI) for $C_{19}H_{33}NBO_3$ $[M+NH_4]^+$:** calculated: 334.2554, found 334.2553.

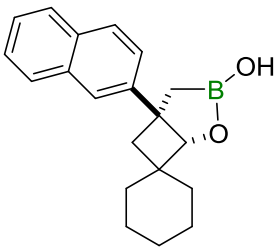
2-(naphthalen-2-yl)-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) methyl) spiro[3.5]nonan-1-ol (25)



25

Flash column chromatography (pentane:diethyl ether 3:2) yielded **25** (208.3 mg, 52% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.79 (d, *J* = 1.9 Hz, 1H), 7.77 – 7.69 (m, 3H), 7.49 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.44 – 7.31 (m, 2H), 3.93 (s, 1H), 2.69 (d, *J* = 12.6 Hz, 1H), 1.64 (d, *J* = 12.7 Hz, 1H), 1.53 (dd, *J* = 5.7, 1.7 Hz, 3H), 1.45 – 1.29 (m, 6H), 1.16 – 1.06 (m, 3H), 0.92 (s, 6H), 0.89 (s, 6H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 141.2, 133.2, 131.9, 127.9, 127.4, 127.3, 126.7, 125.6, 125.3, 84.5, 82.8, 46.8, 41.5, 39.7, 38.0, 30.0, 26.1, 24.7, 24.6, 23.2, 21.9. **^{11}B NMR ($CDCl_3$, 128.3 MHz)** δ 33.7. **HRMS (ESI) for $C_{26}H_{29}NBO_3$ $[M+NH_4]^+$:** calculated: 424.3026, found: 424.3023.

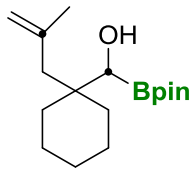
1-(naphthalen-2-yl)-4-oxa-3-boraspiro[bicyclo[3.2.0]heptane-6,1'-cyclohexan]-3-ol (26-*syn-(B-OH)*)



26-*syn-(B-OH)*

Flash column chromatography (pentane:diethyl ether 3:2) yielded **26-***syn-(B-OH)* (78.5 mg, 39% yield) as a colourless oil. **^{1}H NMR (CDCl$_3$, 400 MHz)** δ = 7.72 (dt, *J* = 6.4, 3.4 Hz, 3H), 7.58 (d, *J* = 2.2 Hz, 1H), 7.43 – 7.31 (m, 2H), 7.28 (dd, *J* = 8.5, 2.0 Hz, 1H), 4.64 (d, *J* = 2.4 Hz, 1H), 2.36 – 2.26 (m, 1H), 1.90 (dd, *J* = 12.0, 2.0 Hz, 1H), 1.56 – 1.46 (m, 2H), 1.35 – 1.18 (m, 10H). **^{13}C NMR (CDCl$_3$, 100 MHz)** δ = 147.3, 133.3, 131.6, 128.5, 127.6, 127.5, 126.1, 125.3, 124.6, 122.6, 90.2, 65.8, 46.8, 44.4, 40.7, 36.7, 32.4, 25.8, 22.6, 22.3, 15.2. **^{11}B NMR (CDCl$_3$, 128.3 MHz)** δ = 36.5. **HRMS (ESI) for $C_{20}H_{23}BO_2$ $[M+H]^+$:** calculated: 307.1870, found: 307.1869.

(1-(2-methylallyl)cyclohexyl)(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methanol (29)



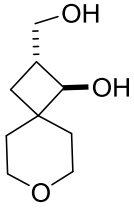
29

Flash column chromatography (pentane:diethyl ether 3:2) yielded **29** (95.4 mg, 32% yield) as a colourless oil. **^{1}H NMR (CDCl$_3$, 400 MHz)** δ = 4.86 – 4.77 (m, 1H), 4.73 (s, 1H), 3.51 (d, *J* = 5.9 Hz, 1H), 2.19 (d, *J* = 13.2 Hz, 1H), 2.10 – 2.01 (m, 1H), 1.75 (s, 3H), 1.60 (d, *J* = 6.0 Hz, 1H), 1.54 – 1.26 (m, 10H), 1.21 (s, 12H). **^{13}C NMR (CDCl$_3$, 100 MHz)** δ = 144.4, 114.7, 84.0, 41.1, 33.1, 31.5, 26.4, 25.5, 25.0, 24.7, 21.8, 21.6. **^{11}B NMR (CDCl$_3$, 128.3 MHz)** δ = 33.0. **HRMS (ESI) for $C_{17}H_{32}BO_3$ $[M]^+$:** calculated: 295.2441, found: 295.2445.

2.7. General procedure for the oxidation of spiroboronate compounds[9]

The oxidation was performed in a reaction vial, $NaBO_3 \cdot H_2O$ (2 mmol) was dissolved in THF/H_2O (3:2, 0.2 M) and the boronate (1 equiv, 0.2 mmol) was then added at room temperature. After stirred for 1.5 h, the reaction mixture was extracted three times with EtOAc, dried ($MgSO_4$), filtered and concentrated in *vacuo*. The crude mixture was further purified by flash column chromatography.

2-(hydroxymethyl)-7-oxaspiro[3.5]nonan-1-ol (30)

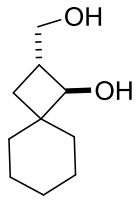


30

Flash column chromatography (pentane:ethyl acetate 100:0 to 0:100) yielded **30** (52.5 mg, 61% yield) as a colourless oil. **^{1}H NMR (CDCl$_3$, 400 MHz)** δ = 3.89 (dt, *J* = 11.3, 4.1 Hz, 1H), 3.73 (m, 3H), 3.59 (m, 2H), 3.43 (td, *J* = 11.1, 2.6 Hz, 1H), 2.33 (m, 1H), 1.88 (m, 2H), 1.77 (m, 1H), 1.50 (m, 1H), 1.40 (m, 1H), 1.09 (t, *J* =

10.1 Hz, 1H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 77.2, 76.6, 64.9, 64.5, 42.6, 40.1, 38.1, 30.4, 29.6, 27.2. **HRMS (ESI) for $C_9H_{17}O_3$ $[M+H]^+$:** calculated: 173.1172, found: 173.1185.

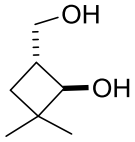
2-(hydroxymethyl)spiro[3.5]nonan-1-ol2-(hydroxymethyl)spiro[3.5]nonan-1-ol (31)



31

Flash column chromatography (pentane:ethyl acetate 100:0 to 0:100) yielded **31** (27.3 mg, 90% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 3.63 (dd, *J* = 10.9, 5.1 Hz, 1H), 3.53 – 3.44 (m, 2H), 3.37 (m, 2H), 2.28 – 2.14 (m, 1H), 1.65 (t, *J* = 10.3 Hz, 1H), 1.62 – 1.24 (m, 8H), 1.24 – 1.09 (m, 2H), 0.85 (t, *J* = 10.2 Hz, 1H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 78.0, 65.7, 42.7, 42.6, 38.7, 29.8, 27.4, 26.3, 23.1, 22.3. **HRMS (ESI) for $C_{10}H_{18}O_2$ $[M]^+$:** calculated: 170.1307, found: 170.1309.

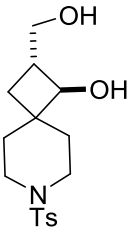
(1R,4R)-4-(hydroxymethyl)-2,2-dimethylcyclobutan-1-ol (32)



32

Flash column chromatography (pentane:ethyl ether:methanol 3:2:1) yielded **32** (73.8 mg, 81 %) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 3.70 – 3.58 (m, 1H), 3.58 – 3.44 (m, 2H), 3.25 (s, 1H), 2.65 (s, 1H), 2.29 – 2.14 (m, 1H), 1.57 – 1.46 (m, 1H), 1.01 (d, *J* = 8.1 Hz, 6H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 65.5, 42.9, 38.3, 30.0, 28.3, 21.0. **HRMS (ESI) for $C_7H_{14}O_2$ $[M]^+$:** calculated: 130.0992, found: 130.0994.

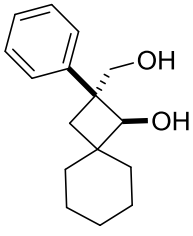
2-(hydroxymethyl)-7-tosyl-7-azaspiro[3.5]nonan-1-ol (33)



33

Flash column chromatography (pentane:ethyl acetate 100:0 to 0:100) yielded **33** (121.9 mg, 75% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.63 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 3.72 (d, *J* = 7.5 Hz, 1H), 3.67 (dd, *J* = 10.9, 5.3 Hz, 1H), 3.59 (dd, *J* = 10.9, 5.3 Hz, 1H), 3.49 (m, 1H), 3.32 (m, 1H), 2.67 (t, *J* = 11.4 Hz, 1H), 2.53 (t, *J* = 11.4 Hz, 1H), 2.43 (s, 3H), 2.27 (m, 1H), 1.90 (m, 1H), 1.78 (m, 1H), 1.64 (m, 1H), 1.59 (t, *J* = 10.8 Hz, 1H), 1.51 (m, 1H), 0.97 (t, *J* = 10.8 Hz, 1H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 143.3, 133.3, 129.6, 127.6, 75.6, 64.4, 43.3, 42.9, 42.4, 40.1, 36.7, 29.2, 26.5, 21.5. **HRMS (ESI) for $C_{16}H_{24}NO_4S$ $[M+H]^+$:** calculated: 326.1421, found: 326.1427.

2-(hydroxymethyl)-2-phenylspiro[3.5]nonan-1-ol (34)

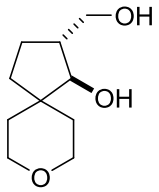


34

Flash column chromatography (pentane:diethyl ether 3:2) yielded **34** (148.7 mg, 76% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.41 – 7.25 (m, 4H), 7.25 – 7.20 (m, 1H), 3.89 (s, 1H), 3.67 (dt, *J* = 10.9, 0.8 Hz, 1H), 3.58 (dd, *J* = 10.9, 0.8 Hz, 1H), 2.33 (d, *J* = 12.5 Hz, 1H), 1.67 (d, *J* = 12.5 Hz, 1H), 1.50 – 1.43 (m, 5H), 1.35 – 1.26 (m, 2H), 1.13 (d, *J* = 3.4 Hz, 2H), 1.11 – 1.04 (m, 1H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 139.0, 128.8, 128.6, 126.8, 77.8,

72.7, 51.1, 41.5, 38.6, 33.2, 30.7, 26.0, 23.0, 21.9. **HRMS (ESI) for $C_{16}H_{22}O_2$ $[M]^+$:**calculated: 246.1620, found: 246.1617.

2-(hydroxymethyl)-8-oxaspiro[4.5]decan-1-ol (35)

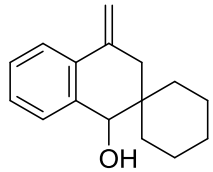


35

Flash column chromatography (pentane:ethyl acetate 3:2) yielded **35** (50 mg, 70% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 3.81 (m, 3H), 3.62 – 3.46 (m, 2H), 3.46 – 3.35 (m, 2H), 1.87 – 1.77 (m, 3H), 1.71 (dtd, *J* = 13.2, 9.1, 5.7 Hz, 1H), 1.36 – 1.29 (m, 1H), 1.25 – 1.05 (m, 4H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 84.8, 66.8, 65.4, 64.4, 45.3, 42.6, 36.3, 31.3, 29.3, 21.9. **HRMS (ESI) for $C_{10}H_{18}O_2$ $[M]^+$:** calculated: 186.1256, found: 186.1252.

2.8. Compound 23

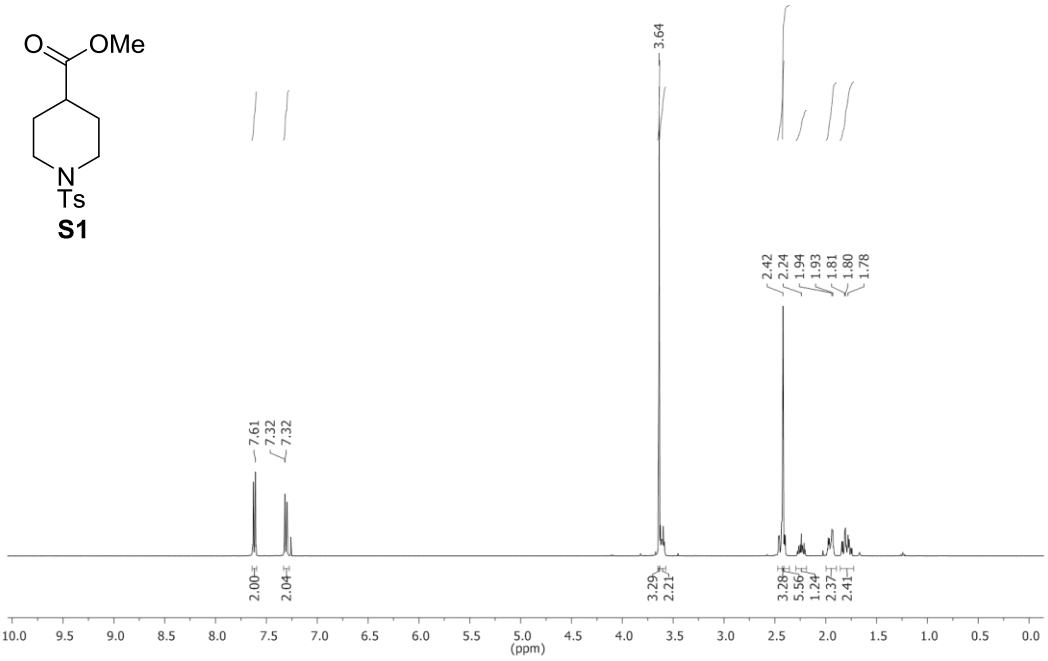
4'-methylene-3',4'-dihydro-1'H-spiro[cyclohexane-1,2'-naphthalen]-1'-ol (23)

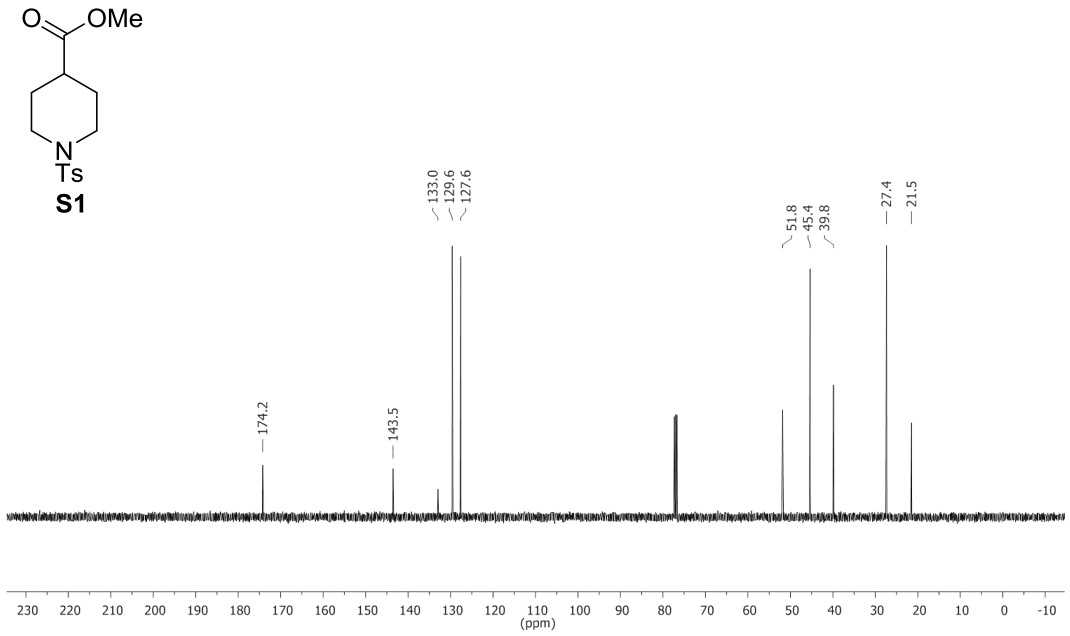


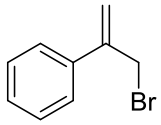
23

Flash column chromatography (pentane: diethyl ether 3:2) yielded **23** (38.8 mg, 34% yield) as a colourless oil. **^{1}H NMR ($CDCl_3$, 400 MHz)** δ = 7.65 – 7.55 (m, 1H), 7.41 – 7.29 (m, 1H), 7.25 – 7.16 (m, 2H), 5.51 (s, 1H), 5.01 (s, 1H), 4.29 (s, 1H), 2.71 – 2.61 (m, 1H), 2.29 – 2.20 (m, 1H), 1.51 – 1.33 (m, 6H), 1.37 – 1.08 (m, 4H). **^{13}C NMR ($CDCl_3$, 100 MHz)** δ = 140.5, 137.4, 133.7, 129.8, 128.4, 127.9, 123.7, 110.0, 37.2, 37.0, 32.6, 31.4, 31.4, 26.2, 24.5. **HRMS (ESI) for $C_{22}H_{32}BO_3$ $[M–H^+$+Bpin$]^+$:** calculated: 355.2445, found: 355.2453.

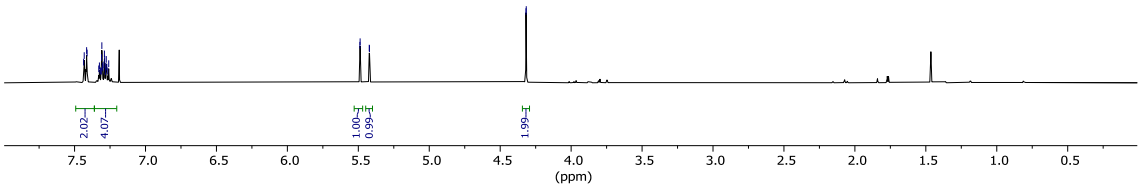
2.9. ^{1}H, ^{13}C and ^{11}B spectra images






Br

S3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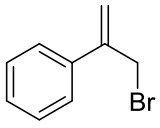
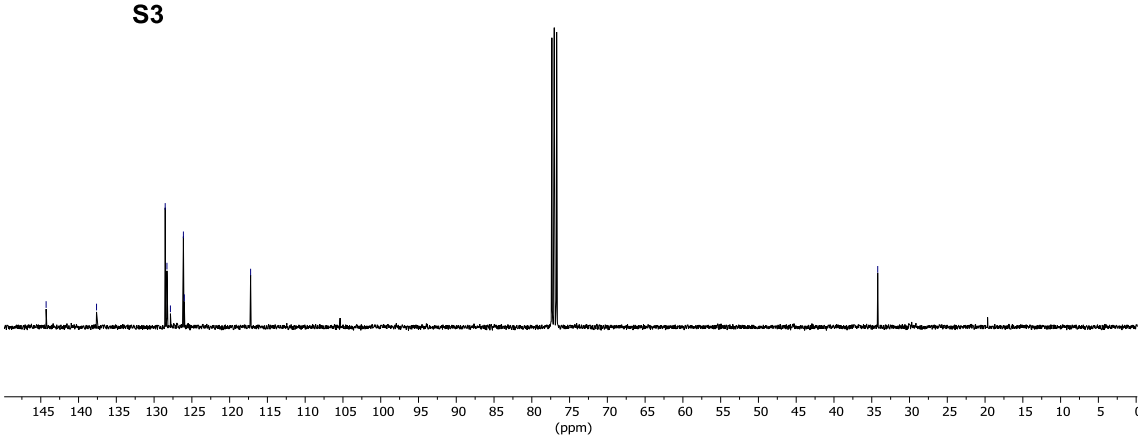
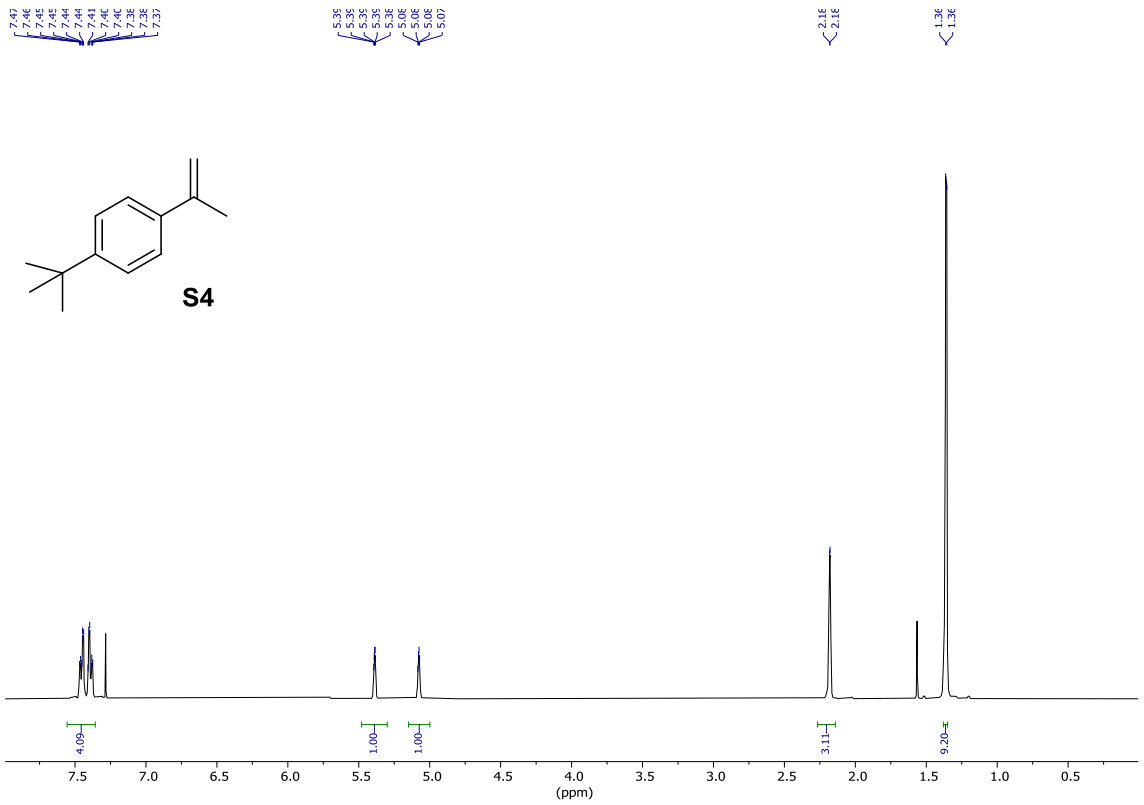
1.99
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


Br

S3


145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
(ppm)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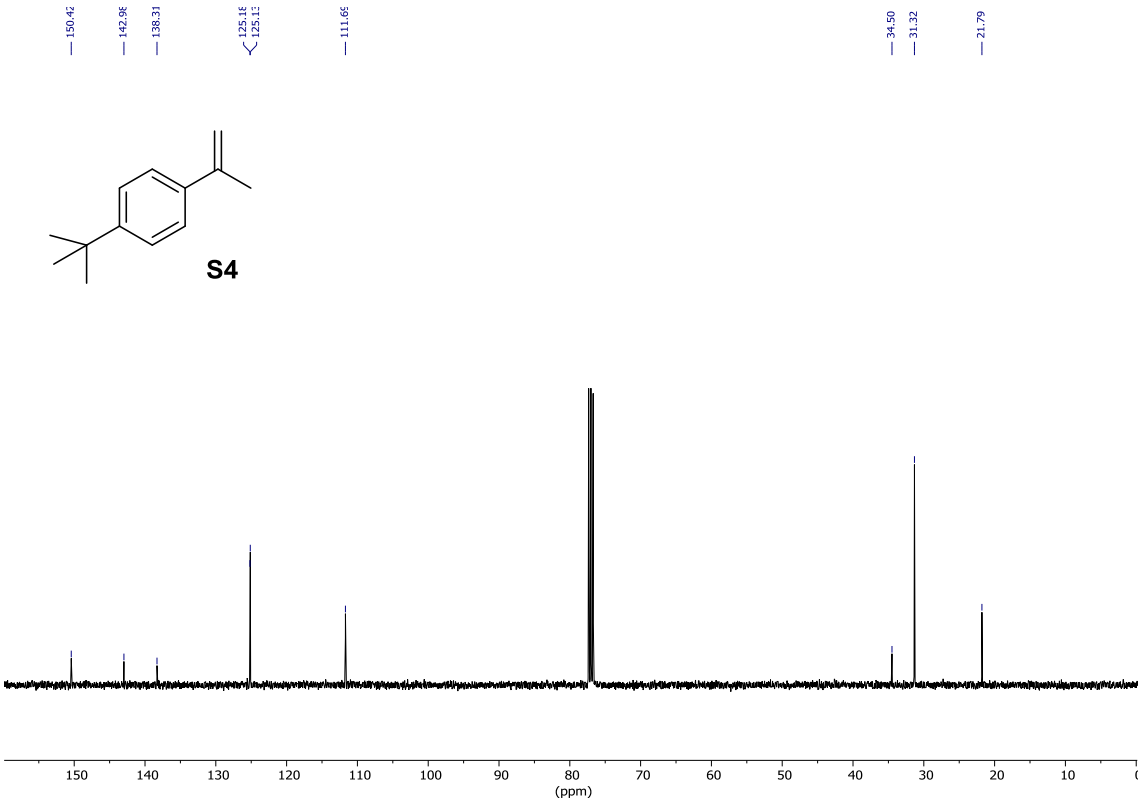
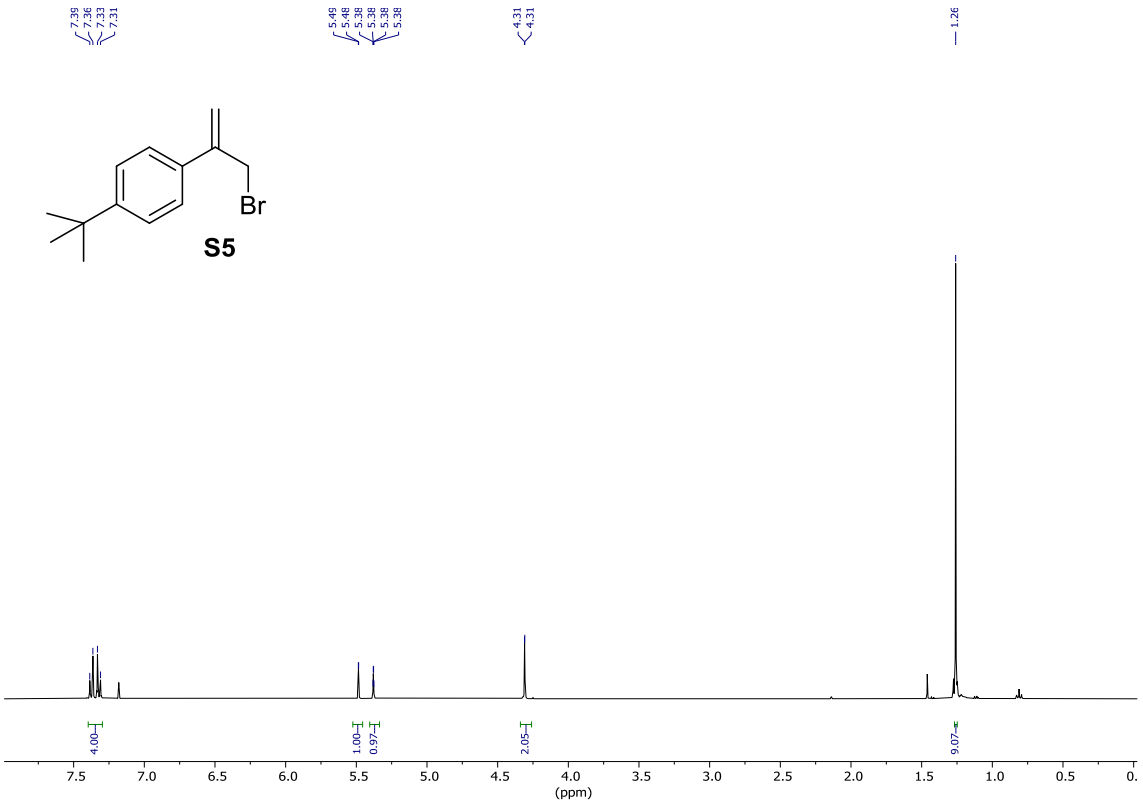
7.46
7.45
7.45
7.44
7.44
7.41
7.40
7.40
7.38
7.38
7.37
5.35
5.35
5.35
5.35
5.38
5.08
5.08
5.08
5.07
2.18
2.18
1.36
1.36
S4
4.09
1.00
1.00
3.11
9.20
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


150.42
142.98
138.31
125.18
125.12
111.65
34.50
31.32
21.79
S4
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)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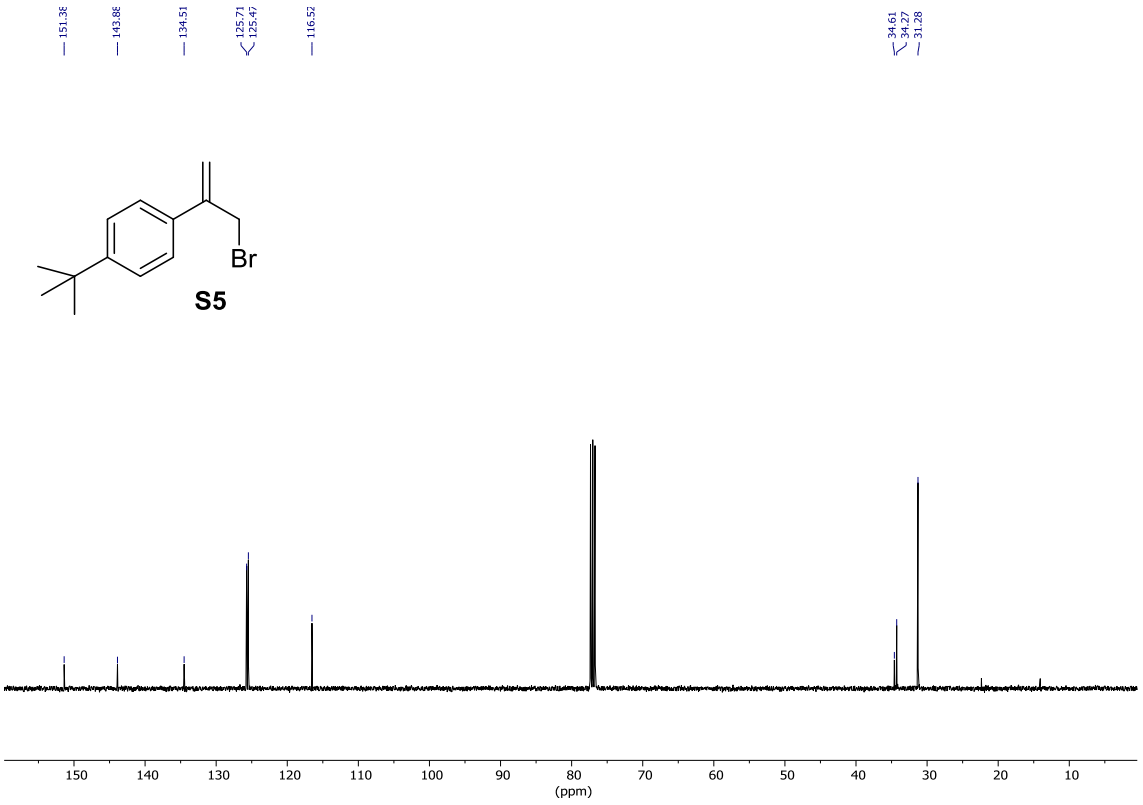
7.36
7.33
7.31
5.49
5.48
5.38
5.38
5.38
5.38
4.31
4.31
1.26
Br
S5
4.00
1.00
0.97
2.05
9.07
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

Br

S5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134.51
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116.52
34.61
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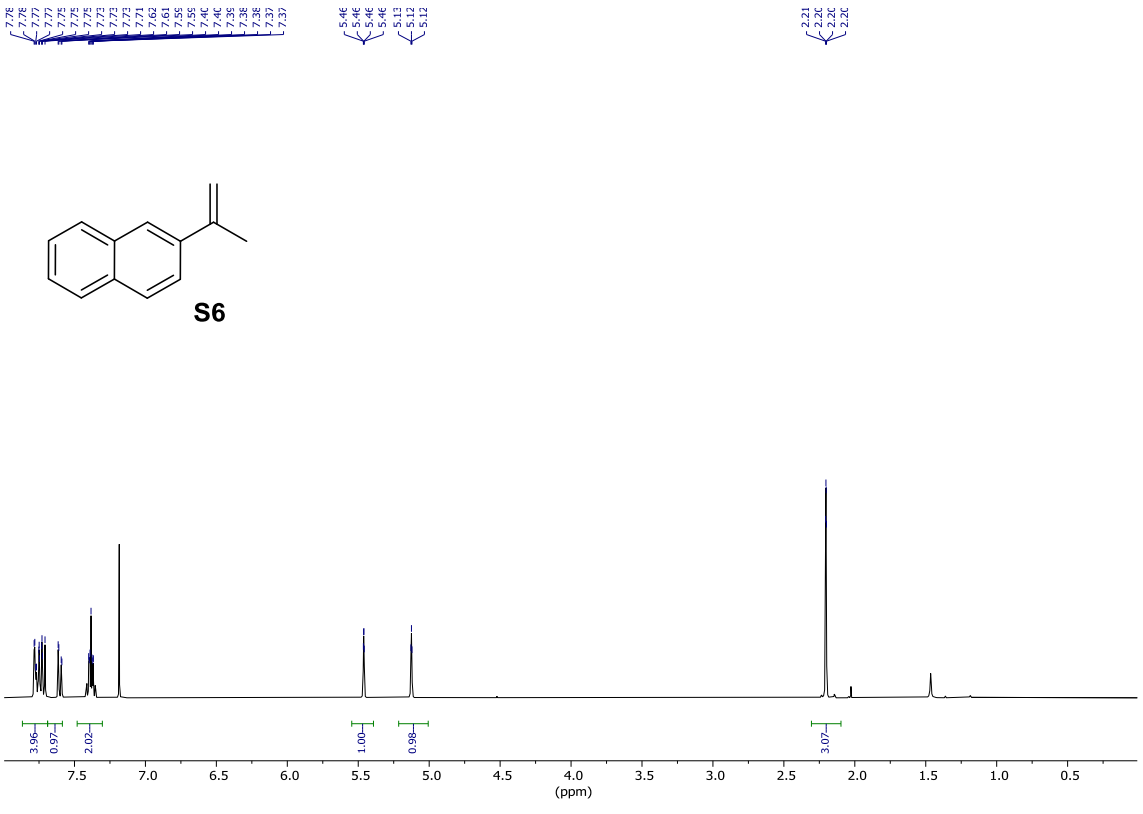
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)


7.78
7.78
7.77
7.77
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7.75
7.73
7.72
7.72
7.71
7.62
7.61
7.55
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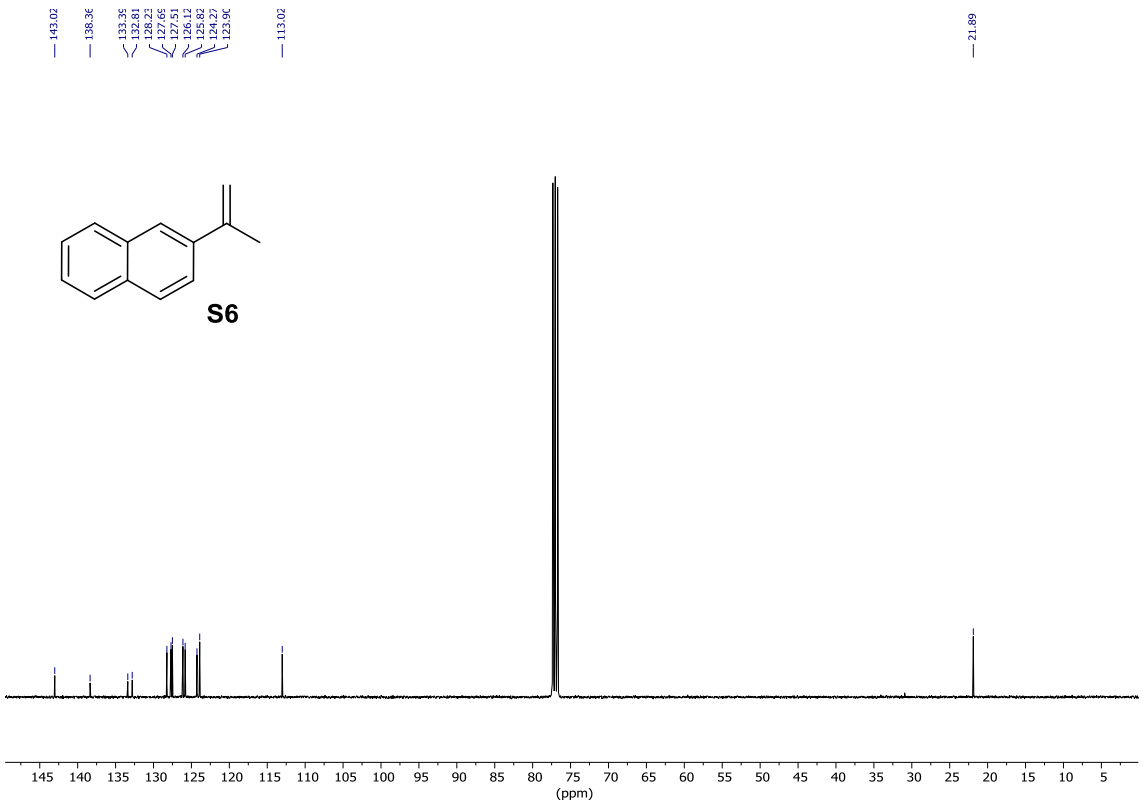
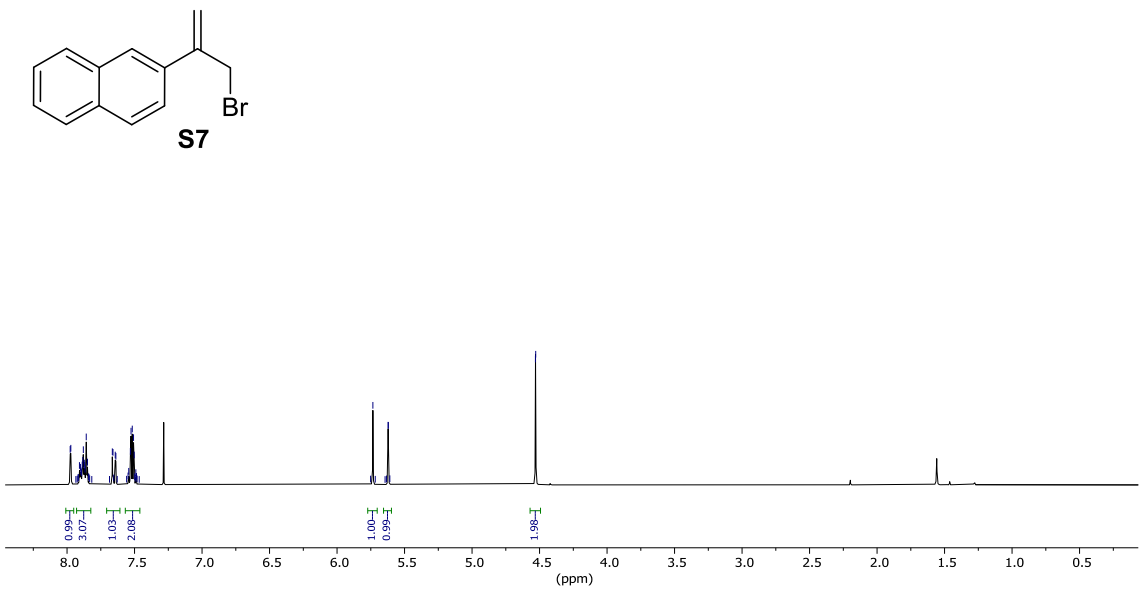
7.38
7.37
7.37
5.46
5.46
5.46
5.46
5.13
5.12
5.12
2.21
2.20
2.20
2.20
3.96
0.97
2.02
1.00
0.98
3.07
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

S6


143.02
138.36
133.35
132.81
128.23
127.65
127.51
126.12
125.82
124.27
123.96
113.02
21.89
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)

S6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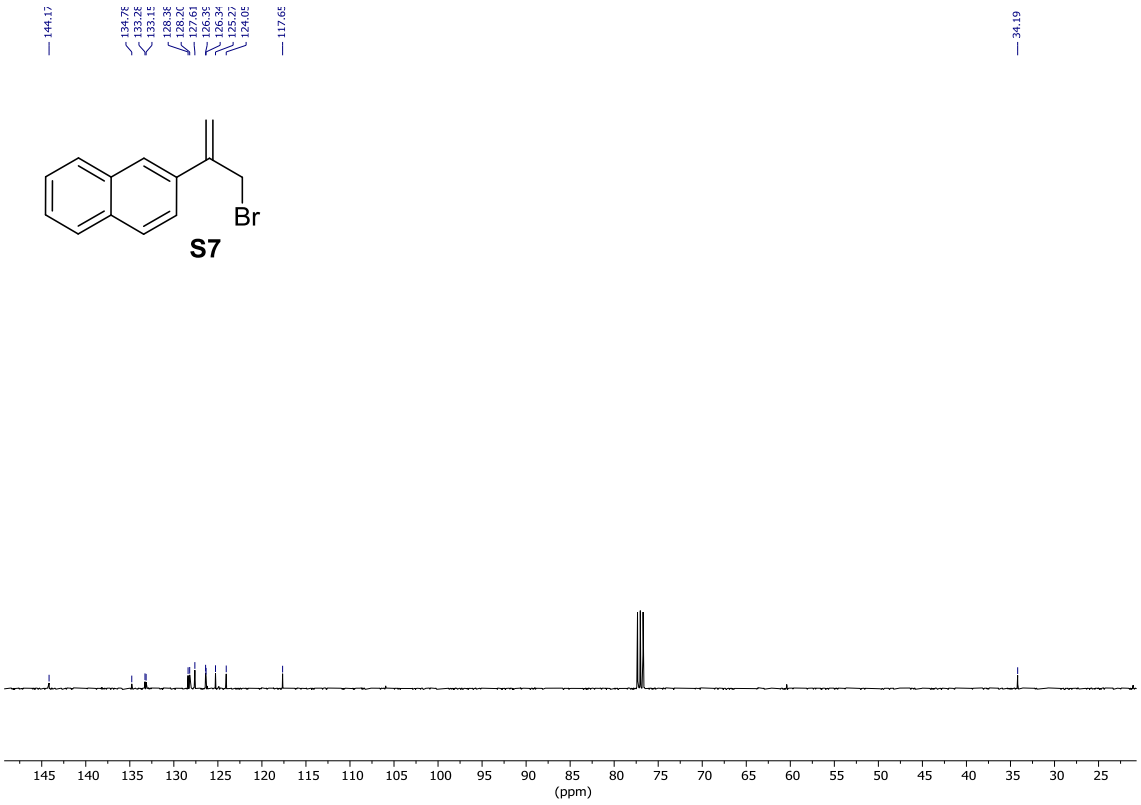
3.07
1.03
2.08
1.00
0.99
1.98
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

S7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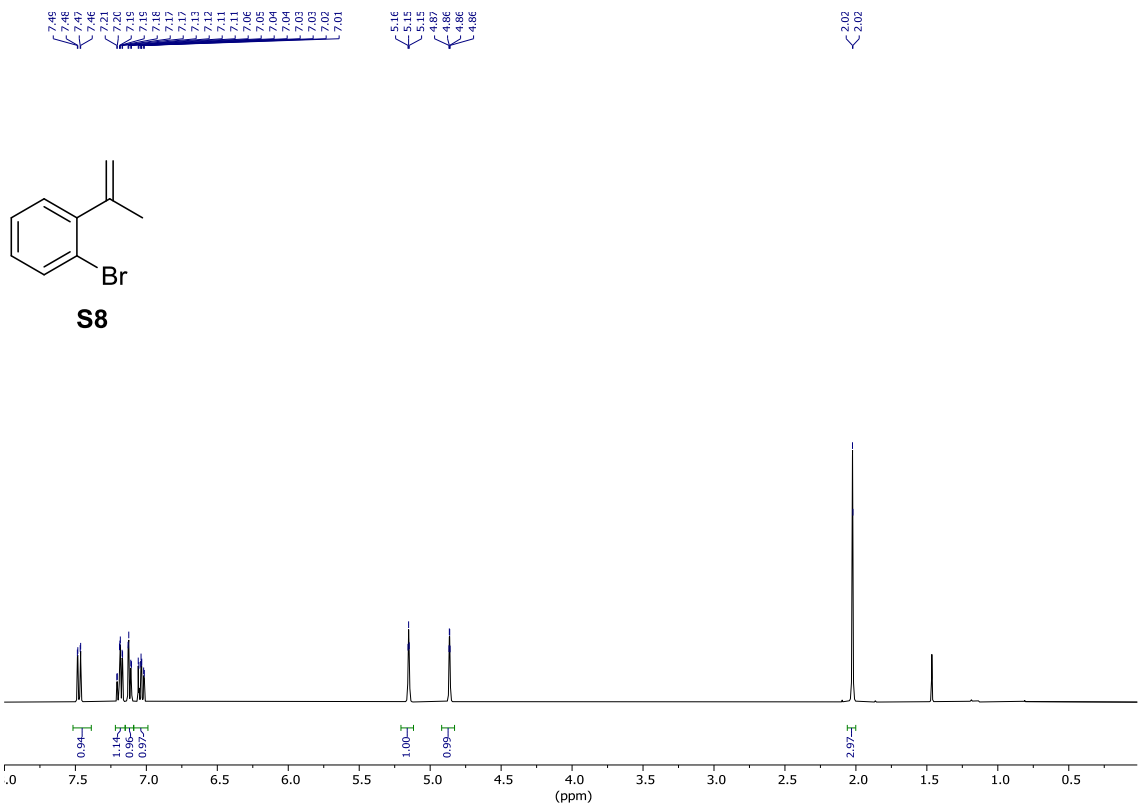
134.78
133.26
133.15
128.38
128.26
127.61
126.35
126.34
125.27
124.05
117.65
34.19
Br
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
(ppm)

S7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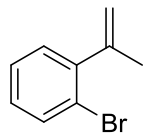
7.47
7.46
7.21
7.20
7.19
7.19
7.18
7.17
7.17
7.13
7.12
7.11
7.11
7.06
7.05
7.04
7.04
7.03
7.03
7.02
7.01
5.16
5.15
5.15
4.87
4.86
4.86
4.86
2.02
2.02
0.94
1.14
0.96
0.97
1.00
0.99
2.97
.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

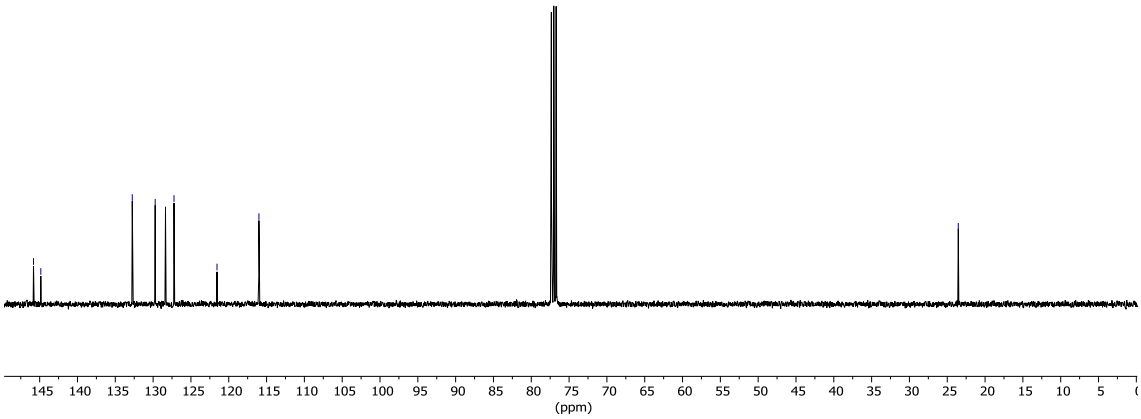
Br

S8

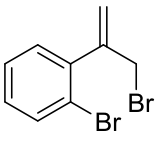

145.81
144.65
132.76
129.73
128.36
127.24
121.55
116.01
23.54


Br

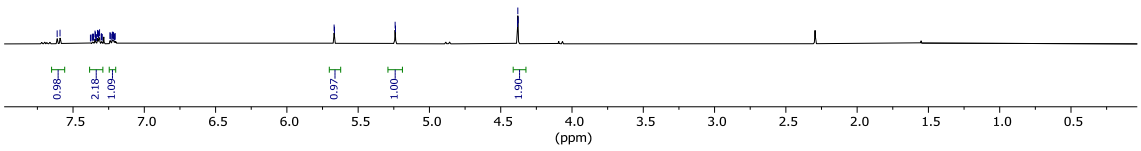
S8


145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)


7.61
7.55
7.38
7.37
7.36
7.24
7.22
7.21
7.20
5.67
5.24
4.38
4.35
4.33


Br
Br

S9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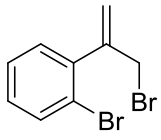
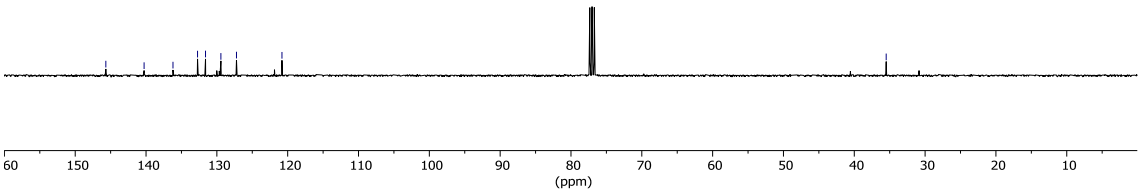
1.09
0.97
1.00
1.90
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)


145.68
140.27
136.26
132.75
131.66
129.43
127.23
120.81
35.49

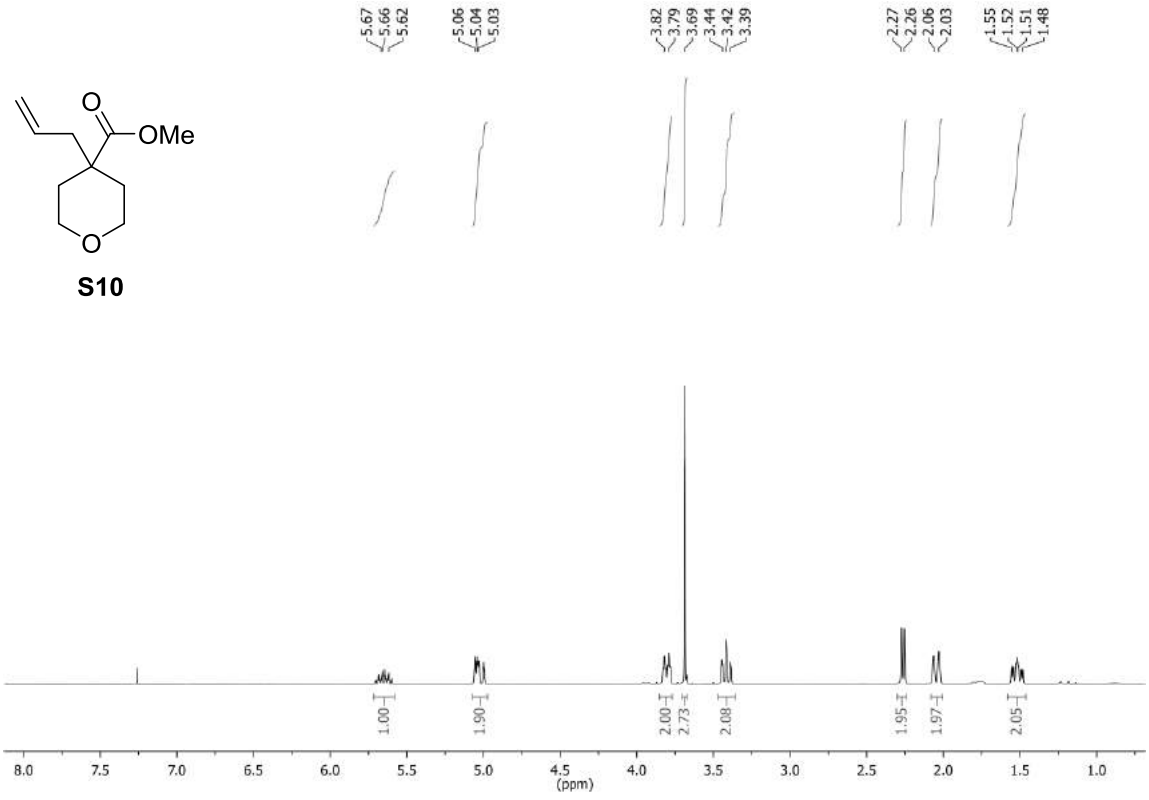

Br
Br

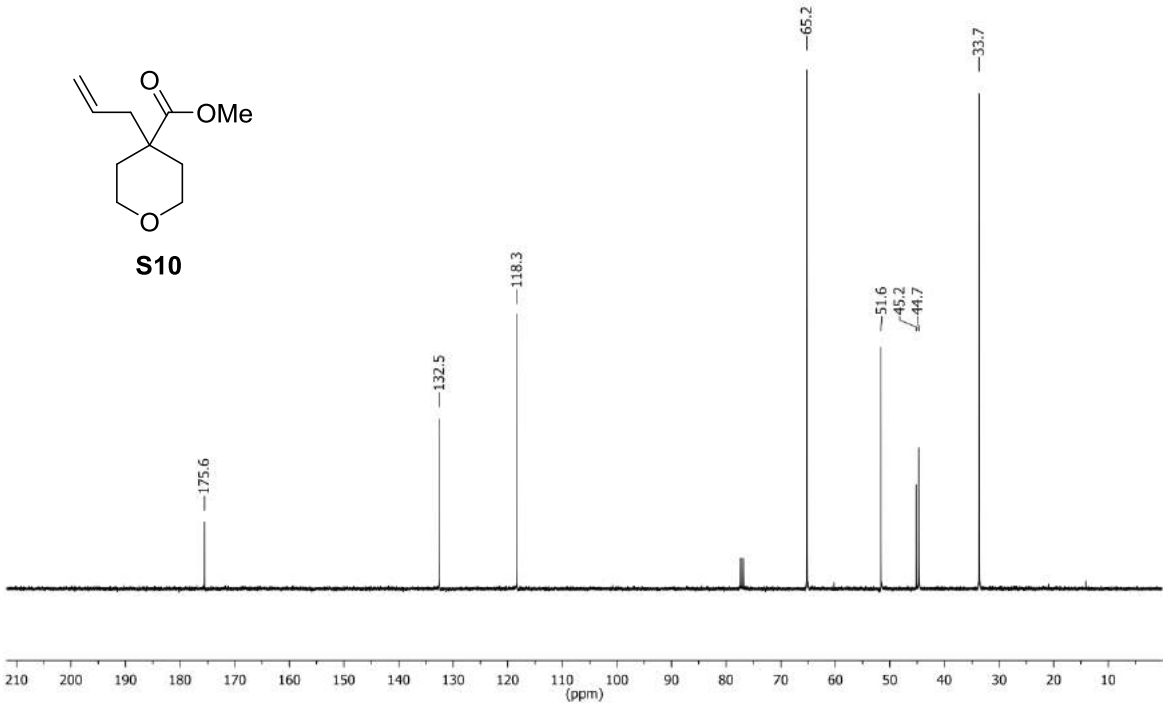
S9

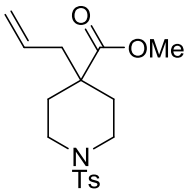

60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)

O
OMe
O

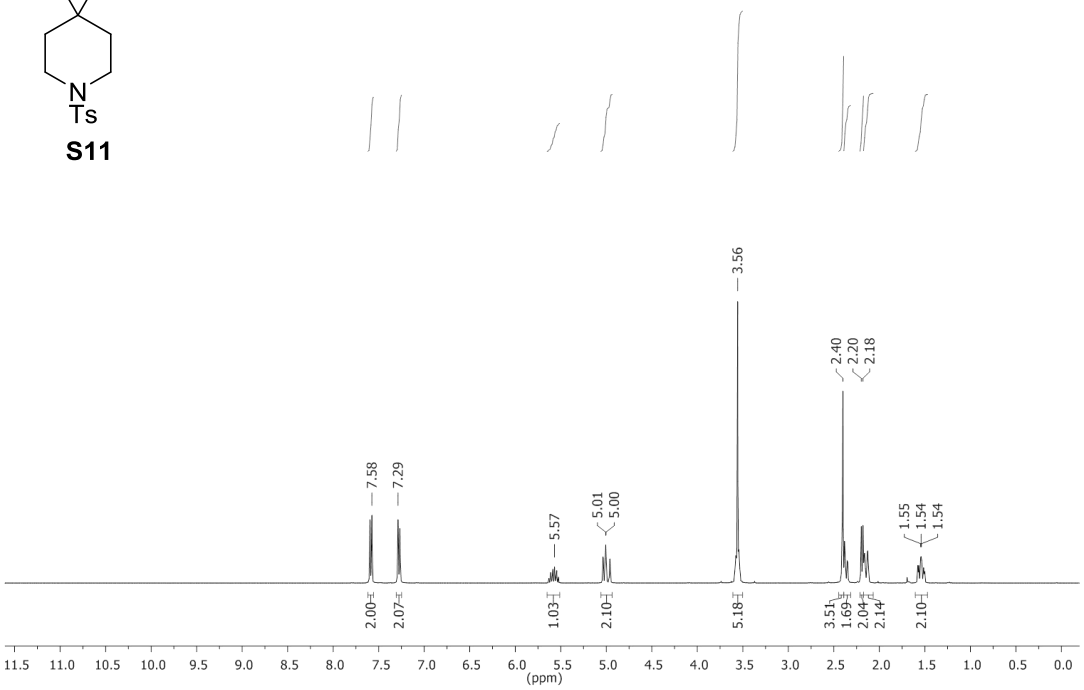
S10


5.67
5.66
5.62
5.06
5.04
5.03
3.82
3.79
3.69
3.44
3.42
3.39
2.27
2.26
2.06
2.03
1.55
1.52
1.51
1.48
1.00
1.90
2.00
2.73
2.08
1.95
1.97
2.05
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)


O
OMe
O
S10
175.6
132.5
118.3
65.2
51.6
45.2
44.7
33.7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)


O
OMe
N
Ts

S11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3.56
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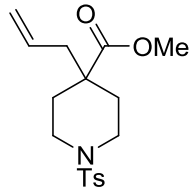
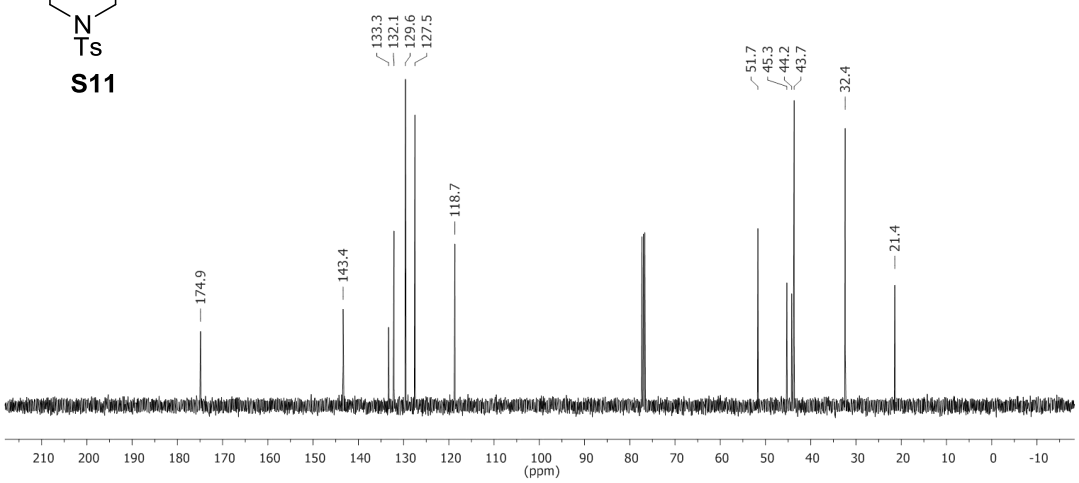
2.20
2.18
1.55
1.54
1.54
2.00
2.07
1.03
2.10
5.18
3.51
1.69
2.04
2.14
2.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

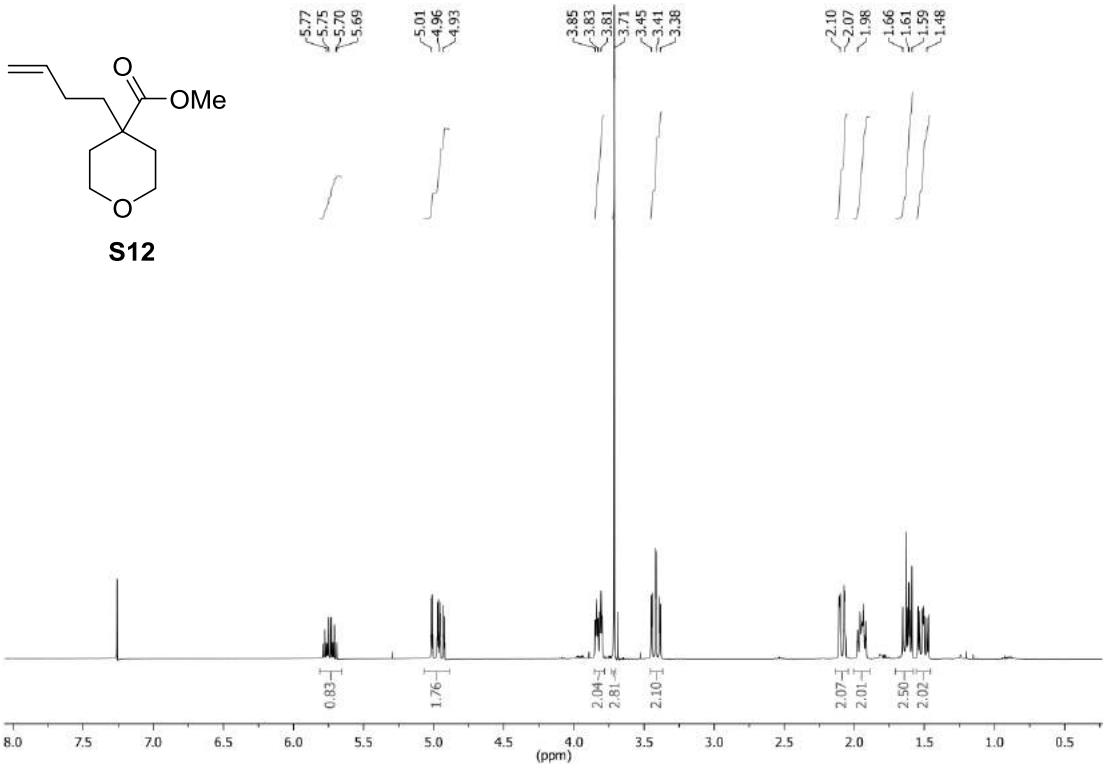

O
OMe
N
Ts

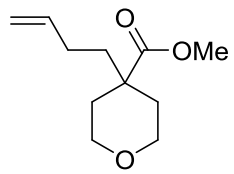
S11


133.3
132.1
129.6
127.5
118.7
143.4
174.9
51.7
45.3
44.2
43.7
32.4
21.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

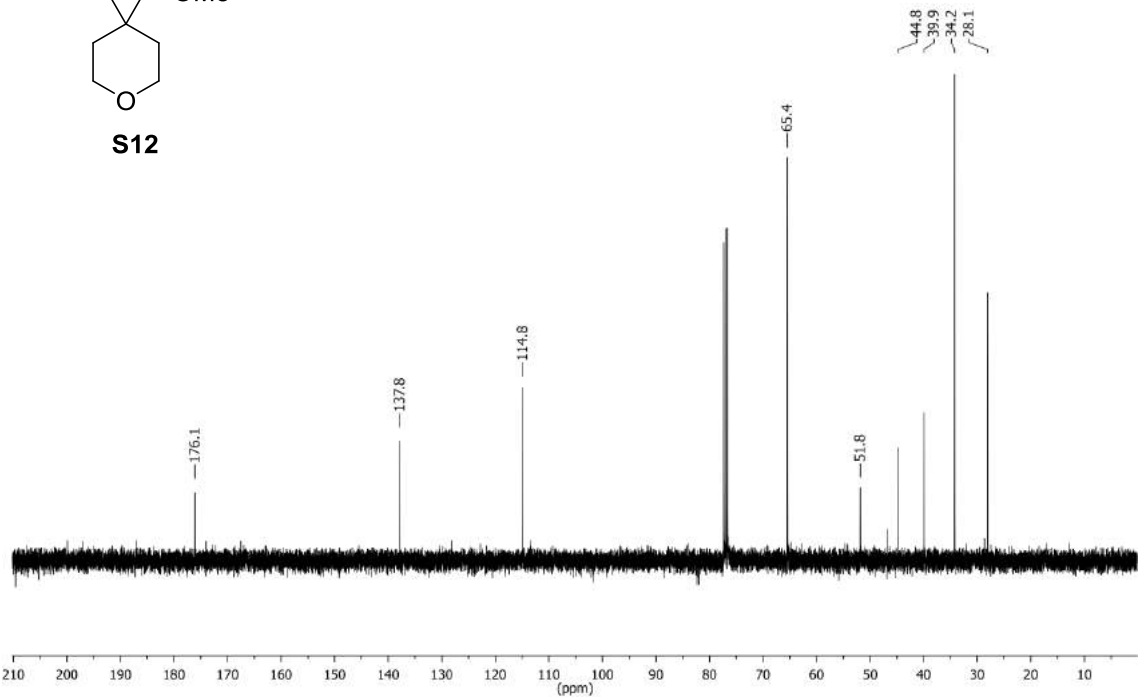
O
OMe
O

S12


5.77
5.75
5.70
5.69
5.01
4.96
4.93
3.85
3.83
3.81
3.71
3.45
3.41
3.38
2.10
2.07
1.98
1.66
1.61
1.59
1.48
0.83
1.76
2.04
2.81
2.10
2.07
2.01
2.50
2.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


O
OMe
O

S12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39.9
34.2
28.1
65.4
114.8
137.8
176.1
51.8
210
200
190
180
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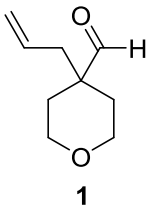
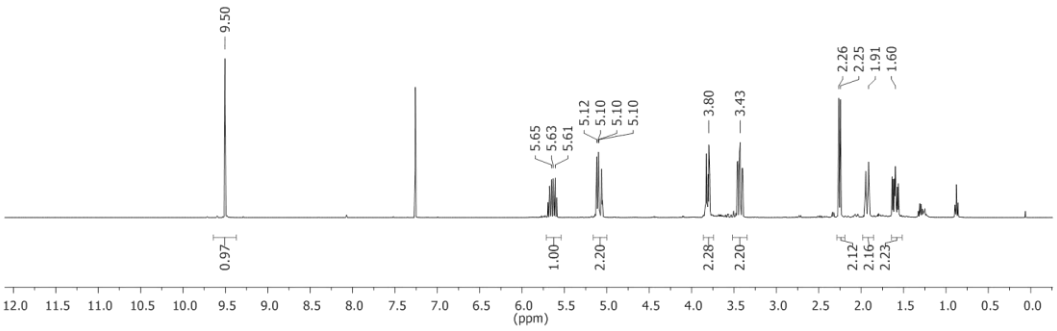
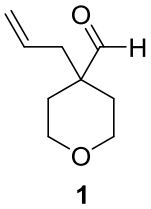
80
70
60
50
40
30
20
10
(ppm)

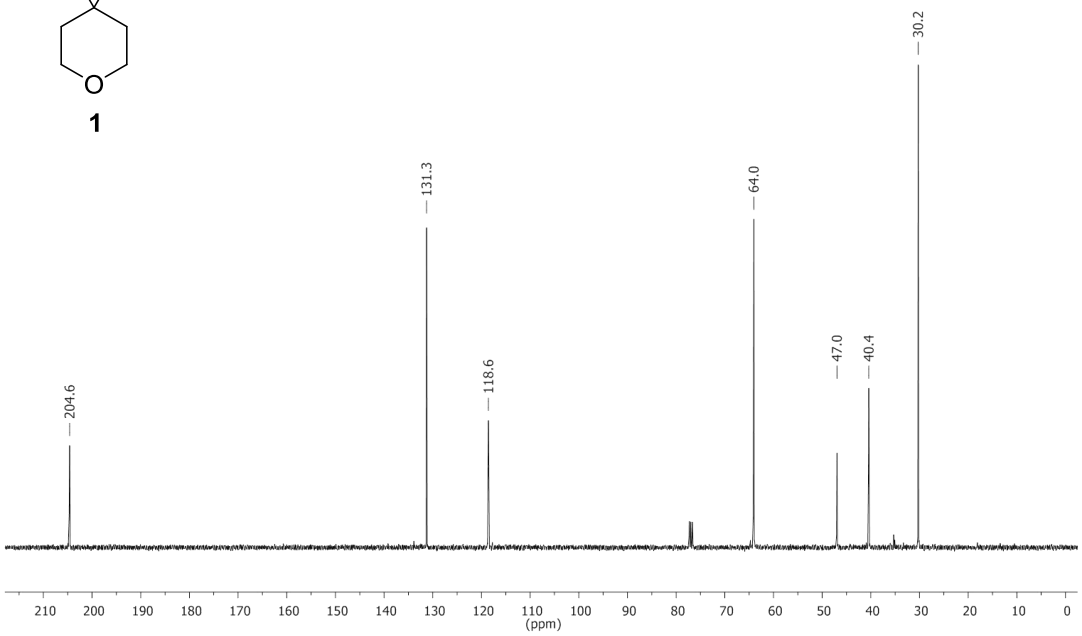


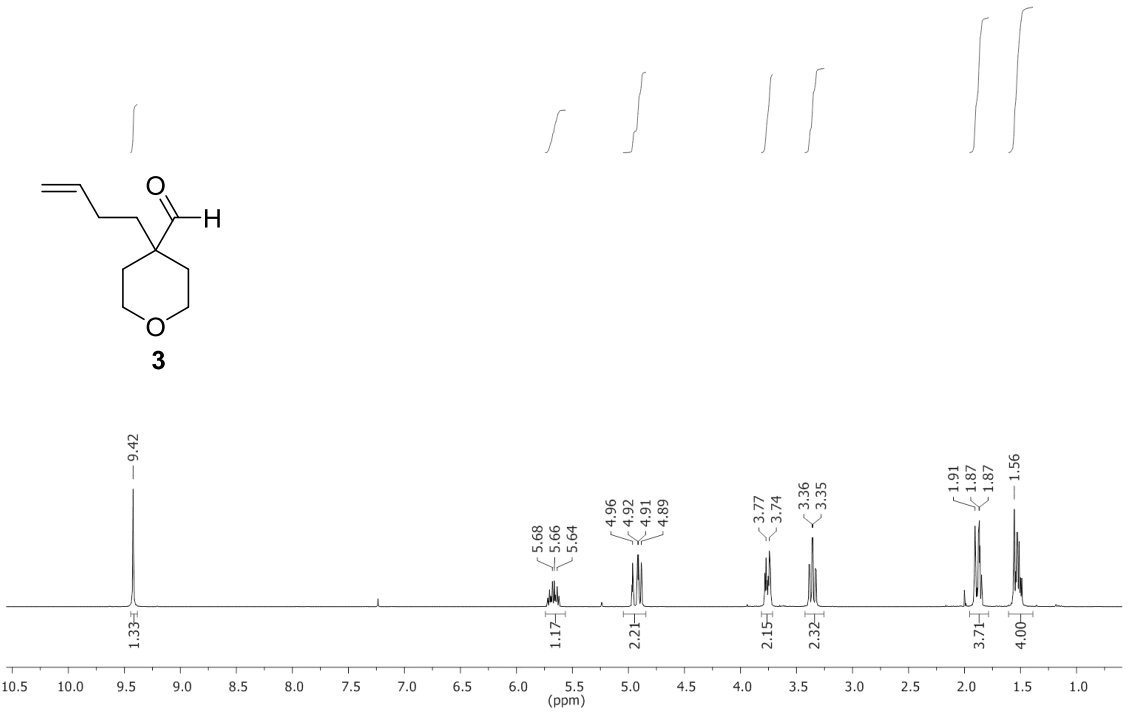
1

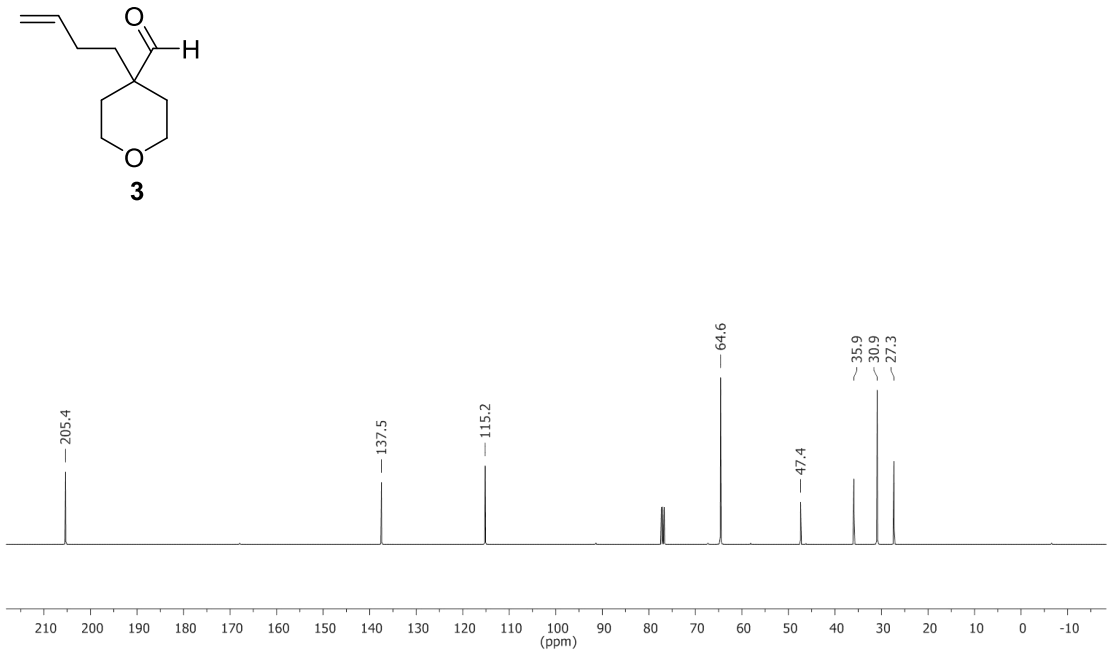

9.50
5.65
5.63
5.61
5.12
5.10
5.10
5.10
3.80
3.43
2.26
2.25
1.91
1.60
0.97
1.00
2.20
2.28
2.20
2.12
2.16
2.23
(ppm)

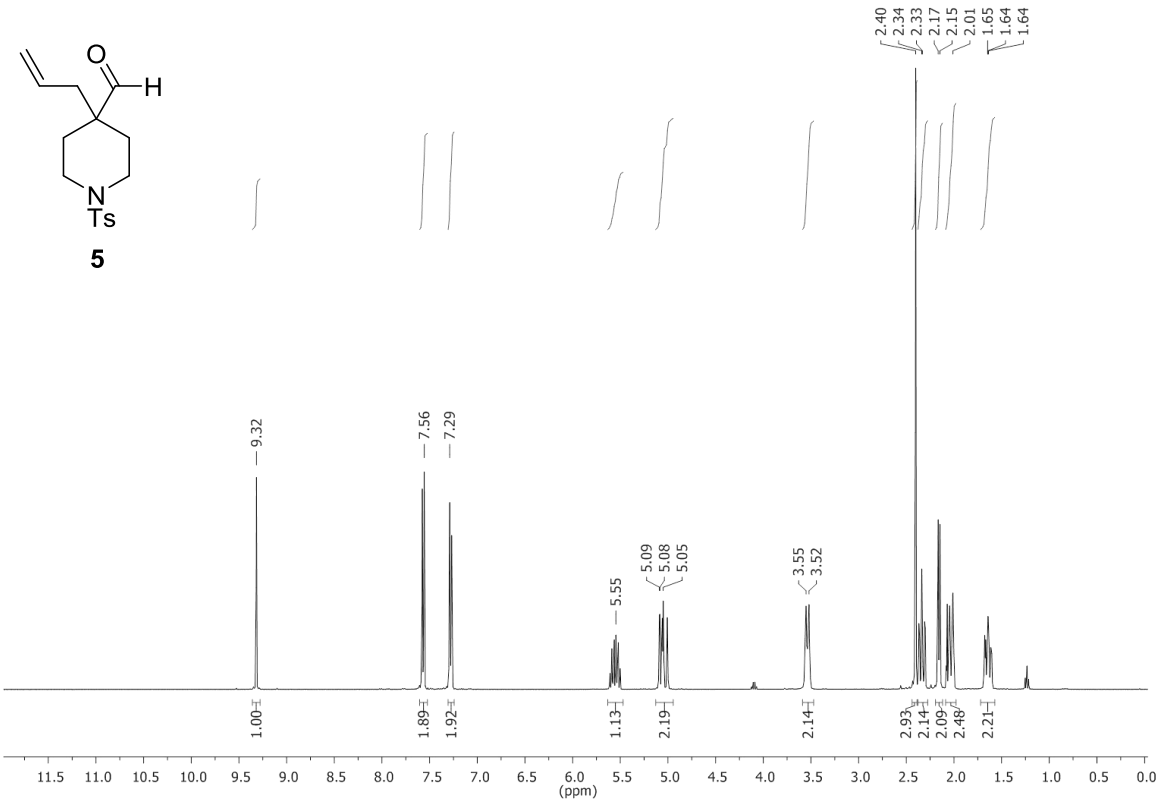


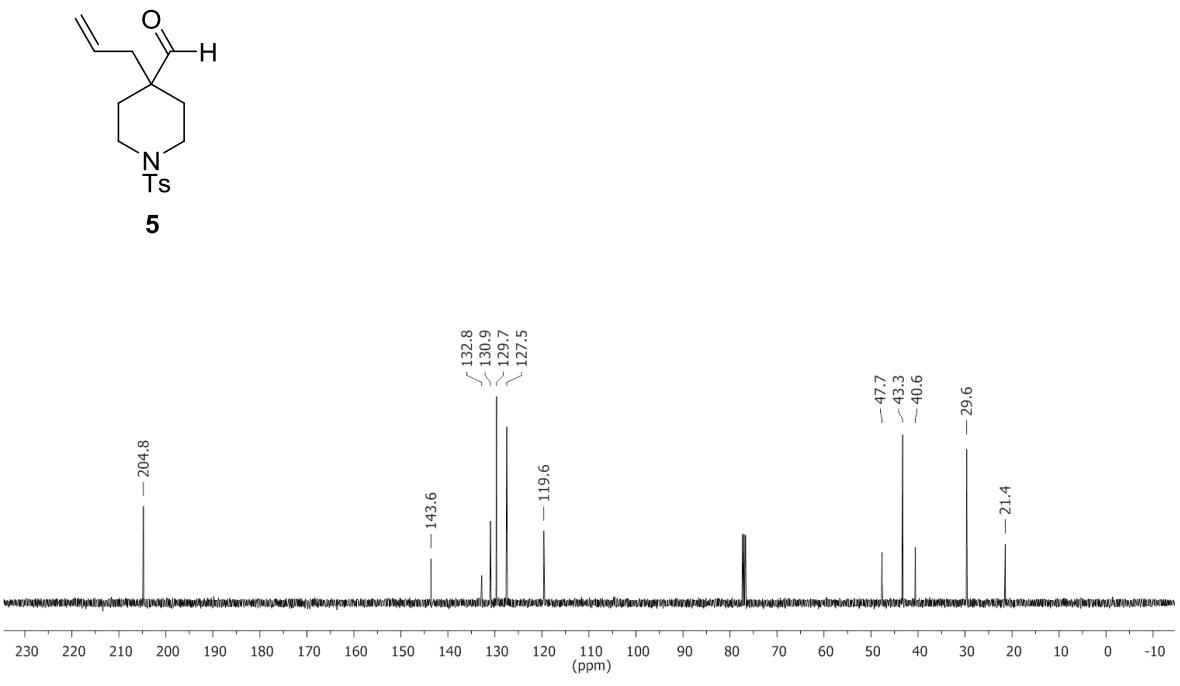
1

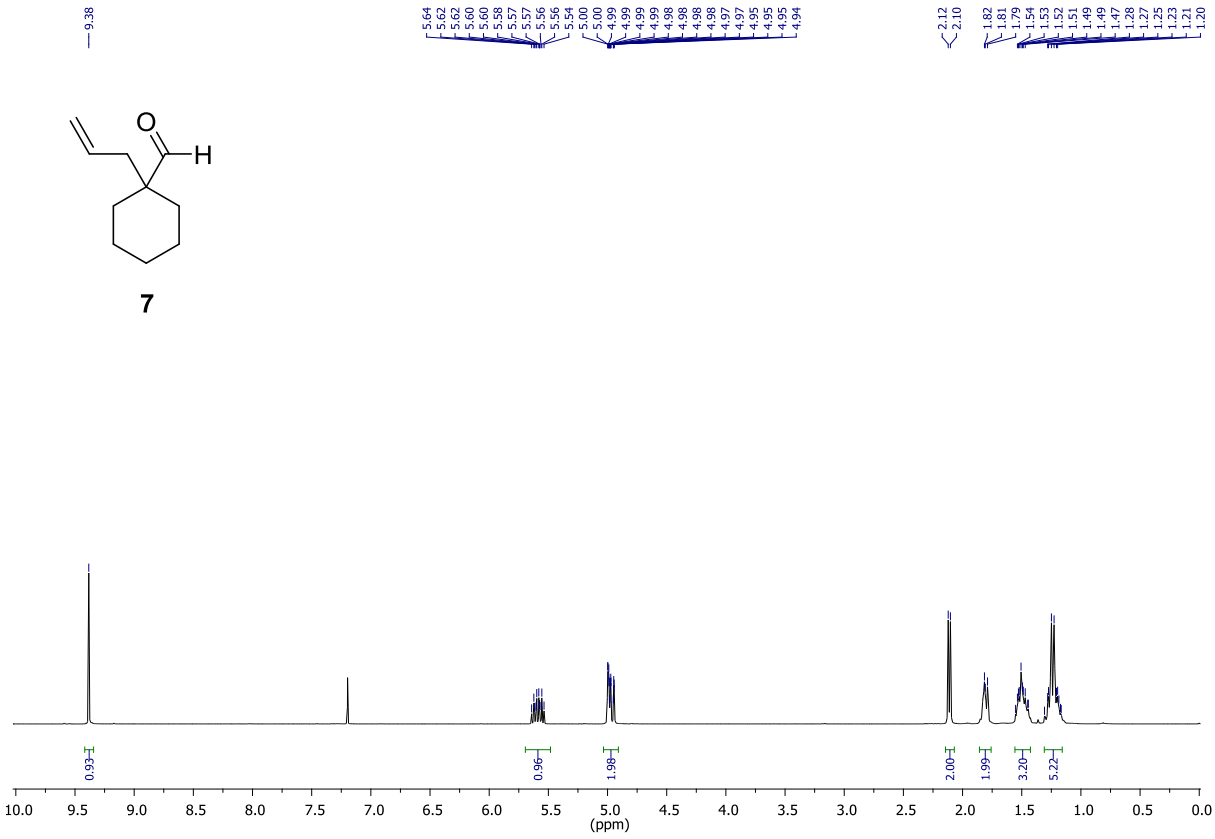

204.6
131.3
118.6
64.0
47.0
40.4
30.2
(ppm)

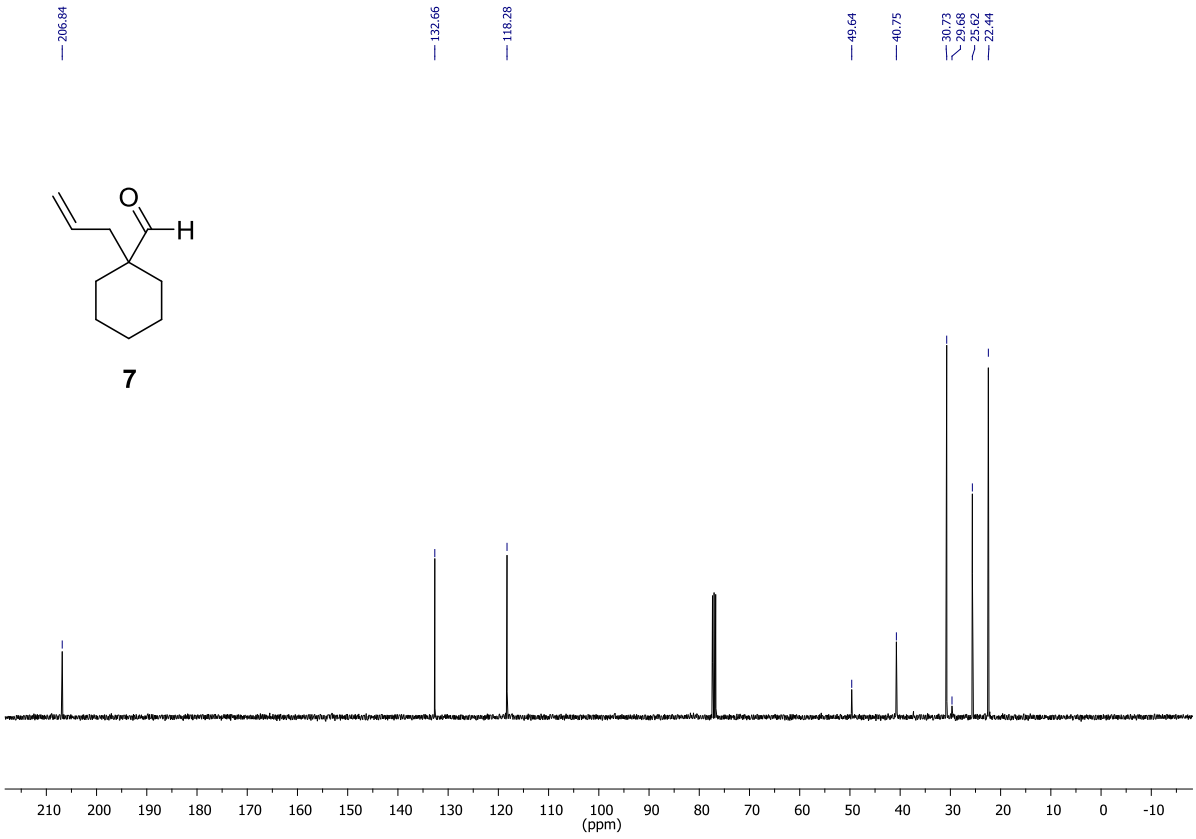

O
H
O
3
9.42
5.68
5.66
5.64
4.96
4.92
4.91
4.89
3.77
3.74
3.36
3.35
1.91
1.87
1.87
1.56
1.33
1.17
2.21
2.15
2.32
3.71
4.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
(ppm)

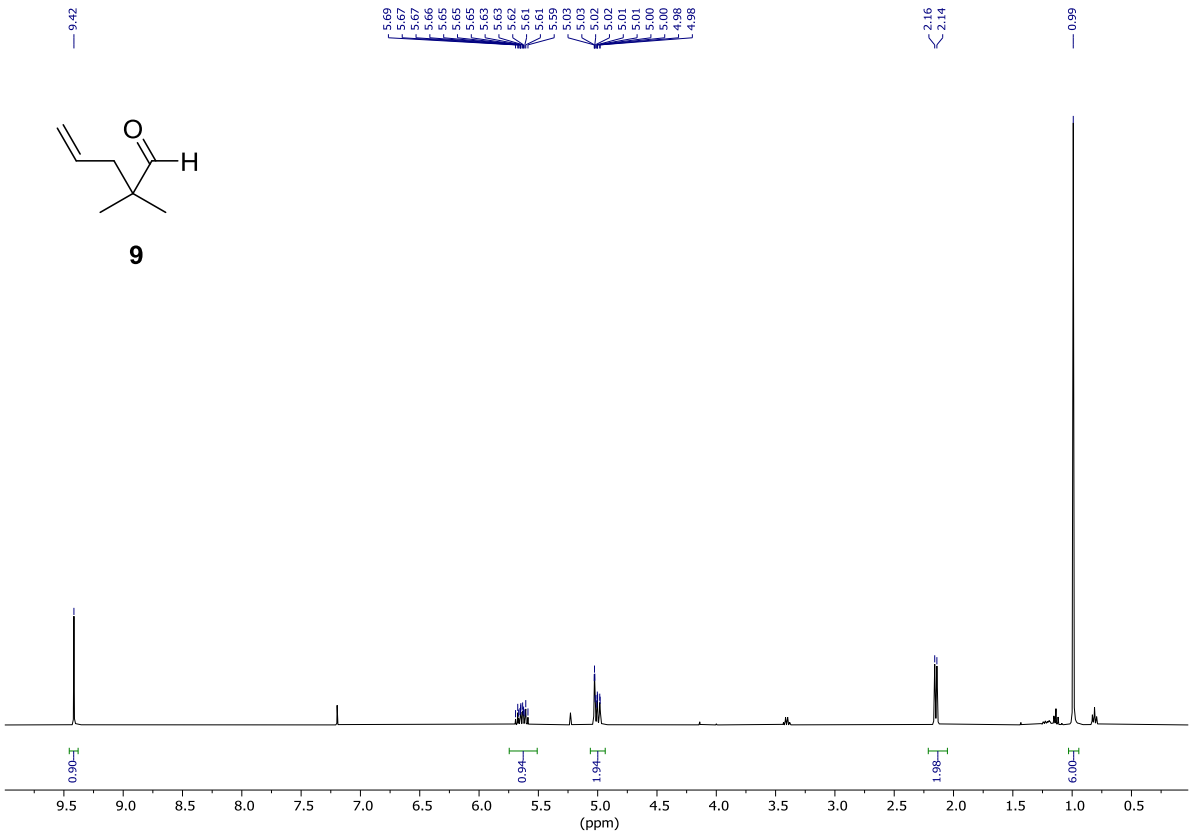

O
H
O
3
205.4
137.5
115.2
64.6
47.4
35.9
30.9
27.3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)


O
H
N
Ts
5
9.32
7.56
7.29
5.55
5.09
5.08
5.05
3.55
3.52
2.40
2.34
2.33
2.17
2.15
2.01
1.65
1.64
1.64
1.00
1.89
1.92
1.13
2.19
2.14
2.93
2.14
2.09
2.48
2.21
(ppm)

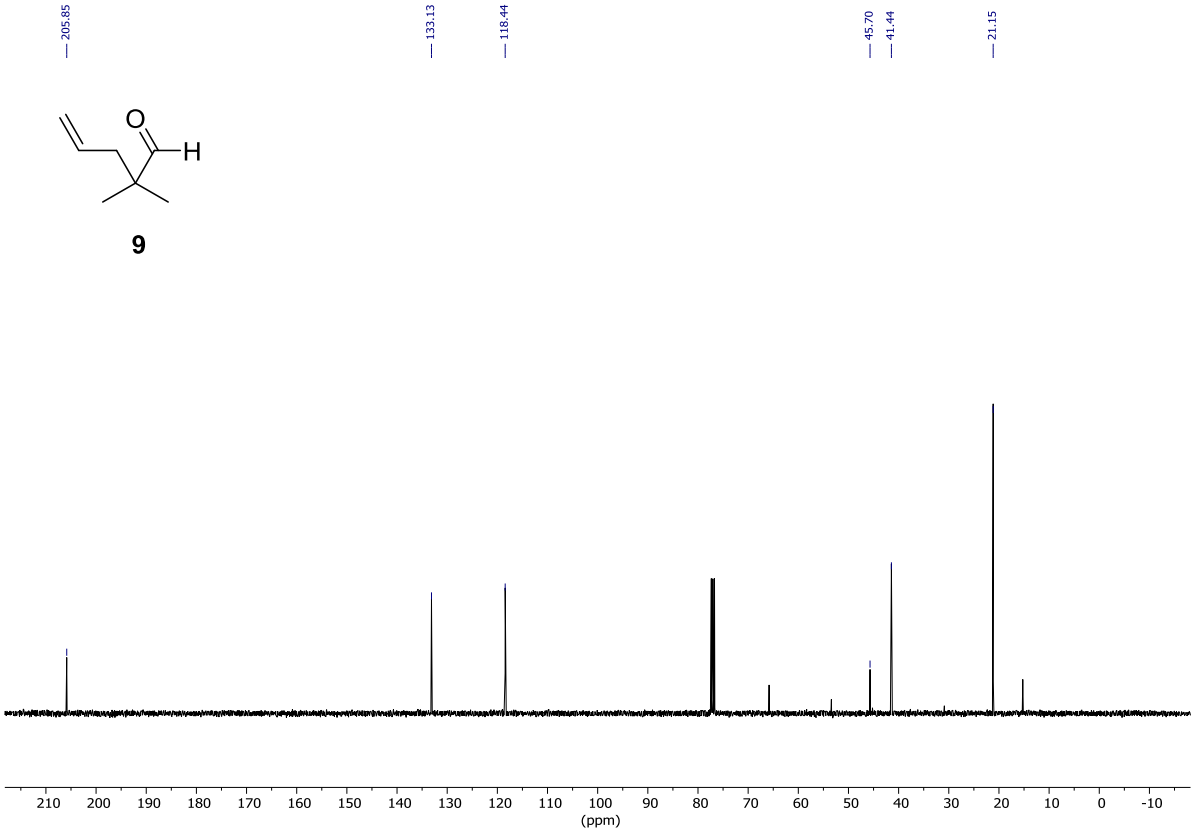

O
H
N
Ts
5
204.8
143.6
132.8
130.9
129.7
127.5
119.6
47.7
43.3
40.6
29.6
21.4
(ppm)


9.38
5.64
5.62
5.62
5.60
5.60
5.58
5.57
5.57
5.56
5.56
5.54
5.00
5.00
4.99
4.99
4.99
4.99
4.98
4.98
4.98
4.98
4.97
4.95
4.95
4.94
2.12
2.10
1.82
1.81
1.79
1.54
1.53
1.52
1.51
1.49
1.49
1.47
1.28
1.27
1.25
1.23
1.21
1.20
O
H
7
0.93
0.96
1.98
2.00
1.99
3.20
5.22
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

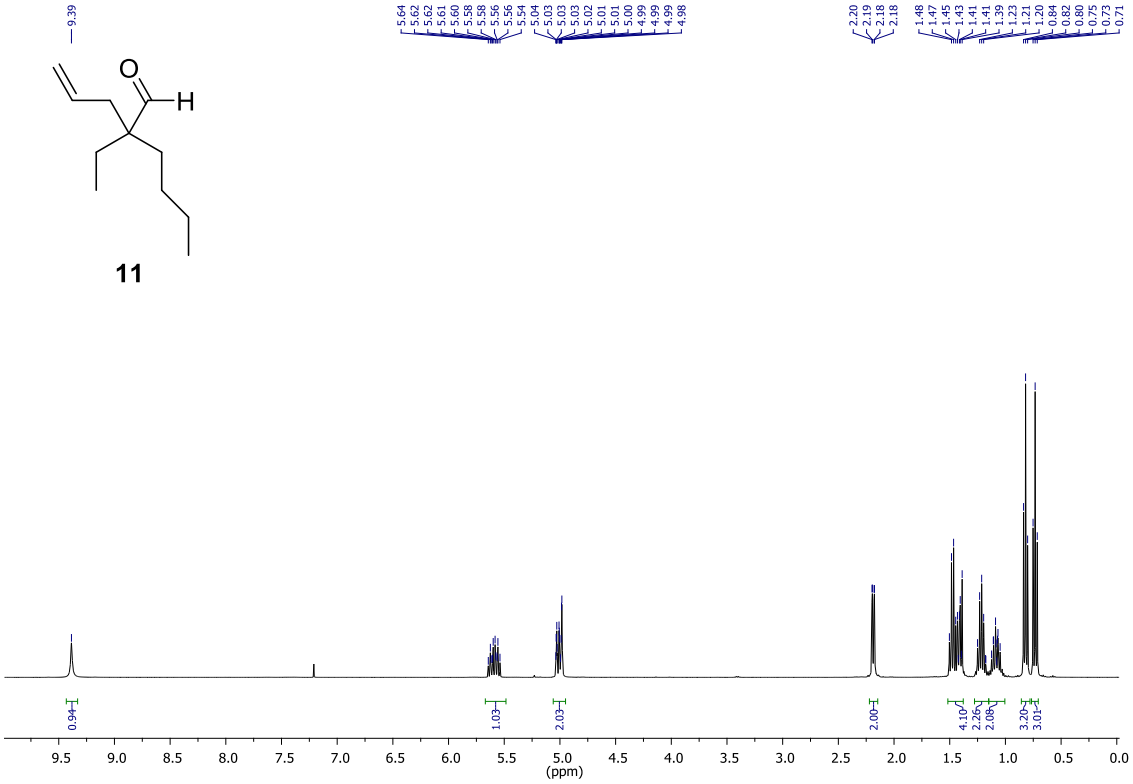

206.84
132.66
118.28
49.64
40.75
30.73
29.68
25.62
22.44
O
H
7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

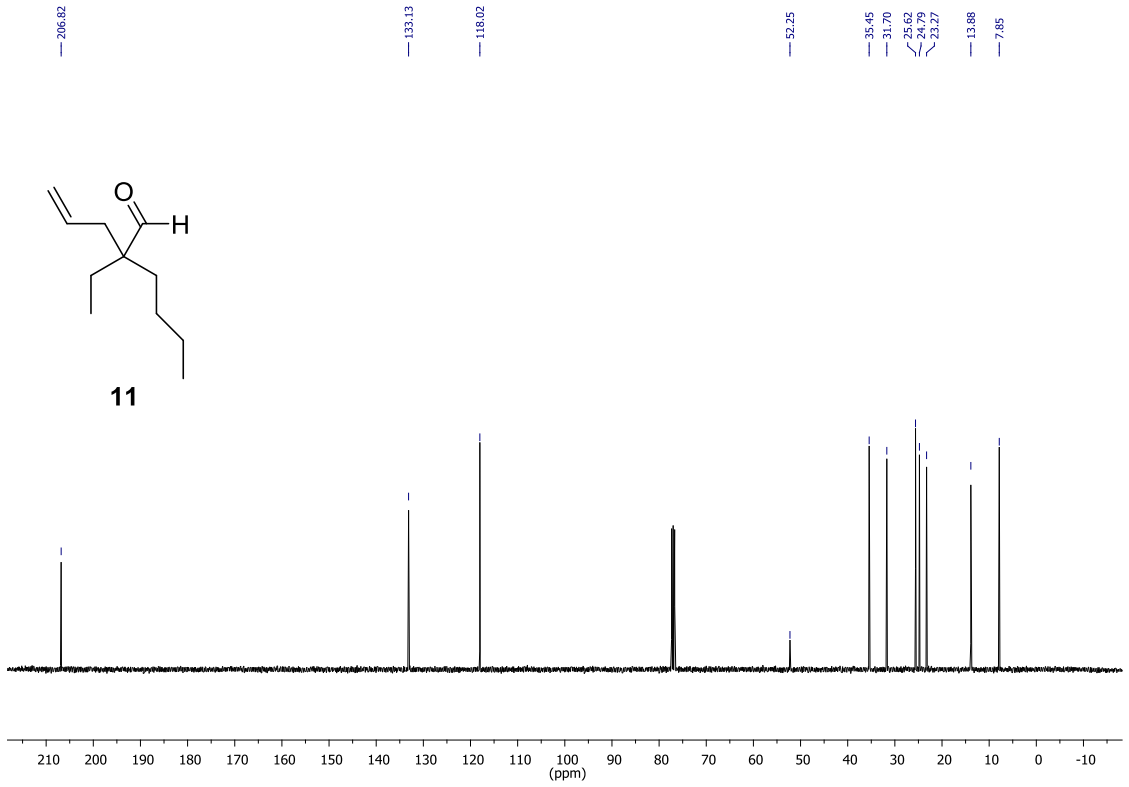

9.42
5.69
5.67
5.67
5.66
5.65
5.65
5.65
5.63
5.63
5.62
5.61
5.61
5.59
5.03
5.03
5.02
5.02
5.01
5.01
5.00
5.00
4.98
4.98
2.16
2.14
0.99
O
H
0.90
0.94
1.94
1.98
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

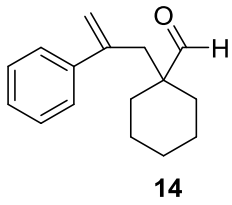
9

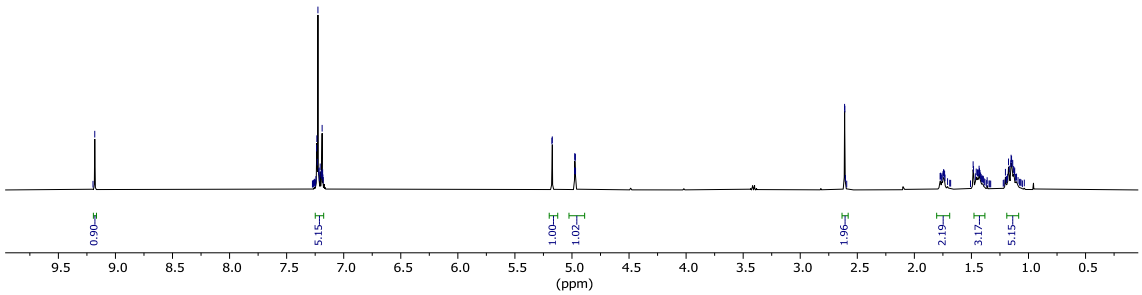

205.85
133.13
118.44
45.70
41.44
21.15
O
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

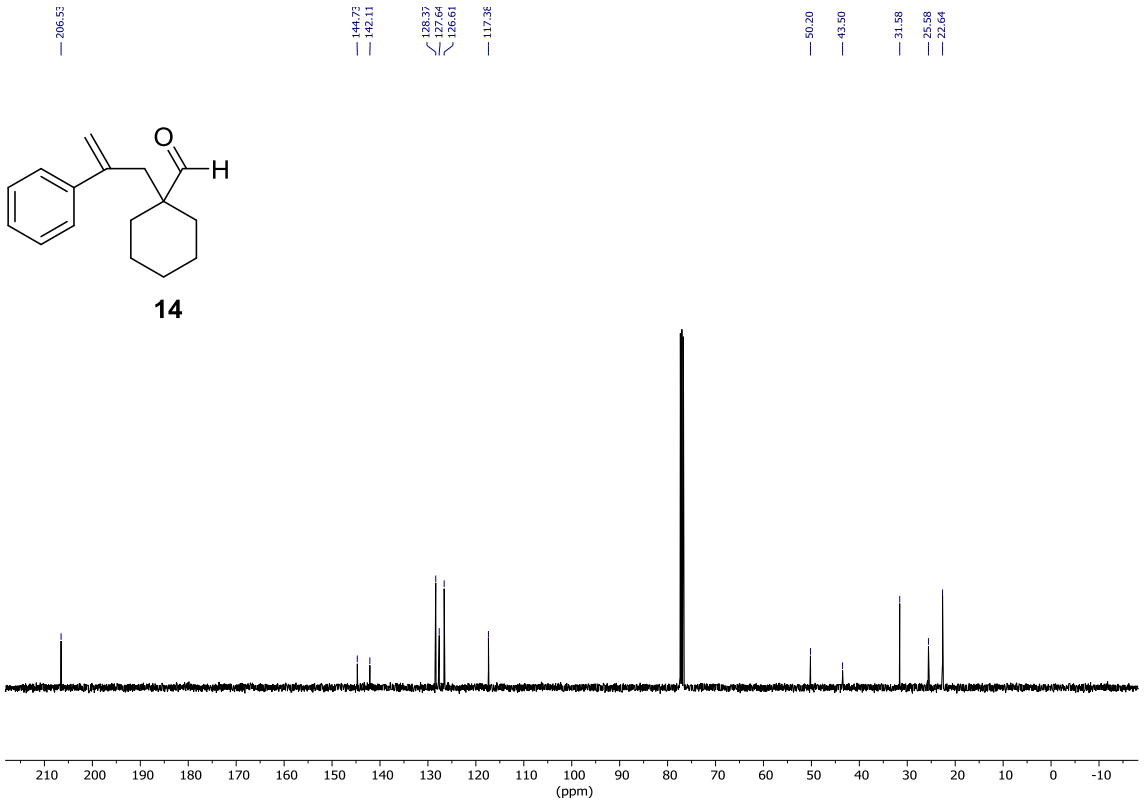
9

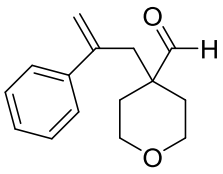

9.39
5.64
5.62
5.62
5.61
5.60
5.58
5.58
5.56
5.55
5.54
5.04
5.03
5.03
5.03
5.02
5.01
5.01
5.00
4.99
4.99
4.99
4.98
2.20
2.19
2.18
2.18
1.48
1.47
1.45
1.43
1.41
1.41
1.39
1.23
1.21
1.20
0.84
0.82
0.80
0.75
0.73
0.71
O
H
11
0.94
1.03
2.03
2.00
4.10
2.26
2.08
3.20
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)


206.82
133.13
118.02
52.25
35.45
31.70
25.62
24.79
23.27
13.88
7.85
O
H
11
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

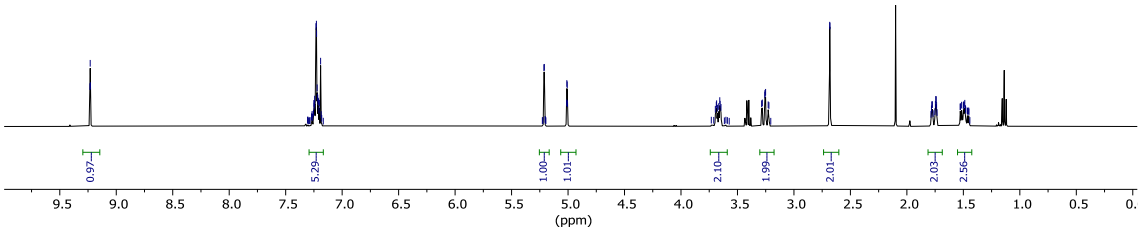

O
H
14

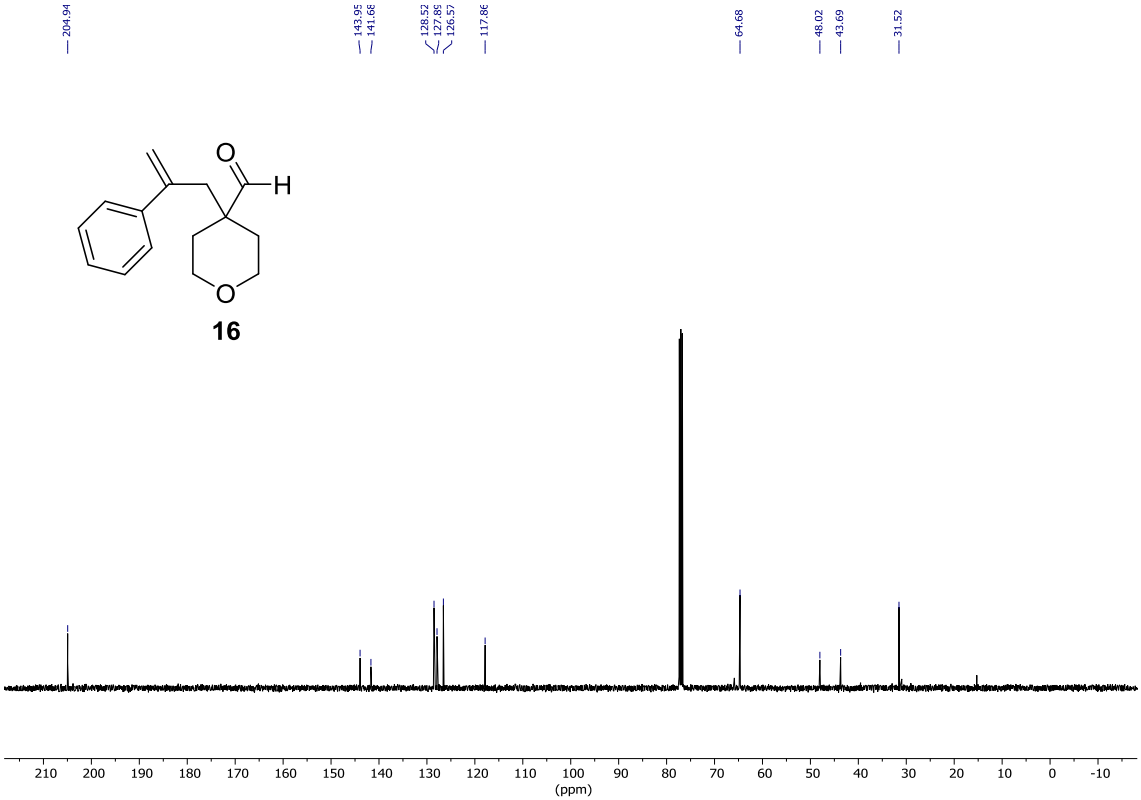

0.90
5.15
1.00
1.02
1.96
2.19
3.17
5.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)


206.53
144.73
142.11
128.37
127.64
126.61
117.38
50.20
43.50
31.58
25.58
22.64
O
H
14
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

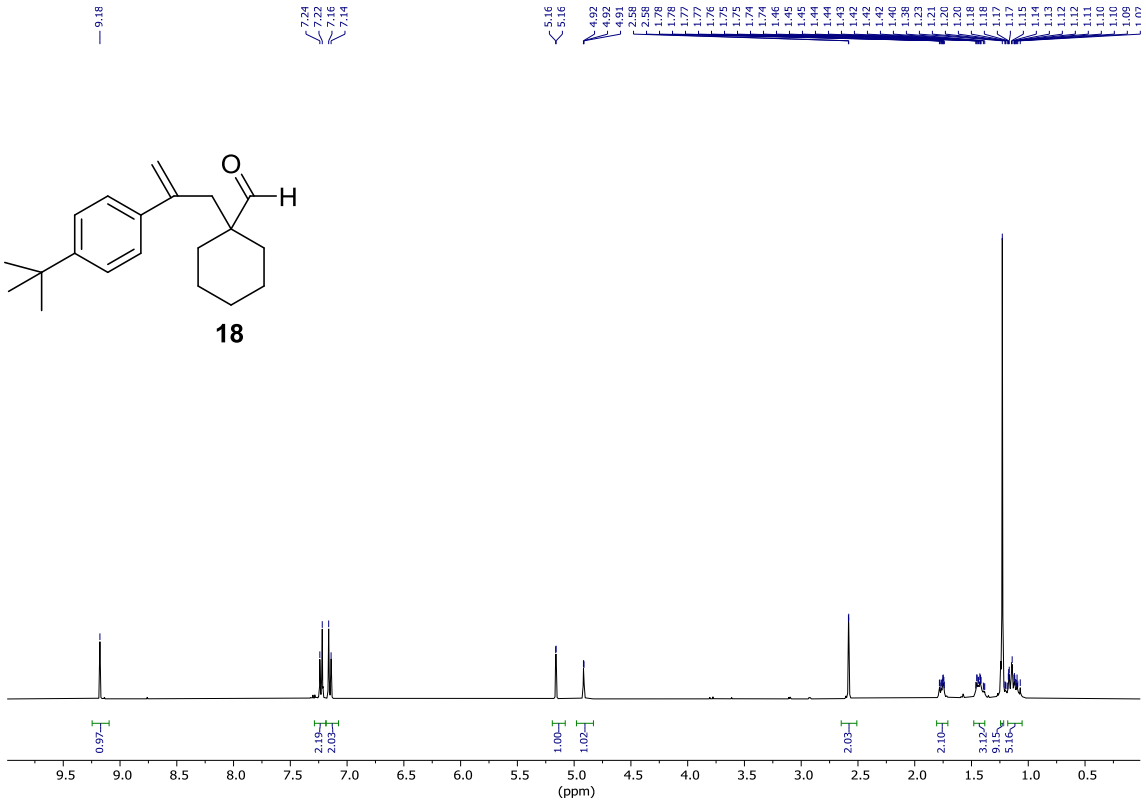


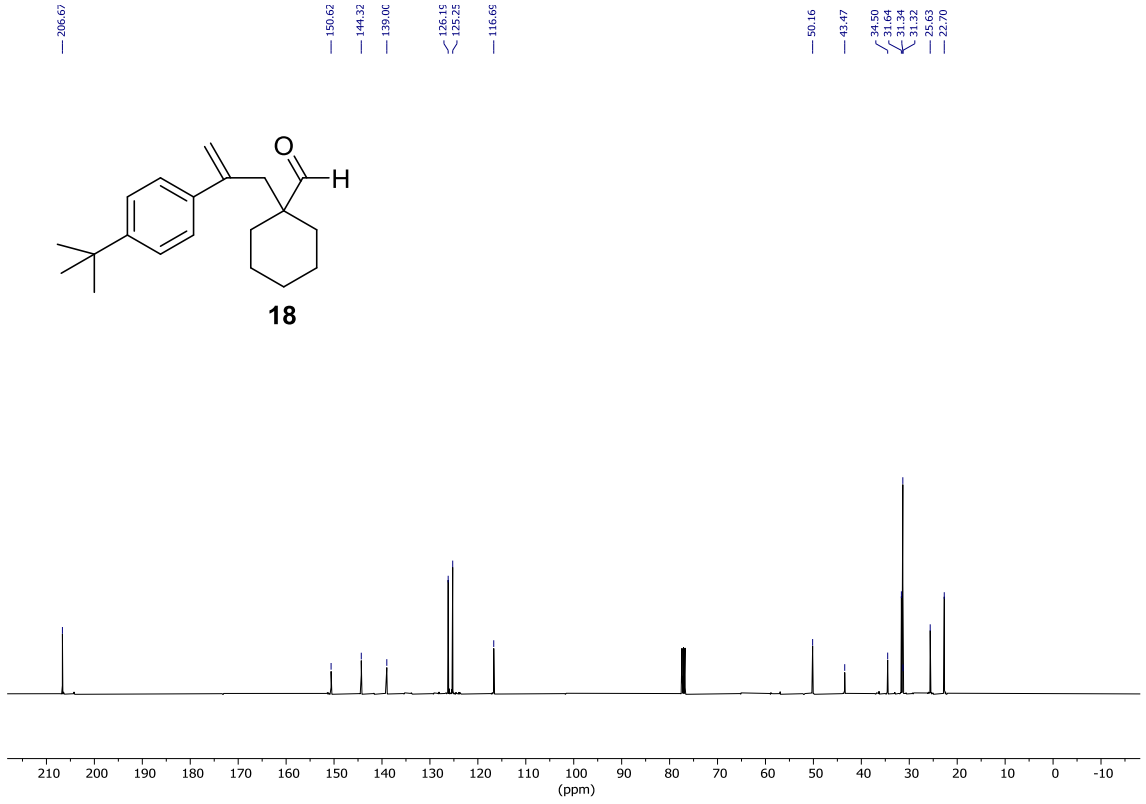
16

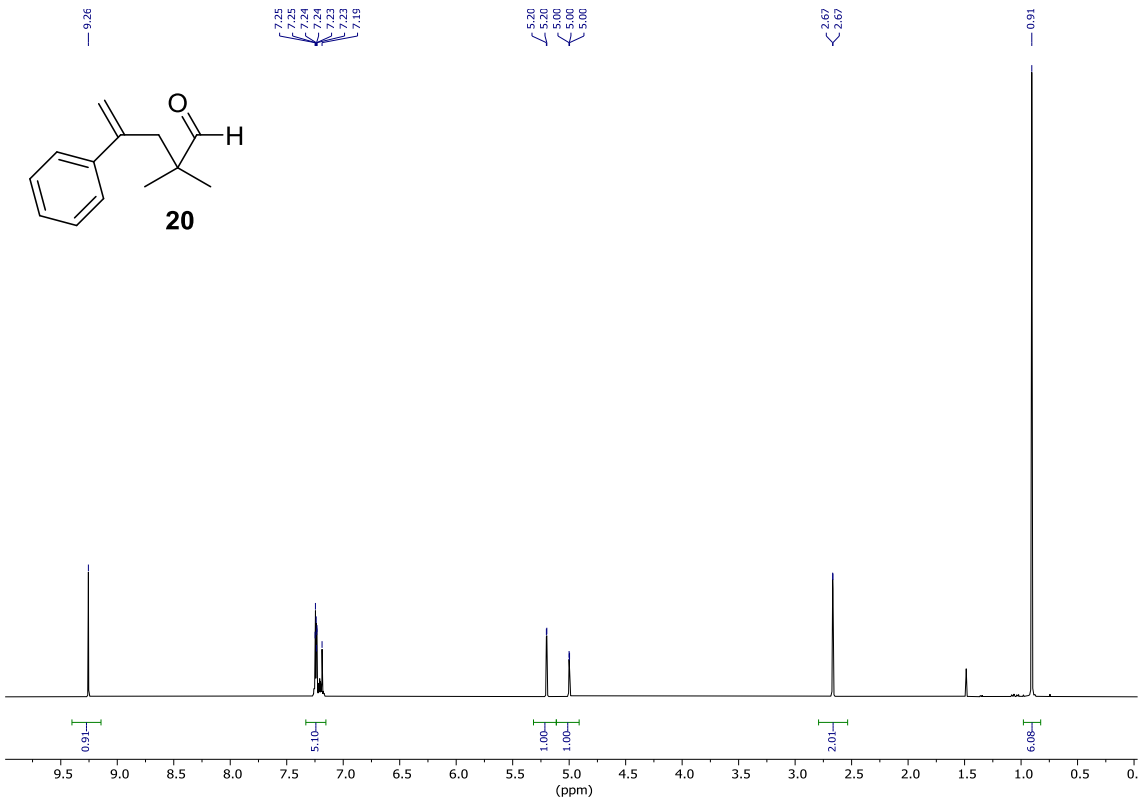


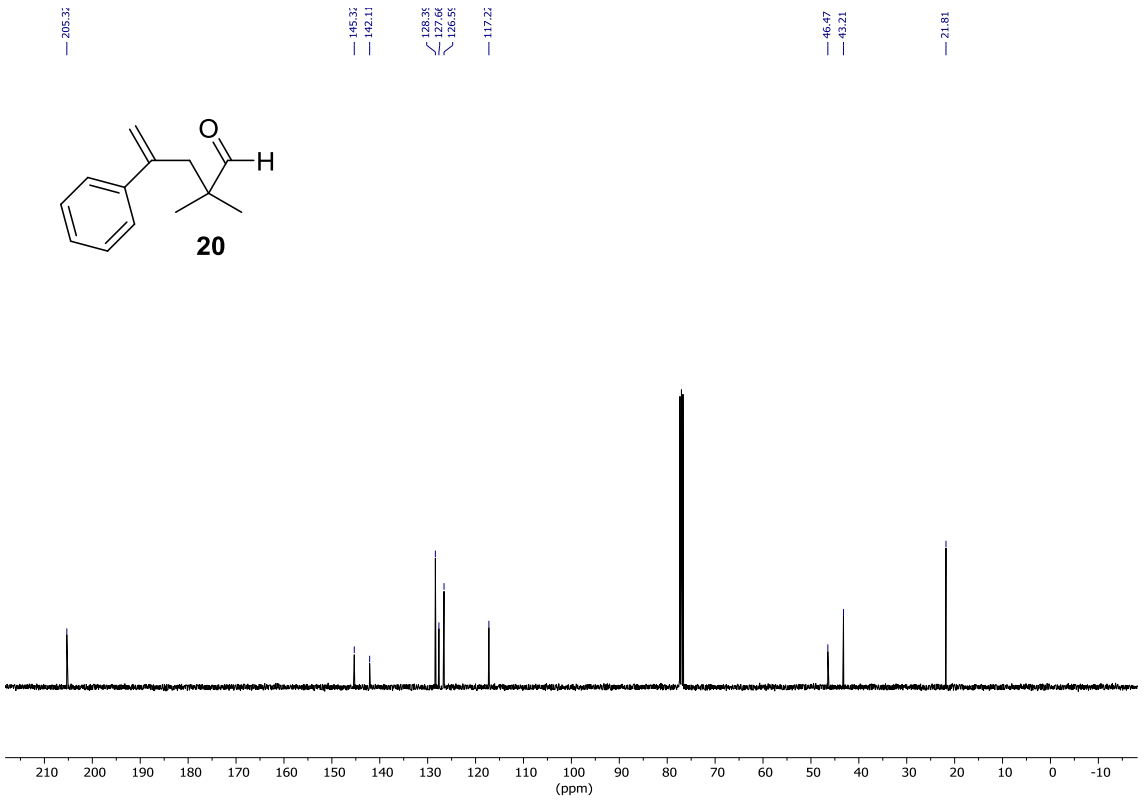


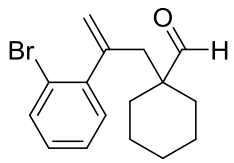
16


9.18
7.24
7.22
7.16
7.14
5.16
5.16
4.92
4.92
4.91
2.58
2.58
1.78
1.78
1.77
1.77
1.76
1.75
1.75
1.74
1.74
1.46
1.45
1.44
1.44
1.43
1.42
1.42
1.42
1.40
1.38
1.23
1.21
1.20
1.20
1.18
1.18
1.17
1.17
1.15
1.14
1.13
1.12
1.12
1.11
1.10
1.10
1.09
1.07
O
H
18
0.97
2.19
2.03
1.00
1.02
2.03
2.10
3.12
9.15
5.16
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

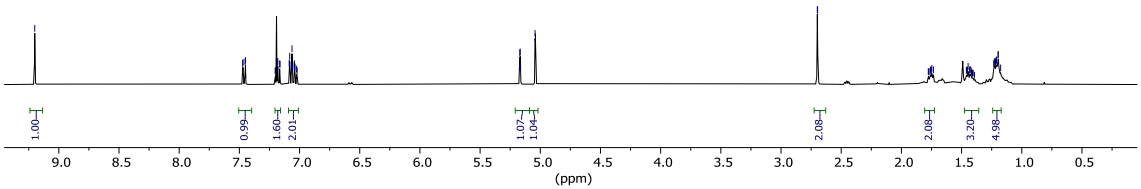

206.67
150.62
144.32
139.00
126.15
125.25
116.65
50.16
43.47
34.50
31.64
31.34
31.32
25.63
22.70
O
H
18
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)

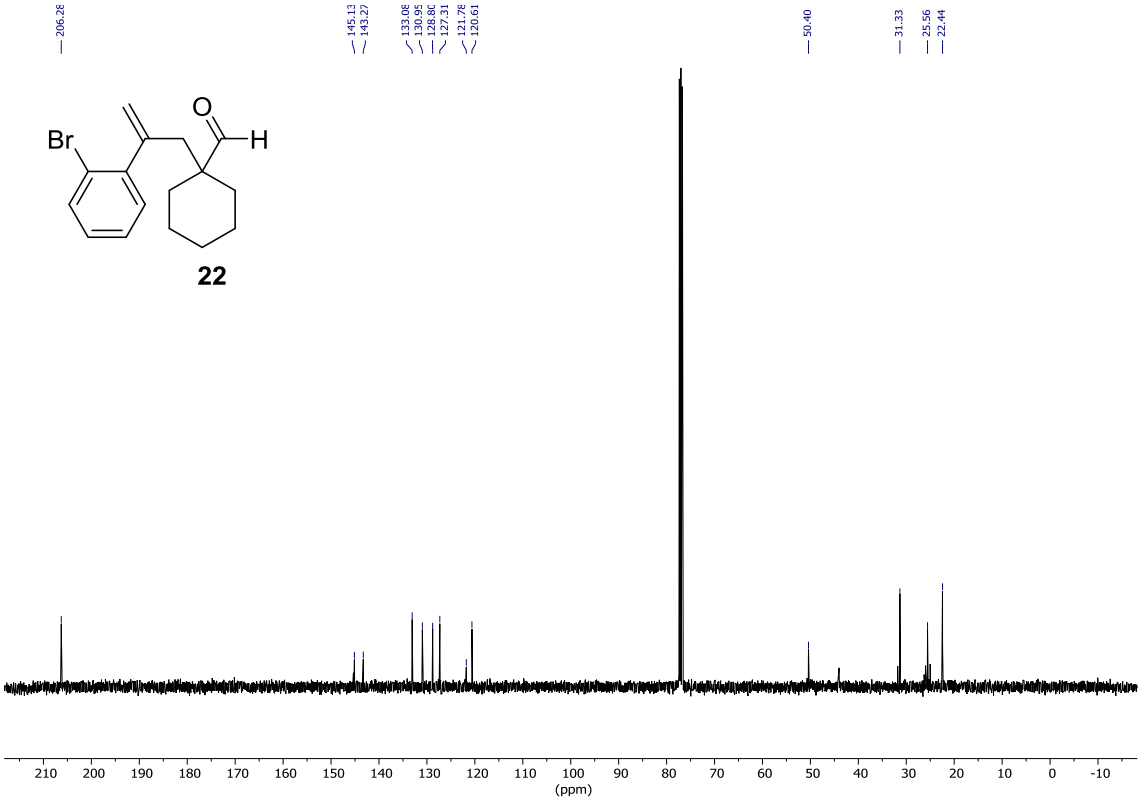

9.26
7.25
7.25
7.24
7.24
7.23
7.23
7.19
5.20
5.20
5.00
5.00
5.00
5.00
2.67
2.67
0.91
O
H
20
0.91
5.10
1.00
1.00
2.01
6.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


205.3
145.3
142.1
128.3
127.6
126.5
117.2
46.47
43.21
21.81
O
H
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)


Br
O
H

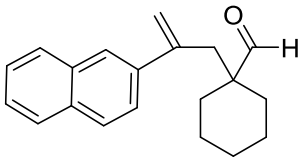
22


1.00
0.99
1.60
2.01
1.07
1.04
2.08
2.08
3.20
4.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

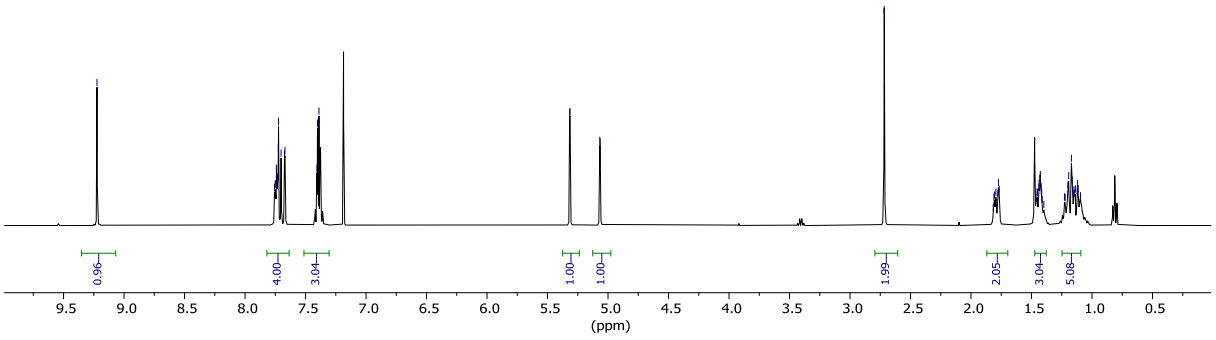

206.28
145.13
143.27
133.08
130.95
128.86
127.31
121.78
120.61
50.40
31.33
25.56
22.44
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)

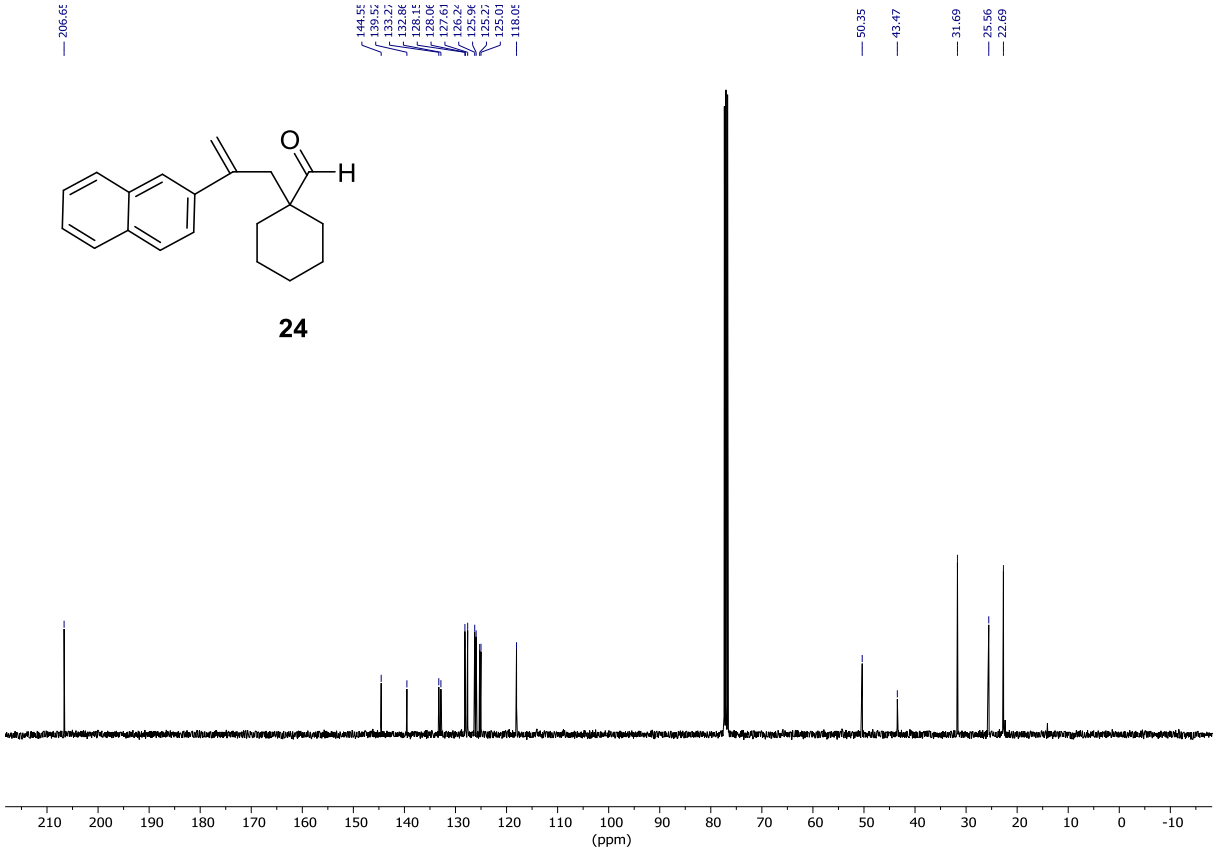
Br
O
H

22

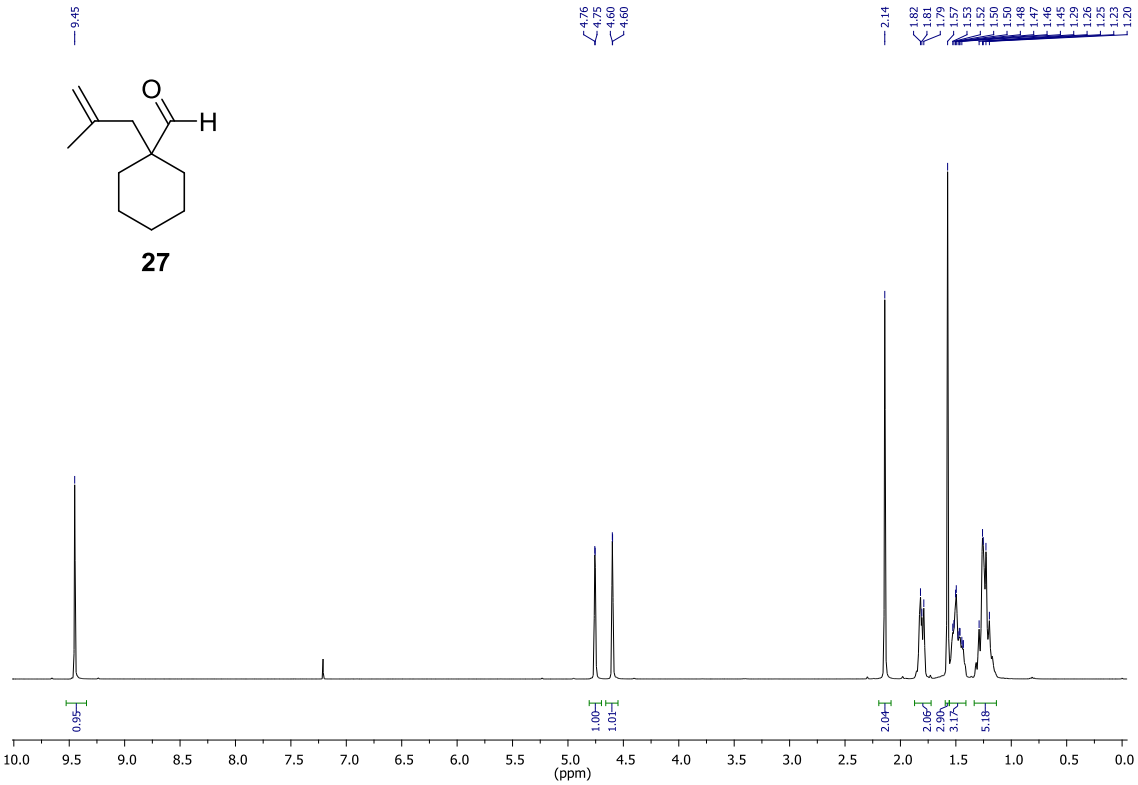

O
H

24

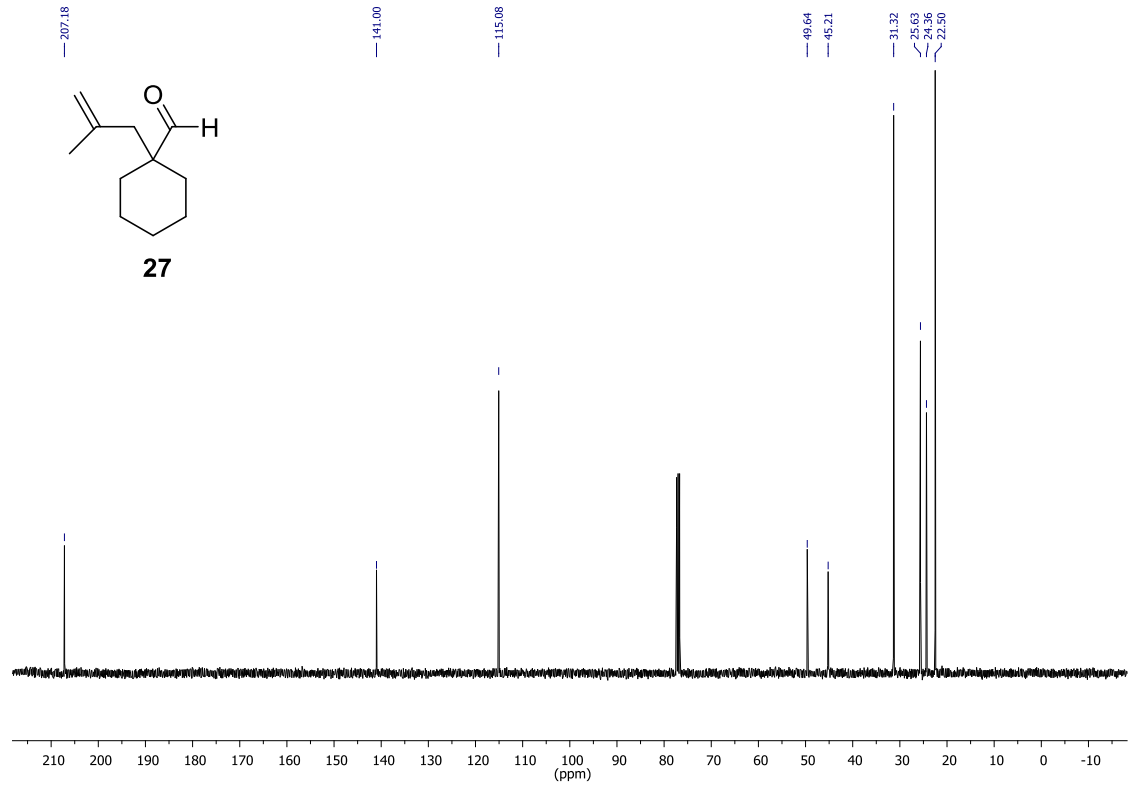

0.96
4.00
3.04
1.00
1.00
1.99
2.05
3.04
5.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


206.65
144.55
139.52
133.22
132.86
128.15
128.06
127.61
126.24
125.96
125.27
125.01
118.05
50.35
43.47
31.69
25.56
22.69
O
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)

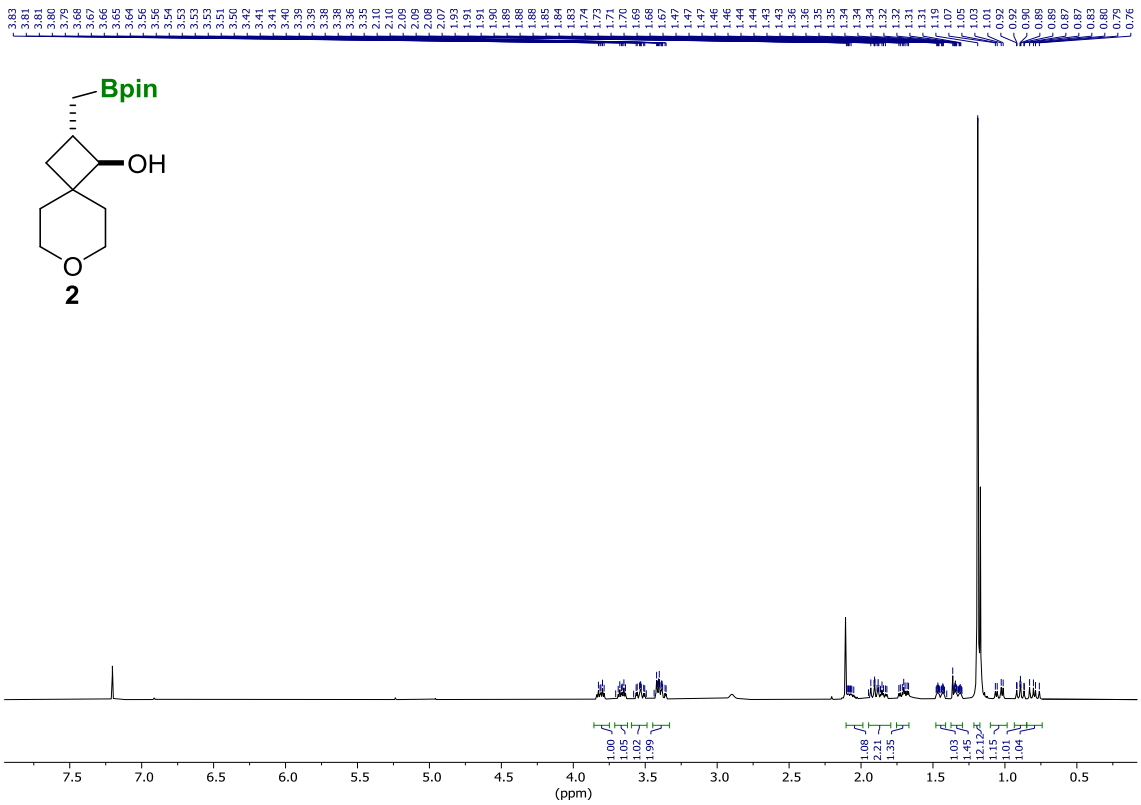
24

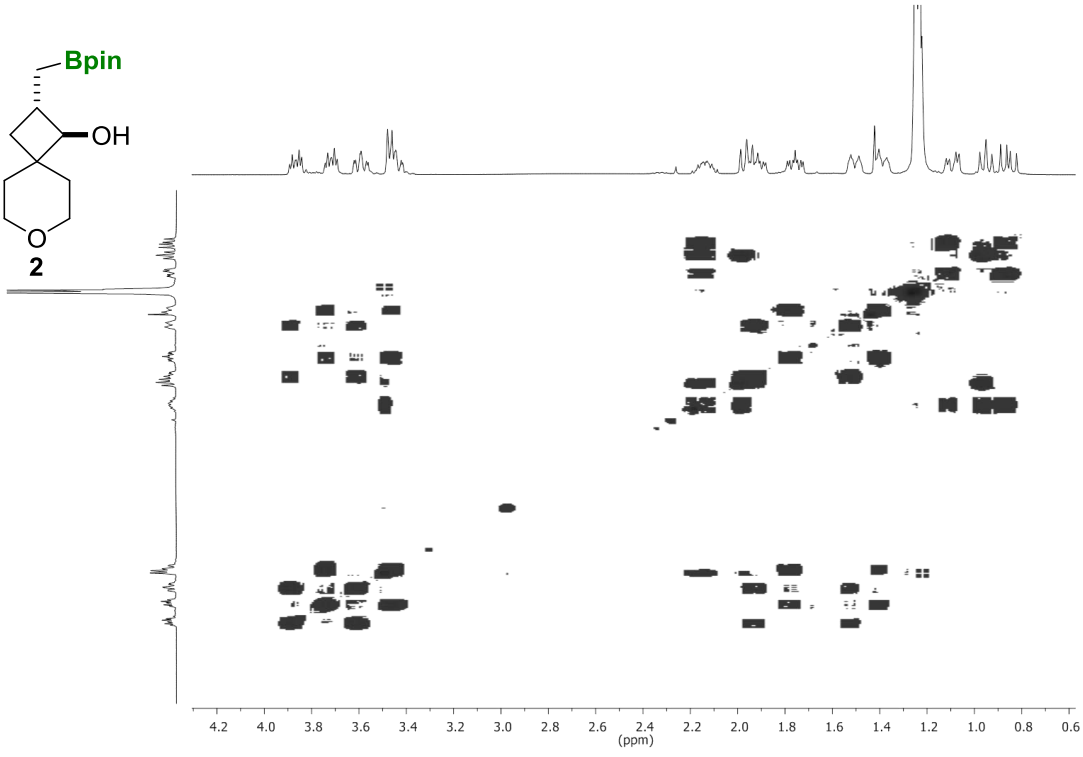

9.45
4.76
4.75
4.60
4.60
2.14
1.82
1.81
1.79
1.57
1.53
1.52
1.50
1.50
1.50
1.48
1.47
1.46
1.45
1.29
1.26
1.25
1.23
1.20
O
H
0.95
1.00
1.01
2.04
2.06
2.90
3.17
5.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

27

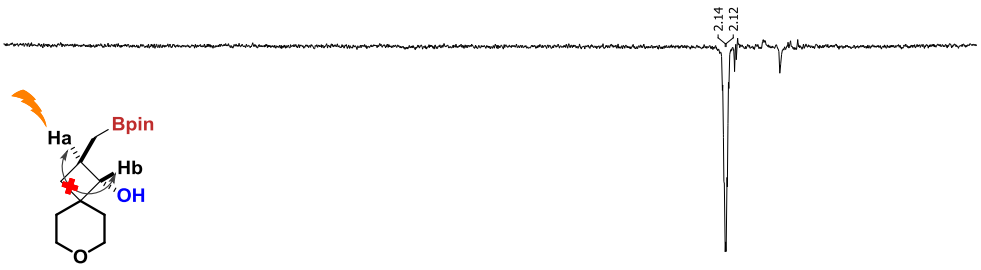

207.18
141.00
115.08
49.64
45.21
31.32
25.63
24.36
22.50
O
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

27

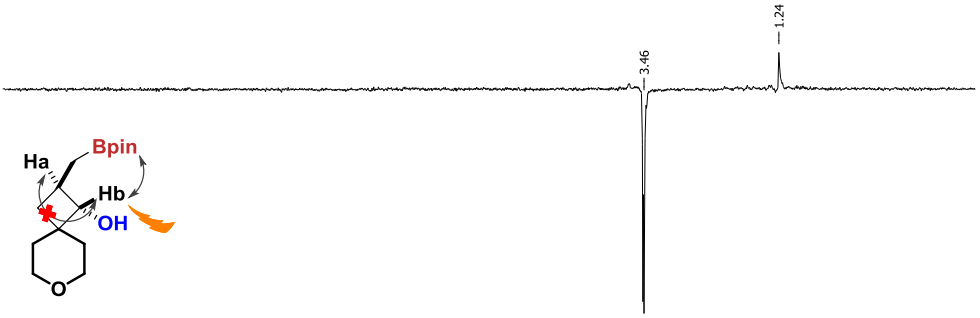

Bpin
OH
O
2
(ppm)

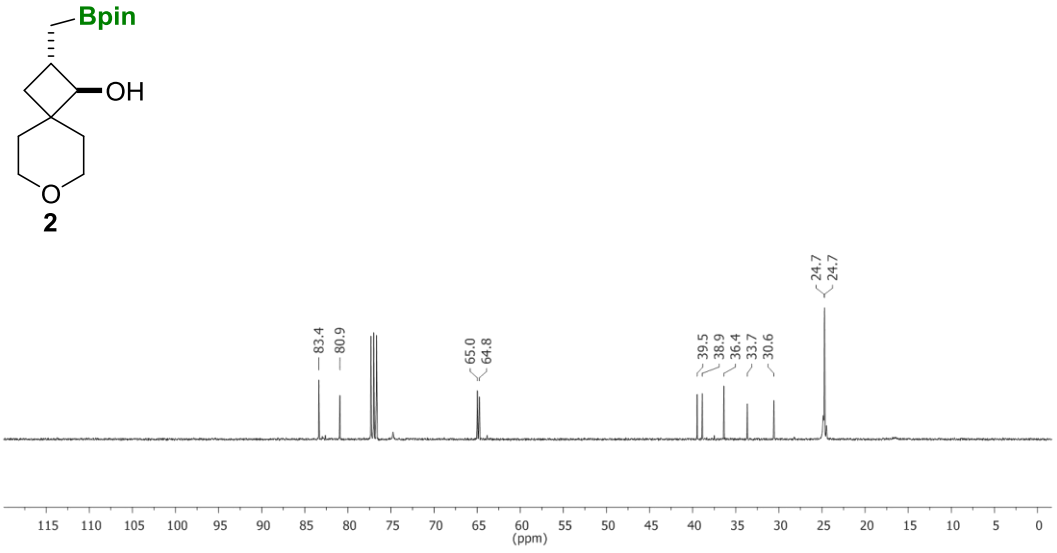

Bpin
OH
O
2
(ppm)

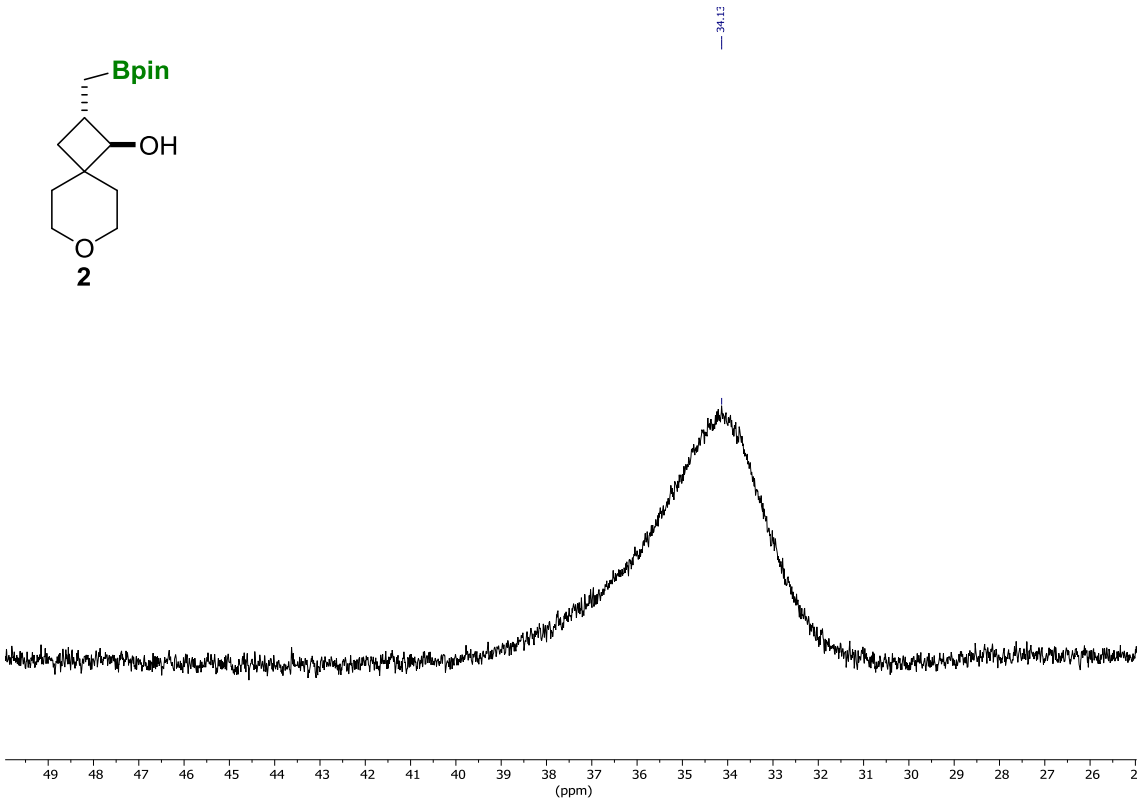
NOE 1


2.14
2.12
Ha
Bpin
Hb
OH
O

NOE 2


3.46
1.24
Ha
Bpin
Hb
OH
O


Bpin
OH
O
2
83.4
80.9
65.0
64.8
39.5
38.9
36.4
33.7
30.6
24.7
24.7
115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
(ppm)


Bpin
OH
O
2
34.13
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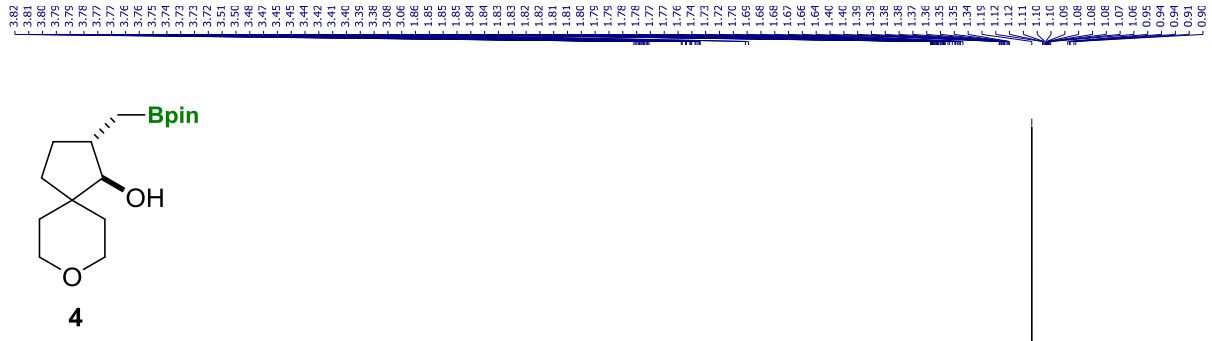
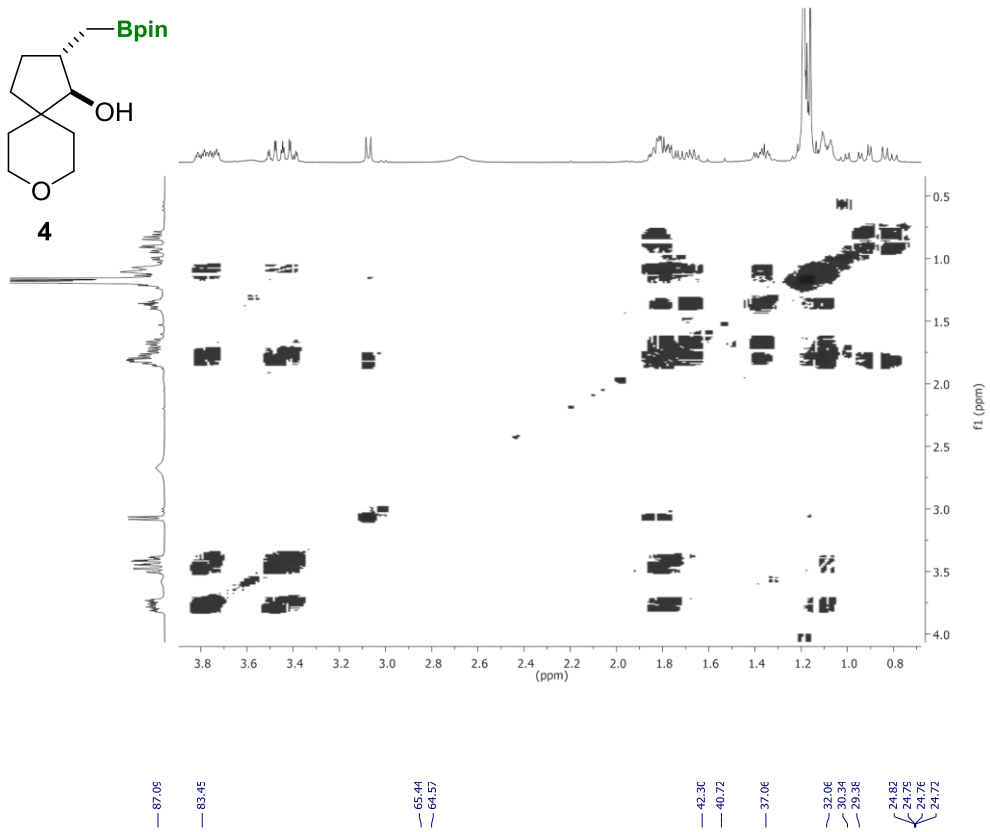
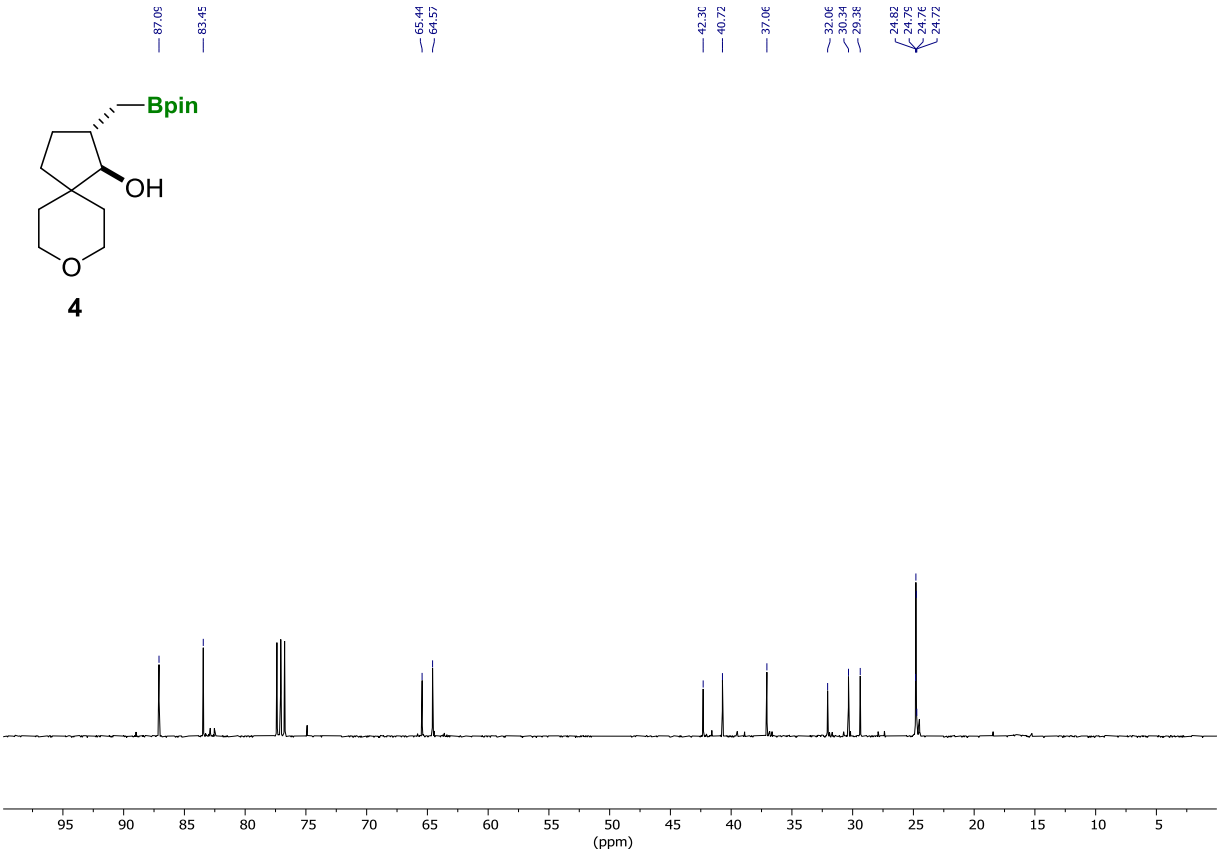
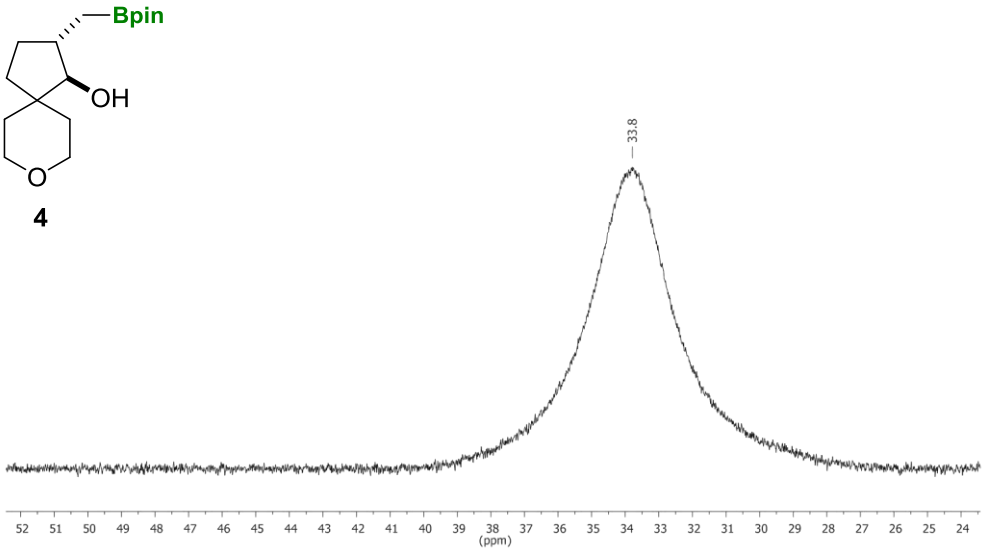
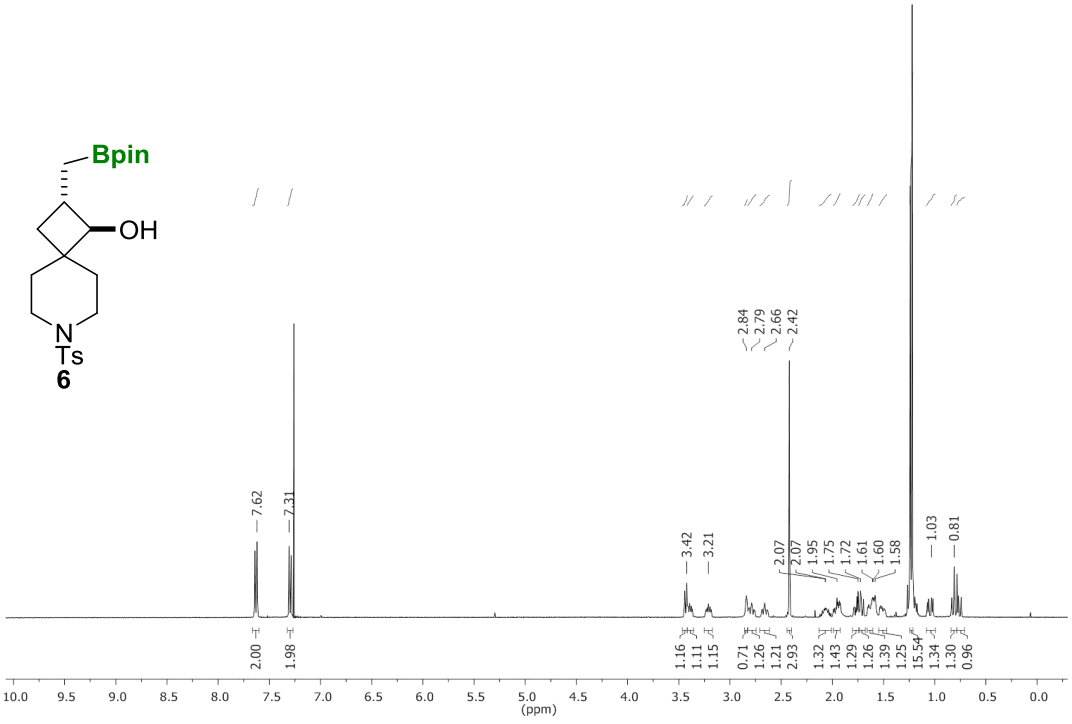
(ppm)

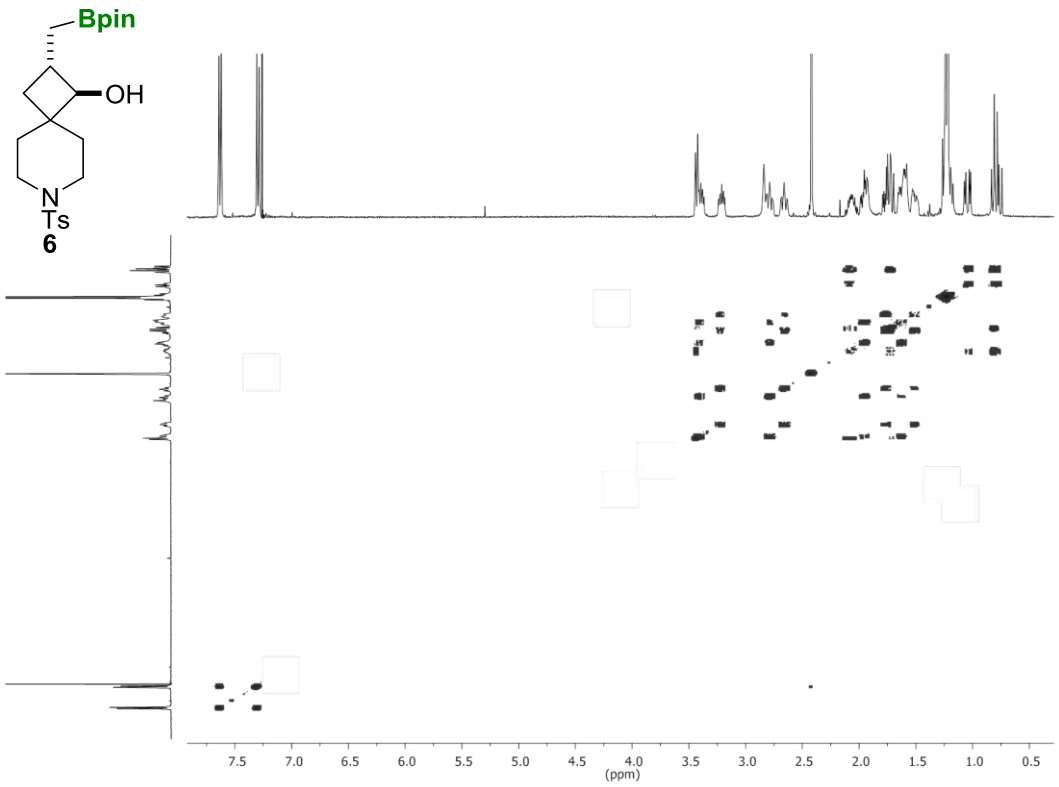

Bpin
OH
O
4
2.44
2.81
1.00
4.16
1.98
1.92
11.93
3.14
1.15
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)


Bpin
OH
O
4
f1 (ppm)
(ppm)


Bpin
OH
O
4
(ppm)


Bpin
OH
O
4
33.8
52 51 50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24
(ppm)


Bpin
OH
N
Ts
6
7.62
7.31
3.42
3.21
2.84
2.79
2.66
2.42
2.07
2.07
1.95
1.75
1.72
1.61
1.60
1.58
1.03
0.81
2.00
1.98
1.16
1.11
1.15
0.71
1.26
1.21
2.93
1.32
1.43
1.29
1.26
1.39
1.25
15.54
1.34
1.30
0.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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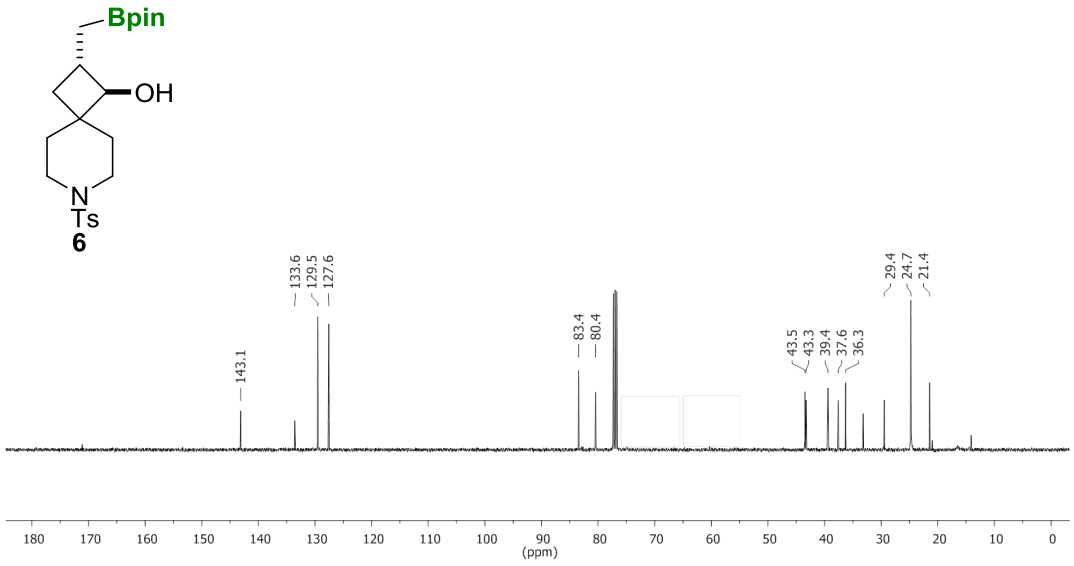
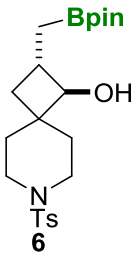
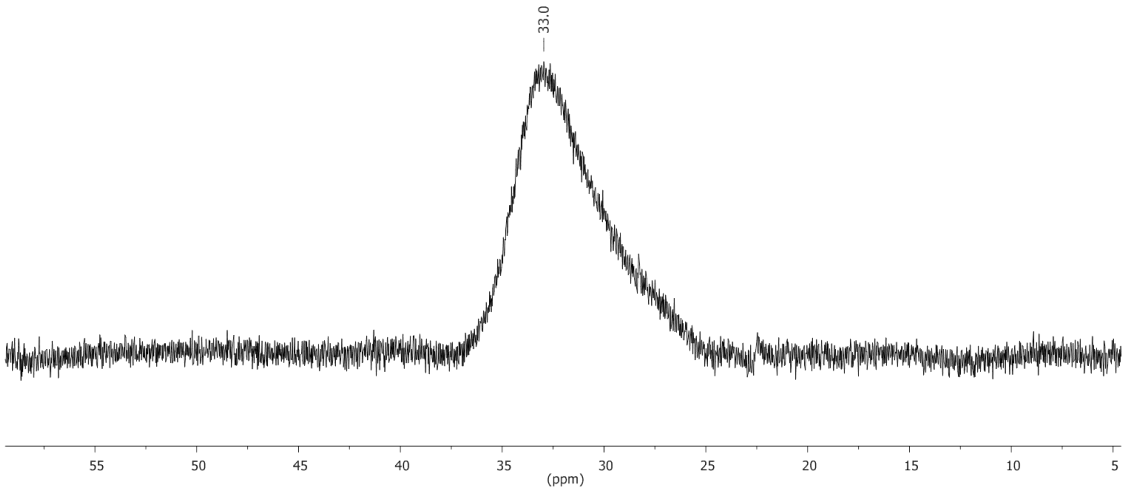
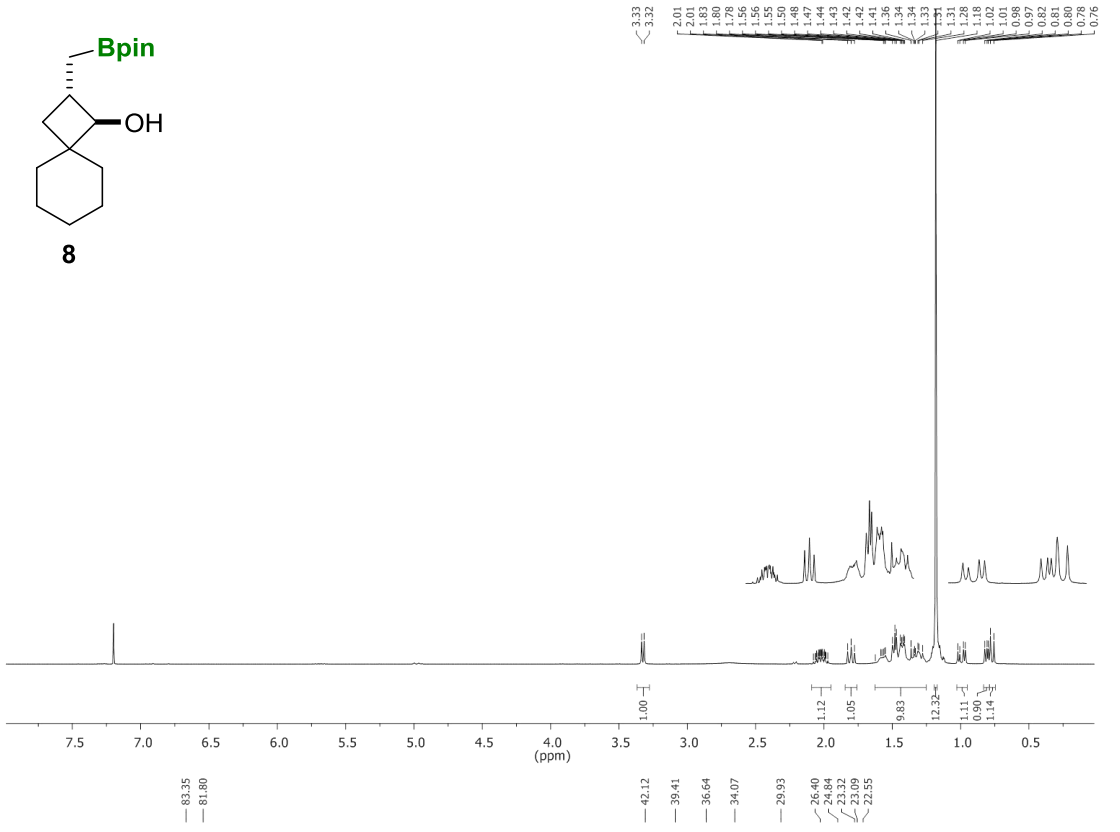
OH
N
Ts
6
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

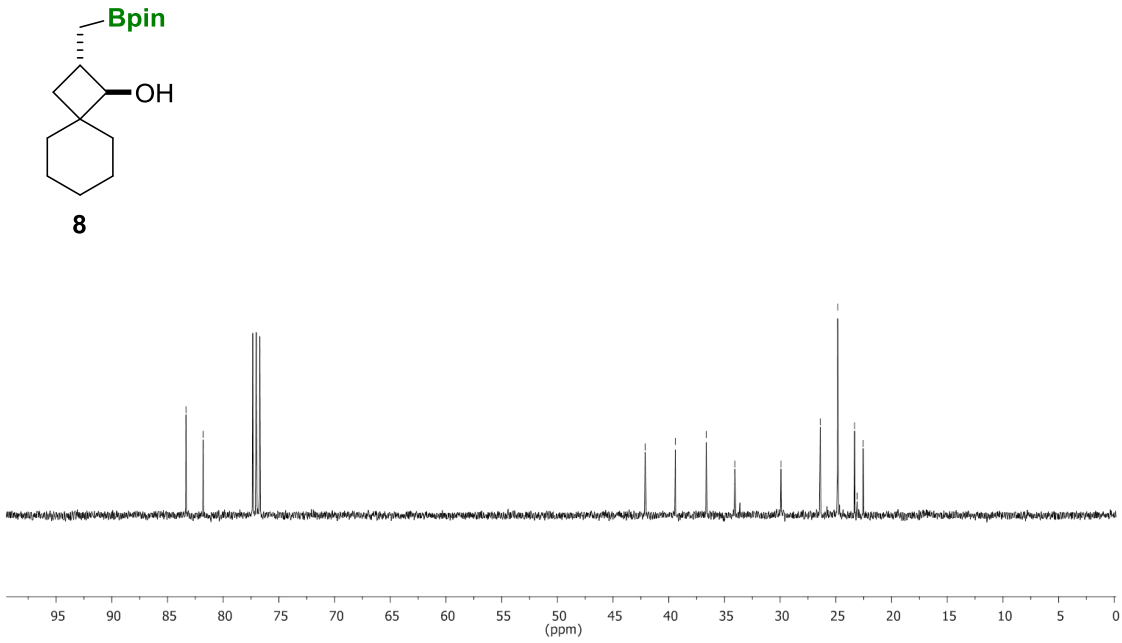

Bpin
OH
N
Ts
6
143.1
133.6
129.5
127.6
83.4
80.4
43.5
43.3
39.4
37.6
36.3
29.4
24.7
21.4
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

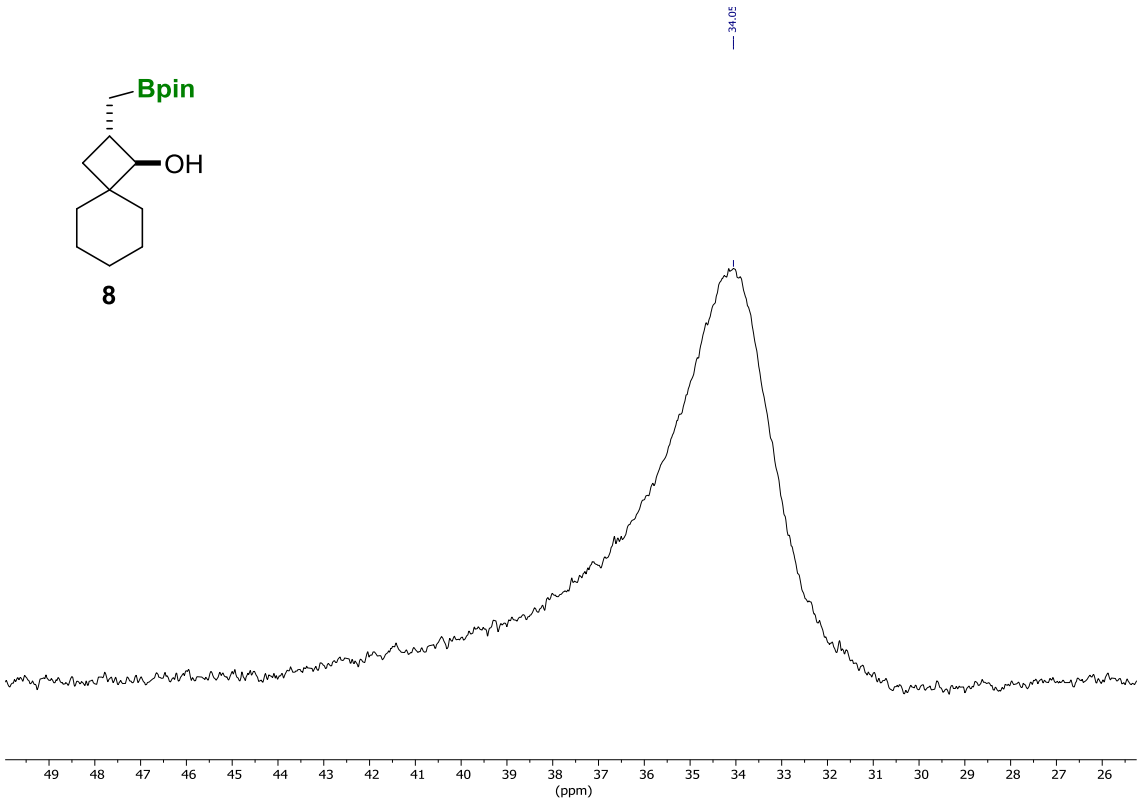


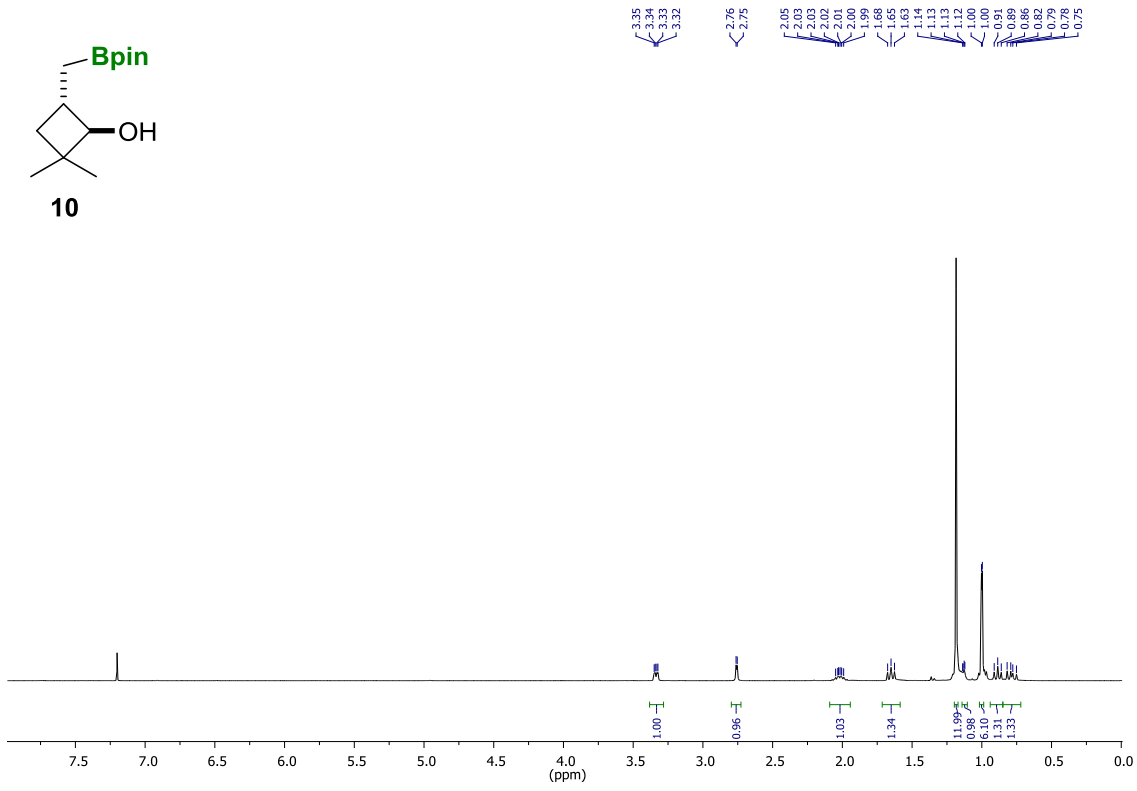
6

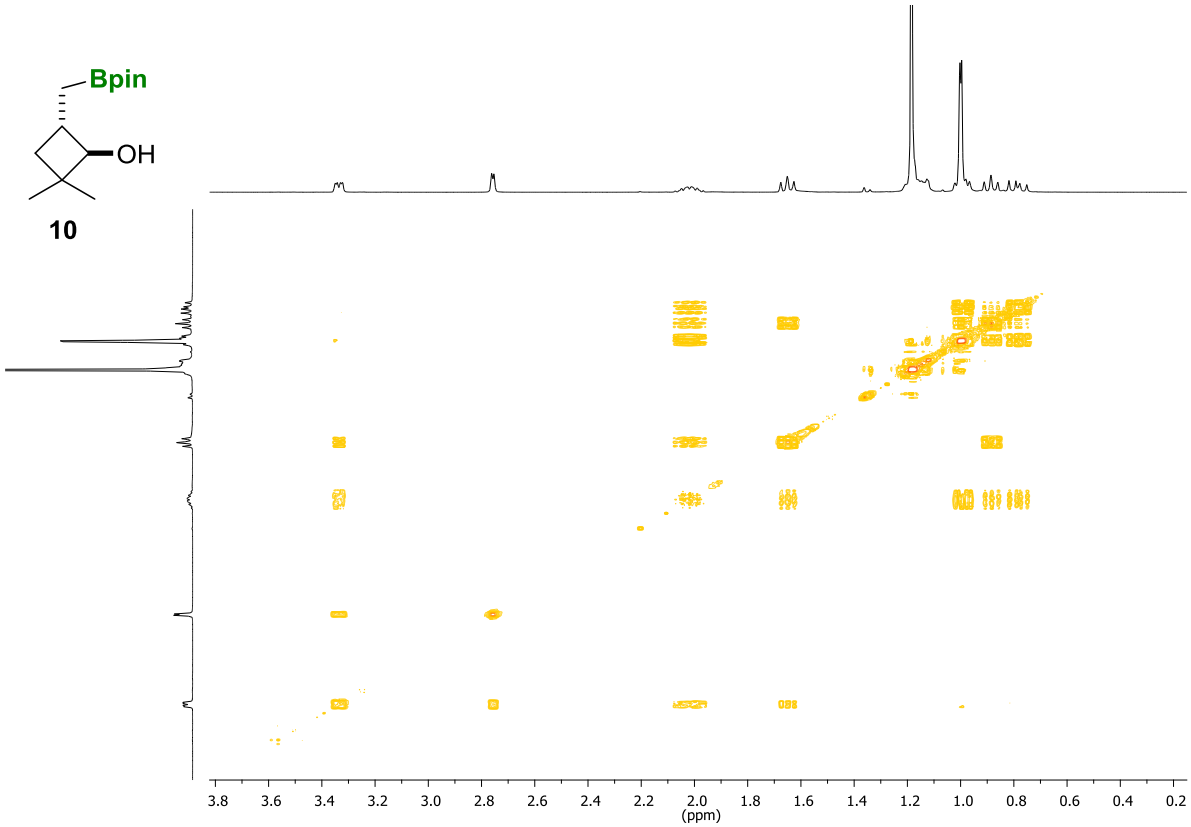


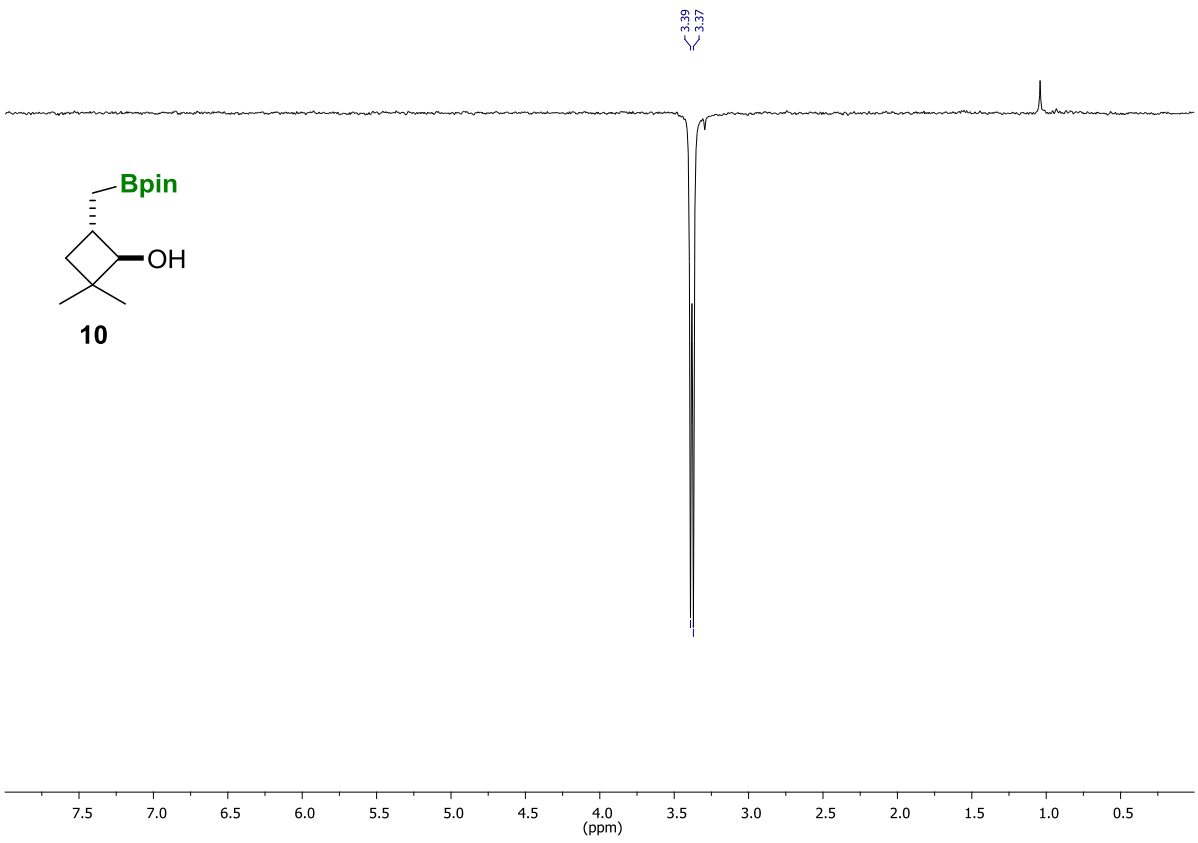

Bpin
OH
8
3.33
3.32
2.01
2.01
1.83
1.80
1.78
1.56
1.56
1.55
1.50
1.48
1.47
1.44
1.43
1.42
1.41
1.36
1.34
1.34
1.33
1.31
1.31
1.28
1.18
1.02
1.01
0.98
0.97
0.82
0.81
0.80
0.78
0.76
1.00
1.12
1.05
9.83
12.32
1.11
0.90
1.14
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)
83.35
81.80
42.12
39.41
36.64
34.07
29.93
26.40
24.84
23.32
23.09
22.55

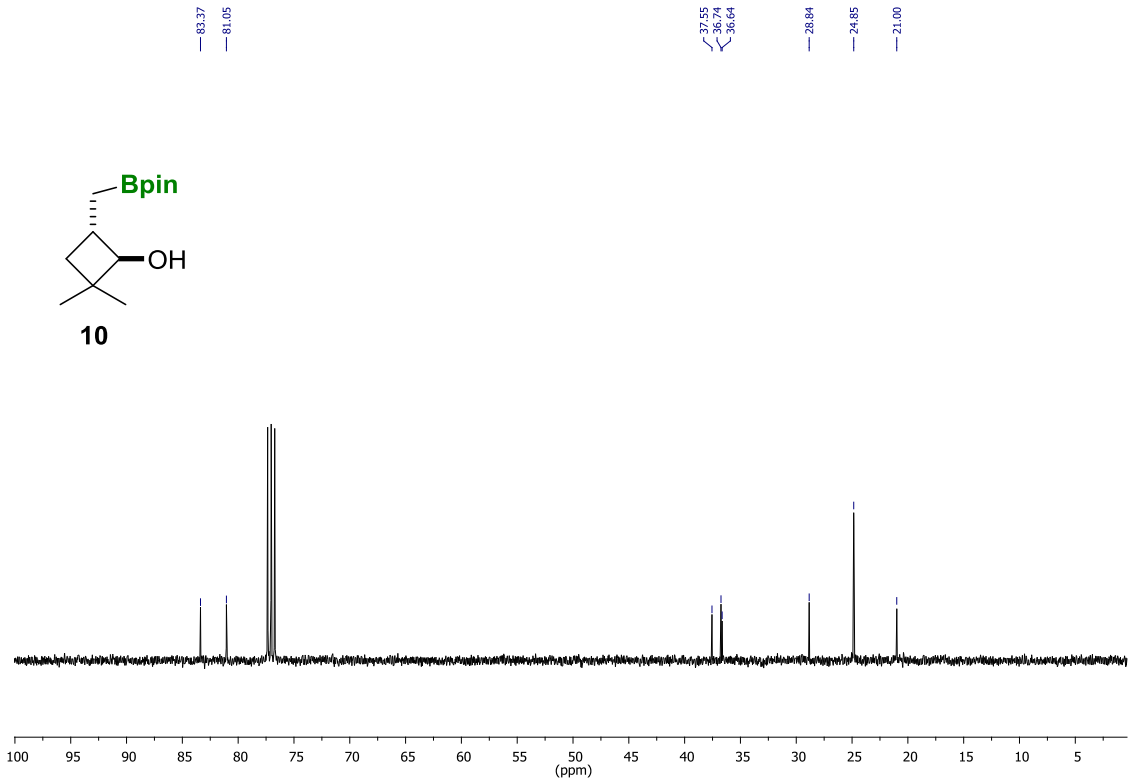

Bpin
OH
8
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
(ppm)

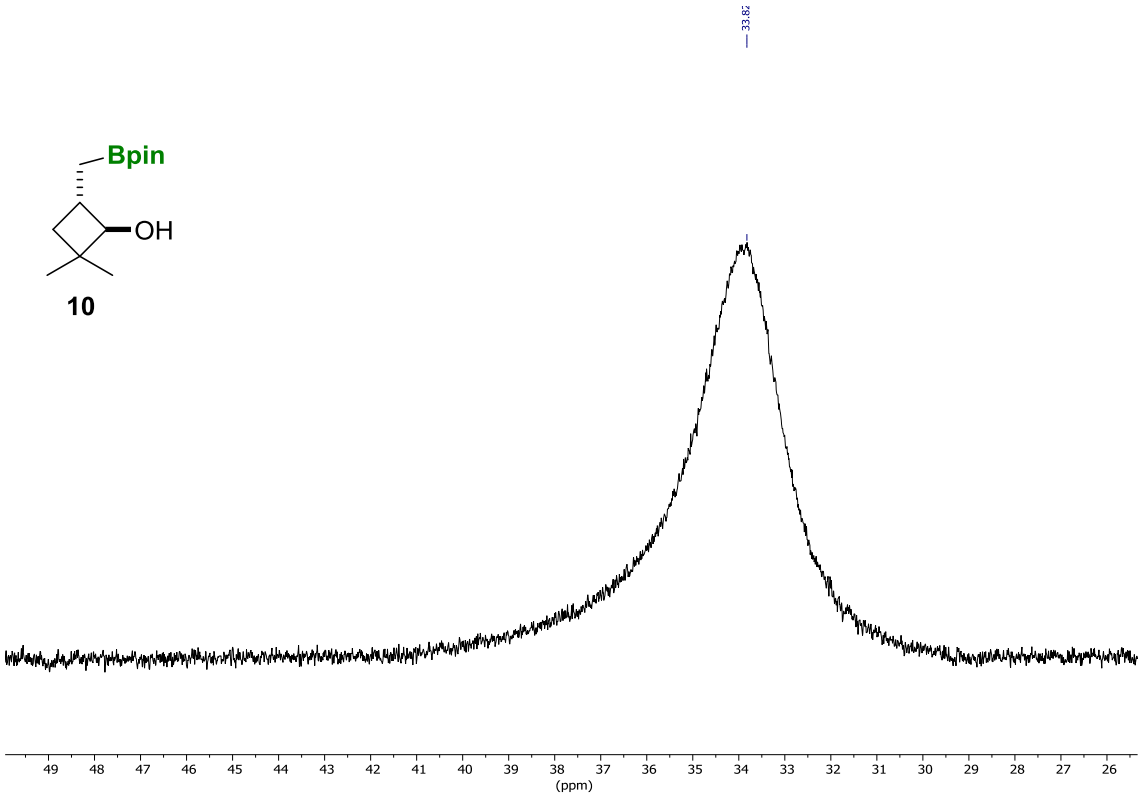

Bpin
OH
8
34.05
49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26
(ppm)

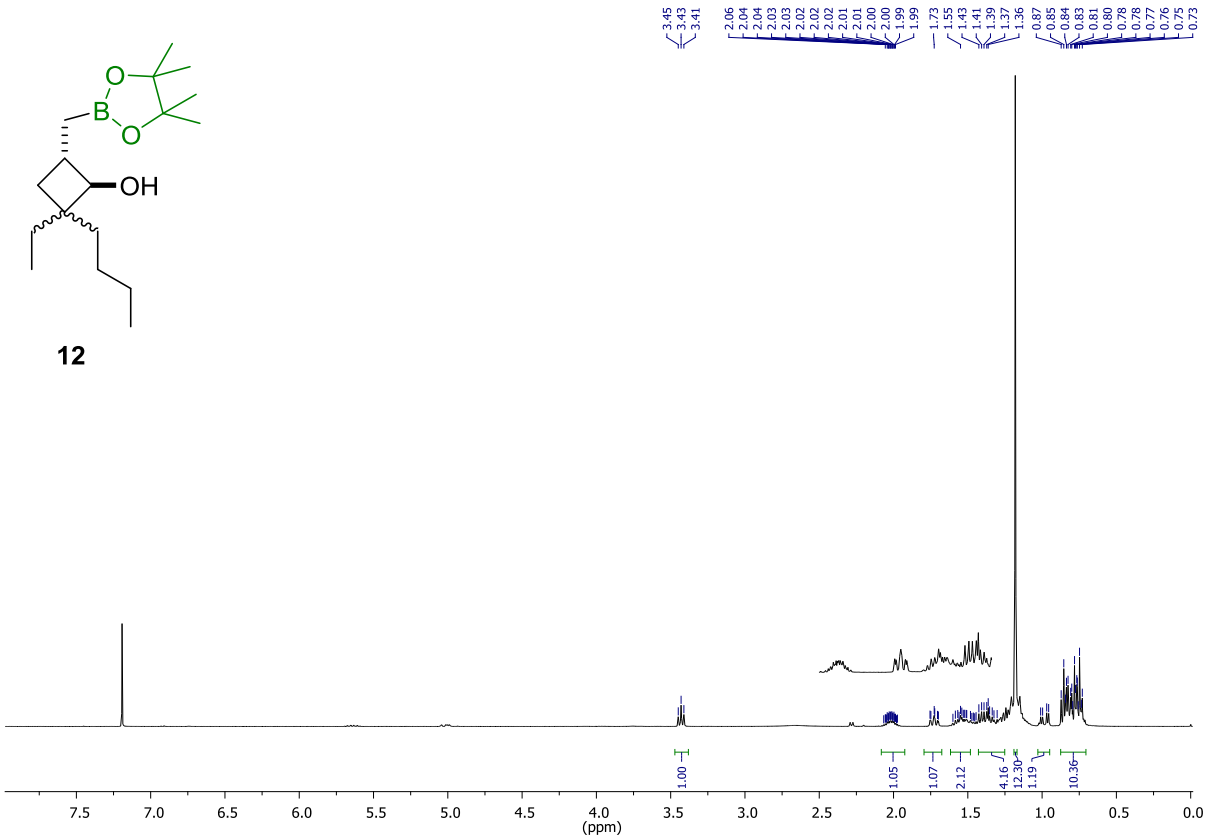

Bpin
OH
10
3.35
3.34
3.33
3.32
2.76
2.75
2.05
2.03
2.03
2.02
2.01
2.00
1.99
1.68
1.65
1.63
1.14
1.13
1.12
1.00
1.00
0.91
0.89
0.86
0.82
0.79
0.78
0.75
1.00
0.96
1.03
1.34
11.99
0.98
6.10
1.31
1.33
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

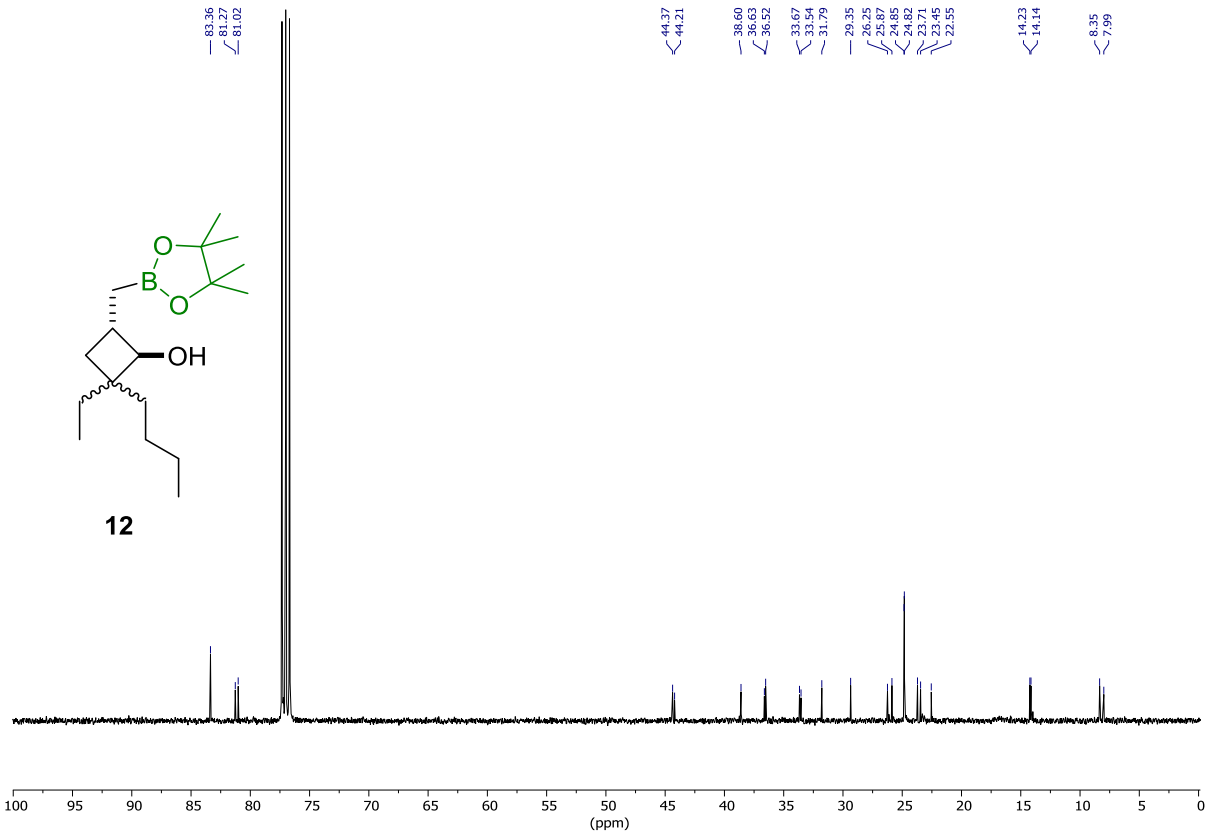

Bpin
OH
10
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
(ppm)

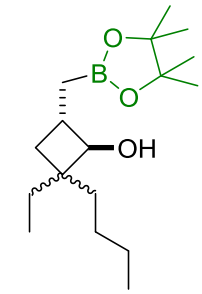

3.39
3.37
Bpin
OH
10
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


83.37
81.05
37.55
36.74
36.64
28.84
24.85
21.00
Bpin
OH
10
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)

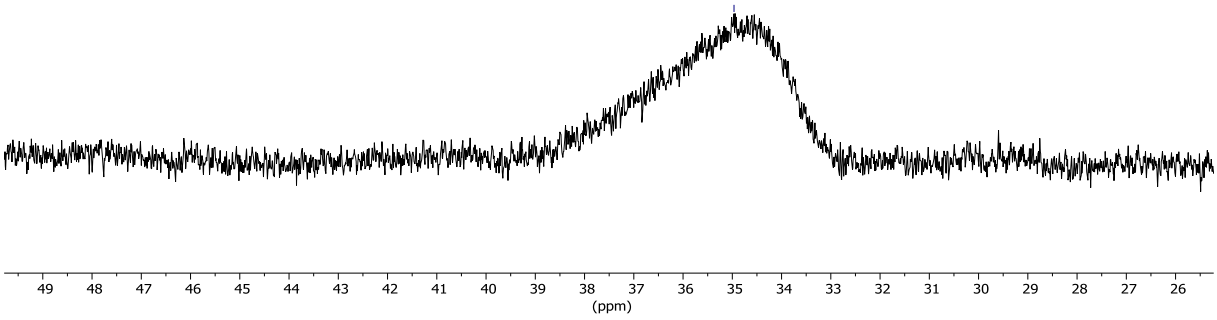

33.82
Bpin
OH
10
49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26
(ppm)

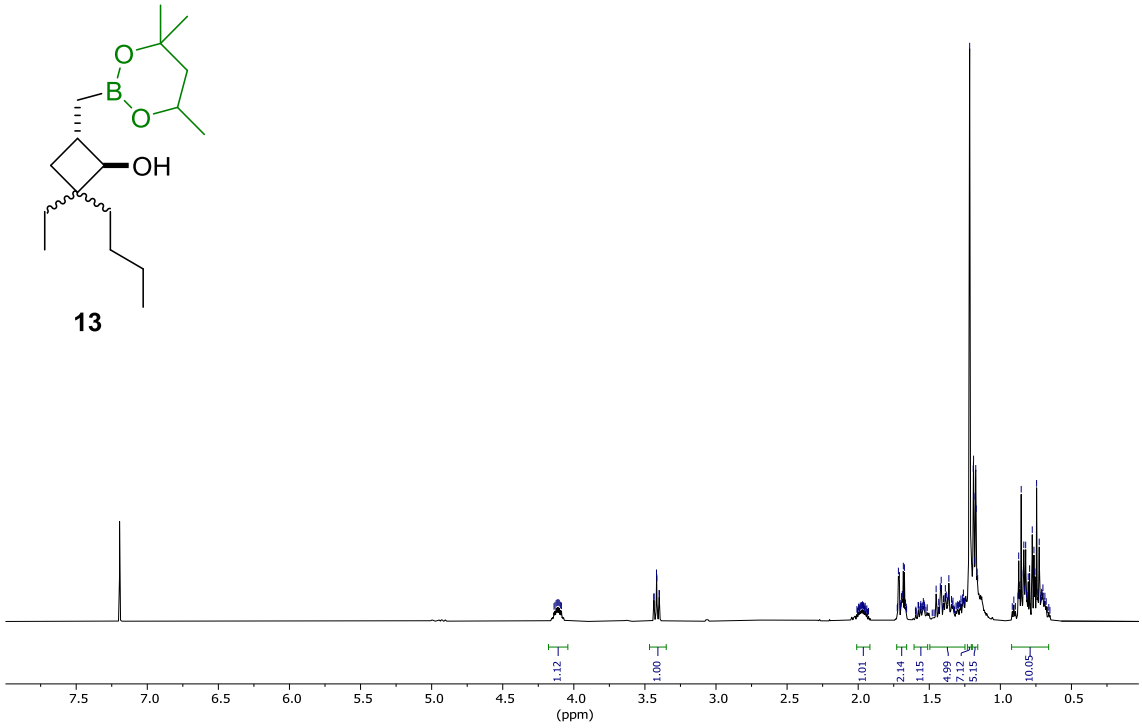

O
B
O
OH
12
3.45
3.43
3.41
2.06
2.04
2.04
2.03
2.03
2.02
2.02
2.02
2.01
2.01
2.00
2.00
1.99
1.99
1.73
1.55
1.43
1.41
1.39
1.37
1.36
0.87
0.85
0.84
0.83
0.81
0.80
0.78
0.78
0.77
0.76
0.75
0.73
1.00
1.05
1.07
2.12
4.16
12.30
1.19
10.36
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)


83.36
81.27
81.02
44.37
44.21
38.60
36.63
36.52
33.67
33.54
31.79
29.35
26.25
25.67
24.85
24.82
23.71
23.45
22.55
14.23
14.14
8.35
7.99
O
B
O
OH
12
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
(ppm)

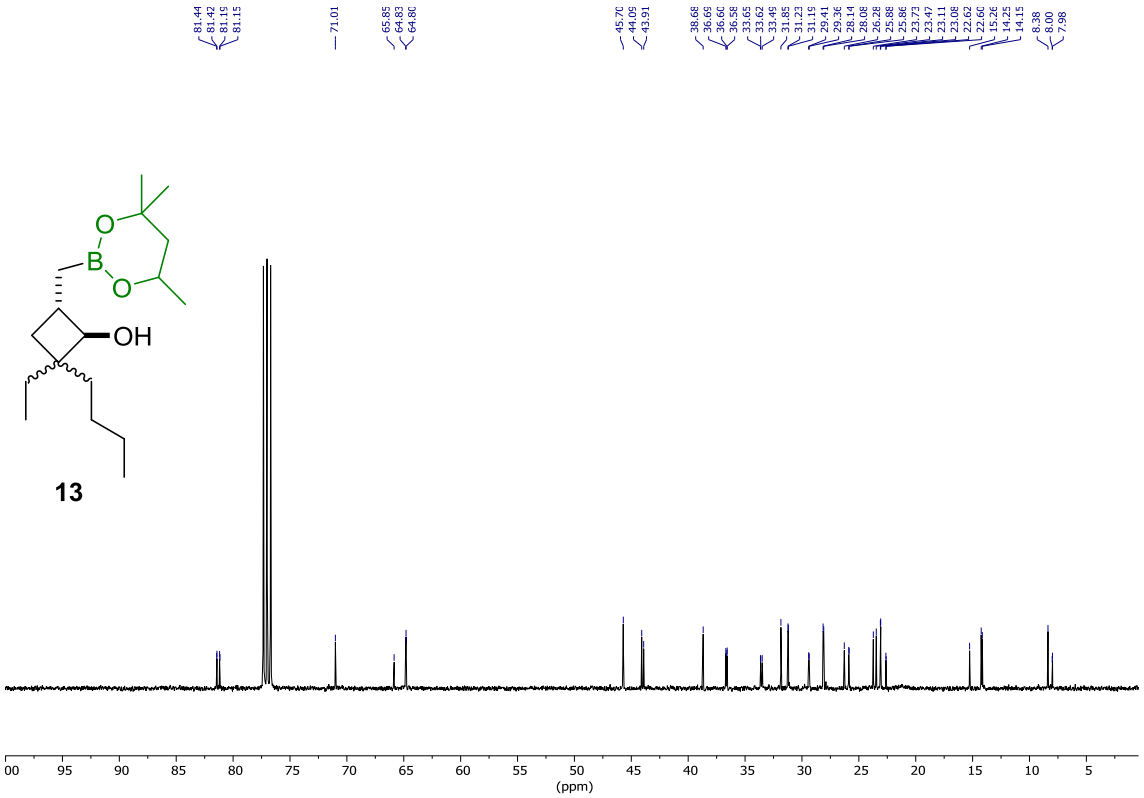

O
B
O
OH

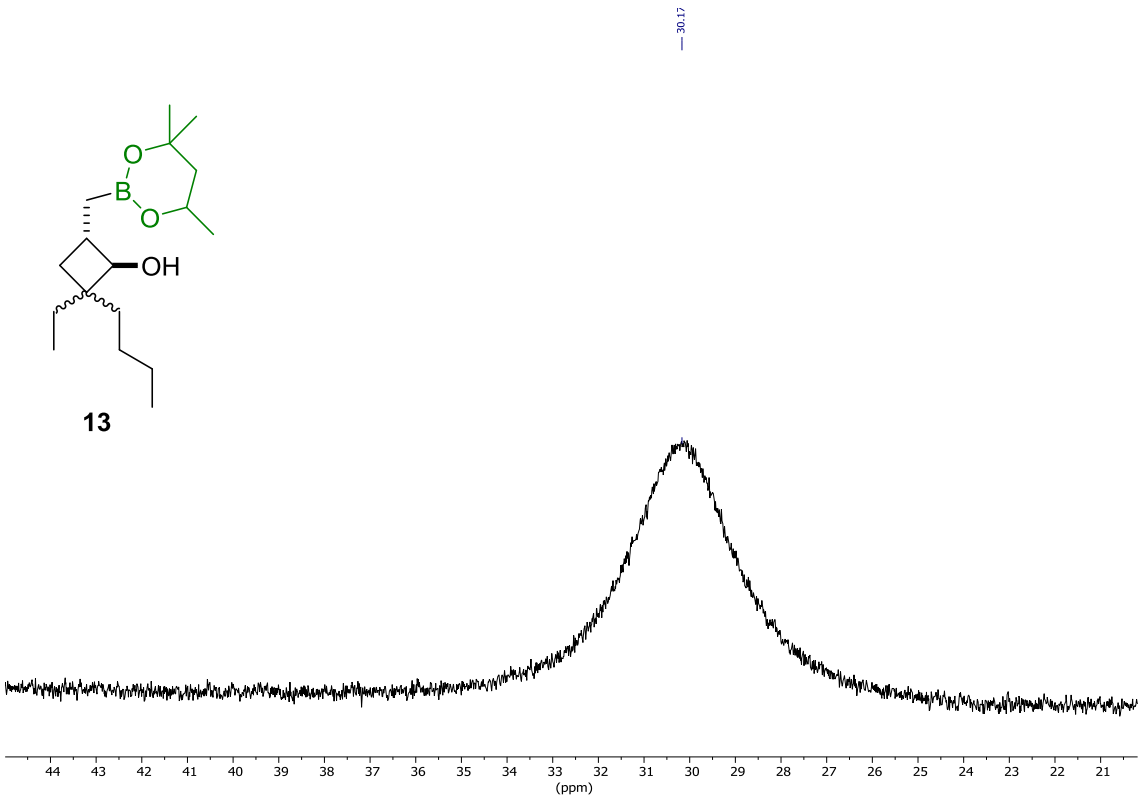
12

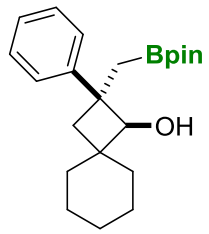

34.97
49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26
(ppm)


O
B
O
OH
1.12
1.00
1.01
2.14
1.15
4.99
7.12
5.15
10.05
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

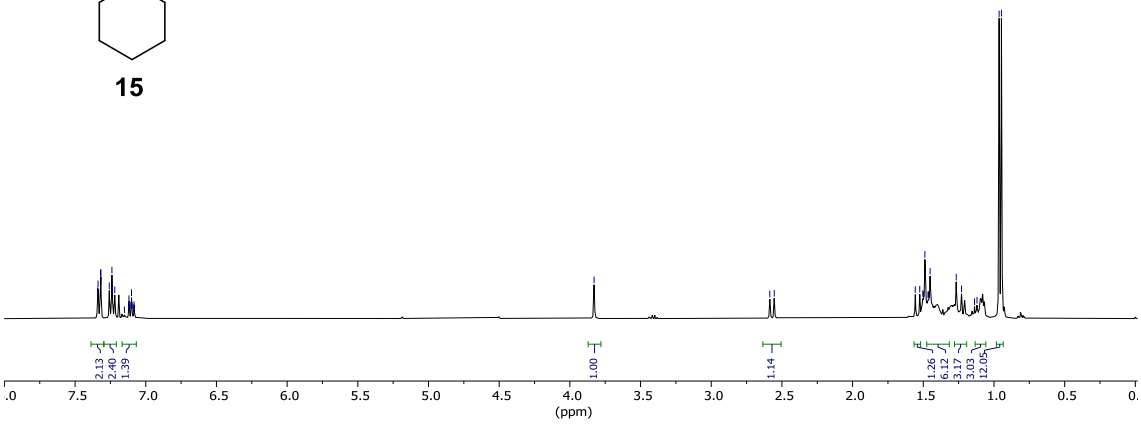
13

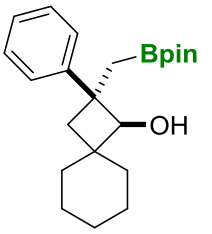

81.44
81.42
81.19
81.15
71.01
65.85
64.83
64.80
45.70
44.05
43.91
38.68
36.69
36.60
36.58
33.65
33.62
33.46
33.45
31.23
31.19
29.41
29.36
28.14
28.08
26.28
25.88
25.86
23.73
23.47
23.08
22.62
22.56
15.26
14.25
14.15
8.38
8.00
7.98
O
B
O
OH
13
00 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)


30.17
O
B
O
OH
13
44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21
(ppm)

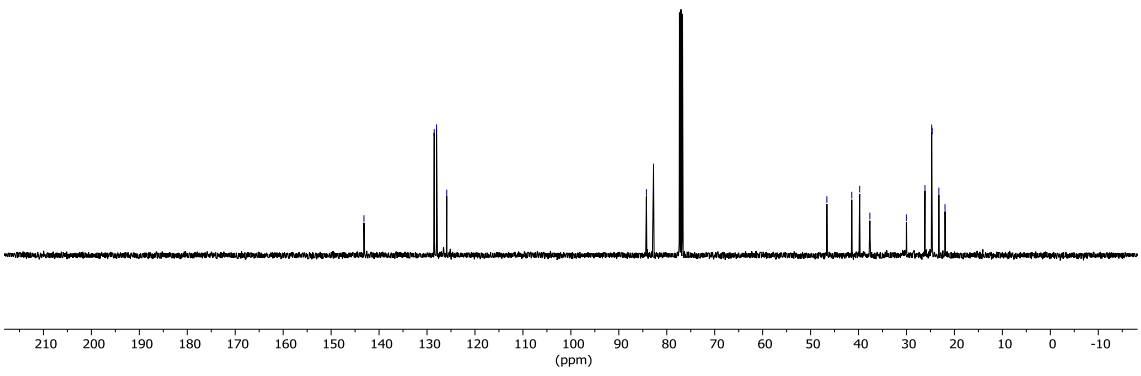


15



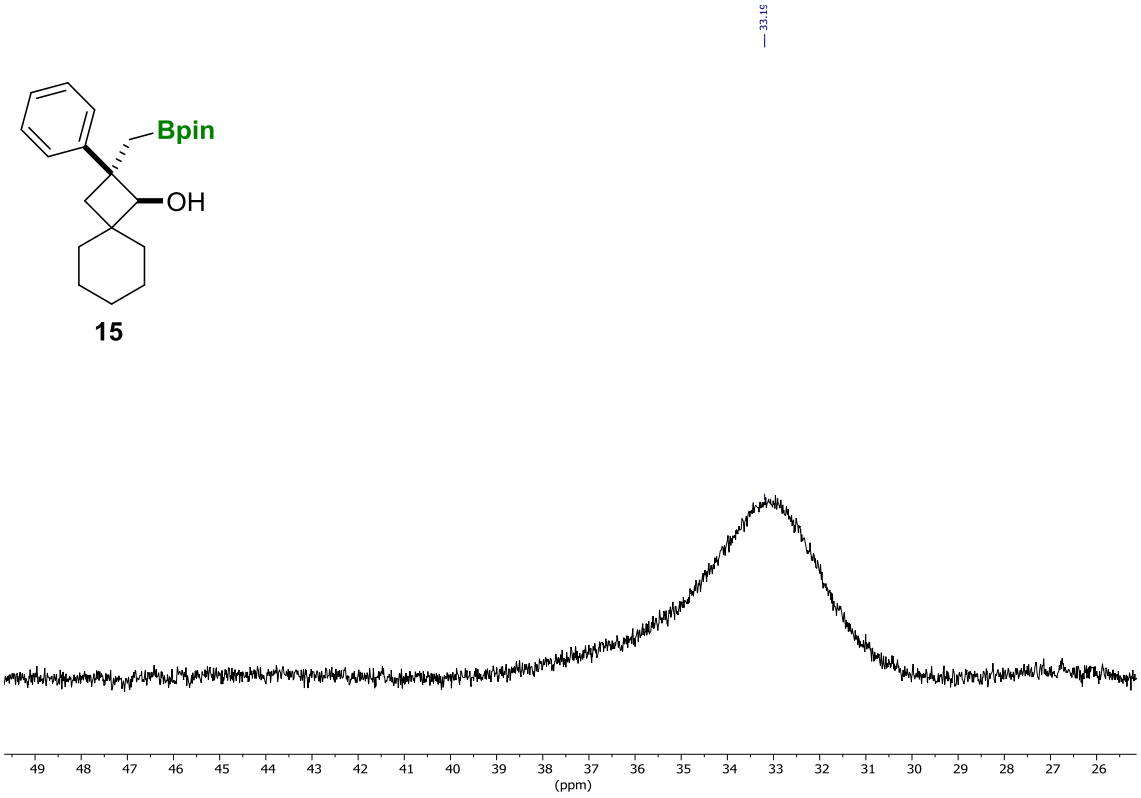


15

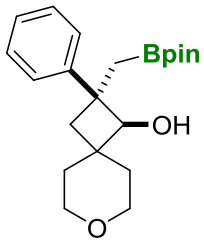


Bpin
OH

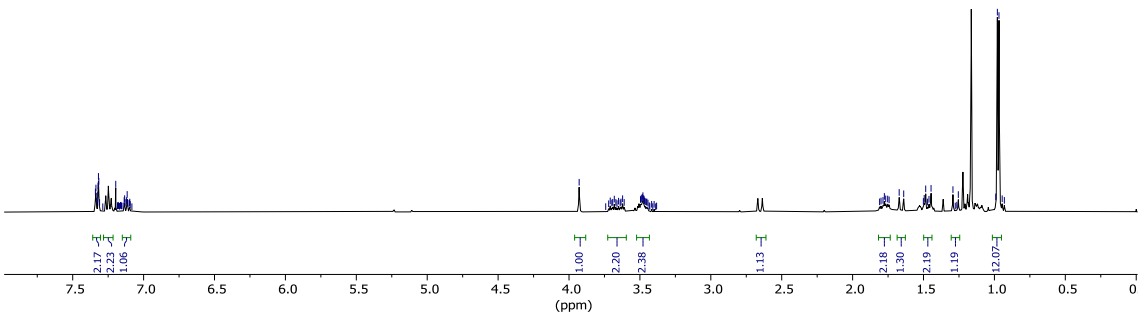
15

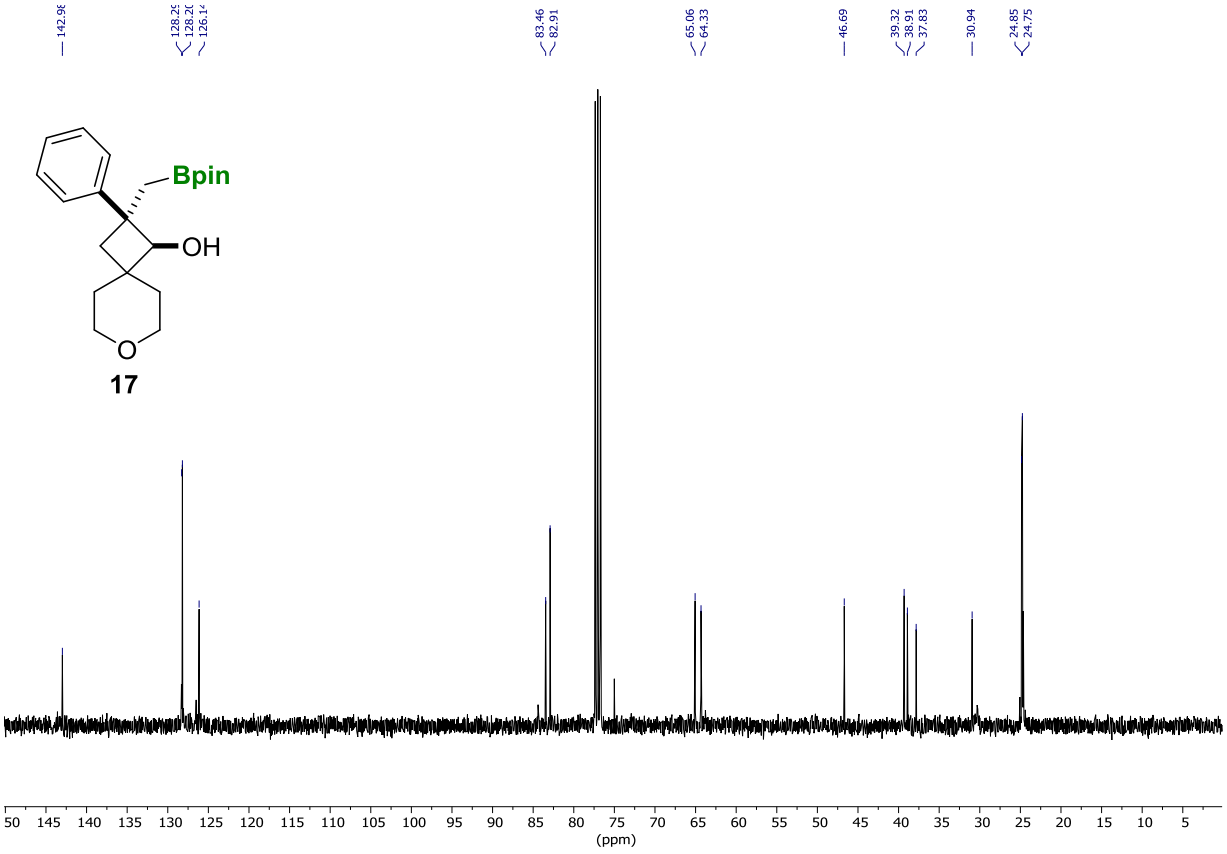

33.15
49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26
(ppm)

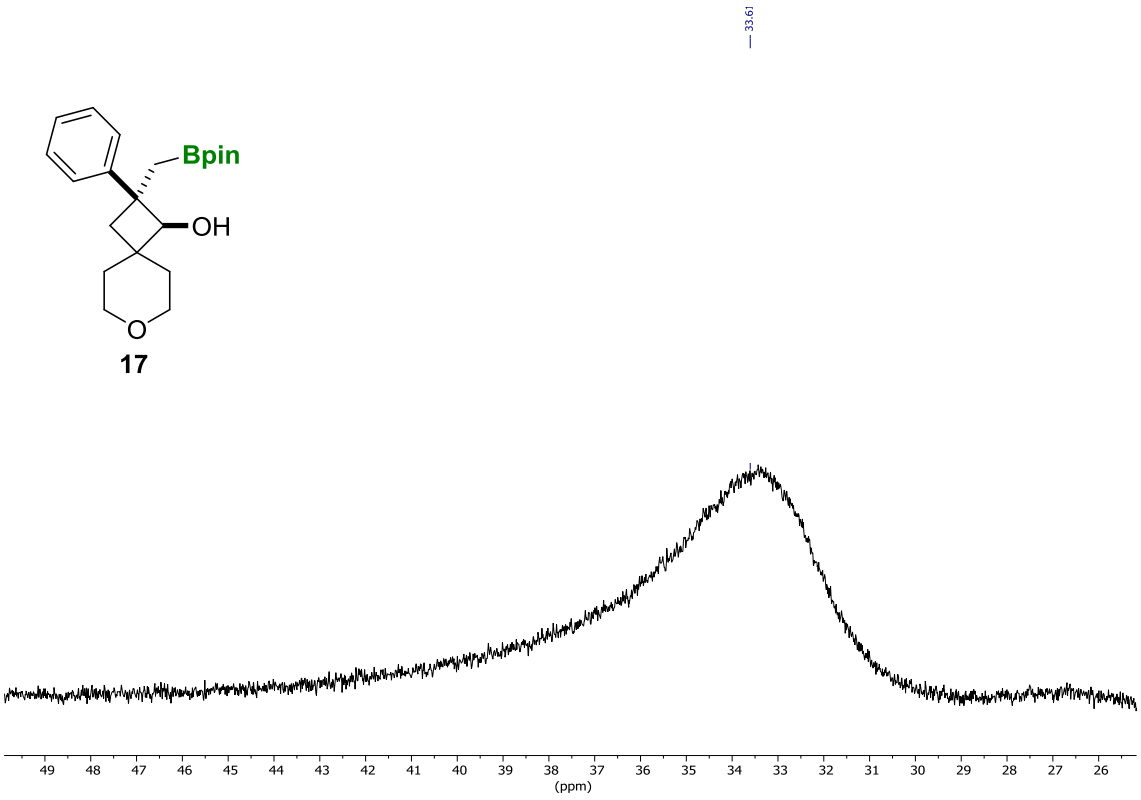

7.34 7.34 7.33 7.32 7.32 7.32 7.32 7.31 7.28 7.20 7.18 7.18 7.18 7.17 7.16 7.16 7.16 7.14 7.14 7.13 7.12 7.12 7.11 7.10 7.06 7.06
3.93 3.74 3.72 3.71 3.70 3.68 3.68 3.67 3.66 3.65 3.64 3.63 3.62 3.61 3.50 3.46 3.46 3.48 3.48 3.47 3.47 3.46 3.45 3.45 3.44 3.43 3.43 3.42 3.41 3.40 3.39 3.38
1.81 1.80 1.79 1.78 1.77 1.75 1.74 1.67 1.64 1.50 1.50 1.48 1.47 1.46 1.45 1.29 1.28 1.27 1.23 0.98 0.98 0.97 0.95 0.93

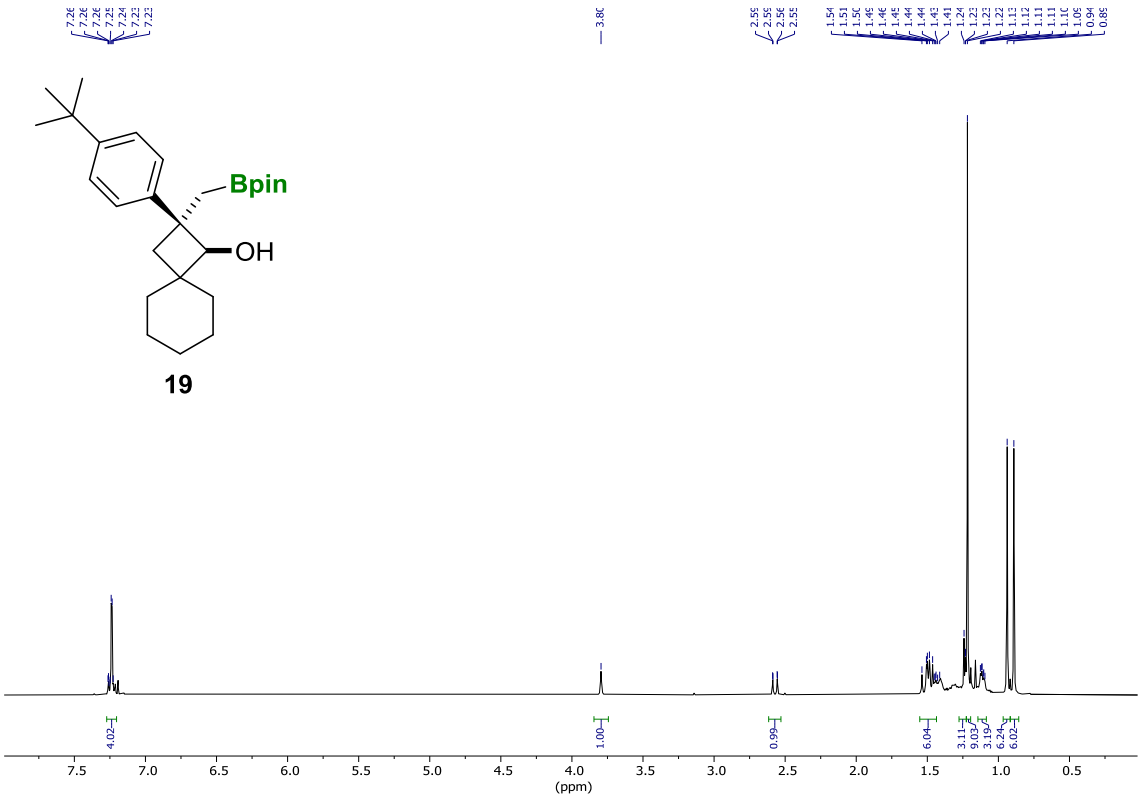

Bpin
OH
O

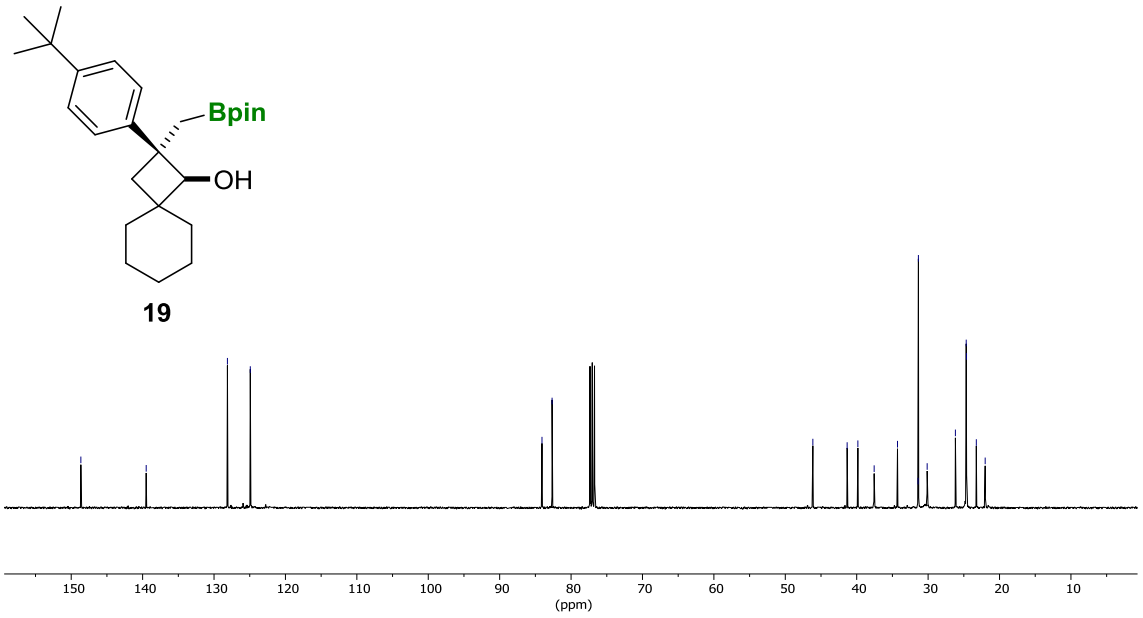
17

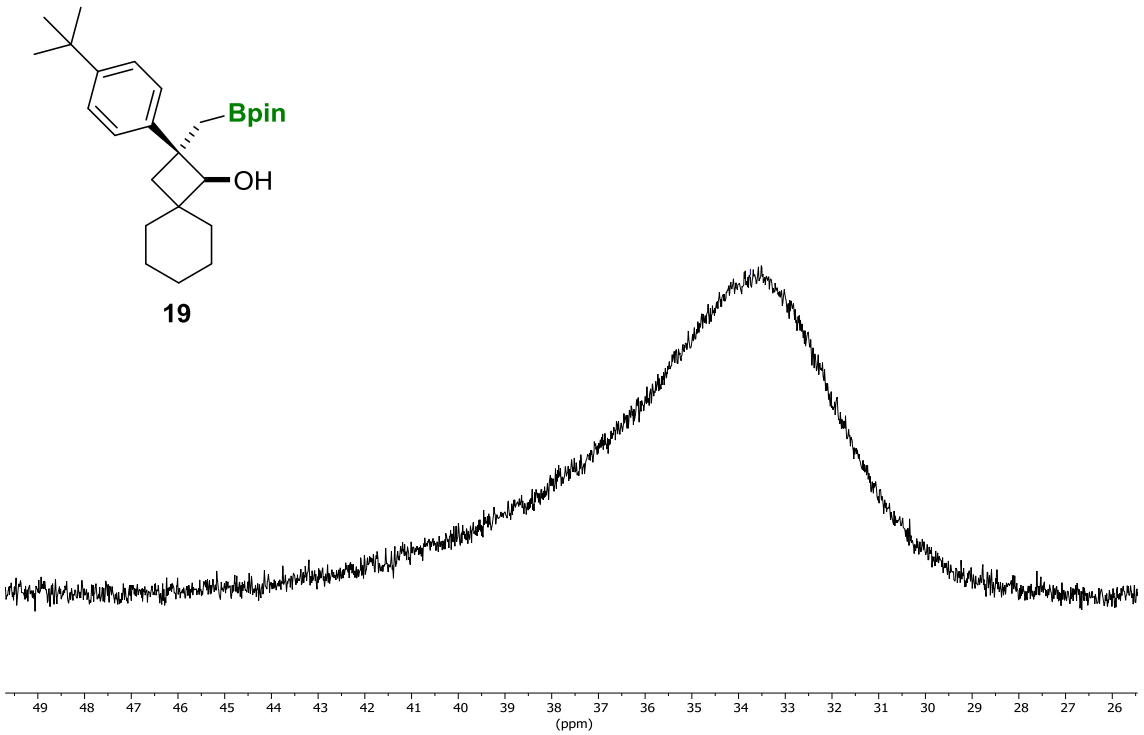

2.17
2.23
1.06
1.00
2.20
2.38
1.13
2.18
1.30
2.19
1.19
12.07
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
(ppm)

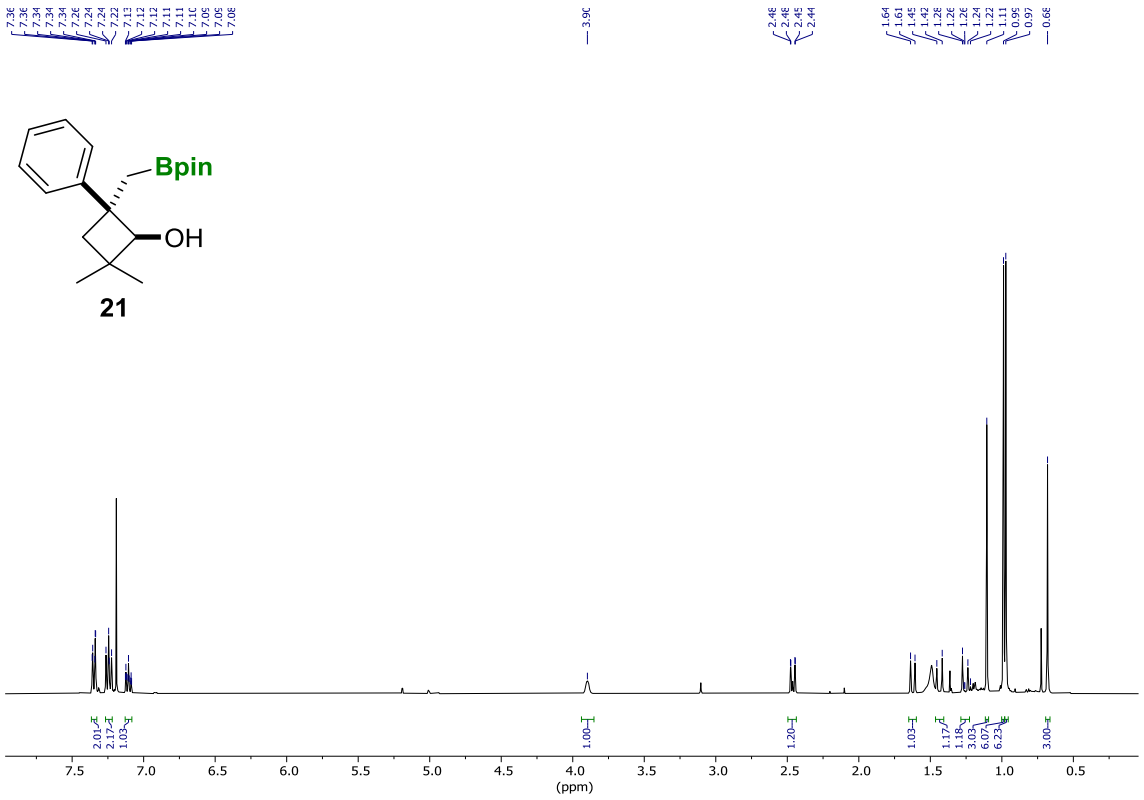

142.98
128.25
128.20
126.14
83.46
82.91
65.06
64.33
46.69
39.32
38.91
37.83
30.94
24.85
24.75
Bpin
OH
O
17
50 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)

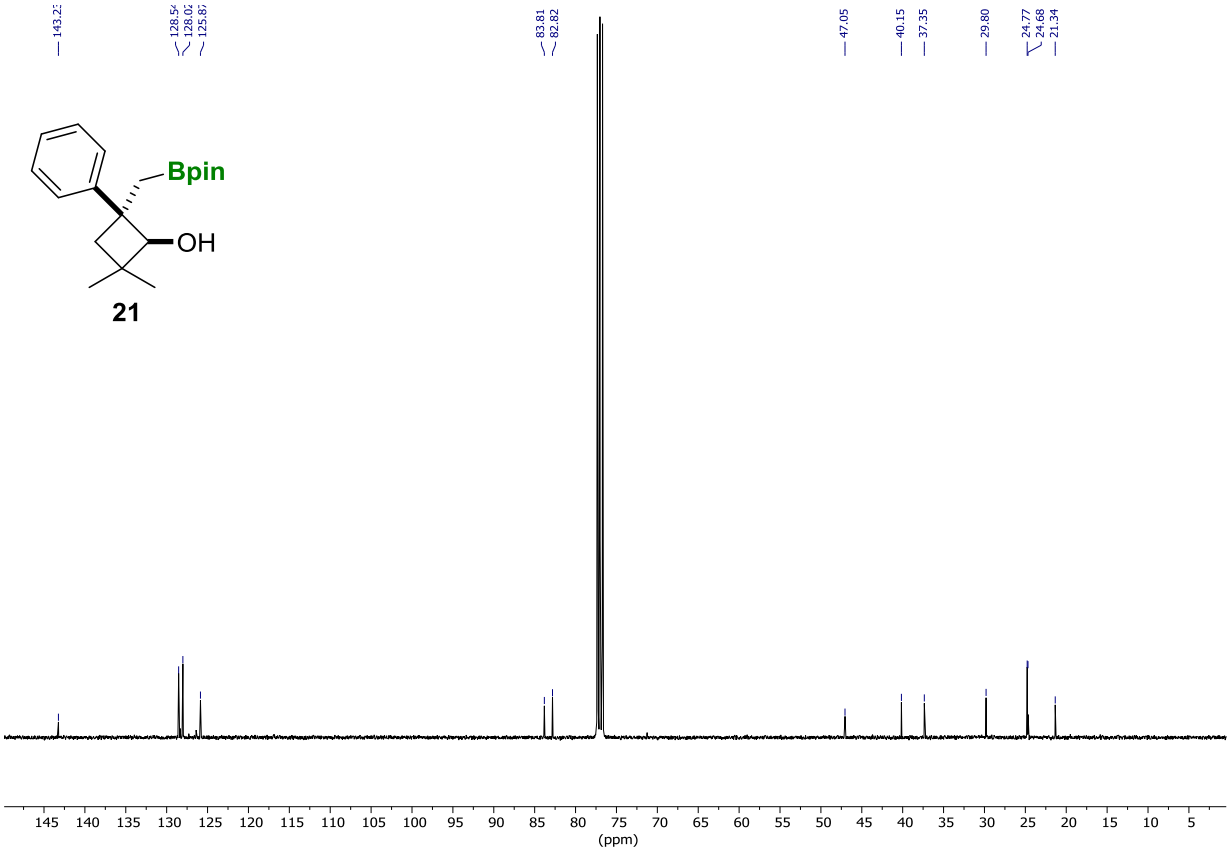

33.61
Bpin
OH
O
17
49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26
(ppm)

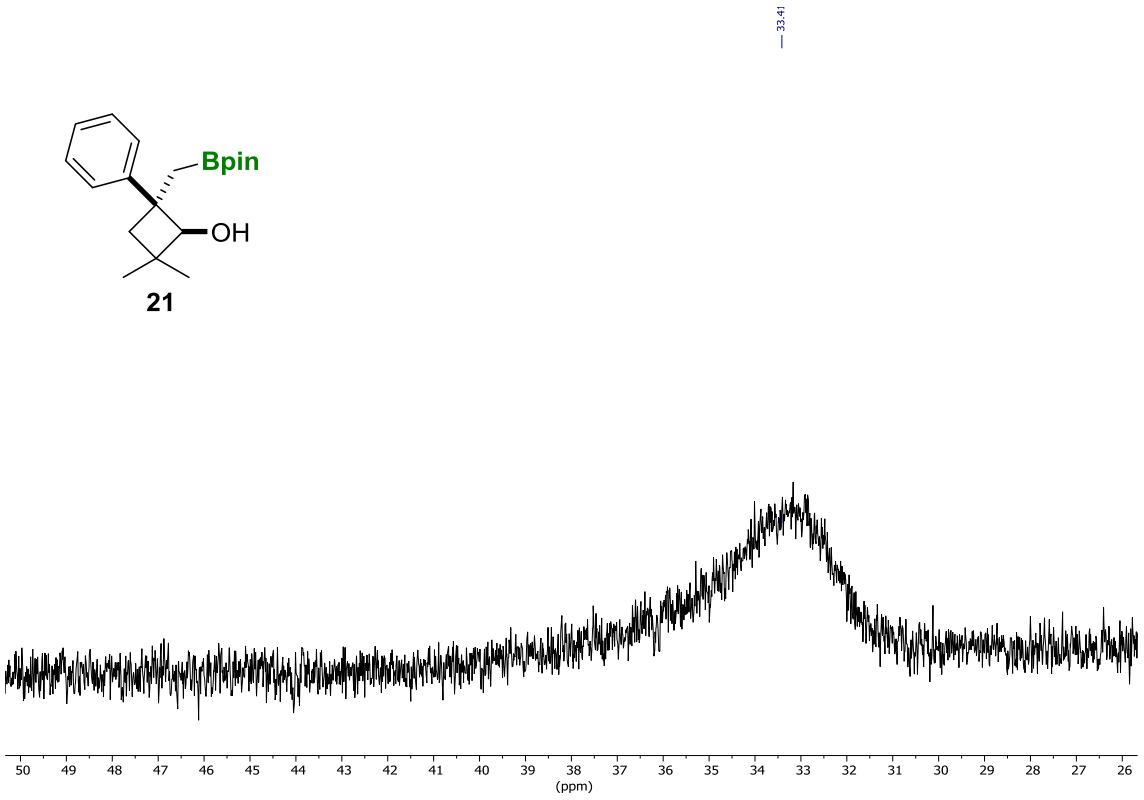

Bpin
OH
19
(ppm)

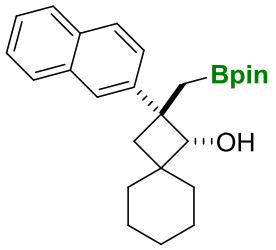

Bpin
OH
19
(ppm)


Bpin
OH
19
33.75
49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26
(ppm)

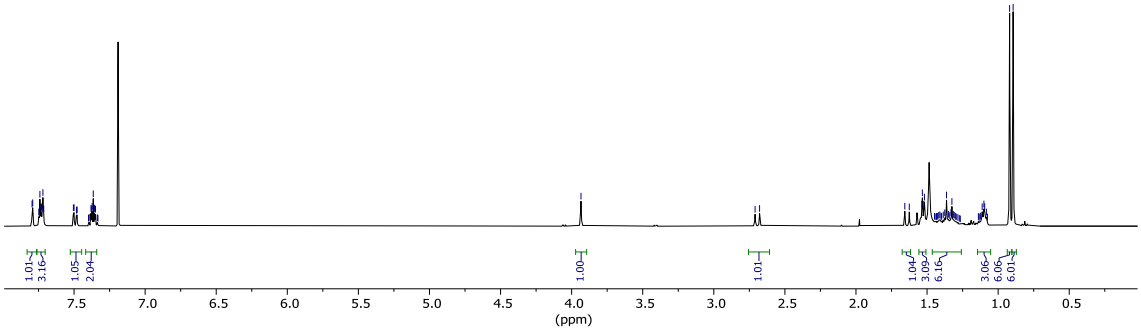

Bpin
OH
21
7.36 7.36 7.34 7.34 7.34 7.24 7.24 7.24 7.22 7.13 7.12 7.12 7.11 7.11 7.10 7.05 7.05 7.04
3.90
2.46 2.46 2.45 2.44
1.64 1.61 1.45 1.43 1.26 1.26 1.24 1.22 1.11 0.95 0.97 0.68
2.01 2.17 1.03 1.00 1.20 1.03 1.17 1.18 3.03 6.07 6.23 3.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

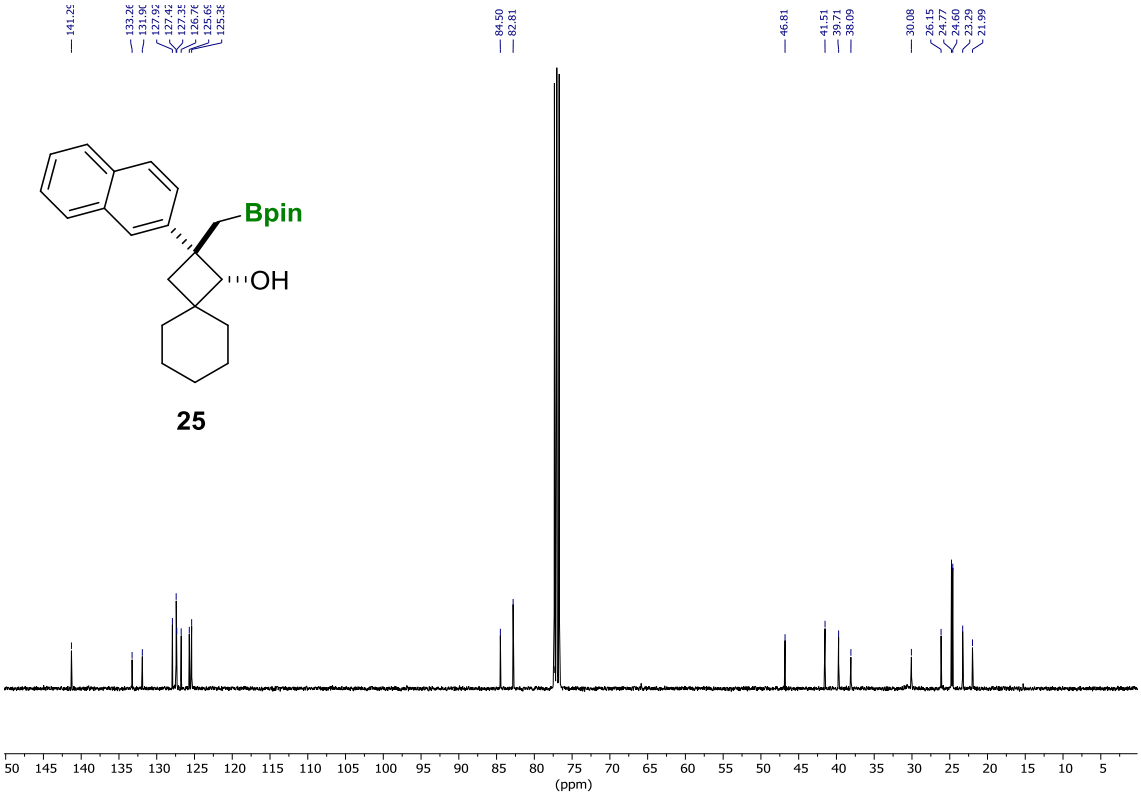

143.22
128.54
128.02
125.87
83.81
82.82
47.05
40.15
37.35
29.80
24.77
24.68
21.34
Bpin
OH
21
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)


33.41
Bpin
OH
21
50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26
(ppm)


Bpin
OH

25

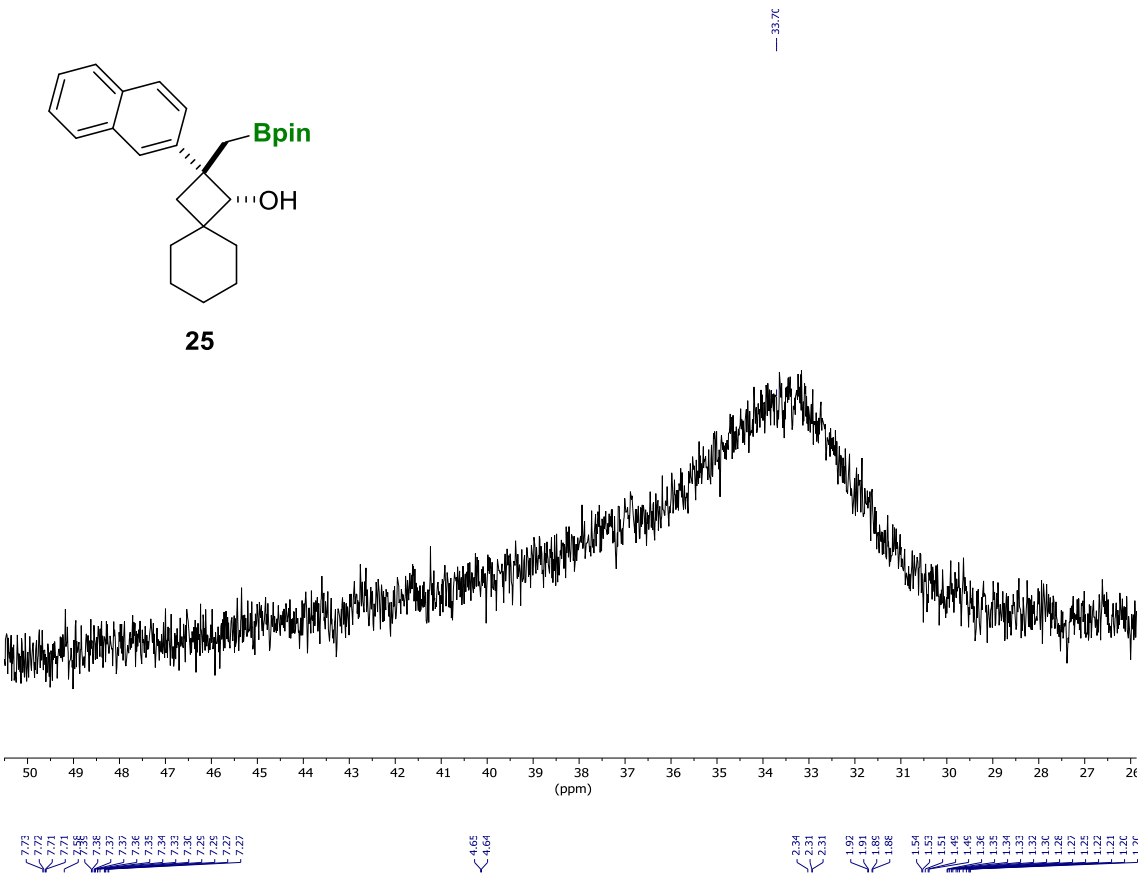

1.01
3.16
1.05
2.04
1.00
1.01
1.04
3.09
6.16
3.06
6.06
6.01
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

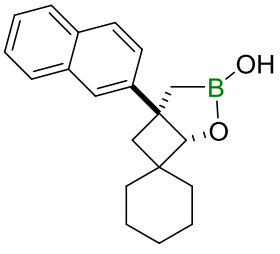

141.2
133.2
131.9
127.9
127.4
127.3
126.7
125.6
125.3
84.50
82.81
46.81
41.51
39.71
38.09
30.08
26.15
24.77
24.60
23.29
21.99
Bpin
OH
50
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
(ppm)

25

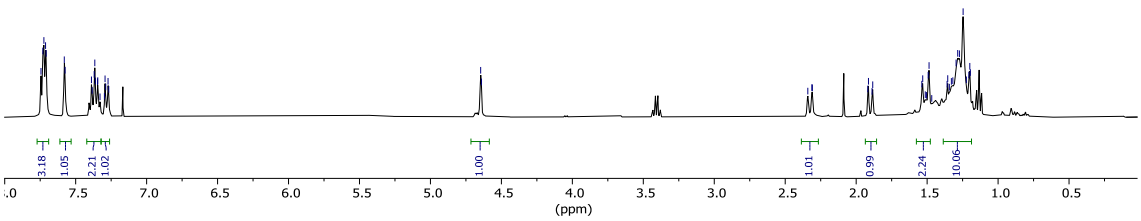
Bpin
OH

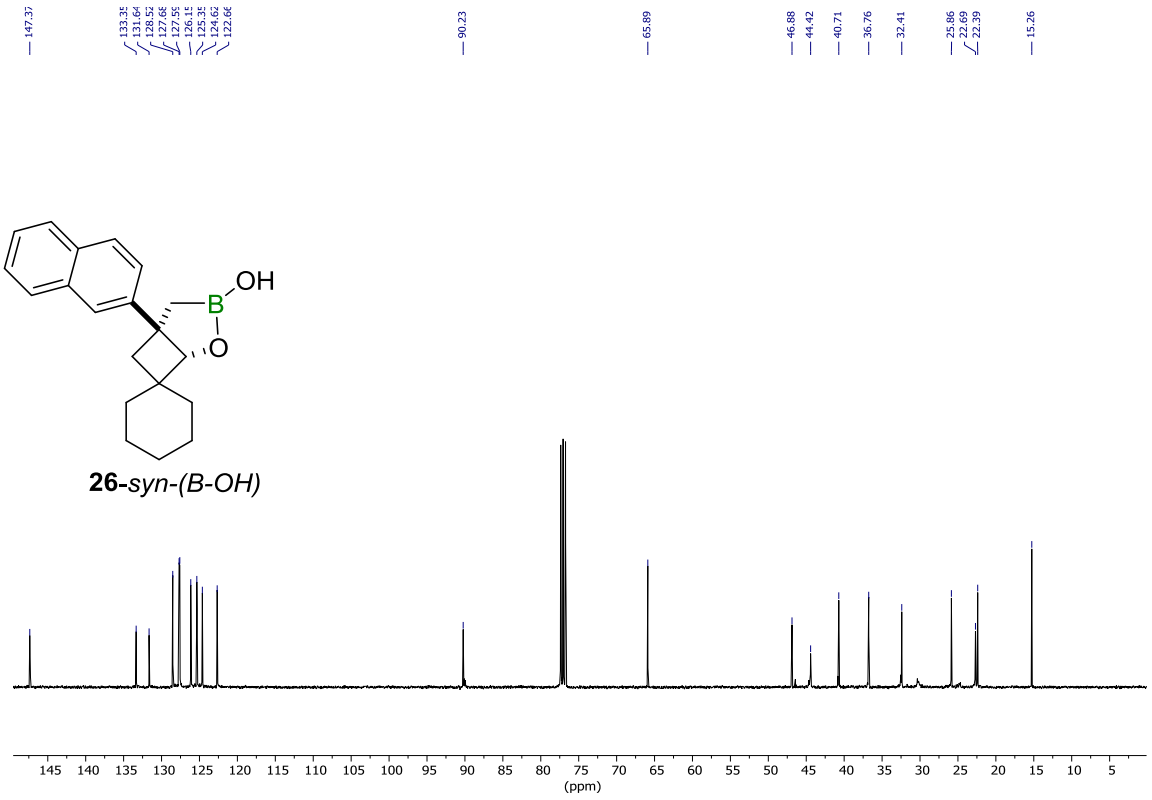
25


50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27
(ppm)

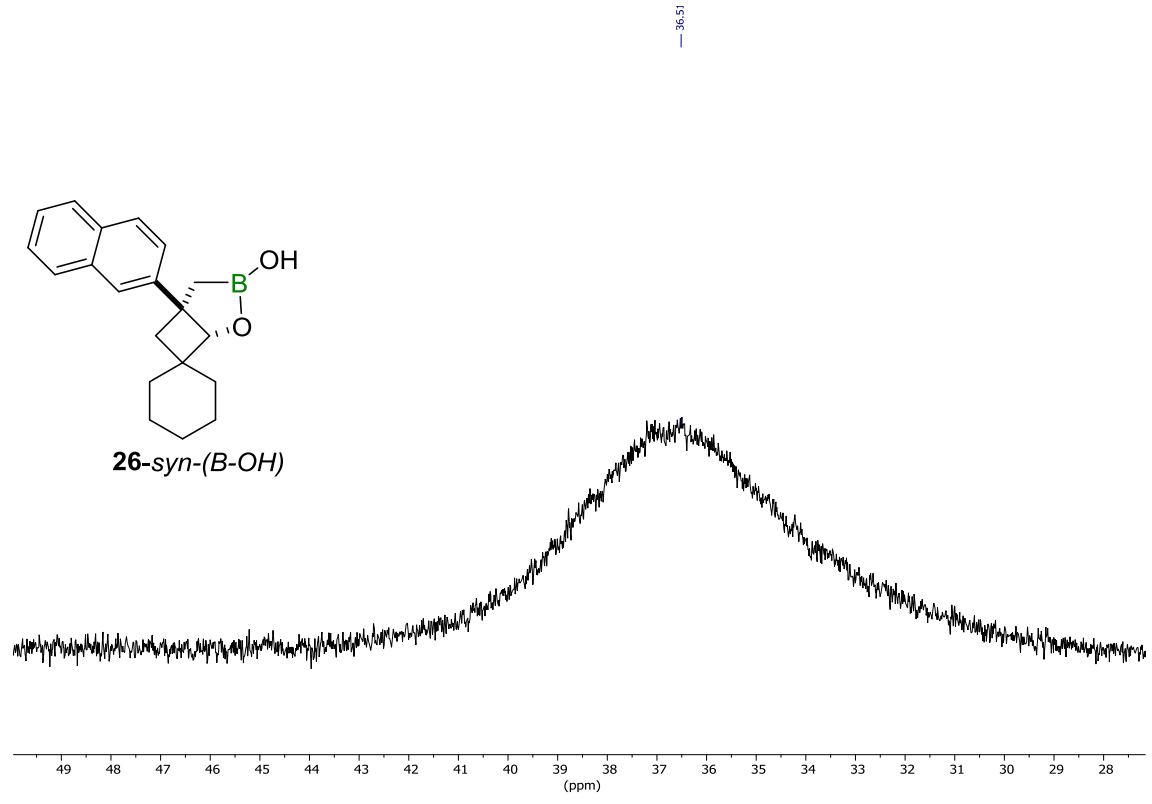

OH
B
O

26-*syn-(B-OH)*

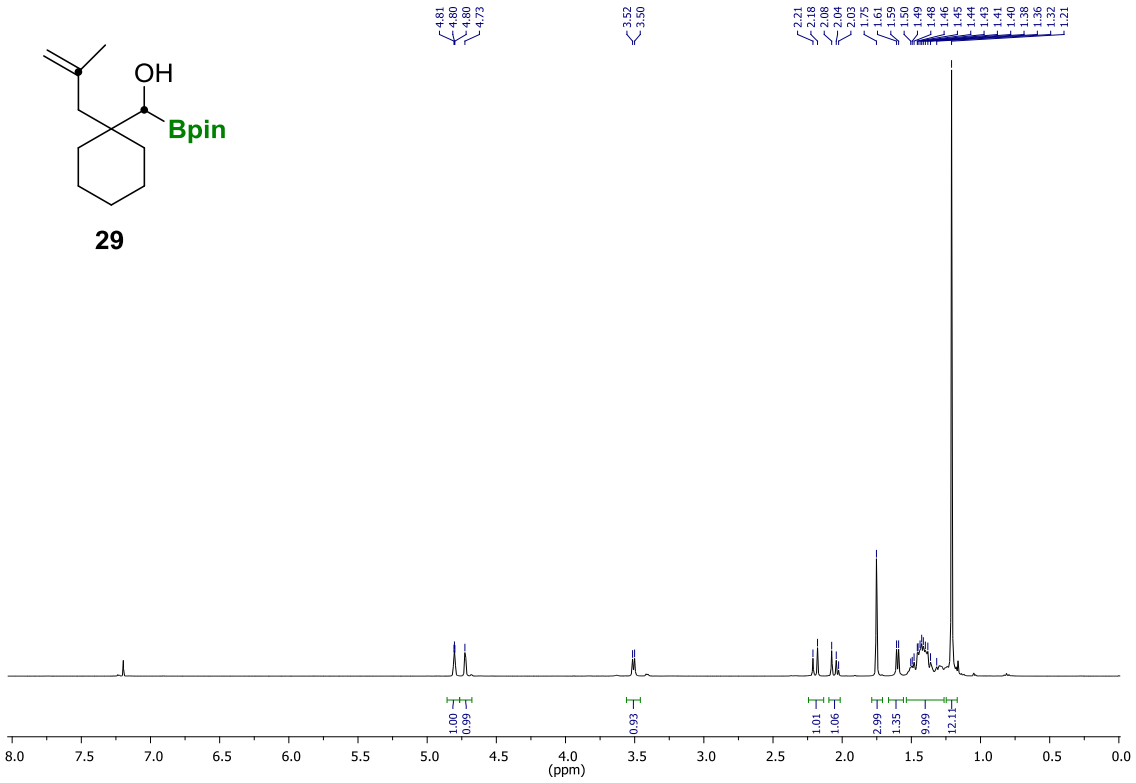

3.18
1.05
2.21
1.02
1.00
1.01
0.99
2.24
10.06
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

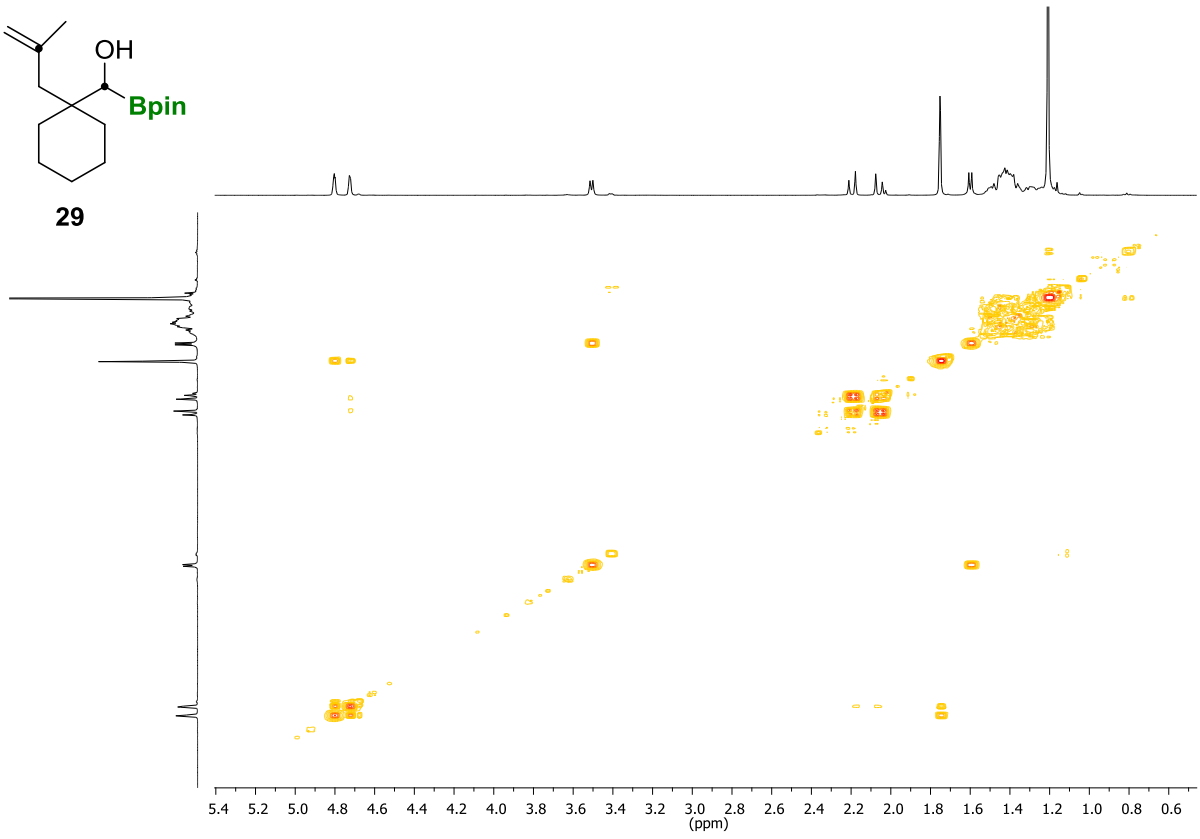


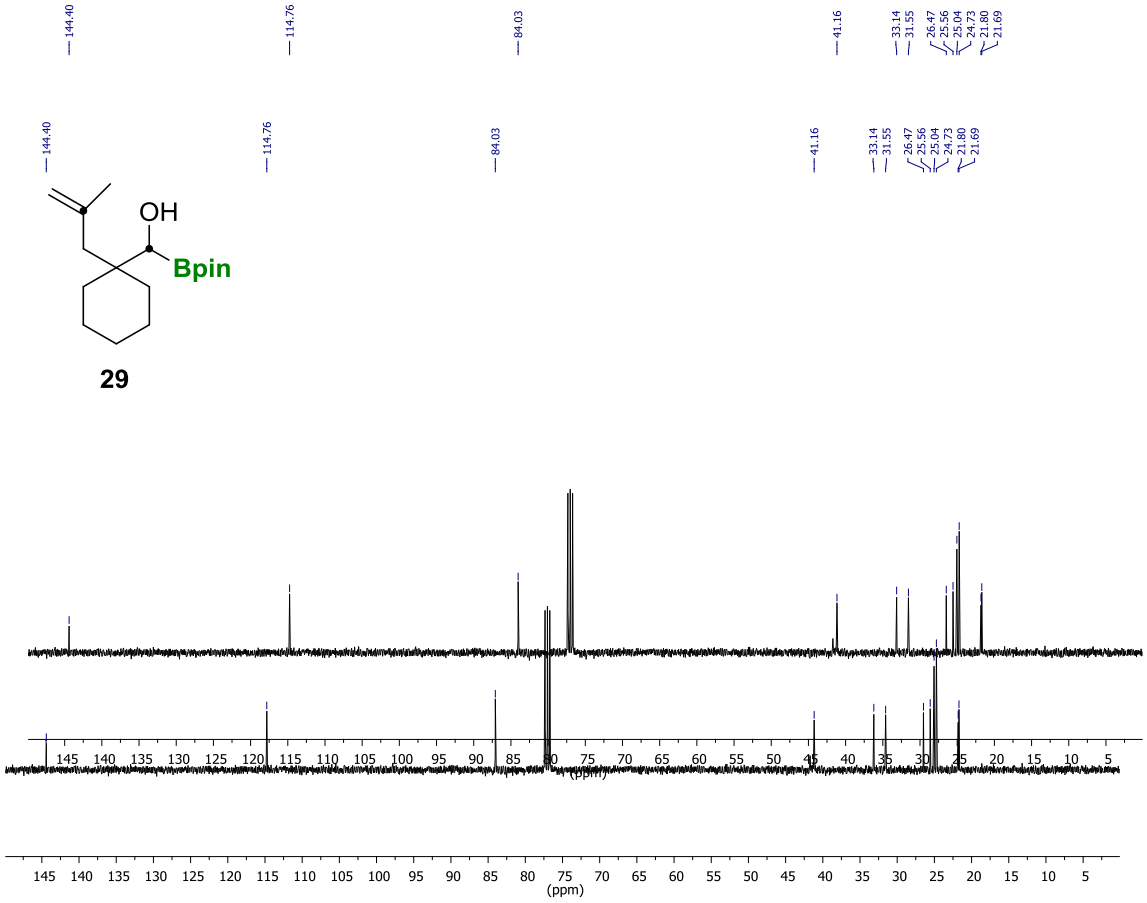
26-*syn-(B-OH)*

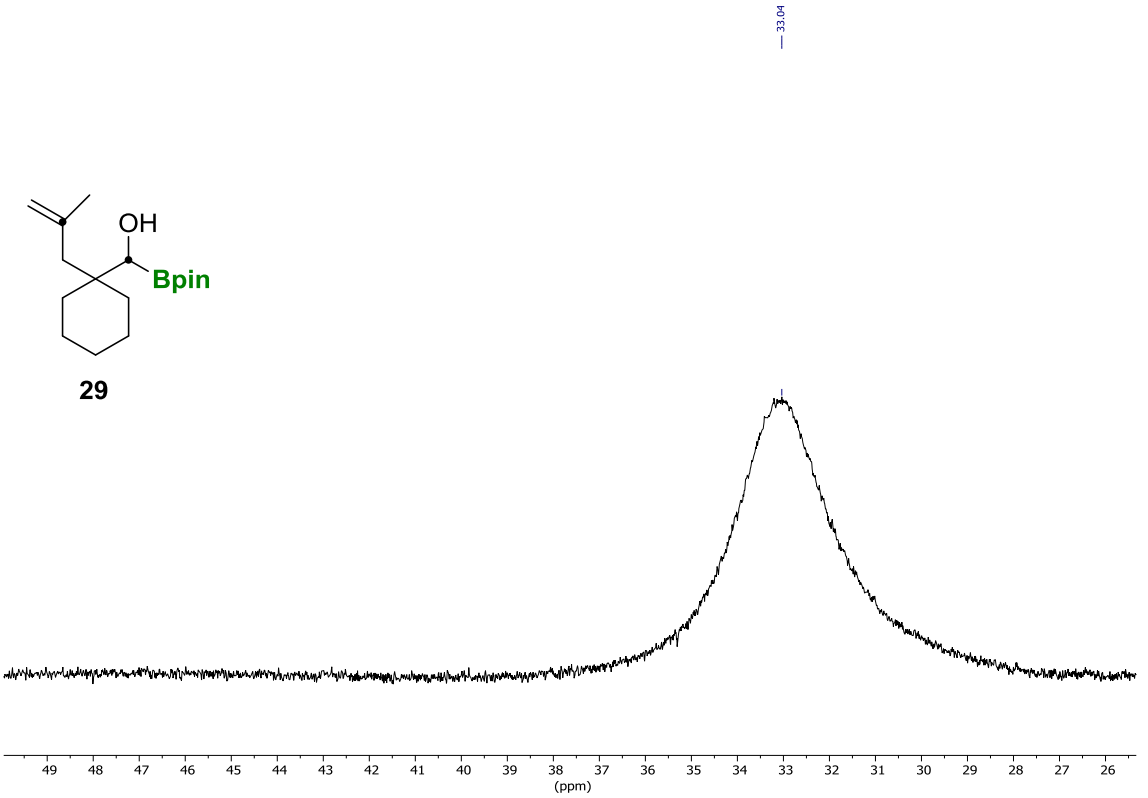


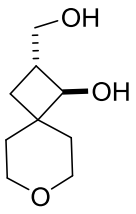
26-*syn-(B-OH)*


OH
Bpin
29
4.81
4.80
4.80
4.73
3.52
3.50
2.21
2.18
2.08
2.04
2.03
1.75
1.61
1.59
1.50
1.49
1.48
1.46
1.45
1.44
1.43
1.41
1.40
1.38
1.36
1.32
1.21
1.00
0.99
0.93
1.01
1.06
2.99
1.35
9.99
12.11
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

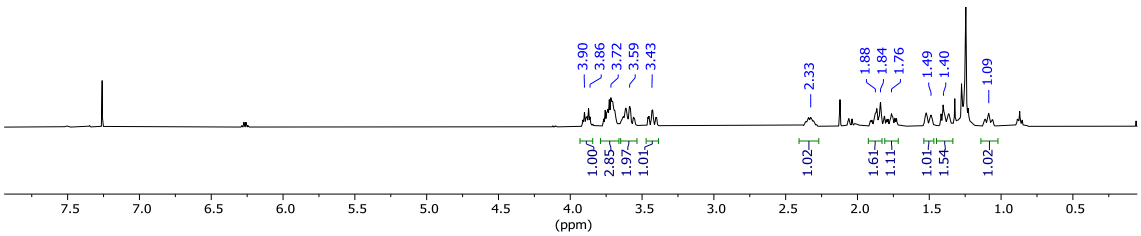

OH
Bpin
29
5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6
(ppm)

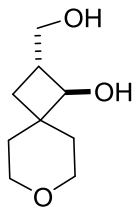

144.40
114.76
84.03
41.16
33.14
31.55
26.47
25.56
25.04
24.73
21.80
21.69
OH
Bpin
29
(ppm)


33.04
OH
Bpin
29
(ppm)

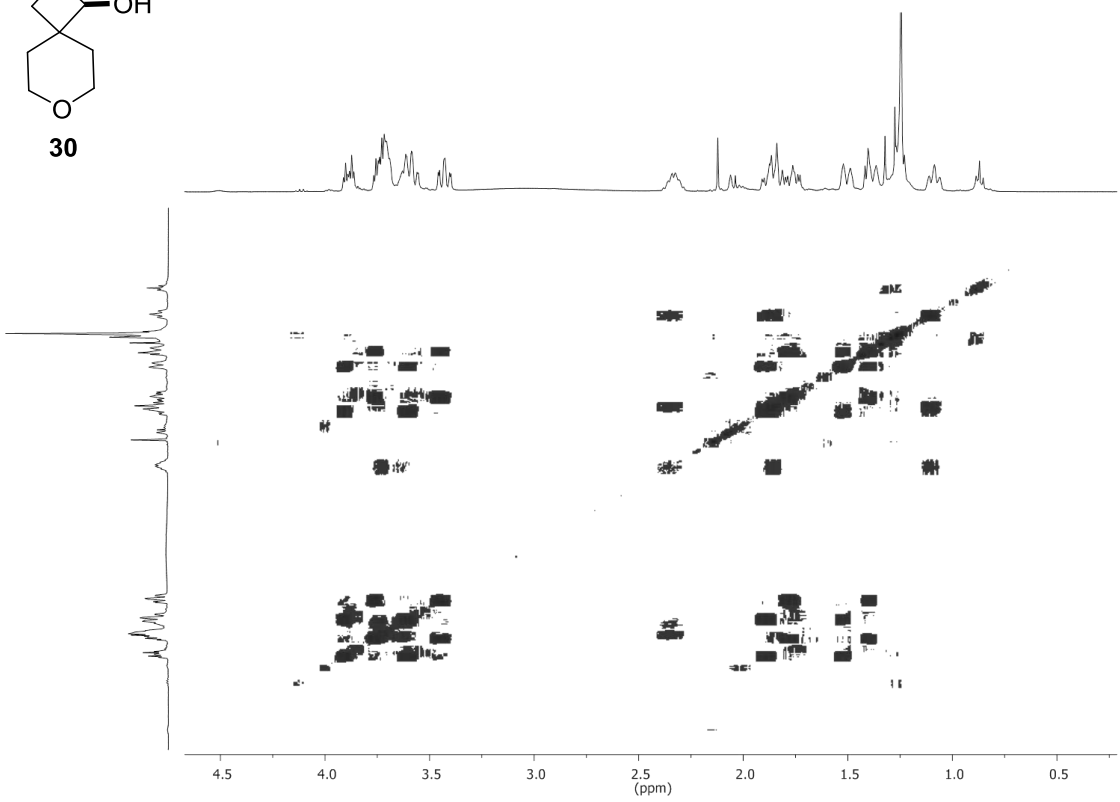

OH
OH
O

30


3.90
3.86
3.72
3.59
3.43
2.33
1.88
1.84
1.76
1.49
1.40
1.09
1.00
2.85
1.97
1.01
1.02
1.61
1.11
1.01
1.54
1.02
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

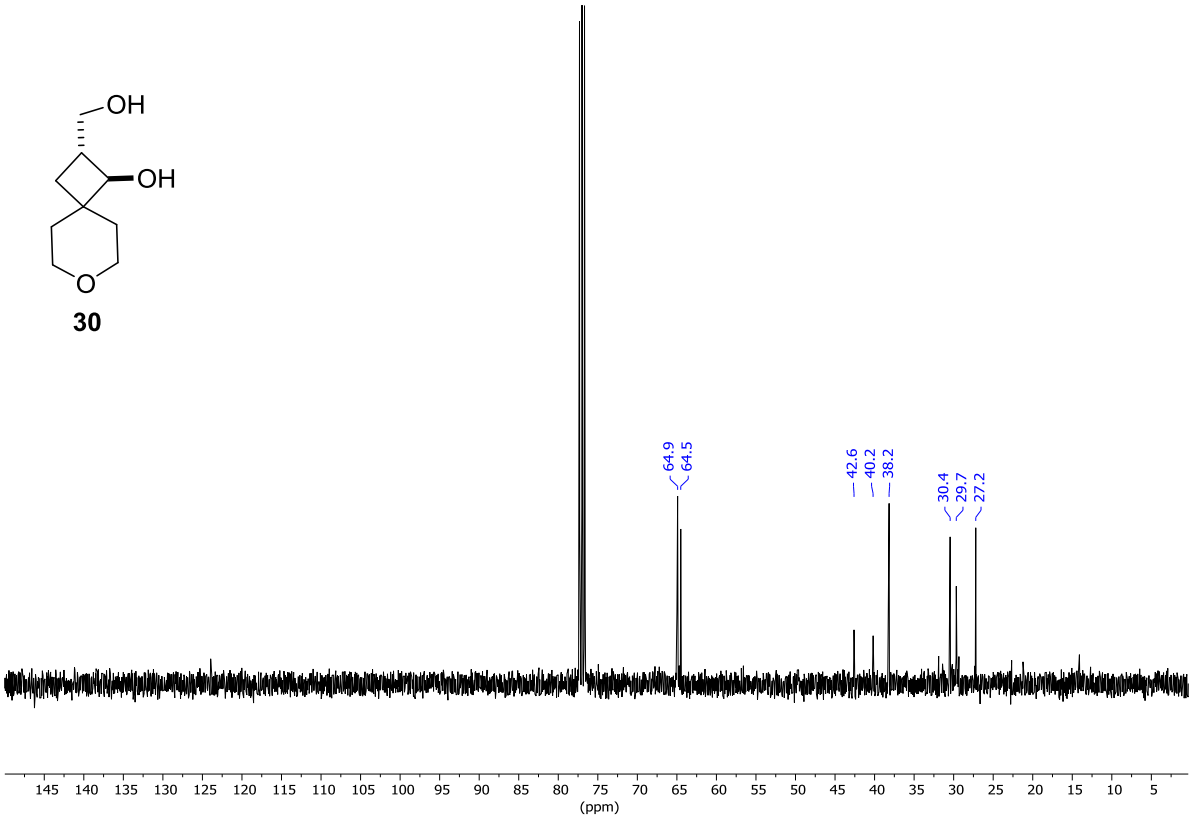

OH
OH
O

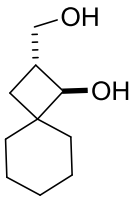
30


4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

OH
OH
O

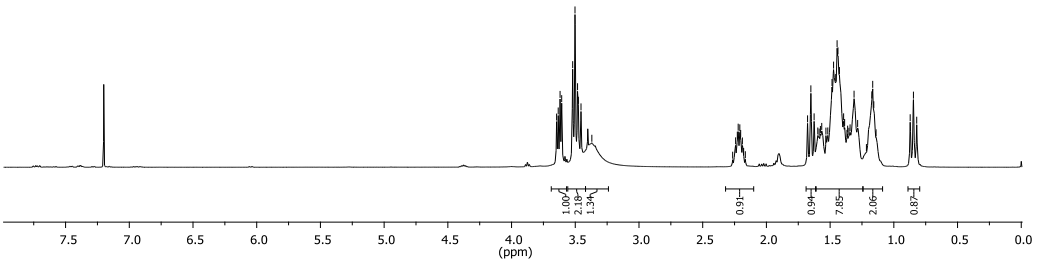
30

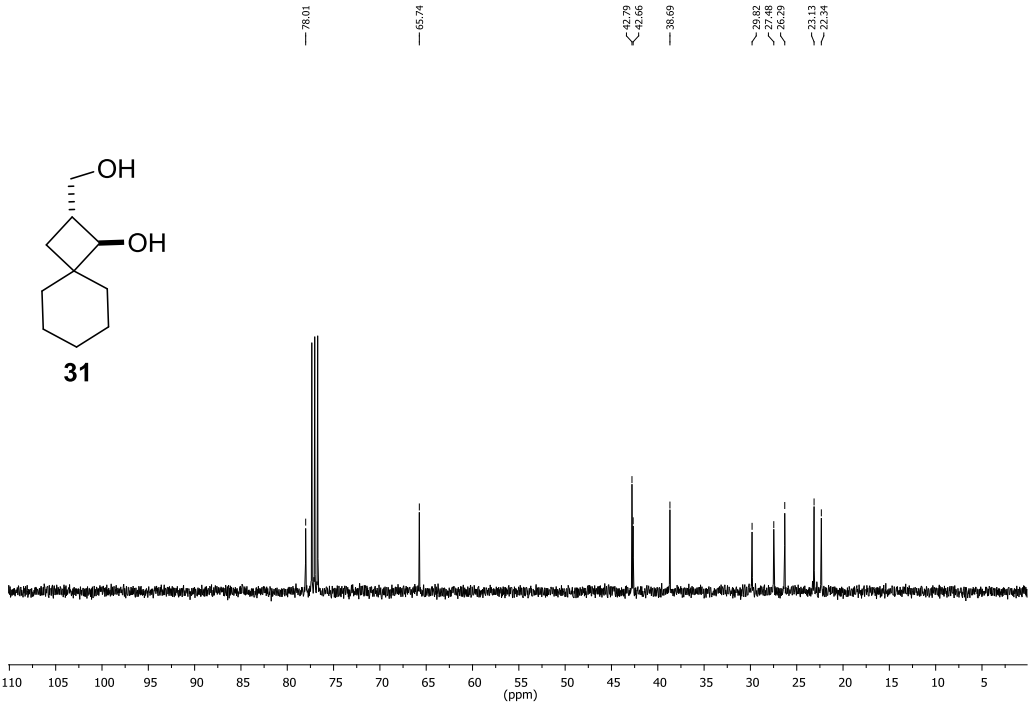

64.9
64.5
42.6
40.2
38.2
30.4
29.7
27.2
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)

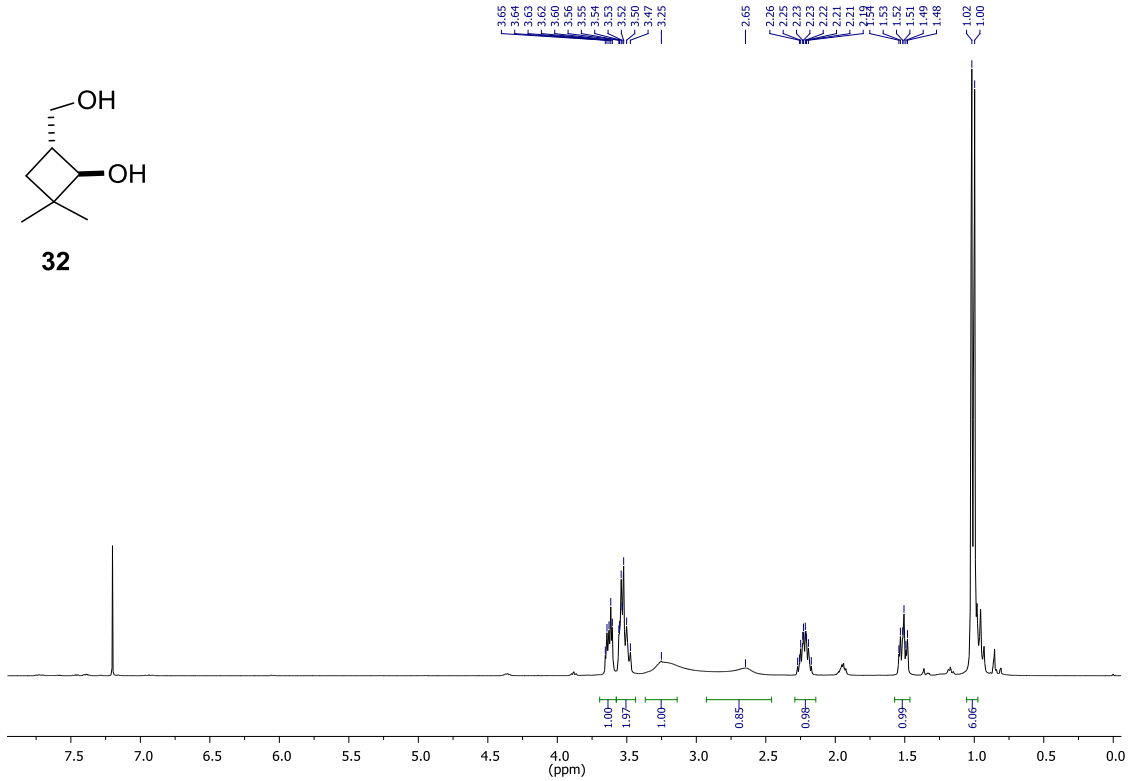

OH
OH

31


3.65
3.63
3.62
3.61
3.52
3.50
3.48
3.48
3.45
3.37
2.26
2.24
2.23
2.22
2.21
2.20
2.19
2.18
2.17
1.65
1.49
1.47
1.46
1.45
1.44
1.43
1.31
1.27
0.87
0.85
0.82

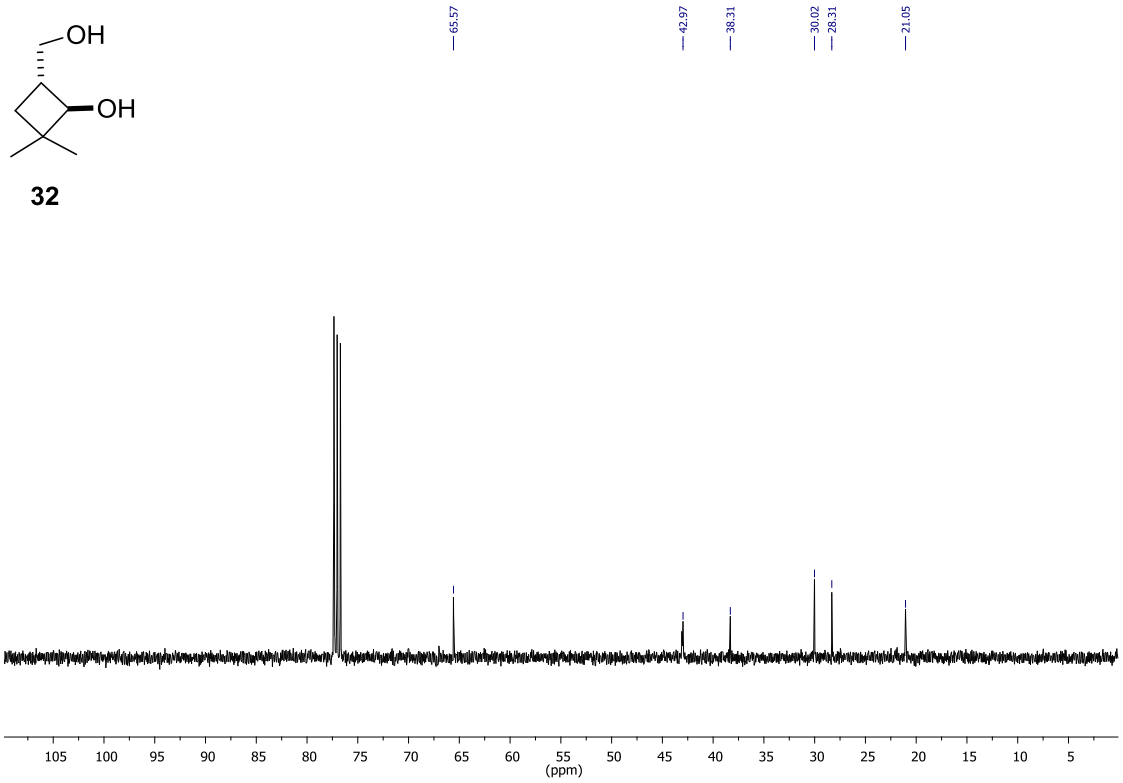

1.09
2.19
1.34
0.91
0.94
7.85
2.06
0.87
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

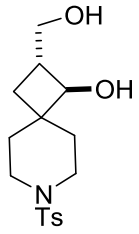

78.01
65.74
42.79
42.66
38.69
29.82
27.48
26.29
23.13
22.34
OH
OH
31
110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)


3.65
3.64
3.63
3.62
3.60
3.56
3.55
3.54
3.53
3.52
3.50
3.47
3.25
2.65
2.26
2.25
2.23
2.23
2.22
2.21
2.21
1.54
1.53
1.52
1.51
1.49
1.48
1.02
1.00
OH
OH
32
1.00
1.97
1.00
0.85
0.98
0.99
6.06
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

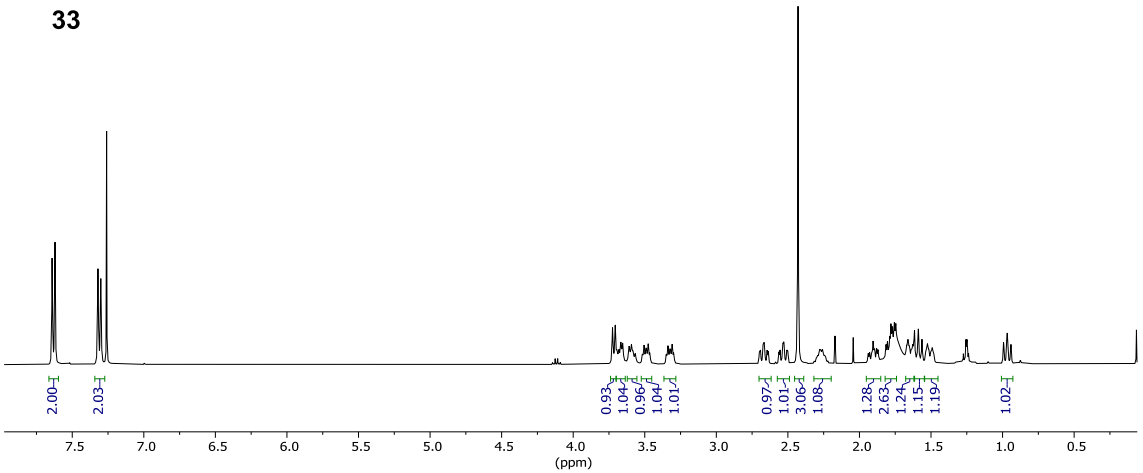
OH
OH

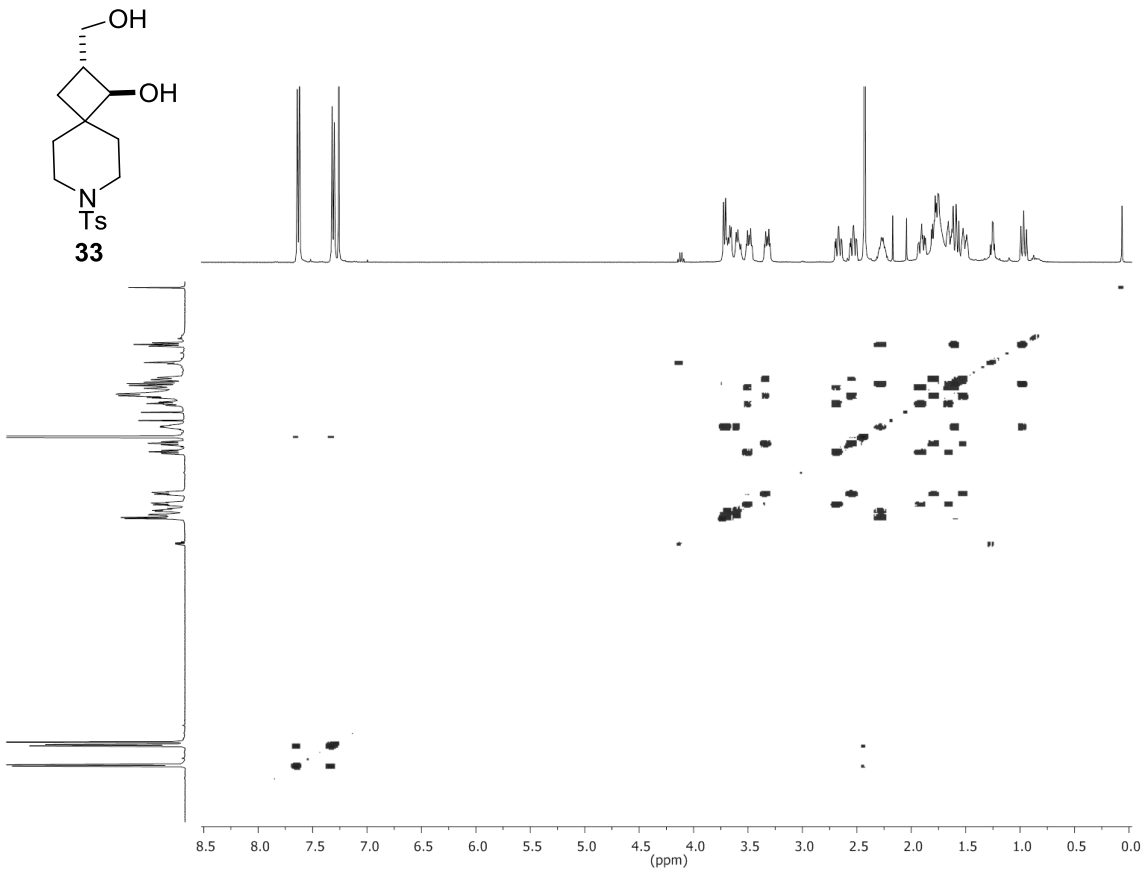
32

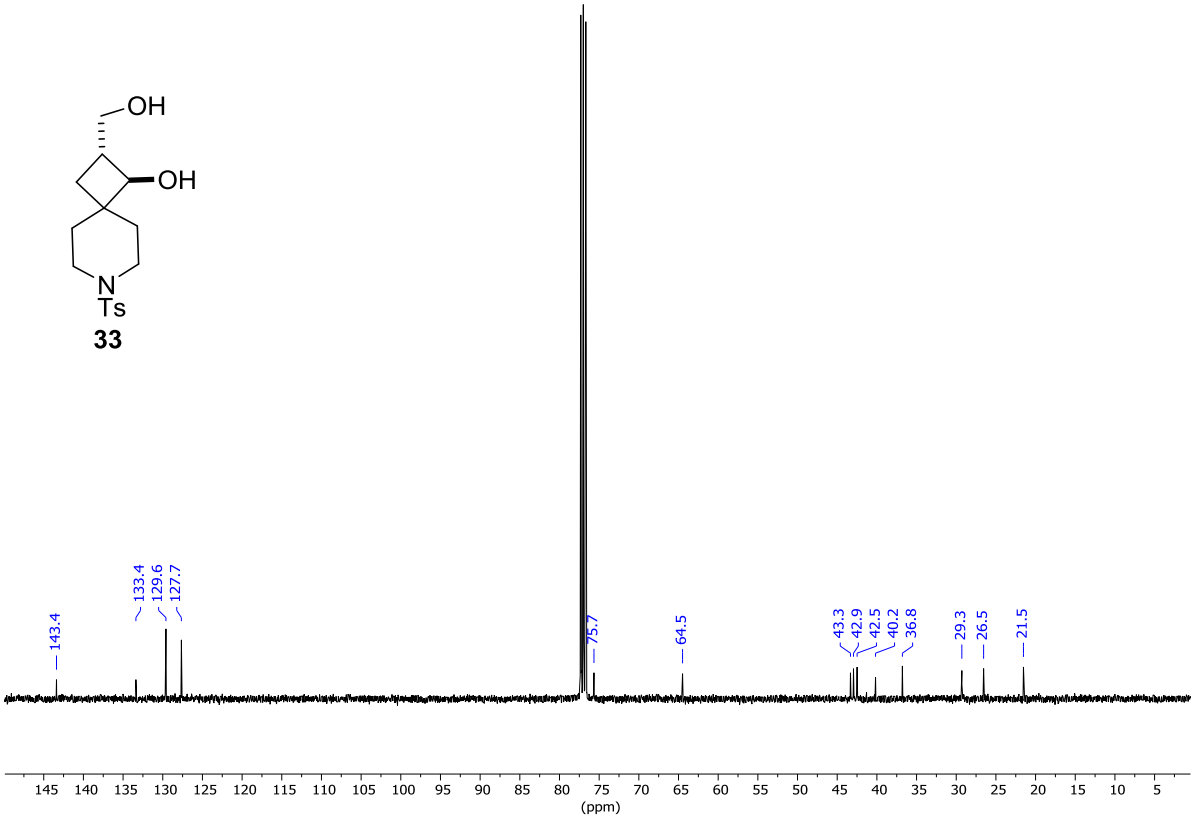

65.57
42.97
38.31
30.02
28.31
21.05
105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)


OH
OH
N
Ts

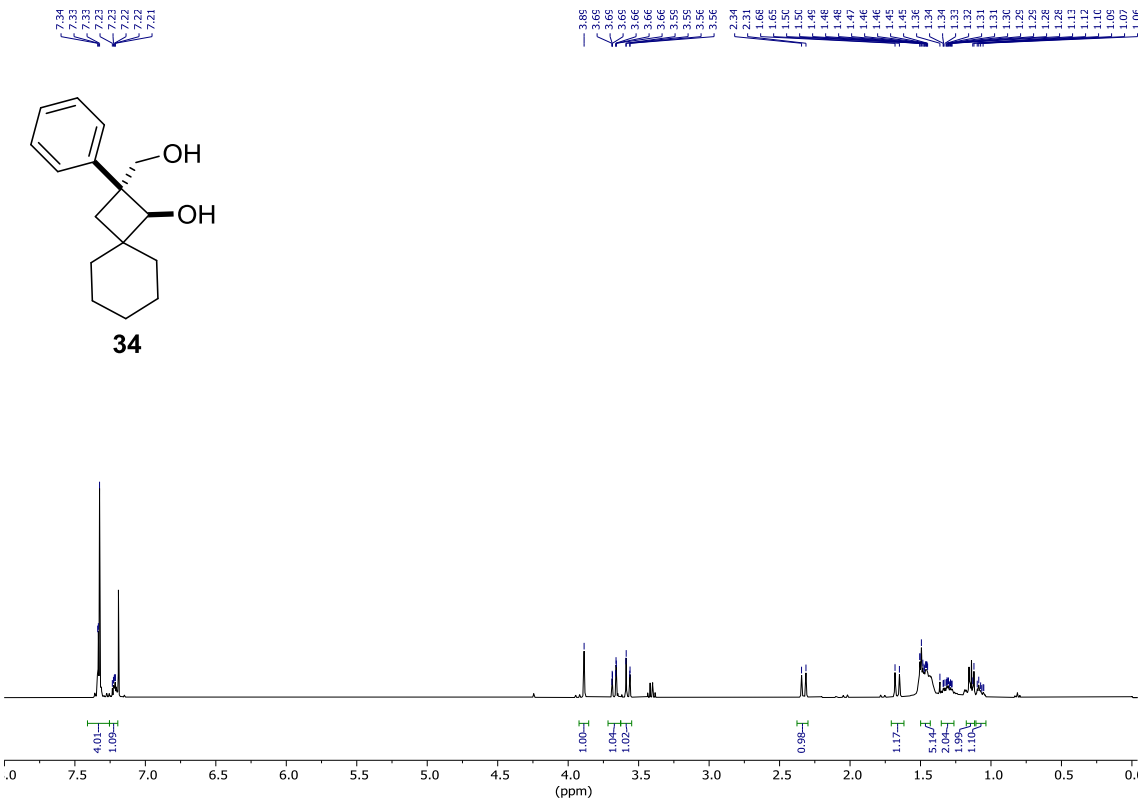
33


2.00
2.03
0.93
1.04
0.96
1.04
1.01
0.97
1.01
3.06
1.08
1.28
2.63
1.24
1.15
1.19
1.02
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

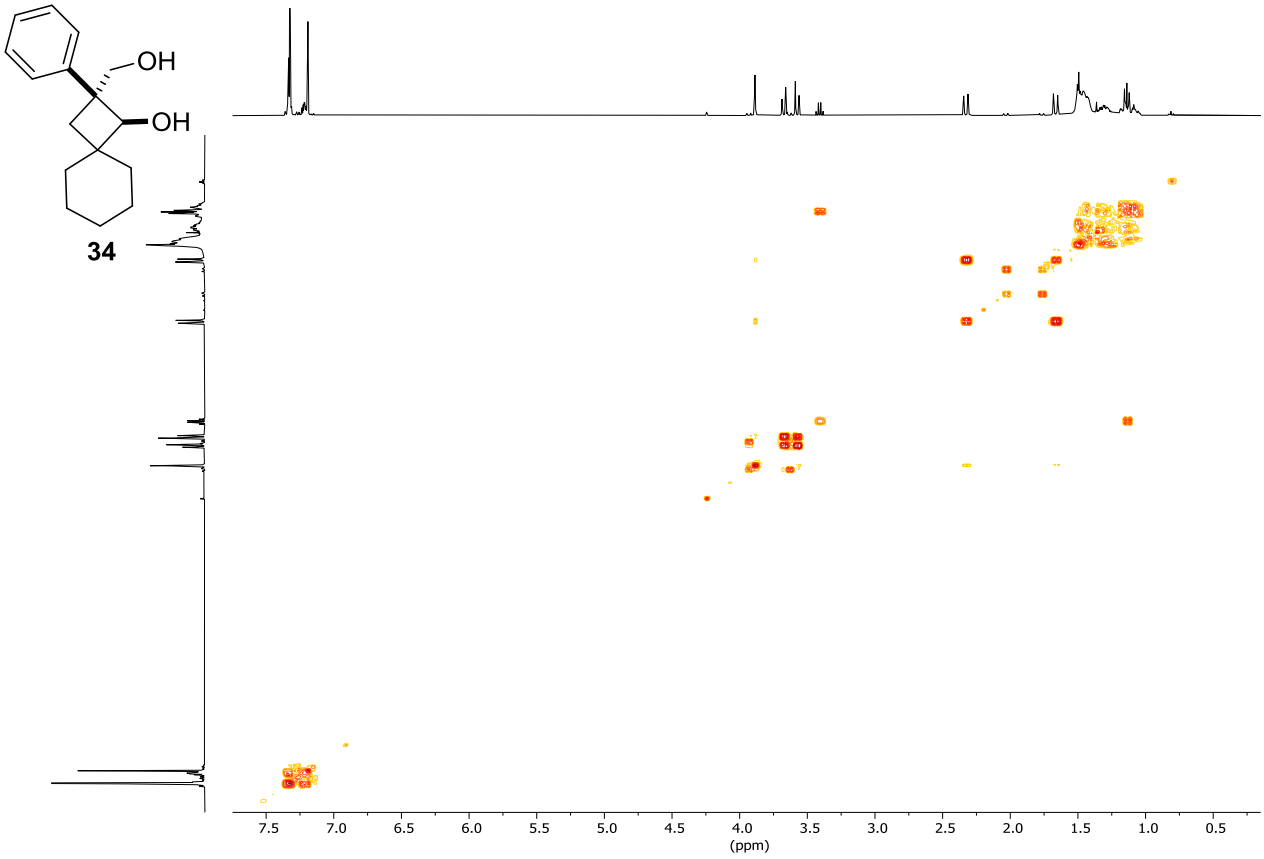

OH
OH
N
Ts
33
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

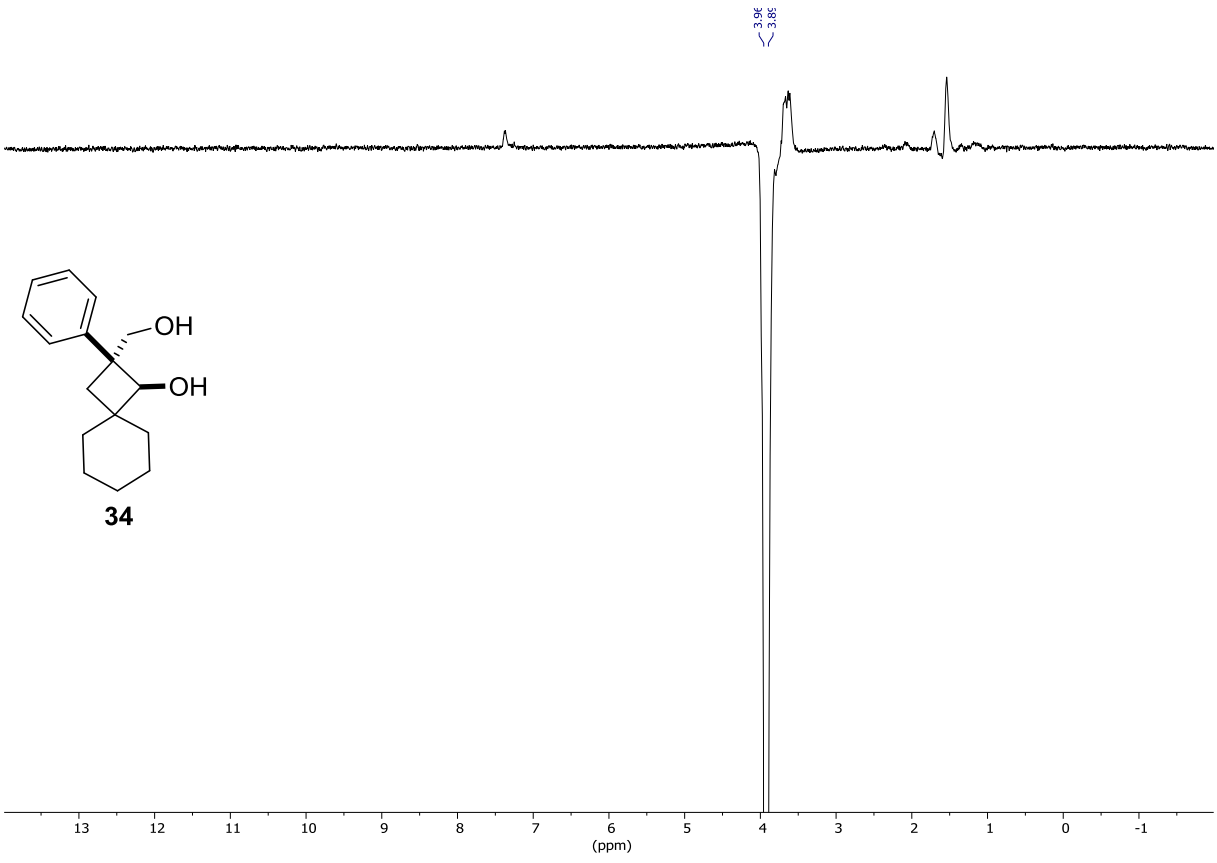

OH
OH
N
Ts
143.4
133.4
129.6
127.7
75.7
64.5
43.3
42.9
42.5
40.2
36.8
29.3
26.5
21.5
(ppm)

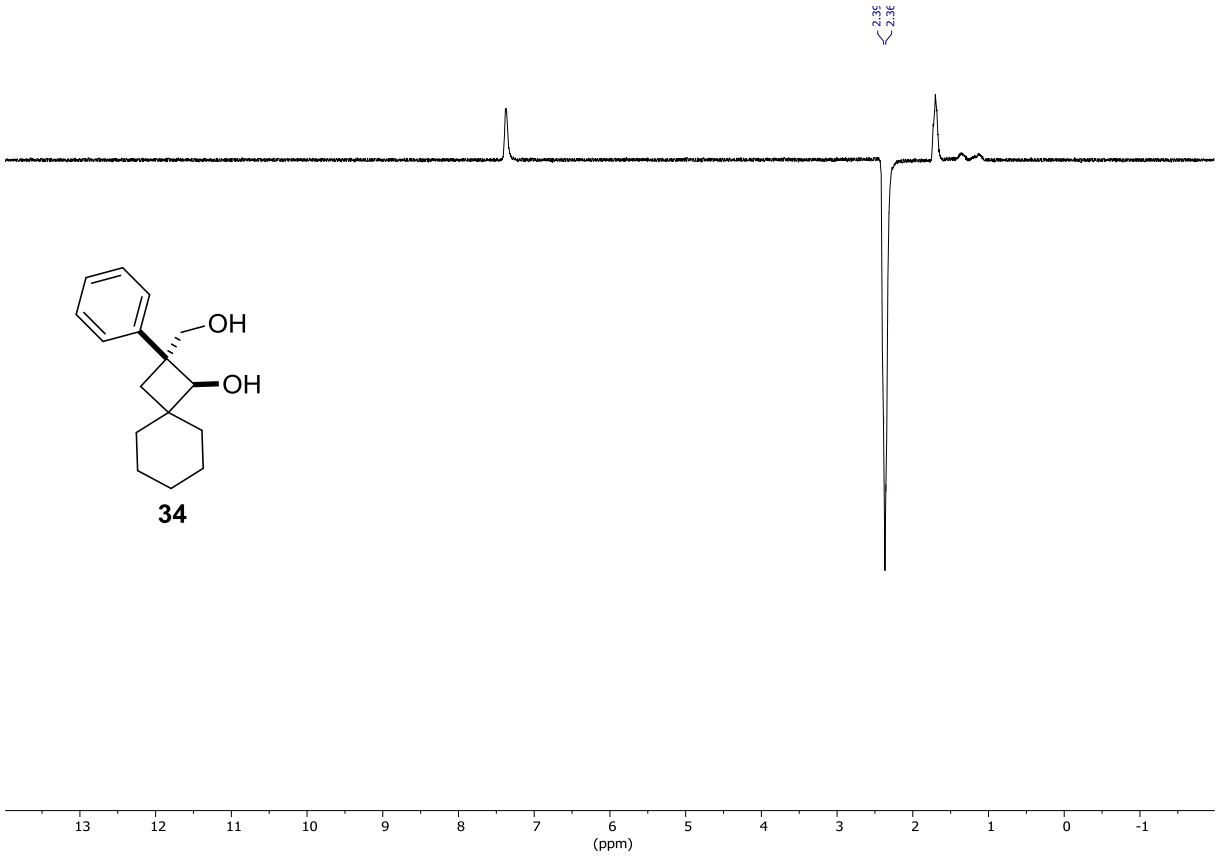
33

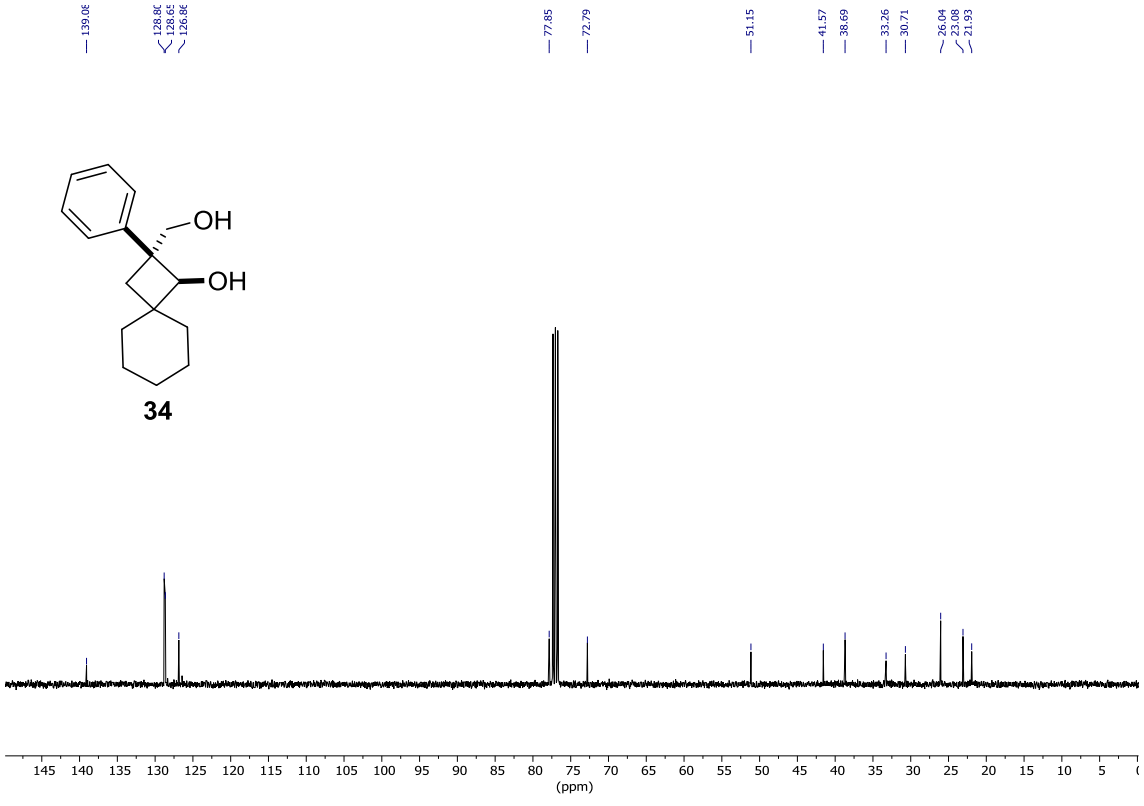

OH
OH
(ppm)

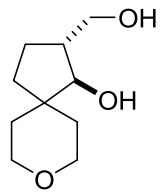
34


OH
OH
34
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

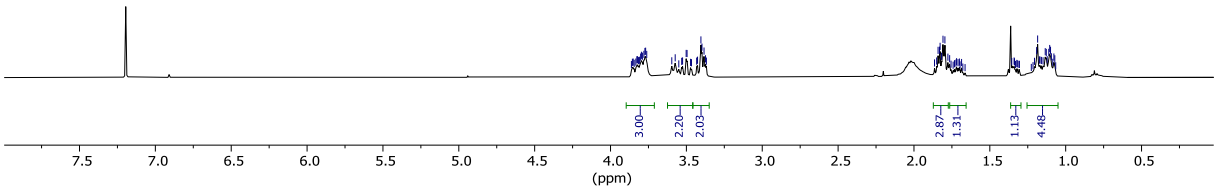

3.96
3.85
OH
OH
34
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
(ppm)

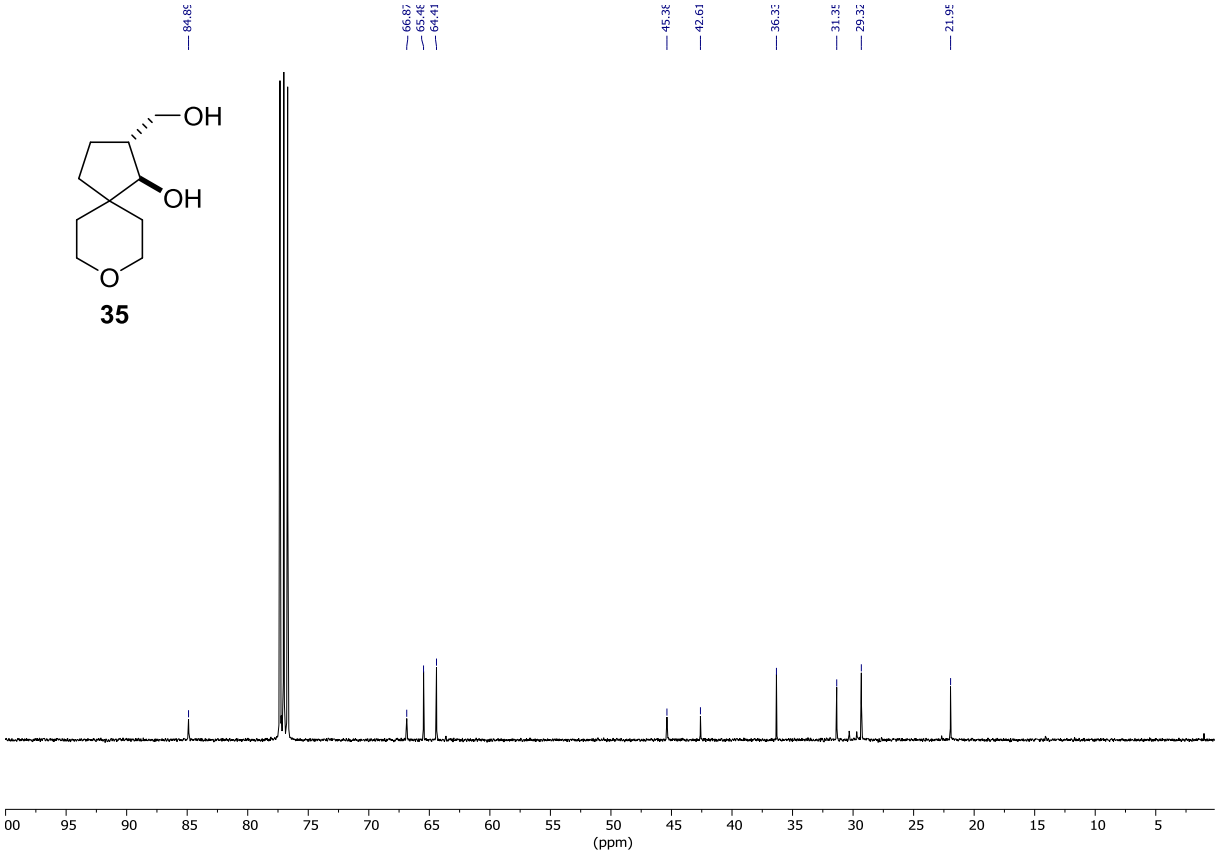

OH
OH
34
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
(ppm)

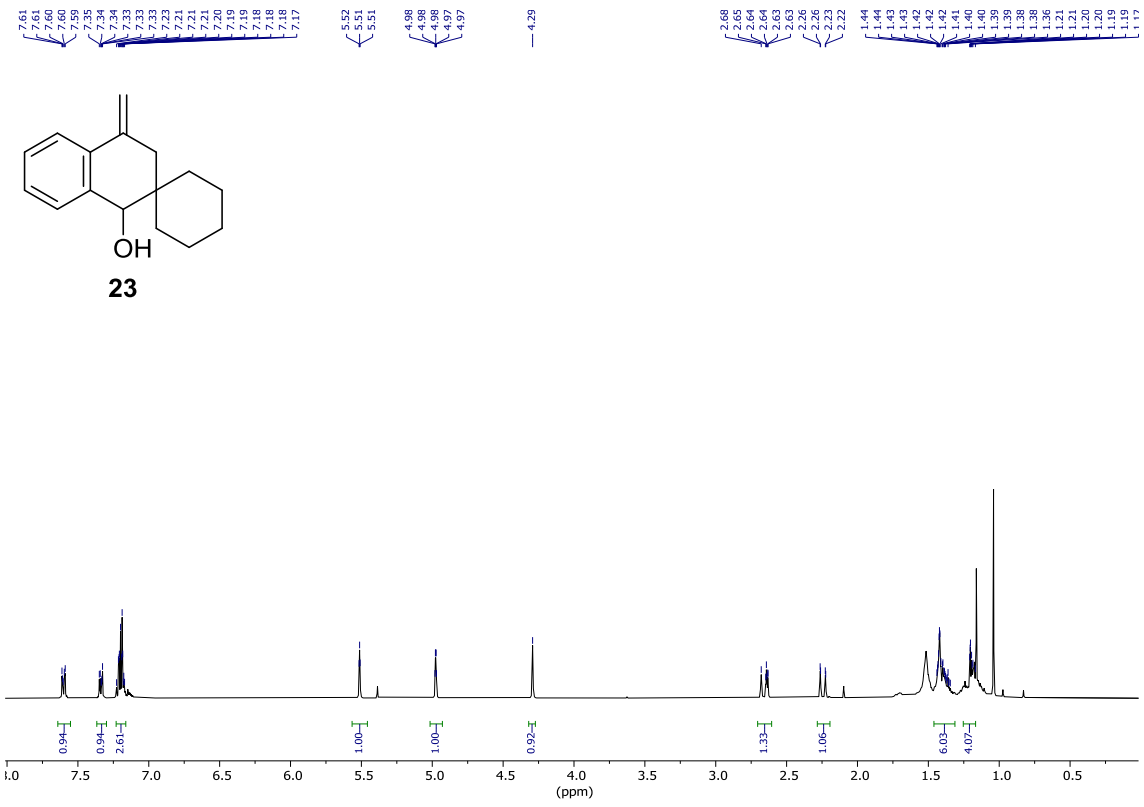

139.08
128.86
126.65
126.64
77.85
72.79
51.15
41.57
38.69
33.26
30.71
26.04
23.08
21.93
OH
OH
34
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)

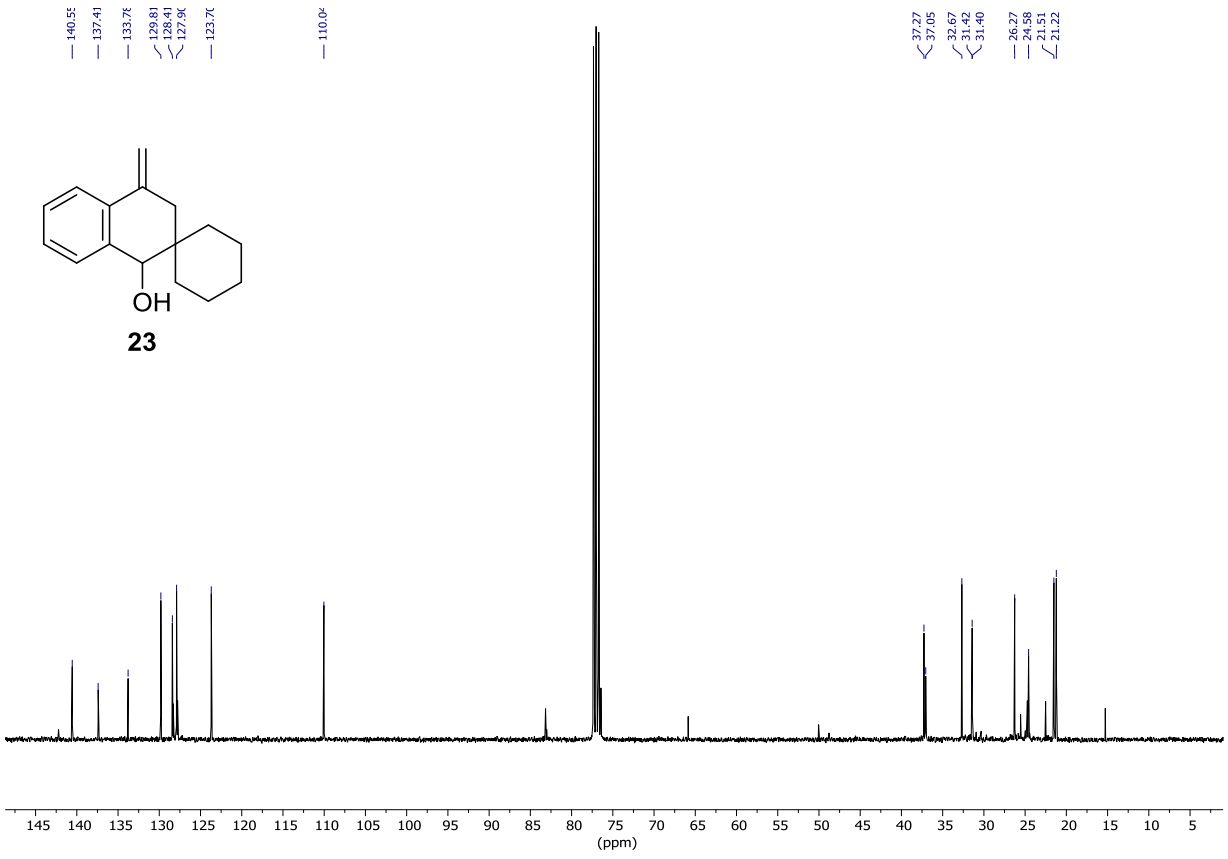

OH
OH
O

35


3.00
2.20
2.03
2.87
1.31
1.13
4.48
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


OH
OH
O
35
(ppm)


OH
23
(ppm)


140.55
137.41
133.78
129.81
128.41
127.90
123.76
110.04
37.27
37.05
32.67
31.42
31.40
26.27
24.58
21.51
21.22
OH
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
(ppm)

23

3. Computational Studies

3.1. Computational Details.

Geometry optimizations and transition state searches were performed with Gaussian 16[10] package. The quantum mechanics calculations were performed within the framework of Density Functional Theory (DFT)[11] by using the ωB97X-D functional.[12] Two different basis set were used. The first one (Basis set I) was used for geometry optimizations and frequency calculations, where we defined effective core potentials (ECPs) with double-ζ valence basis set (LANDL2DZ)[13] were employed for Cu and P, supplemented with polarized shells with the following exponents: Cu (f = 3.525) and P (d = 0.387).[14] For all other electrons of all other atoms 6-31G(d) basis set was used.[15] All calculation was performed within solvent (THF) represented via the SMD model.[16] Potential energies were refined through single point calculations with a larger basis set II, which consisted of LANL2TZ(f) for Cu,[13,14,17] LANL08(d) for P[13,14,17] and 6-311++G(d,p)[15] for other atoms. Free energy corrections were considered at a concentration of 1 M and a temperature of 298.15 K.

3.2. Computed free-energy profiles.

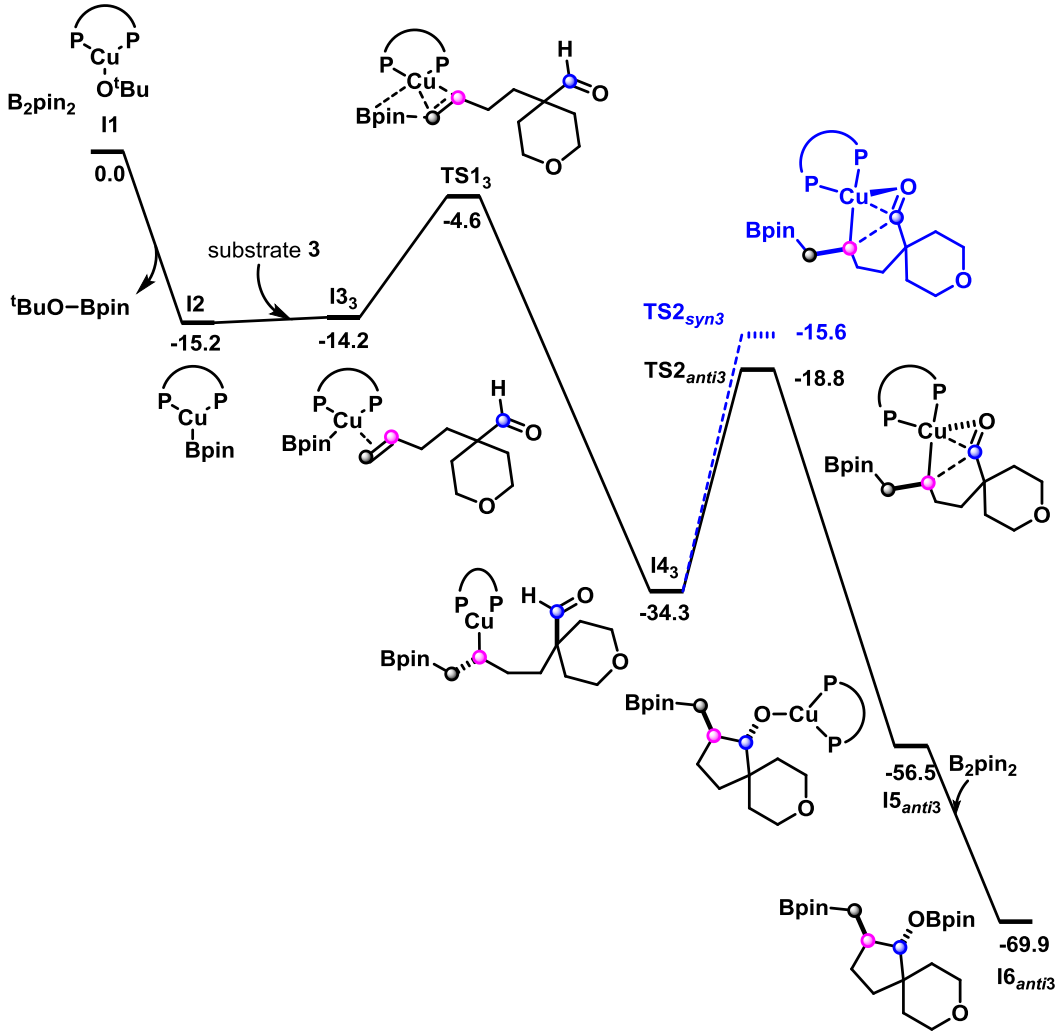


Figure S1. Computed free energy profile (in kcal·mol^{-1}) for the formation of 5-membered ring spirocyclic product **4**. Dashed blue line represents alternative path related to *syn* diastereoselecivity. P-P= Xantphos.

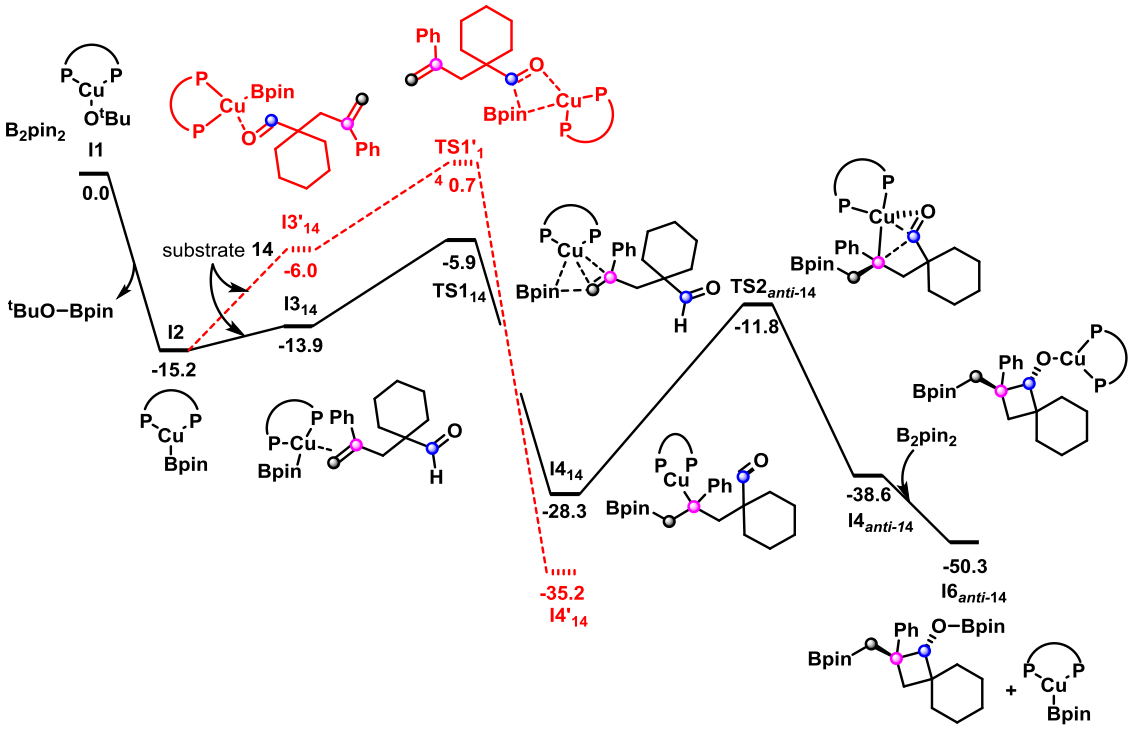


Figure S2. Computed free energy profile (in kcal·mol^{-1}) for the formation of 4-membered ring spirocyclic product **15**. Dashed red lines represent alternative paths related to chemoselectivity. P-P= Xantphos.

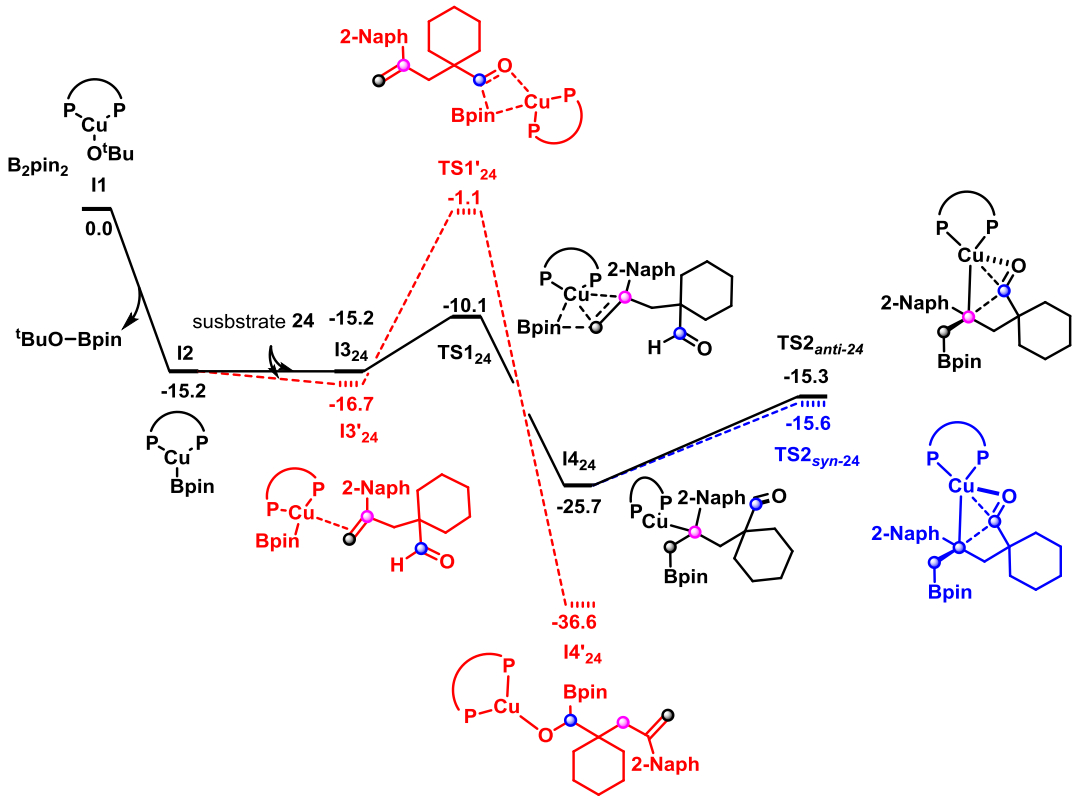


Figure S3. Computed free energy profile (in kcal·mol^{-1}) for the formation of 4-membered ring spirocyclic product **24**. Dashed lines represent alternative paths related to chemoselectivity (red lines) and diastereoselectivity (blue lines). P-P= Xantphos.

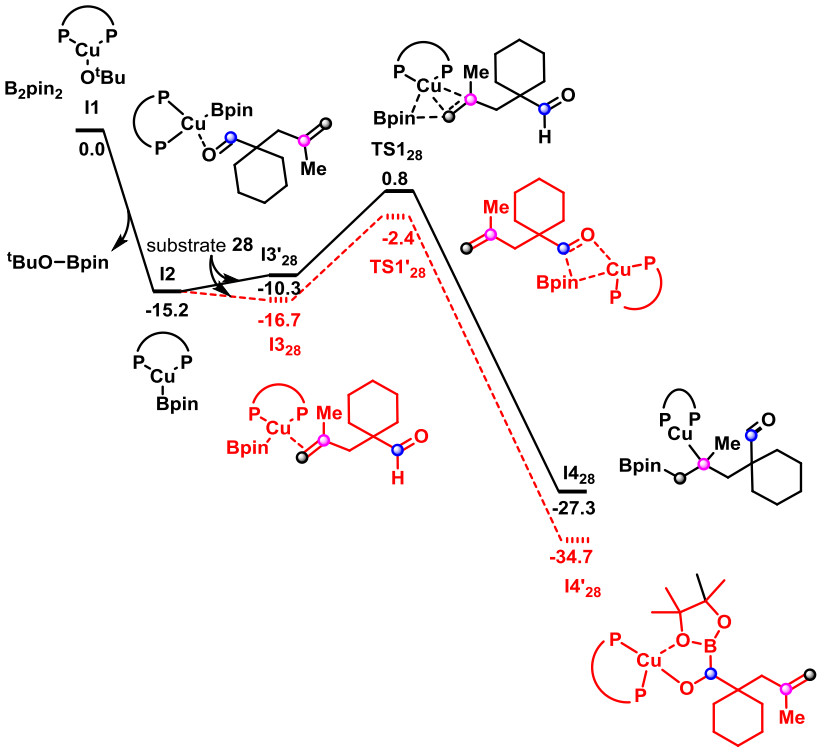


Figure S4. Computed free energy profile (in kcal·mol^{-1}) for the formation of 4-membered ring spirocyclic product **28**. Dashed red lines represent alternative paths related to chemoselectivity. P-P= Xantphos.

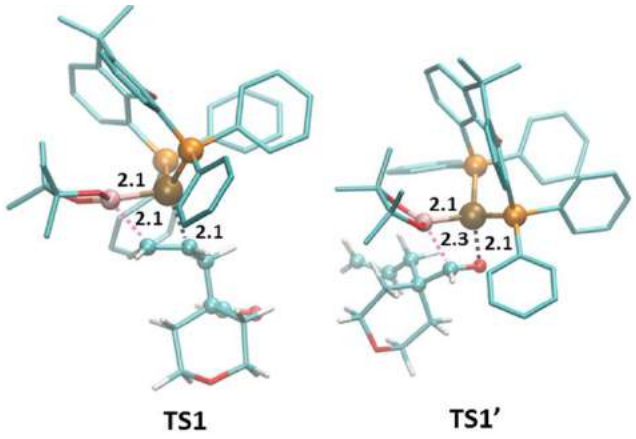


Figure S5. Molecular structures and main geometric parameters (Å) of the key transition states (**TS1** and **TS1'**) for the chemoselectivity of the borylative 4-membered ring closing reaction of substrate **1**.

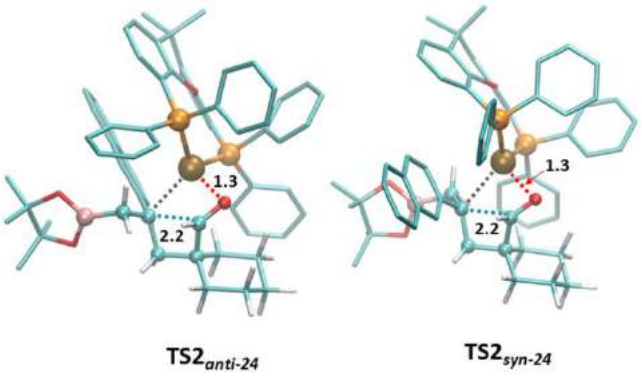


Figure S6. Molecular structures and main geometric parameters (Å) of transition states **TS2**$_{anti\text{-}24}$ and **TS2**$_{syn\text{-}24}$ for the ring closing step of substrate **24**.

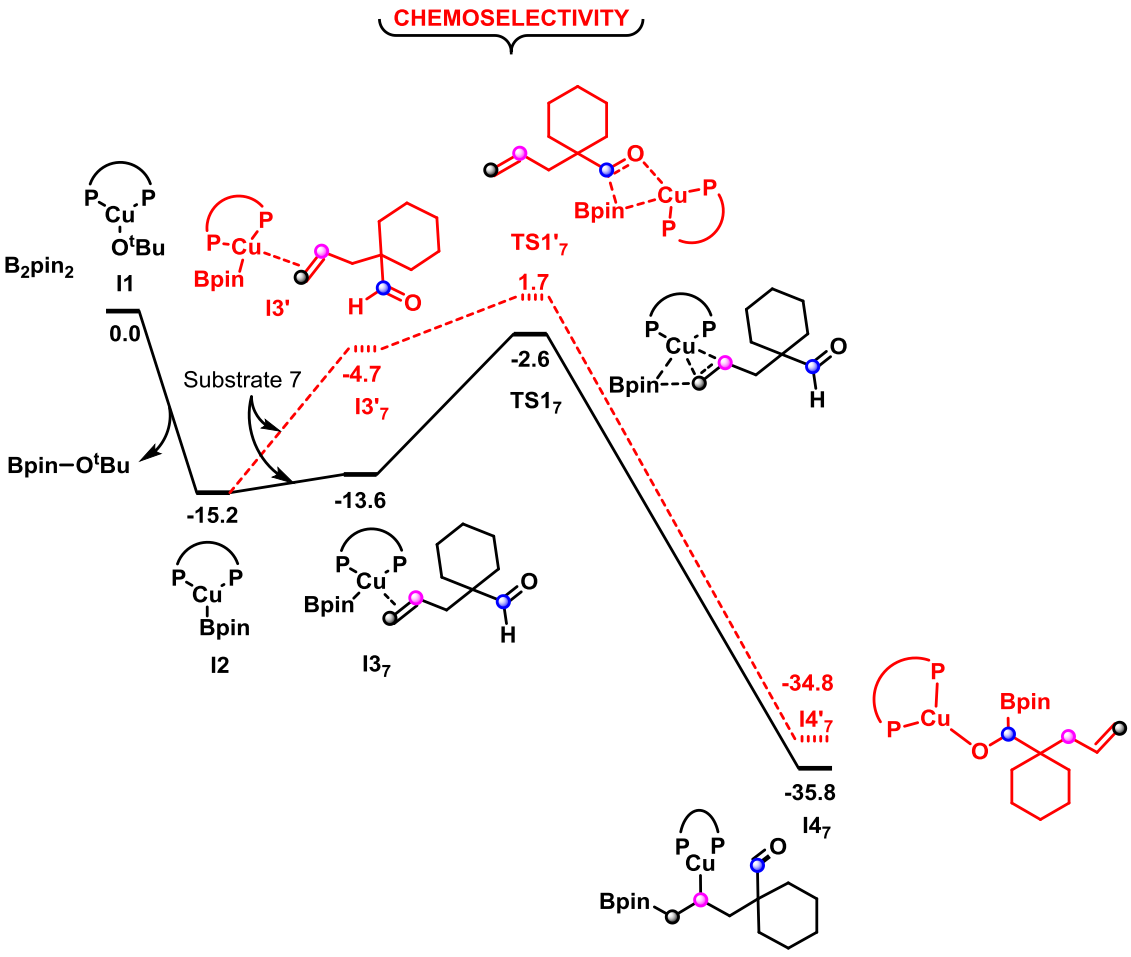


Figure S7. Computed free energy profile (in kcal·mol^{-1}) for the first steps of the formation of 4-membered ring spirocyclic product **7**. Dashed red lines represent alternative paths related to chemoselectivity. P-P= Xantphos.

SUBSTRATE 7

C	-1.029794	1.340416	-2.195205
H	-1.299889	0.587697	-2.933439
H	-0.134288	1.923793	-2.391394
C	-1.761079	1.531653	-1.099211
H	-1.452493	2.292011	-0.383155
C	-3.004038	0.756016	-0.766411
H	-3.069853	-0.125296	-1.415453
H	-2.929812	0.392684	0.267973
O	-6.162694	-0.031113	-1.040982
C	-5.387548	0.616902	-0.374276
H	-5.377701	0.510247	0.734265
C	-4.329219	1.566136	-0.912035
C	-4.314730	2.826766	-0.025135
C	-4.596187	1.932288	-2.378120
C	-5.582953	3.667096	-0.198036
H	-3.447293	3.438267	-0.298934
H	-4.180625	2.538297	1.025540
C	-5.836898	2.813597	-2.557738
H	-3.715599	2.462848	-2.760308
H	-4.698091	1.013941	-2.966161
H	-5.520136	4.561955	0.430600
H	-6.457209	3.099094	0.151328
H	-5.926060	3.106519	-3.609717
H	-6.733225	2.230549	-2.315193
C	-5.785081	4.055182	-1.664491
H	-6.703052	4.642194	-1.779042
H	-4.952665	4.698650	-1.981885

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Cu	-0.201590	0.067914	-1.034194
C	-1.848661	0.802384	-2.410344
H	-1.929921	0.065224	-3.205032
H	-1.362307	1.741506	-2.658962
C	-2.495188	0.629882	-1.229373
H	-2.500690	1.443785	-0.508608
P	0.570603	2.124492	0.114778
P	-0.410415	-1.603542	0.617193
B	1.434953	-0.496195	-2.161329
O	1.662083	-1.613376	-2.976750
O	2.650618	0.167156	-1.974288
C	3.081340	-1.838652	-3.088628
C	3.668706	-0.419819	-2.798305
C	-2.477543	-0.911992	4.712699
C	-2.002897	-0.230831	2.448787
C	-1.035520	-2.259972	3.323052
C	-1.669373	-2.035703	4.541222
C	-2.643378	-0.009219	3.666239
H	-0.406617	-3.136889	3.195844
H	-1.532668	-2.738013	5.357995
H	-2.971001	-0.738598	5.664335
C	-0.315456	2.780381	1.590644
C	-1.859559	3.530683	3.810929
C	0.202004	2.675741	2.884045
C	-1.621664	3.264754	1.424961
C	-2.385339	3.642817	2.524115
C	-0.566984	3.045581	3.985840
H	-2.040664	3.362644	0.426343
H	-3.391207	4.024203	2.375372
H	-2.455719	3.819437	4.671177

C	2.331681	2.035010	0.653703
C	5.038758	1.619084	1.245616
C	3.276789	3.024886	0.379810
C	2.783425	0.859981	1.254784
C	4.121740	0.617821	1.562421
C	4.620613	2.816138	0.670095
H	2.965945	3.953249	-0.087839
H	5.348397	3.588633	0.443247
H	6.092624	1.475572	1.457786
C	1.228582	-2.302515	1.076878
C	3.833523	-3.124571	1.688946
C	1.572591	-3.653426	1.019615
C	2.214913	-1.394546	1.466773
C	3.521056	-1.767156	1.779481
C	2.869406	-4.059556	1.321023
H	0.831443	-4.386907	0.719127
H	3.132463	-5.110837	1.264502
H	4.837600	-3.465183	1.916860
C	-1.284039	-3.051865	-0.107280
C	-2.679440	-5.065880	-1.460807
C	-0.892116	-3.442207	-1.396424
C	-2.376792	-3.680609	0.494104
C	-3.075733	-4.678097	-0.184192
C	-1.581339	-4.451139	-2.061656
H	-0.054205	-2.944508	-1.881598
H	-2.700056	-3.383941	1.487201
H	-3.932210	-5.149916	0.287956
H	-1.268249	-4.748020	-3.058278
H	-3.226117	-5.841525	-1.988493
C	0.621903	3.552408	-1.050164
C	0.793667	5.593044	-2.960701
C	0.336010	4.875380	-0.699775
C	1.004076	3.263166	-2.367380
C	1.093371	4.278844	-3.314594
C	0.416289	5.888749	-1.652893
H	0.052967	5.121758	0.318866
H	1.246126	2.238050	-2.636623
H	1.394302	4.041443	-4.330675
H	0.188877	6.912113	-1.369574
H	0.856841	6.384965	-3.701039
H	-2.114314	0.486752	1.641297
H	1.210132	2.304673	3.040913
H	-3.258189	0.875828	3.795967
H	-0.150154	2.954429	4.984286
O	1.831588	-0.082110	1.551523
C	4.476983	-0.684789	2.279494
C	-3.382056	-0.548933	-0.933646
H	-3.208004	-1.329254	-1.684020
H	-3.123373	-0.979470	0.038135
C	-1.203815	-1.361815	2.262639
O	-6.158064	-2.260372	-1.299642
C	-5.533808	-1.553031	-0.541476
H	-5.338496	-1.886064	0.503395
C	-4.901498	-0.213621	-0.885351
C	-5.201793	0.767191	0.266954
C	-5.415720	0.329718	-2.223061
C	-6.679159	1.164447	0.318551
H	-4.598421	1.672124	0.128392
H	-4.885524	0.321294	1.219307
C	-6.883615	0.765493	-2.164778
H	-4.795440	1.190387	-2.502030
H	-5.275283	-0.430308	-2.999170
H	-6.838520	1.886109	1.127288
H	-7.292601	0.284215	0.558241

H	-7.168583	1.216571	-3.121701
H	-7.518300	-0.118078	-2.029658
C	3.793920	0.453617	-4.048507
H	4.015223	1.480196	-3.740590
H	4.597436	0.112266	-4.708970
H	2.856841	0.464864	-4.613596
C	4.980940	-0.414397	-2.024206
H	5.772117	-0.922810	-2.586196
H	5.297194	0.617637	-1.844029
H	4.868462	-0.902650	-1.053419
C	3.394072	-2.393654	-4.471040
H	4.475277	-2.501511	-4.610144
H	2.939016	-3.382611	-4.584664
H	3.003920	-1.749508	-5.262153
C	3.450859	-2.863888	-2.015609
H	2.844248	-3.763488	-2.157114
H	4.506481	-3.149455	-2.066749
H	3.242293	-2.470577	-1.018049
C	5.942223	-1.074109	2.065083
H	6.180765	-1.993917	2.605272
H	6.169313	-1.223119	1.004812
H	6.608976	-0.302518	2.458386
C	4.223748	-0.485512	3.792768
H	4.438819	-1.410515	4.337818
H	4.869718	0.308279	4.182064
H	3.183422	-0.207659	3.988262
C	-7.135827	1.749612	-1.019933
H	-8.198051	2.014504	-0.975553
H	-6.582901	2.680107	-1.210833

TS1$_7$

Cu	-0.501080	0.394587	-0.091743
C	-1.927071	1.005608	-1.461883
H	-2.272548	0.219075	-2.132873
H	-1.838708	1.969819	-1.965450
C	-2.497843	0.999678	-0.123109
H	-2.635325	1.979327	0.334194
P	0.972851	1.688934	1.104874
P	-0.175890	-1.878835	0.287873
B	0.066244	0.707032	-2.072613
O	0.152565	-0.234652	-3.088955
O	0.798046	1.837631	-2.401414
C	1.212564	0.167372	-3.982663
C	1.250612	1.714886	-3.765188
C	-0.211282	-3.222393	4.716517
C	-0.833632	-1.674719	2.975145
C	0.503902	-3.613813	2.444890
C	0.476261	-3.996197	3.782663
C	-0.868833	-2.063883	4.311510
H	1.039041	-4.221826	1.720972
H	0.991675	-4.898931	4.096519
H	-0.230463	-3.521446	5.760246
C	1.027114	1.365484	2.917383
C	0.912630	0.832147	5.663430
C	2.128361	0.818104	3.575561
C	-0.137069	1.639593	3.647614
C	-0.189621	1.387160	5.012874
C	2.066383	0.544303	4.941658
H	-1.007224	2.051471	3.141801
H	-1.095076	1.613194	5.568077
H	0.868894	0.622955	6.727965
C	2.726822	1.556061	0.554203
C	5.275703	1.179815	-0.555926

C	3.519037	2.652867	0.209363
C	3.258272	0.283139	0.336654
C	4.524392	0.058813	-0.203966
C	4.779782	2.464467	-0.347633
H	3.140119	3.659041	0.353088
H	5.380698	3.325153	-0.623030
H	6.261991	1.057329	-0.989913
C	1.379053	-2.582033	-0.397444
C	3.828267	-3.363901	-1.511152
C	1.455531	-3.713659	-1.211377
C	2.561005	-1.885364	-0.142778
C	3.793814	-2.239478	-0.687017
C	2.673157	-4.100122	-1.763660
H	0.558236	-4.284065	-1.428272
H	2.721929	-4.978018	-2.399832
H	4.763543	-3.676873	-1.962121
C	-1.492493	-2.889539	-0.503426
C	-3.674251	-4.108373	-1.763089
C	-1.732478	-2.676553	-1.868894
C	-2.349987	-3.720524	0.220301
C	-3.439274	-4.323041	-0.407918
C	-2.813052	-3.289427	-2.494129
H	-1.079086	-2.015540	-2.434468
H	-2.184456	-3.888511	1.279873
H	-4.105892	-4.958590	0.167104
H	-2.990267	-3.118126	-3.551839
H	-4.525297	-4.576005	-2.249005
C	0.652269	3.498397	1.038774
C	0.106201	6.232416	0.830865
C	1.072366	4.380577	2.040663
C	-0.041053	3.997863	-0.067672
C	-0.309906	5.360422	-0.172028
C	0.799157	5.741247	1.936395
H	1.612511	4.003962	2.904443
H	-0.347210	3.317524	-0.855348
H	-0.848260	5.738803	-1.035856
H	1.127049	6.418395	2.719292
H	-0.108739	7.294003	0.752868
H	-1.326037	-0.759860	2.654980
H	3.043449	0.605366	3.031856
H	-1.398417	-1.453973	5.036423
H	2.927872	0.110829	5.440573
O	2.468791	-0.788107	0.679937
C	5.007059	-1.387940	-0.316220
C	-3.508256	-0.056962	0.259824
H	-3.234018	-0.999170	-0.228383
H	-3.476035	-0.253940	1.340026
C	-0.151394	-2.448710	2.033488
C	-5.694648	-1.074000	0.242617
H	-5.525247	-1.875578	-0.513020
O	-6.318179	-1.317266	1.254277
C	-5.011399	0.233918	-0.090711
C	-5.563179	1.392188	0.748597
C	-5.190770	0.511704	-1.591723
C	-6.997970	1.775428	0.371642
H	-4.908574	2.260495	0.599810
H	-5.510385	1.125783	1.809825
C	-6.636601	0.864685	-1.952590
H	-4.537523	1.348250	-1.864943
H	-4.847684	-0.356952	-2.170083
H	-7.310369	2.652332	0.950207
H	-7.674251	0.957276	0.648276
H	-6.708662	1.085734	-3.023562
H	-7.289513	-0.000468	-1.766523

C	6.138773	-1.534831	-1.335937
H	7.003000	-0.933189	-1.042631
H	6.482297	-2.571467	-1.383690
H	5.821671	-1.225996	-2.337121
C	5.515486	-1.839249	1.073134
H	5.841719	-2.883600	1.033858
H	6.362997	-1.219892	1.384305
H	4.731519	-1.754990	1.831705
C	0.247929	2.468608	-4.638831
H	0.181889	3.503719	-4.290756
H	0.553104	2.478497	-5.689471
H	-0.749391	2.022809	-4.570526
C	2.631603	2.343081	-3.878250
H	2.561179	3.421739	-3.707929
H	3.320059	1.930490	-3.137226
H	3.049737	2.183509	-4.877716
C	2.487158	-0.532161	-3.509870
H	2.775827	-0.189082	-2.512944
H	2.303474	-1.608971	-3.457219
H	3.322593	-0.354665	-4.194261
C	0.862943	-0.275593	-5.394959
H	-0.124969	0.079279	-5.696285
H	1.602604	0.099371	-6.109944
H	0.863439	-1.368544	-5.449790
C	-7.131566	2.054768	-1.127284
H	-8.172677	2.286786	-1.379113
H	-6.535781	2.941445	-1.386152

$I4_7$

Cu	0.759883	-0.072407	-0.751967
C	1.033381	-1.591608	-3.357733
H	0.829148	-0.713810	-3.987771
H	1.626716	-2.278749	-3.994575
C	1.828785	-1.195571	-2.089232
H	1.999295	-2.133059	-1.539533
P	0.300337	-0.917397	1.526590
P	-0.350567	2.022642	-0.794836
B	-0.317952	-2.279837	-2.986189
O	-1.557018	-1.870315	-3.420312
O	-0.398791	-3.371346	-2.147011
C	-2.546493	-2.563128	-2.628625
C	-1.765303	-3.832602	-2.142773
C	0.349519	4.930417	2.755301
C	1.152329	3.292367	1.172031
C	-1.164289	3.966748	1.141487
C	-0.927540	4.828165	2.209624
C	1.388004	4.165682	2.230174
H	-2.163929	3.901128	0.722496
H	-1.743240	5.420769	2.613158
H	0.533852	5.600957	3.589367
C	0.892215	0.178553	2.881817
C	1.924643	1.897902	4.835098
C	0.043421	0.775921	3.816171
C	2.262168	0.464932	2.924629
C	2.776244	1.309061	3.902135
C	0.558510	1.636466	4.783608
H	2.930557	0.039204	2.182526
H	3.841894	1.516421	3.924874
H	2.323550	2.565392	5.593059
C	-1.428838	-1.331611	2.018896
C	-4.145753	-1.915894	2.411132
C	-1.817182	-2.546486	2.590497
C	-2.437200	-0.423932	1.694988

C	-3.796661	-0.680553	1.868006
C	-3.164755	-2.834565	2.780519
H	-1.065768	-3.281277	2.859759
H	-3.455120	-3.786672	3.212786
H	-5.189975	-2.170540	2.556744
C	-2.183797	1.907629	-0.903949
C	-4.963970	1.539005	-0.873938
C	-2.966395	2.367715	-1.963428
C	-2.835485	1.259309	0.144728
C	-4.214335	1.078032	0.208157
C	-4.345429	2.171119	-1.950858
H	-2.498906	2.871257	-2.803434
H	-4.945277	2.522303	-2.784252
H	-6.040514	1.407492	-0.885390
C	0.094251	3.051181	-2.254484
C	0.828955	4.500572	-4.529597
C	0.742455	2.417242	-3.318703
C	-0.178379	4.421527	-2.336518
C	0.187751	5.141441	-3.469400
C	1.105806	3.138316	-4.454317
H	0.968221	1.356215	-3.246900
H	-0.674144	4.927528	-1.512789
H	-0.025434	6.204663	-3.525027
H	1.609212	2.635392	-5.274461
H	1.115661	5.066002	-5.411213
C	1.175277	-2.507192	1.837706
C	2.485054	-4.965234	2.109594
C	1.850866	-2.819485	3.021050
C	1.153944	-3.441390	0.794578
C	1.799620	-4.666333	0.933861
C	2.508125	-4.040981	3.151814
H	1.872610	-2.109629	3.841937
H	0.635393	-3.213233	-0.133375
H	1.775297	-5.380419	0.115950
H	3.037035	-4.270529	4.072012
H	3.000574	-5.915259	2.214072
H	1.969315	2.682303	0.794125
H	-1.022263	0.570409	3.802255
H	2.384326	4.231695	2.656082
H	-0.112866	2.098478	5.501044
O	-2.038296	0.772903	1.152939
C	-4.777546	0.422873	1.469579
C	3.209025	-0.696610	-2.527072
H	3.733405	-1.472039	-3.117348
H	3.096128	0.158896	-3.214270
C	-0.126430	3.190863	0.615408
C	3.614605	1.027108	-0.826577
H	3.171547	1.709489	-1.585203
O	3.692304	1.390660	0.332542
C	4.159113	-0.261667	-1.396112
C	4.309657	-1.361508	-0.329076
C	5.542501	0.097532	-2.006146
C	5.443517	-1.141751	0.677816
H	4.486607	-2.306983	-0.861010
H	3.358290	-1.480179	0.200565
C	6.631517	0.350626	-0.962456
H	5.844323	-0.746920	-2.639510
H	5.436367	0.963788	-2.672574
H	5.534017	-2.031001	1.312766
H	5.189268	-0.301732	1.332160
H	7.581135	0.552646	-1.470848
H	6.389099	1.247412	-0.377583
C	-6.194253	-0.113076	1.258432
H	-6.578929	-0.555739	2.181117

H	-6.875875	0.699687	0.993512
H	-6.229507	-0.868939	0.467688
C	-4.802964	1.483489	2.596070
H	-5.472753	2.305465	2.323413
H	-5.162423	1.034758	3.527702
H	-3.807571	1.899965	2.777660
C	-1.844912	-5.002310	-3.122968
H	-1.129396	-5.771256	-2.817803
H	-2.843868	-5.447794	-3.135300
H	-1.590955	-4.686710	-4.139489
C	-2.123346	-4.295040	-0.738196
H	-1.523712	-5.170583	-0.471000
H	-1.933177	-3.515392	0.001494
H	-3.180063	-4.576269	-0.682840
C	-2.917815	-1.621003	-1.488464
H	-2.038830	-1.384453	-0.879839
H	-3.298312	-0.688023	-1.911470
H	-3.686202	-2.046722	-0.837166
C	-3.766046	-2.852674	-3.489638
H	-3.500409	-3.395643	-4.399084
H	-4.497095	-3.444523	-2.929351
H	-4.243313	-1.912206	-3.780775
C	6.772610	-0.844662	-0.017929
H	7.556455	-0.653849	0.723976
H	7.089029	-1.724045	-0.596988

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Cu	-0.511198	0.021490	0.071185
C	-3.378861	0.186790	1.815747
H	-3.786476	-0.357264	2.692272
P	0.476334	2.012385	-0.749063
P	0.822170	-0.825161	1.846980
B	-1.064300	-1.419983	-1.287498
O	-1.404803	-2.746310	-0.972375
O	-1.021299	-1.305670	-2.683929
C	-1.300418	-3.559718	-2.153308
C	-1.516364	-2.513012	-3.289092
C	3.494289	1.898087	4.480332
C	1.401871	1.406702	3.386312
C	3.240920	-0.145007	3.219434
C	4.023833	0.702741	3.999281
C	2.180018	2.246555	4.177276
H	3.660399	-1.076732	2.850694
H	5.048491	0.428009	4.231584
H	4.106507	2.559352	5.086254
C	1.284338	3.291638	0.298238
C	2.422475	5.159569	2.048952
C	2.657722	3.542128	0.270011
C	0.487717	3.979224	1.224311
C	1.049322	4.919049	2.080945
C	3.223953	4.464250	1.148640
H	-0.580450	3.781107	1.272665
H	0.417043	5.453453	2.783675
H	2.864922	5.882676	2.727377
C	1.795319	1.481292	-1.927619
C	3.583545	0.327259	-3.752695
C	1.913141	1.988103	-3.224226
C	2.633101	0.421044	-1.571105
C	3.521408	-0.187623	-2.458631
C	2.801155	1.416264	-4.127972
H	1.286563	2.816793	-3.536744
H	2.876252	1.812865	-5.135331
H	4.256530	-0.114182	-4.479524

C	2.006947	-1.933140	0.978527
C	3.700245	-3.462744	-0.645740
C	2.155009	-3.300586	1.207761
C	2.730977	-1.368823	-0.073344
C	3.592868	-2.092899	-0.892585
C	2.991148	-4.060085	0.393336
H	1.602796	-3.775964	2.012170
H	3.093474	-5.125942	0.570765
H	4.349318	-4.075259	-1.261829
C	-0.006960	-1.958669	3.031675
C	-1.396151	-3.696910	4.724400
C	-1.136353	-2.644927	2.566491
C	0.416253	-2.146940	4.350075
C	-0.278759	-3.010881	5.193791
C	-1.821161	-3.515166	3.409311
H	-1.465153	-2.499775	1.539360
H	1.288265	-1.618037	4.723278
H	0.055325	-3.148099	6.217958
H	-2.694160	-4.044819	3.040786
H	-1.937209	-4.370047	5.382901
C	-0.650972	2.963259	-1.854587
C	-2.505823	4.224628	-3.529028
C	-0.766316	4.354827	-1.857252
C	-1.464605	2.206229	-2.709940
C	-2.381406	2.835717	-3.544759
C	-1.695608	4.981278	-2.686810
H	-0.137506	4.957780	-1.209848
H	-1.378534	1.120863	-2.716297
H	-3.006650	2.238580	-4.202027
H	-1.781301	6.063758	-2.675315
H	-3.229624	4.714630	-4.173440
H	0.385831	1.692583	3.127771
H	3.293378	3.020378	-0.439078
H	1.765244	3.181214	4.541140
H	4.294590	4.642983	1.121408
O	2.557337	-0.020529	-0.274754
C	4.402460	-1.322893	-1.935337
C	-4.344635	0.359878	0.659644
C	1.923084	0.201342	2.905576
C	-5.000692	-2.147637	0.841554
H	-5.956937	-1.983247	1.339047
C	-4.474307	-1.033004	-0.016893
C	-2.992726	-2.281049	-3.619721
H	-3.077566	-1.396710	-4.258771
H	-3.431005	-3.131704	-4.151209
H	-3.575251	-2.098397	-2.711690
C	-0.734308	-2.785403	-4.566797
H	-1.021392	-3.749073	-5.001587
H	-0.945582	-2.005097	-5.304704
H	0.342229	-2.791194	-4.382251
C	-2.343558	-4.666918	-2.095416
H	-2.344808	-5.249496	-3.023148
H	-2.115086	-5.348416	-1.269715
H	-3.346942	-4.265893	-1.933909
C	0.107657	-4.163046	-2.152737
H	0.253120	-4.718061	-1.221608
H	0.258610	-4.850725	-2.991225
H	0.870495	-3.379604	-2.196381
C	4.892082	-2.233681	-3.064453
H	5.538378	-3.022281	-2.670183
H	4.057127	-2.699843	-3.596649
H	5.493532	-1.671070	-3.783086
C	5.626206	-0.696523	-1.225391
H	6.264815	-1.482648	-0.809313

H	6.214844	-0.108048	-1.936833
H	5.318423	-0.037544	-0.407677
O	-2.227251	0.574913	1.841847
C	-4.380356	-3.318075	0.982942
H	-3.426180	-3.506969	0.493923
H	-4.808288	-4.119064	1.580304
H	-3.497007	-1.322165	-0.416742
H	-5.151245	-0.889736	-0.871004
C	-5.716889	0.840359	1.209456
H	-6.519021	0.342134	0.653543
H	-5.826032	0.520049	2.253881
C	-3.797681	1.356602	-0.368638
H	-2.860891	0.968403	-0.779331
H	-4.512972	1.390174	-1.199765
C	-3.586301	2.770535	0.200437
H	-2.560219	2.867178	0.566004
H	-3.699257	3.495483	-0.613549
C	-5.899974	2.366319	1.118213
H	-6.292939	2.634349	0.129461
H	-6.648794	2.689462	1.848738
C	-4.574317	3.095091	1.335562
H	-4.732557	4.176323	1.404332
H	-4.154020	2.783212	2.301605

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Cu	0.501804	0.067297	-0.661185
C	2.460325	0.994867	-1.028038
P	-1.169300	1.776636	-0.908200
P	-0.398954	-2.053350	-0.503617
B	1.591482	0.630950	1.045858
O	1.944009	-0.318844	1.991798
O	1.313192	1.835126	1.661618
C	1.618486	0.178439	3.309839
C	1.509381	1.733516	3.086756
C	-3.255135	-3.188102	-3.963160
C	-1.340308	-1.993066	-3.113623
C	-2.652965	-3.378027	-1.633754
C	-3.494826	-3.706859	-2.691996
C	-2.175154	-2.335126	-4.173890
H	-2.840400	-3.791998	-0.647324
H	-4.337250	-4.371007	-2.524102
H	-3.912827	-3.445663	-4.787879
C	-2.317291	1.427237	-2.301685
C	-3.905426	0.844362	-4.530468
C	-3.685587	1.200422	-2.151133
C	-1.747327	1.349203	-3.579668
C	-2.539648	1.077426	-4.688484
C	-4.473313	0.898802	-3.261302
H	-0.678418	1.506534	-3.703045
H	-2.088044	1.031815	-5.674900
H	-4.522750	0.617078	-5.394289
C	-2.252312	1.999333	0.563796
C	-3.697396	2.146853	2.963173
C	-2.514757	3.234997	1.159764
C	-2.747274	0.858762	1.199335
C	-3.483295	0.896545	2.383772
C	-3.221106	3.305669	2.355480
H	-2.146241	4.144974	0.698781
H	-3.405226	4.270721	2.816307
H	-4.251090	2.226324	3.892205
C	-1.368220	-2.375350	1.030300
C	-2.797683	-2.617087	3.429238
C	-1.190249	-3.490185	1.852622

C	-2.305496	-1.421109	1.429038
C	-3.032766	-1.509592	2.615935
C	-1.894579	-3.604863	3.046238
H	-0.483818	-4.263008	1.571067
H	-1.737574	-4.469020	3.683469
H	-3.329547	-2.723849	4.368110
C	0.824153	-3.426037	-0.485630
C	2.779183	-5.422030	-0.375582
C	1.813938	-3.393394	0.505694
C	0.825275	-4.461535	-1.421959
C	1.805234	-5.452037	-1.368963
C	2.779014	-4.392422	0.564441
H	1.828189	-2.578048	1.225796
H	0.064884	-4.501555	-2.195733
H	1.800854	-6.250554	-2.104795
H	3.538536	-4.361560	1.339352
H	3.539799	-6.195824	-0.334734
C	-0.630488	3.507457	-1.251160
C	0.266939	6.129135	-1.663231
C	-1.259793	4.332718	-2.188388
C	0.445712	4.014176	-0.511563
C	0.888472	5.317931	-0.716417
C	-0.808975	5.634428	-2.395952
H	-2.104184	3.964171	-2.761890
H	0.920325	3.391891	0.241878
H	1.723780	5.698001	-0.135605
H	-1.303882	6.262756	-3.130425
H	0.617501	7.143690	-1.827652
H	-0.509640	-1.310223	-3.271401
H	-4.147806	1.264494	-1.170751
H	-1.989201	-1.922623	-5.160260
H	-5.535760	0.716278	-3.131069
O	-2.487000	-0.346934	0.593636
C	-4.059907	-0.417780	2.907012
C	-1.570907	-2.516237	-1.838862
C	2.782312	2.505319	3.430937
H	2.675402	3.536976	3.082648
H	2.954475	2.525238	4.511256
H	3.661726	2.076284	2.946605
C	0.314161	2.392169	3.767144
H	0.380171	2.291937	4.855358
H	0.300198	3.458918	3.524201
H	-0.630967	1.961018	3.429999
C	2.714149	-0.256219	4.272682
H	2.530079	0.143281	5.275119
H	2.727463	-1.348233	4.340607
H	3.700648	0.074748	3.940815
C	0.292016	-0.469773	3.704617
H	0.395469	-1.557522	3.659939
H	-0.006732	-0.192411	4.720041
H	-0.505658	-0.180642	3.017192
C	-4.411955	-0.339718	4.394170
H	-4.848146	-1.281451	4.737134
H	-3.532780	-0.117506	5.007003
H	-5.165083	0.432535	4.570659
C	-5.343344	-0.734180	2.102463
H	-5.768484	-1.687592	2.432498
H	-6.088307	0.053168	2.256531
H	-5.136319	-0.805687	1.030399
O	1.865298	0.595930	-2.117475
H	2.387074	2.073471	-0.795841
C	3.867896	-1.049897	-0.759433
H	3.476795	-1.326098	0.223752
H	3.117226	-1.351388	-1.501963

C	5.120336	-1.829757	-1.026496
H	5.482889	-1.830766	-2.054542
C	5.775381	-2.551644	-0.117636
H	6.660848	-3.128154	-0.372364
H	5.447252	-2.584427	0.919851
C	3.916848	0.493914	-0.814055
C	4.510675	1.117949	0.463324
C	4.664012	1.042524	-2.062492
H	4.119650	0.586470	1.335423
H	4.352443	0.466828	-2.939711
C	6.192444	1.092904	-1.958294
H	6.613976	0.082091	-1.951977
H	6.590025	1.592473	-2.849926
C	6.039943	1.148069	0.537128
H	6.428748	0.126195	0.615652
H	6.343193	1.674404	1.450404
H	4.145845	2.154008	0.534556
H	4.313733	2.070742	-2.233363
C	6.644878	1.820202	-0.693249
H	7.739063	1.831019	-0.628336
H	6.315868	2.868562	-0.735054

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Cu	-0.447612	0.053906	0.620606
C	-3.235959	-0.591367	0.310417
P	0.785411	2.034621	0.393340
P	0.972219	-1.785418	0.917274
B	-2.647454	-0.723911	-1.154394
O	-2.939618	-1.698172	-2.078910
O	-1.642529	0.114897	-1.604695
C	-1.922546	-1.653740	-3.107702
C	-1.394853	-0.183455	-2.995278
C	3.783114	-0.848993	4.479284
C	1.624294	-0.758645	3.408363
C	3.477232	-1.831122	2.295274
C	4.299227	-1.526719	3.377811
C	2.442486	-0.470331	4.495532
H	3.888474	-2.364261	1.443051
H	5.344008	-1.822079	3.359496
H	4.425243	-0.610431	5.321752
C	1.779031	2.442256	1.886514
C	3.164423	2.958437	4.262779
C	3.173690	2.398776	1.912881
C	1.081776	2.730767	3.067405
C	1.771093	3.002199	4.243743
C	3.861410	2.647764	3.099239
H	-0.005420	2.752548	3.064143
H	1.218986	3.237920	5.148509
H	3.703315	3.159720	5.183656
C	1.968737	2.169557	-1.017158
C	3.574766	2.119707	-3.319327
C	2.004195	3.265194	-1.885193
C	2.777245	1.075911	-1.332546
C	3.589137	1.018369	-2.466077
C	2.796554	3.237093	-3.027221
H	1.391346	4.136298	-1.681248
H	2.805097	4.090528	-3.697405
H	4.179698	2.115970	-4.219351
C	2.088943	-2.256139	-0.464434
C	3.671552	-2.696291	-2.734704
C	2.163288	-3.527474	-1.036896
C	2.837060	-1.235791	-1.052623
C	3.641752	-1.419243	-2.174942

C	2.943198	-3.740748	-2.169474
H	1.591629	-4.345805	-0.611677
H	2.985348	-4.729206	-2.615257
H	4.273232	-2.887649	-3.616557
C	0.196333	-3.387502	1.373396
C	-1.089545	-5.797795	1.966498
C	-1.112197	-3.617724	0.938868
C	0.855642	-4.374321	2.114273
C	0.213671	-5.573348	2.409447
C	-1.752237	-4.819690	1.229733
H	-1.635891	-2.851276	0.376432
H	1.870592	-4.205424	2.462949
H	0.730364	-6.333524	2.987448
H	-2.769687	-4.983892	0.887974
H	-1.588648	-6.733162	2.201234
C	-0.263077	3.522598	0.142475
C	-1.949115	5.685006	-0.394813
C	0.050536	4.796093	0.628148
C	-1.424064	3.341034	-0.615706
C	-2.261758	4.419958	-0.886728
C	-0.793243	5.871449	0.362237
H	0.951419	4.949847	1.214790
H	-1.673687	2.347039	-0.978235
H	-3.170041	4.265431	-1.461358
H	-0.547328	6.856674	0.746894
H	-2.607413	6.524834	-0.596045
H	0.585383	-0.437420	3.413846
H	3.734050	2.175923	1.010246
H	2.036890	0.067245	5.346409
H	4.946281	2.604857	3.108322
O	2.740031	0.005795	-0.472434
C	4.459644	-0.223352	-2.657929
C	2.133079	-1.449153	2.303406
C	4.918469	-0.386505	-4.108343
H	5.522954	0.469771	-4.418930
H	5.552924	-1.270651	-4.212777
H	4.070487	-0.482154	-4.793544
C	5.704262	-0.090297	-1.748282
H	6.333937	-0.981210	-1.839758
H	6.292690	0.785191	-2.041103
H	5.422480	0.022137	-0.696971
C	-2.211755	0.818041	-3.810358
H	-1.919915	1.832214	-3.521716
H	-2.032035	0.701331	-4.882955
H	-3.283905	0.704661	-3.622337
C	0.088990	-0.010432	-3.275092
H	0.366773	1.042033	-3.165668
H	0.692409	-0.597349	-2.580107
H	0.329966	-0.323221	-4.296073
C	-0.866789	-2.689340	-2.724700
H	-0.401633	-2.436086	-1.768522
H	-1.343507	-3.668156	-2.620470
H	-0.079556	-2.764429	-3.480245
C	-2.552275	-2.004663	-4.445787
H	-3.414493	-1.371050	-4.664041
H	-1.821166	-1.892532	-5.252822
H	-2.888407	-3.045590	-4.434661
O	-2.327352	0.033979	1.159275
H	-3.436467	-1.633706	0.641869
C	-4.395916	1.569039	-0.159569
H	-4.084472	1.516867	-1.215421
H	-3.540205	1.951547	0.403787
C	-5.546516	2.525701	-0.057889
H	-6.449526	2.279456	-0.618659

C	-5.526883	3.654349	0.650844
H	-6.381290	4.325983	0.683992
H	-4.648747	3.944421	1.225162
C	-4.635363	0.124417	0.337657
C	-5.153025	0.153055	1.788460
C	-5.664813	-0.595723	-0.556672
C	-5.559237	-1.225402	2.318302
H	-6.024300	0.820278	1.846099
H	-4.367625	0.585986	2.416324
C	-6.074034	-1.979348	-0.038897
H	-6.572519	0.021451	-0.615737
H	-5.279158	-0.679415	-1.580490
H	-5.968841	-1.124606	3.330728
H	-4.673303	-1.867470	2.405690
H	-6.848712	-2.401163	-0.690774
H	-5.219685	-2.665451	-0.087857
C	-6.584459	-1.898897	1.402147
H	-6.834686	-2.899262	1.775306
H	-7.515426	-1.313579	1.417173

4. X-Ray Diffraction data of Compound 25

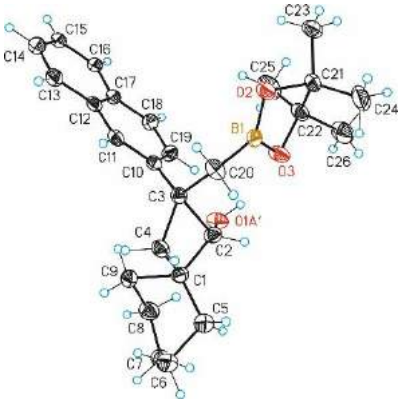

Table 1. Crystal data and structure refinement for mo_RJ452FB_0m (**25**).

Identification code	mo_RJ452FB_0m	
Empirical formula	C26 H35 B O3	
Formula weight	406.35	
Temperature	100(2)K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 17.9052(16)Å	α= 90°.
	b = 6.4987(6)Å	β = 100.138(3)°.
	c = 19.8249(16)Å	γ = 90°.
Volume	2270.8(3) $Å^3$	
Z	4	
Density (calculated)	1.189 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	880	
Crystal size	0.040 x 0.020 x 0.020 mm^3	
Theta range for data collection	1.155 to 26.119°.	
Index ranges	-20<=h<=22,-8<=k<=8,-23<=l<=24	
Reflections collected	29583	
Independent reflections	4488[R(int) = 0.0626]	
Completeness to theta =26.119°	99.6%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.74 and 0.53	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4488/ 1424/ 550	
Goodness-of-fit on F^2	1.025	

Final R indices [I>2sigma(I)]	R1 = 0.0663, wR2 = 0.1626
R indices (all data)	R1 = 0.1147, wR2 = 0.1886
Largest diff. peak and hole	0.249 and -0.287 e.Å^{-3}

Table 2. Bond lengths [Å] and angles [°] for mo_RJ452FB_0m.

Bond lengths----

C1	C2	1.494(9)
C1	C4	1.520(9)
C1	C5	1.539(8)
C1	C9	1.621(9)
O1A	C4	1.462(12)
O1A'	C2	1.430(12)
C2	C3	1.811(16)
C3	C10	1.492(17)
C3	C20	1.525(18)
C3	C4	1.601(17)
C5	C6	1.518(9)
C6	C7	1.657(10)
C7	C8	1.538(9)
C8	C9	1.541(8)
C1'	C5'	1.531(7)
C1'	C4'	1.535(8)
C1'	C2'	1.547(9)
C1'	C9'	1.715(10)
O1B	C4'	1.390(9)
O1B'	C2'	1.352(18)
C2'	C3'	1.287(15)
C3'	C10'	1.46(2)
C3'	C20	1.563(17)
C3'	C4'	1.655(18)
C5'	C6'	1.534(9)
C6'	C7'	1.833(10)
C7'	C8'	1.521(9)
C8'	C9'	1.509(9)
C10	C11	1.364(5)
C10	C19	1.416(5)

C11 C12 1.424(6)
C12 C17 1.399(6)
C12 C13 1.402(5)
C13 C14 1.395(6)
C14 C15 1.404(6)
C15 C16 1.359(6)
C16 C17 1.447(7)
C17 C18 1.405(5)
C18 C19 1.363(4)
C10' C11' 1.358(13)
C10' C19' 1.433(14)
C11' C12' 1.447(13)
C12' C17' 1.378(13)
C12' C13' 1.382(13)
C13' C14' 1.399(15)
C14' C15' 1.384(9)
C15' C16' 1.344(15)
C16' C17' 1.461(15)
C17' C18' 1.400(14)
C18' C19' 1.349(12)
C20 B1 1.562(4)
O2 B1 1.364(8)
O2 C21 1.516(10)
O3 B1 1.314(7)
O3 C22 1.524(8)
C21 C23 1.511(9)
C21 C24 1.516(7)
C21 C22 1.552(7)
C22 C25 1.497(8)
C22 C26 1.525(9)
O2' B1 1.316(15)
O2' C21' 1.598(19)
O3' B1 1.466(14)
O3' C22' 1.626(18)
C21' C22' 1.495(15)
C21' C24' 1.503(18)
C21' C23' 1.533(14)
C22' C26' 1.541(15)

C22' C25' 1.607(16)

Angles----------

C2 C1 C4 88.6(5)

C2 C1 C5 115.3(5)

C4 C1 C5 115.7(5)

C2 C1 C9 124.5(6)

C4 C1 C9 91.5(5)

C5 C1 C9 114.2(5)

O1A' C2 C1 117.2(8)

O1A' C2 C3 116.3(9)

C1 C2 C3 91.3(7)

C10 C3 C20 113.1(9)

C10 C3 C4 125.7(13)

C20 C3 C4 117.8(12)

C10 C3 C2 107.0(10)

C20 C3 C2 106.5(10)

C4 C3 C2 75.9(6)

O1A C4 C1 119.4(7)

O1A C4 C3 105.3(8)

C1 C4 C3 99.0(7)

C6 C5 C1 111.5(5)

C5 C6 C7 84.8(5)

C8 C7 C6 114.3(5)

C7 C8 C9 112.4(5)

C8 C9 C1 89.2(5)

C5' C1' C4' 114.8(5)

C5' C1' C2' 116.9(5)

C4' C1' C2' 86.4(5)

C5' C1' C9' 109.8(5)

C4' C1' C9' 128.4(5)

C2' C1' C9' 95.8(5)

C3' C2' O1B' 118.8(11)

C3' C2' C1' 96.4(9)

O1B' C2' C1' 124.1(9)

C2' C3' C10' 136.1(15)

C2' C3' C20 121.7(13)

C10' C3' C20 98.7(10)

C2' C3' C4' 90.8(9)
C10' C3' C4' 91.6(10)
C20 C3' C4' 109.1(10)
O1B C4' C1' 119.6(6)
O1B C4' C3' 132.4(7)
C1' C4' C3' 83.2(6)
C1' C5' C6' 112.1(5)
C5' C6' C7' 93.4(5)
C8' C7' C6' 110.8(4)
C9' C8' C7' 110.1(6)
C8' C9' C1' 97.9(5)
C11 C10 C19 117.5(4)
C11 C10 C3 117.6(6)
C19 C10 C3 124.5(6)
C10 C11 C12 122.2(3)
C17 C12 C13 119.1(4)
C17 C12 C11 118.8(4)
C13 C12 C11 122.1(4)
C14 C13 C12 118.8(4)
C13 C14 C15 121.8(4)
C16 C15 C14 121.1(5)
C15 C16 C17 117.5(6)
C12 C17 C18 118.9(4)
C12 C17 C16 121.8(4)
C18 C17 C16 119.3(4)
C19 C18 C17 120.7(3)
C18 C19 C10 121.8(3)
C11' C10' C19' 117.0(12)
C11' C10' C3' 123.7(12)
C19' C10' C3' 119.2(11)
C10' C11' C12' 122.1(12)
C17' C12' C13' 118.9(11)
C17' C12' C11' 118.1(11)
C13' C12' C11' 123.0(11)
C12' C13' C14' 114.2(12)
C15' C14' C13' 128.9(17)
C16' C15' C14' 117.0(15)
C15' C16' C17' 116.4(12)

C12' C17' C18' 120.2(12)
C12' C17' C16' 124.5(12)
C18' C17' C16' 115.3(12)
C19' C18' C17' 120.6(10)
C18' C19' C10' 121.9(10)
C3 C20 B1 117.2(6)
B1 C20 C3' 113.4(6)
B1 O2 C21 103.6(5)
B1 O3 C22 106.7(5)
C23 C21 C24 110.2(4)
C23 C21 O2 101.6(5)
C24 C21 O2 116.9(5)
C23 C21 C22 114.7(5)
C24 C21 C22 113.9(5)
O2 C21 C22 98.6(5)
C25 C22 O3 117.3(5)
C25 C22 C26 115.2(5)
O3 C22 C26 102.2(5)
C25 C22 C21 113.2(5)
O3 C22 C21 95.5(4)
C26 C22 C21 111.5(6)
B1 O2' C21' 104.0(11)
B1 O3' C22' 94.1(8)
C22' C21' C24' 118.6(12)
C22' C21' C23' 114.8(10)
C24' C21' C23' 108.5(9)
C22' C21' O2' 89.0(9)
C24' C21' O2' 99.6(10)
C23' C21' O2' 125.4(9)
C21' C22' C26' 112.2(11)
C21' C22' C25' 113.8(10)
C26' C22' C25' 112.4(9)
C21' C22' O3' 95.7(9)
C26' C22' O3' 127.7(9)
C25' C22' O3' 93.3(9)
O3 B1 O2 113.0(5)
O2' B1 O3' 112.1(9)
O3 B1 C20 123.7(4)

O2' B1 C20 124.0(8)

O2 B1 C20 123.3(4)

O3' B1 C20 123.9(6)

Table 3. Torsion angles [°] for mo_RJ452FB_0m.

C4 C1 C2 O1A' -137.3(8)

C5 C1 C2 O1A' 104.7(9)

C9 C1 C2 O1A' -46.4(11)

C4 C1 C2 C3 -16.7(8)

C5 C1 C2 C3 -134.7(8)

C9 C1 C2 C3 74.2(9)

O1A' C2 C3 C10 14.2(14)

C1 C2 C3 C10 -107.2(9)

O1A' C2 C3 C20 -107.0(11)

C1 C2 C3 C20 131.6(9)

O1A' C2 C3 C4 137.7(9)

C1 C2 C3 C4 16.3(7)

C2 C1 C4 O1A 132.5(7)

C5 C1 C4 O1A -109.9(7)

C9 C1 C4 O1A 8.0(8)

C2 C1 C4 C3 19.2(9)

C5 C1 C4 C3 136.8(8)

C9 C1 C4 C3 -105.3(8)

C10 C3 C4 O1A -39.1(14)

C20 C3 C4 O1A 118.3(10)

C2 C3 C4 O1A -140.1(8)

C10 C3 C4 C1 84.8(11)

C20 C3 C4 C1 -117.8(9)

C2 C3 C4 C1 -16.2(7)

C2 C1 C5 C6 177.7(6)

C4 C1 C5 C6 76.3(7)

C9 C1 C5 C6 -28.1(8)

C1 C5 C6 C7 78.1(6)

C5 C6 C7 C8 -56.5(6)

C6 C7 C8 C9 -18.5(8)

C7 C8 C9 C1 70.2(6)

C2 C1 C9 C8 101.4(7)
C4 C1 C9 C8 -169.2(5)
C5 C1 C9 C8 -50.0(6)
C5' C1' C2' C3' -131.2(10)
C4' C1' C2' C3' -15.1(10)
C9' C1' C2' C3' 113.1(9)
C5' C1' C2' O1B' 97.4(11)
C4' C1' C2' O1B' -146.5(11)
C9' C1' C2' O1B' -18.2(12)
O1B' C2' C3' C10' 56(2)
C1' C2' C3' C10' -79.1(19)
O1B' C2' C3' C20 -98.1(16)
C1' C2' C3' C20 127.0(12)
O1B' C2' C3' C4' 148.8(11)
C1' C2' C3' C4' 14.0(9)
C5' C1' C4' O1B -94.7(7)
C2' C1' C4' O1B 147.2(6)
C9' C1' C4' O1B 52.7(9)
C5' C1' C4' C3' 129.8(8)
C2' C1' C4' C3' 11.7(7)
C9' C1' C4' C3' -82.8(9)
C2' C3' C4' O1B -138.4(9)
C10' C3' C4' O1B -2.2(15)
C20 C3' C4' O1B 97.5(12)
C2' C3' C4' C1' -14.1(9)
C10' C3' C4' C1' 122.1(10)
C20 C3' C4' C1' -138.1(8)
C4' C1' C5' C6' -177.8(5)
C2' C1' C5' C6' -78.8(7)
C9' C1' C5' C6' 28.9(7)
C1' C5' C6' C7' -74.0(5)
C5' C6' C7' C8' 48.2(7)
C6' C7' C8' C9' 26.5(8)
C7' C8' C9' C1' -75.5(7)
C5' C1' C9' C8' 50.5(6)
C4' C1' C9' C8' -98.1(7)
C2' C1' C9' C8' 171.9(5)
C20 C3 C10 C11 -80.5(11)

C4 C3 C10 C11 77.9(12)
C2 C3 C10 C11 162.5(6)
C20 C3 C10 C19 92.2(9)
C4 C3 C10 C19 -109.4(11)
C2 C3 C10 C19 -24.8(13)
C19 C10 C11 C12 0.7(6)
C3 C10 C11 C12 173.9(8)
C10 C11 C12 C17 -2.0(7)
C10 C11 C12 C13 179.8(4)
C17 C12 C13 C14 0.0(6)
C11 C12 C13 C14 178.2(4)
C12 C13 C14 C15 -1.1(6)
C13 C14 C15 C16 2.0(8)
C14 C15 C16 C17 -1.7(10)
C13 C12 C17 C18 -179.8(4)
C11 C12 C17 C18 2.0(6)
C13 C12 C17 C16 0.2(8)
C11 C12 C17 C16 -178.0(5)
C15 C16 C17 C12 0.6(9)
C15 C16 C17 C18 -179.4(5)
C12 C17 C18 C19 -0.7(5)
C16 C17 C18 C19 179.3(5)
C17 C18 C19 C10 -0.7(5)
C11 C10 C19 C18 0.7(6)
C3 C10 C19 C18 -172.0(8)
C2' C3' C10' C11' -49(3)
C20 C3' C10' C11' 109.0(16)
C4' C3' C10' C11' -141.5(15)
C2' C3' C10' C19' 134.3(18)
C20 C3' C10' C19' -68.0(15)
C4' C3' C10' C19' 41.6(15)
C19' C10' C11' C12' 3(2)
C3' C10' C11' C12' -174.1(13)
C10' C11' C12' C17' -2(2)
C10' C11' C12' C13' 177.4(13)
C17' C12' C13' C14' 3(2)
C11' C12' C13' C14' -176.4(16)
C12' C13' C14' C15' -2(4)

C13' C14' C15' C16' 0(4)
C14' C15' C16' C17' 2(3)
C13' C12' C17' C18' -178.9(14)
C11' C12' C17' C18' 0(2)
C13' C12' C17' C16' -1(3)
C11' C12' C17' C16' 178.3(15)
C15' C16' C17' C12' -2(3)
C15' C16' C17' C18' 176.4(16)
C12' C17' C18' C19' 0(2)
C16' C17' C18' C19' -178.5(13)
C17' C18' C19' C10' 1.6(19)
C11' C10' C19' C18' -3(2)
C3' C10' C19' C18' 174.3(12)
C10 C3 C20 B1 -55.1(10)
C4 C3 C20 B1 144.6(7)
C2 C3 C20 B1 62.1(9)
C2' C3' C20 B1 75.9(14)
C10' C3' C20 B1 -86.0(9)
C4' C3' C20 B1 179.2(6)
B1 O2 C21 C23 155.7(4)
B1 O2 C21 C24 -84.2(6)
B1 O2 C21 C22 38.2(6)
B1 O3 C22 C25 -81.0(6)
B1 O3 C22 C26 152.1(5)
B1 O3 C22 C21 38.7(6)
C23 C21 C22 C25 -28.4(6)
C24 C21 C22 C25 -156.7(4)
O2 C21 C22 C25 78.7(5)
C23 C21 C22 O3 -151.3(5)
C24 C21 C22 O3 80.4(5)
O2 C21 C22 O3 -44.2(6)
C23 C21 C22 C26 103.4(7)
C24 C21 C22 C26 -24.9(7)
O2 C21 C22 C26 -149.5(5)
B1 O2' C21' C22' -52.8(10)
B1 O2' C21' C24' -171.6(9)
B1 O2' C21' C23' 67.4(13)
C24' C21' C22' C26' 26.7(14)

C23' C21' C22' C26' 157.3(8)

O2' C21' C22' C26' -73.6(10)

C24' C21' C22' C25' -102.3(14)

C23' C21' C22' C25' 28.3(13)

O2' C21' C22' C25' 157.4(10)

C24' C21' C22' O3' 161.6(10)

C23' C21' C22' O3' -67.9(10)

O2' C21' C22' O3' 61.2(10)

B1 O3' C22' C21' -53.7(9)

B1 O3' C22' C26' 70.1(13)

B1 O3' C22' C25' -168.0(7)

C22 O3 B1 O2 -16.5(6)

C22 O3 B1 C20 165.4(4)

C21' O2' B1 O3' 19.4(11)

C21' O2' B1 C20 -161.8(6)

C21 O2 B1 O3 -14.7(6)

C21 O2 B1 C20 163.4(4)

C22' O3' B1 O2' 19.6(9)

C22' O3' B1 C20 -159.2(5)

C3 C20 B1 O3 -50.2(7)

C3' C20 B1 O2' 162.5(8)

C3 C20 B1 O2 131.9(7)

C3' C20 B1 O3' -18.7(9)

Symetry operations

---

1 'x, y, z'

2 '-x, y+1/2, -z+1/2'

3 '-x, -y, -z'

4 'x, -y-1/2, z-1/2'

5. X-Ray Diffraction data of Compound 26-*syn-(B-OH)*

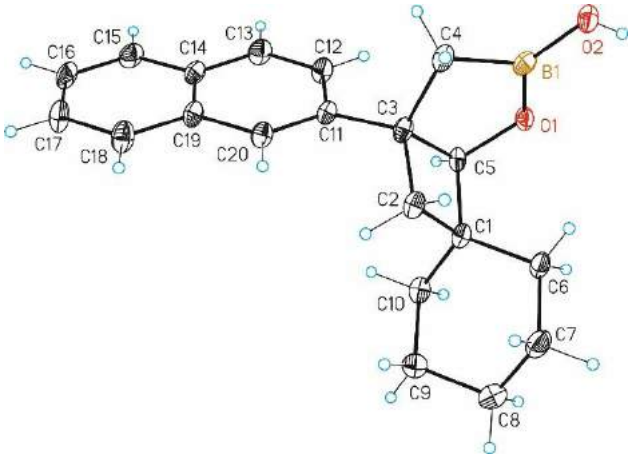

Table 1. Crystal data and structure refinement for mo_RJ452FD_0m_5 (**26-syn-(B-OH)**)

Identification code	mo_RJ452FD_0m_5	
Empirical formula	C20 H23 B O2	
Formula weight	306.19	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 25.557(9)Å	α= 90°.
	b = 5.612(2)Å	β = 113.817(8)°.
	c = 25.398(9)Å	γ = 90°.
Volume	3333(2) $Å^3$	
Z	8	
Density (calculated)	1.221 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	1312	
Crystal size	0.50 x 0.20 x 0.03 mm^3	
Theta range for data collection	1.742 to 31.382°.	
Index ranges	-36<=h<=33,0<=k<=7,0<=l<=36	
Reflections collected	7160	
Independent reflections	7160[R(int) = ?]	
Completeness to theta =31.382°	91.1%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.998 and 0.768	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7160/ 0/ 210	

Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0704, wR2 = 0.1672
R indices (all data)	R1 = 0.1340, wR2 = 0.1981
Largest diff. peak and hole	0.400 and -0.482 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for mo_RJ452FD_0m_5.

Bond lengths----	
O1-B1	1.390(3)
O1-C5	1.446(3)
B1-O2	1.344(3)
B1-C4	1.572(3)
C1-C10	1.523(3)
C1-C6	1.531(3)
C1-C5	1.552(3)
C1-C2	1.558(3)
C2-C3	1.553(3)
C3-C11	1.513(3)
C3-C4	1.545(3)
C3-C5	1.568(3)
C6-C7	1.529(4)
C7-C8	1.525(4)
C8-C9	1.533(3)
C9-C10	1.523(4)
C11-C20	1.373(3)
C11-C12	1.423(3)
C12-C13	1.369(3)
C13-C14	1.420(3)
C14-C19	1.418(3)
C14-C15	1.421(3)
C15-C16	1.364(4)
C16-C17	1.410(4)
C17-C18	1.372(3)
C18-C19	1.418(3)
C19-C20	1.424(3)
Angles----------	
B1-O1-C5	111.26(18)

O2-B1-O1	121.3(2)
O2-B1-C4	128.1(2)
O1-B1-C4	110.6(2)
C10-C1-C6	110.6(2)
C10-C1-C5	111.81(19)
C6-C1-C5	115.90(19)
C10-C1-C2	112.57(19)
C6-C1-C2	115.60(19)
C5-C1-C2	88.87(17)
C3-C2-C1	91.15(17)
C11-C3-C4	111.99(19)
C11-C3-C2	117.4(2)
C4-C3-C2	114.70(19)
C11-C3-C5	116.31(18)
C4-C3-C5	105.41(18)
C2-C3-C5	88.45(17)
O1-C5-C1	113.84(17)
O1-C5-C3	108.20(18)
C1-C5-C3	90.80(17)
C3-C4-B1	103.47(19)
C7-C6-C1	111.0(2)
C8-C7-C6	111.0(2)
C7-C8-C9	110.8(2)
C10-C9-C8	110.7(2)
C1-C10-C9	111.8(2)
C20-C11-C12	118.3(2)
C20-C11-C3	122.8(2)
C12-C11-C3	118.7(2)
C13-C12-C11	121.6(2)
C12-C13-C14	120.8(2)
C19-C14-C13	118.3(2)
C19-C14-C15	118.8(2)
C13-C14-C15	122.8(2)
C16-C15-C14	121.0(2)
C15-C16-C17	120.3(2)
C18-C17-C16	119.9(2)
C17-C18-C19	121.1(2)
C18-C19-C14	118.7(2)

C18-C19-C20	121.9(2)
C14-C19-C20	119.4(2)
C11-C20-C19	121.6(2)

Table 3. Torsion angles [°] for mo_RJ452FD_0m_5.

C5-O1-B1-O2	174.7(2)
C5-O1-B1-C4	-6.8(3)
C10-C1-C2-C3	-106.7(2)
C6-C1-C2-C3	124.9(2)
C5-C1-C2-C3	6.51(17)
C1-C2-C3-C11	112.6(2)
C1-C2-C3-C4	-112.7(2)
C1-C2-C3-C5	-6.44(17)
B1-O1-C5-C1	-99.0(2)
B1-O1-C5-C3	0.3(2)
C10-C1-C5-O1	-142.17(19)
C6-C1-C5-O1	-14.2(3)
C2-C1-C5-O1	103.9(2)
C10-C1-C5-C3	107.5(2)
C6-C1-C5-C3	-124.5(2)
C2-C1-C5-C3	-6.44(17)
C11-C3-C5-O1	130.9(2)
C4-C3-C5-O1	6.2(2)
C2-C3-C5-O1	-109.01(19)
C11-C3-C5-C1	-113.6(2)
C4-C3-C5-C1	121.68(18)
C2-C3-C5-C1	6.46(17)
C11-C3-C4-B1	-136.8(2)
C2-C3-C4-B1	86.1(2)
C5-C3-C4-B1	-9.4(2)
O2-B1-C4-C3	-171.3(2)
O1-B1-C4-C3	10.3(3)
C10-C1-C6-C7	-55.8(3)
C5-C1-C6-C7	175.6(2)
C2-C1-C6-C7	73.6(3)
C1-C6-C7-C8	56.5(3)

C6-C7-C8-C9	-56.5(3)
C7-C8-C9-C10	56.0(3)
C6-C1-C10-C9	55.9(3)
C5-C1-C10-C9	-173.37(19)
C2-C1-C10-C9	-75.1(2)
C8-C9-C10-C1	-56.0(3)
C4-C3-C11-C20	-105.7(3)
C2-C3-C11-C20	30.2(3)
C5-C3-C11-C20	133.0(2)
C4-C3-C11-C12	69.9(3)
C2-C3-C11-C12	-154.2(2)
C5-C3-C11-C12	-51.4(3)
C20-C11-C12-C13	-0.5(4)
C3-C11-C12-C13	-176.3(2)
C11-C12-C13-C14	-0.3(4)
C12-C13-C14-C19	1.1(4)
C12-C13-C14-C15	-179.0(3)
C19-C14-C15-C16	1.3(4)
C13-C14-C15-C16	-178.7(3)
C14-C15-C16-C17	-0.6(4)
C15-C16-C17-C18	-0.3(4)
C16-C17-C18-C19	0.4(4)
C17-C18-C19-C14	0.3(4)
C17-C18-C19-C20	-179.9(3)
C13-C14-C19-C18	178.9(2)
C15-C14-C19-C18	-1.1(4)
C13-C14-C19-C20	-1.0(4)
C15-C14-C19-C20	179.0(2)
C12-C11-C20-C19	0.5(4)
C3-C11-C20-C19	176.2(2)
C18-C19-C20-C11	-179.6(2)
C14-C19-C20-C11	0.2(4)

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6. X-Ray Diffraction data of Compound 33

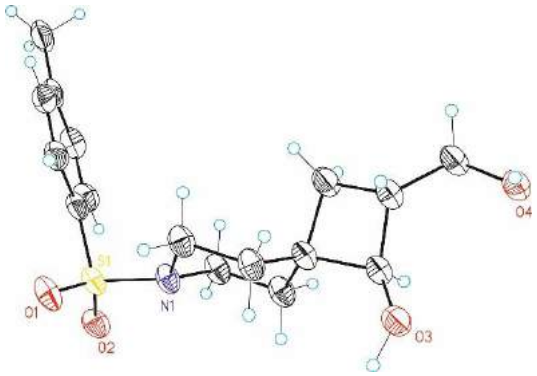

Table 1. Crystal data and structure refinement for mo_JRB919_EE5 (**33**).

Identification code	mo_JRB919_EE5
Empirical formula	$C_{16}H_{25}NO_5S$
Formula weight	343.43
Temperature	100(2)K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	a = 6.567(2)Å α= 78.857(7)°.
	b = 7.546(3)Å β = 84.145(8)°.
	c = 18.576(7)Å γ = 72.132(7)°.
Volume	858.7(6) $Å^3$
Z	2
Density (calculated)	1.328 Mg/m^3
Absorption coefficient	0.213 mm^{-1}
F(000)	368
Crystal size	0.100 x 0.100 x 0.020 mm^3
Theta range for data collection	1.118 to 28.324°.
Index ranges	-8<=h<=8,-9<=k<=10,0<=l<=24
Reflections collected	17003
Independent reflections	17003[R(int) = ?]
Completeness to theta =28.324°	99.0%
Absorption correction	Multi-scan
Max. and min. transmission	0.74 and 0.29
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17003/ 583/ 395
Goodness-of-fit on F^2	1.005
Final R indices [I>2sigma(I)]	R1 = 0.0879, wR2 = 0.2351

R indices (all data)	R1 = 0.1089, wR2 = 0.2528
Largest diff. peak and hole	0.410 and -0.726 e.Å^{-3}

Table 2. Bond lengths [Å] and angles [°] for mo_JRB919_EE5.

Bond lengths----		
O1	S1	1.441(5)
O2	S1	1.442(5)
O3	C13	1.424(6)
O4	C16	1.432(5)
S1	N1	1.642(4)
S1	C6	1.753(5)
N1	C12	1.483(6)
N1	C8	1.482(6)
C1	C2	1.386(7)
C1	C6	1.396(6)
C2	C3	1.396(8)
C3	C4	1.380(8)
C3	C7	1.506(7)
C4	C5	1.384(7)
C5	C6	1.389(6)
C8	C9	1.519(6)
C9	C10	1.530(6)
C10	C11	1.530(6)
C10	C13	1.553(6)
C10	C15	1.556(10)
C11	C12	1.529(6)
C13	C14	1.538(6)
C14	C16	1.528(9)
C14	C15	1.555(11)
O1'	S1'	1.42(3)
O2'	S1'	1.47(3)
O3'	C13'	1.429(10)
O4'	C16'	1.432(10)
S1'	N1'	1.645(16)
S1'	C6'	1.744(15)
N1'	C8'	1.472(19)
N1'	C12'	1.49(4)

C1'	C2'	1.3900
C1'	C6'	1.3900
C2'	C3'	1.3900
C3'	C4'	1.3900
C3'	C7'	1.509(17)
C4'	C5'	1.3900
C5'	C6'	1.3900
C8'	C9'	1.528(18)
C9'	C10'	1.53(2)
C10'	C11'	1.54(4)
C10'	C15'	1.56(7)
C10'	C13'	1.58(4)
C11'	C12'	1.48(4)
C13'	C14'	1.40(4)
C14'	C16'	1.54(2)
C14'	C15'	1.59(7)

Angles----------

O1	S1	O2	119.9(3)
O1	S1	N1	106.8(3)
O2	S1	N1	106.2(3)
O1	S1	C6	107.9(3)
O2	S1	C6	107.5(4)
N1	S1	C6	108.1(3)
C12	N1	C8	113.6(4)
C12	N1	S1	117.5(3)
C8	N1	S1	116.1(4)
C2	C1	C6	119.5(5)
C1	C2	C3	121.1(5)
C4	C3	C2	117.9(5)
C4	C3	C7	122.2(5)
C2	C3	C7	119.8(6)
C3	C4	C5	122.5(5)
C4	C5	C6	118.8(5)
C5	C6	C1	120.2(5)
C5	C6	S1	119.2(4)
C1	C6	S1	120.6(4)
N1	C8	C9	108.8(4)

C8	C9	C10	111.5(4)
C11	C10	C9	109.6(3)
C11	C10	C13	114.1(4)
C9	C10	C13	115.3(4)
C11	C10	C15	111.8(6)
C9	C10	C15	118.1(6)
C13	C10	C15	86.5(4)
C12	C11	C10	111.0(3)
N1	C12	C11	109.3(4)
O3	C13	C14	117.2(5)
O3	C13	C10	119.9(6)
C14	C13	C10	90.0(3)
C16	C14	C13	118.4(5)
C16	C14	C15	115.7(6)
C13	C14	C15	87.0(5)
C14	C15	C10	89.2(4)
O4	C16	C14	110.5(9)
O1'	S1'	O2'	118(2)
O1'	S1'	N1'	105.9(19)
O2'	S1'	N1'	104(2)
O1'	S1'	C6'	109.9(19)
O2'	S1'	C6'	110(2)
N1'	S1'	C6'	108.6(17)
C8'	N1'	C12'	111(3)
C8'	N1'	S1'	119.0(17)
C12'	N1'	S1'	114.2(18)
C2'	C1'	C6'	120.0
C3'	C2'	C1'	120.0
C2'	C3'	C4'	120.0
C2'	C3'	C7'	119.6(18)
C4'	C3'	C7'	120.4(18)
C5'	C4'	C3'	120.0
C4'	C5'	C6'	120.0
C5'	C6'	C1'	120.0
C5'	C6'	S1'	119.6(15)
C1'	C6'	S1'	120.4(15)
N1'	C8'	C9'	111.7(19)
C10'	C9'	C8'	111(2)

C9'	C10'	C11'	110(2)
C9'	C10'	C15'	113(4)
C11'	C10'	C15'	117(4)
C9'	C10'	C13'	115(2)
C11'	C10'	C13'	115(2)
C15'	C10'	C13'	85(3)
C12'	C11'	C10'	111(2)
C11'	C12'	N1'	109(2)
C14'	C13'	O3'	125(4)
C14'	C13'	C10'	93(2)
O3'	C13'	C10'	120(4)
C13'	C14'	C16'	120(4)
C13'	C14'	C15'	90(3)
C16'	C14'	C15'	118(4)
C10'	C15'	C14'	87(3)
O4'	C16'	C14'	115(5)

Table 3. Torsion angles [°] for mo_JRB919_EE5.

O1	S1	N1	C12	-42.8(5)
O2	S1	N1	C12	-171.9(5)
C6	S1	N1	C12	73.0(5)
O1	S1	N1	C8	177.9(5)
O2	S1	N1	C8	48.8(6)
C6	S1	N1	C8	-66.3(5)
C6	C1	C2	C3	1.8(7)
C1	C2	C3	C4	-1.3(7)
C1	C2	C3	C7	178.3(6)
C2	C3	C4	C5	0.1(7)
C7	C3	C4	C5	-179.4(6)
C3	C4	C5	C6	0.6(7)
C4	C5	C6	C1	-0.1(6)
C4	C5	C6	S1	178.9(5)
C2	C1	C6	C5	-1.1(7)
C2	C1	C6	S1	180.0(6)
O1	S1	C6	C5	33.7(5)
O2	S1	C6	C5	164.3(5)
N1	S1	C6	C5	-81.5(5)

O1	S1	C6	C1	-147.4(5)
O2	S1	C6	C1	-16.8(6)
N1	S1	C6	C1	97.5(5)
C12	N1	C8	C9	59.0(7)
S1	N1	C8	C9	-160.1(4)
N1	C8	C9	C10	-56.8(6)
C8	C9	C10	C11	56.1(5)
C8	C9	C10	C13	-173.5(4)
C8	C9	C10	C15	-73.4(7)
C9	C10	C11	C12	-55.4(5)
C13	C10	C11	C12	173.6(4)
C15	C10	C11	C12	77.5(6)
C8	N1	C12	C11	-58.9(6)
S1	N1	C12	C11	160.9(3)
C10	C11	C12	N1	56.1(5)
C11	C10	C13	O3	29.9(7)
C9	C10	C13	O3	-98.3(6)
C15	C10	C13	O3	142.2(8)
C11	C10	C13	C14	-92.0(4)
C9	C10	C13	C14	139.9(4)
C15	C10	C13	C14	20.3(6)
O3	C13	C14	C16	97.9(9)
C10	C13	C14	C16	-138.0(6)
O3	C13	C14	C15	-144.4(8)
C10	C13	C14	C15	-20.3(5)
C16	C14	C15	C10	140.5(6)
C13	C14	C15	C10	20.3(6)
C11	C10	C15	C14	94.5(6)
C9	C10	C15	C14	-137.0(5)
C13	C10	C15	C14	-20.1(6)
C13	C14	C16	O4	-67.5(9)
C15	C14	C16	O4	-168.7(8)
O1'	S1'	N1'	C8'	170(3)
O2'	S1'	N1'	C8'	45(4)
C6'	S1'	N1'	C8'	72(3)
O1'	S1'	N1'	C12'	-57(3)
O2'	S1'	N1'	C12'	179(3)
C6'	S1'	N1'	C12'	61(3)

C6' C1' C2' C3'	0.0
C1' C2' C3' C4'	0.0
C1' C2' C3' C7'	178(4)
C2' C3' C4' C5'	0.0
C7' C3' C4' C5'	-178(4)
C3' C4' C5' C6'	0.0
C4' C5' C6' C1'	0.0
C4' C5' C6' S1'	-179(3)
C2' C1' C6' C5'	0.0
C2' C1' C6' S1'	179(3)
O1' S1' C6' C5'	29(3)
O2' S1' C6' C5'	160(3)
N1' S1' C6' C5'	-86(3)
O1' S1' C6' C1'	-150(3)
O2' S1' C6' C1'	-19(3)
N1' S1' C6' C1'	95(2)
C12' N1' C8' C9'	59(4)
S1' N1' C8' C9' -	166(2)
N1' C8' C9' C10'	-54(4)
C8' C9' C10' C11'	51(3)
C8' C9' C10' C15'	-82(4)
C8' C9' C10' C13'	-177(3)
C9' C10' C11' C12'	-55(3)
C15' C10' C11' C12'	75(4)
C13' C10' C11' C12'	173(2)
C10' C11' C12' N1'	60(3)
C8' N1' C12' C11'	-62(3)
S1' N1' C12' C11'	160(2)
C9' C10' C13' C14'	95(3)
C11' C10' C13' C14'	-135(3)
C15' C10' C13' C14'	-18(4)
C9' C10' C13' O3'	-39(5)
C11' C10' C13' O3'	91(4)
C15' C10' C13' O3'	-152(5)
O3' C13' C14' C16'	-90(6)
C10' C13' C14' C16'	140(4)
O3' C13' C14' C15'	148(5)
C10' C13' C14' C15'	17(4)

C9' C10' C15' C14'	-99(4)
C11' C10' C15' C14'	131(3)
C13' C10' C15' C14'	15(3)
C13' C14' C15' C10'	-17(4)
C16' C14' C15' C10'	-142(5)
C13' C14' C16' O4'	55(7)
C15' C14' C16' O4'	163(6)

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7. X-Ray Diffraction data of Compound 34

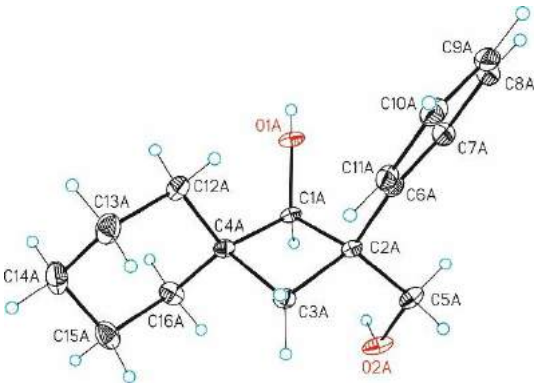

Table 1. Crystal data and structure refinement for mo_RJ414_0m (**34**)

Identification code	mo_RJ414_0m	
Empirical formula	C32 H44 N0 O4	
Formula weight	492.67	
Temperature	100(2)K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.5197(4)Å	α= 90.2804(18)°.
	b = 11.8799(6)Å	β = 92.9933(18)°.
	c = 18.0068(10)Å	γ = 92.9301(19)°.
Volume	1390.92(13) $Å^3$	
Z	2	
Density (calculated)	1.176 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	536	
Crystal size	0.400 x 0.050 x 0.020 mm^3	
Theta range for data collection	1.132 to 30.572°.	
Index ranges	-9<=h<=5,-16<=k<=16,-24<=l<=25	
Reflections collected	16263	
Independent reflections	8025[R(int) = 0.0278]	
Completeness to theta =30.572°	94.1%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.74 and 0.64	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8025/ 0/ 341	
Goodness-of-fit on F^2	1.021	

Final R indices [I>2sigma(I)]	R1 = 0.0484, wR2 = 0.1130
R indices (all data)	R1 = 0.0675, wR2 = 0.1236
Largest diff. peak and hole	0.419 and -0.268 e.Å^{-3}

Table 2. Bond lengths [Å] and angles [°] for mo_RJ414_0m.

Bond lengths----

O1A C1A 1.4127(13)
O2A C5A 1.4251(16)
C1A C4A 1.5463(17)
C1A C2A 1.5679(16)
C2A C6A 1.5169(17)
C2A C5A 1.5401(17)
C2A C3A 1.5557(17)
C3A C4A 1.5603(16)
C4A C16A 1.5263(18)
C4A C12A 1.5310(17)
C6A C11A 1.3958(17)
C6A C7A 1.4038(17)
C7A C8A 1.3876(19)
C8A C9A 1.386(2)
C9A C10A 1.384(2)
C10A C11A 1.3947(18)
C12A C13A 1.5334(19)
C13A C14A 1.528(2)
C14A C15A 1.526(2)
C15A C16A 1.5238(19)
O1B C1B 1.4154(13)
O2B C5B 1.4244(15)
C1B C4B 1.5501(16)
C1B C2B 1.5704(17)
C2B C6B 1.5159(16)
C2B C5B 1.5390(16)
C2B C3B 1.5564(16)
C3B C4B 1.5547(17)
C4B C16B 1.5257(17)
C4B C12B 1.5327(17)

C6B C11B 1.3956(17)
C6B C7B 1.4033(17)
C7B C8B 1.3898(18)
C8B C9B 1.385(2)
C9B C10B 1.384(2)
C10B C11B 1.3944(19)
C12B C13B 1.5366(18)
C13B C14B 1.526(2)
C14B C15B 1.529(2)
C15B C16B 1.5293(18)

Angles----------
O1A C1A C4A 120.13(10)
O1A C1A C2A 120.42(10)
C4A C1A C2A 90.98(8)
C6A C2A C5A 109.31(10)
C6A C2A C3A 117.55(10)
C5A C2A C3A 113.15(9)
C6A C2A C1A 113.73(9)
C5A C2A C1A 114.30(10)
C3A C2A C1A 87.56(9)
C2A C3A C4A 90.91(9)
C16A C4A C12A 110.92(10)
C16A C4A C1A 113.13(10)
C12A C4A C1A 114.55(10)
C16A C4A C3A 115.10(10)
C12A C4A C3A 113.37(10)
C1A C4A C3A 88.17(9)
O2A C5A C2A 112.67(11)
C11A C6A C7A 117.42(12)
C11A C6A C2A 123.71(11)
C7A C6A C2A 118.87(11)
C8A C7A C6A 121.24(13)
C9A C8A C7A 120.61(13)
C10A C9A C8A 118.95(13)
C9A C10A C11A 120.67(13)
C10A C11A C6A 121.08(12)
C4A C12A C13A 111.17(10)

C14A C13A C12A 111.42(12)
C15A C14A C13A 111.14(11)
C16A C15A C14A 110.59(11)
C15A C16A C4A 111.72(11)
O1B C1B C4B 120.14(10)
O1B C1B C2B 121.33(10)
C4B C1B C2B 90.70(8)
C6B C2B C5B 107.94(10)
C6B C2B C3B 116.81(10)
C5B C2B C3B 113.44(9)
C6B C2B C1B 115.60(9)
C5B C2B C1B 115.07(9)
C3B C2B C1B 87.09(9)
C4B C3B C2B 91.05(8)
C16B C4B C12B 110.44(11)
C16B C4B C1B 114.83(10)
C12B C4B C1B 114.07(9)
C16B C4B C3B 114.99(9)
C12B C4B C3B 113.13(10)
C1B C4B C3B 87.86(9)
O2B C5B C2B 112.74(10)
C11B C6B C7B 117.57(11)
C11B C6B C2B 122.96(11)
C7B C6B C2B 119.39(11)
C8B C7B C6B 121.13(13)
C9B C8B C7B 120.45(13)
C10B C9B C8B 119.23(13)
C9B C10B C11B 120.51(13)
C10B C11B C6B 121.08(13)
C4B C12B C13B 111.25(10)
C14B C13B C12B 112.03(12)
C13B C14B C15B 111.26(12)
C14B C15B C16B 111.01(11)
C4B C16B C15B 111.33(10)

Table 3. Torsion angles [°] for mo_RJ414_0m.

O1A	C1A	C2A	C6A	18.84(15)
C4A	C1A	C2A	C6A	-107.47(10)
O1A	C1A	C2A	C5A	-107.66(12)
C4A	C1A	C2A	C5A	126.03(10)
O1A	C1A	C2A	C3A	137.98(11)
C4A	C1A	C2A	C3A	11.66(8)
C6A	C2A	C3A	C4A	104.04(10)
C5A	C2A	C3A	C4A	-127.02(10)
C1A	C2A	C3A	C4A	-11.56(8)
O1A	C1A	C4A	C16A	105.23(12)
C2A	C1A	C4A	C16A	-128.23(10)
O1A	C1A	C4A	C12A	-23.23(15)
C2A	C1A	C4A	C12A	103.31(10)
O1A	C1A	C4A	C3A	-138.17(11)
C2A	C1A	C4A	C3A	-11.63(8)
C2A	C3A	C4A	C16A	126.48(11)
C2A	C3A	C4A	C12A	-104.32(11)
C2A	C3A	C4A	C1A	11.72(9)
C6A	C2A	C5A	O2A	-174.27(10)
C3A	C2A	C5A	O2A	52.67(13)
C1A	C2A	C5A	O2A	-45.51(14)
C5A	C2A	C6A	C11A	-119.67(12)
C3A	C2A	C6A	C11A	11.07(16)
C1A	C2A	C6A	C11A	111.26(13)
C5A	C2A	C6A	C7A	60.13(13)
C3A	C2A	C6A	C7A	-169.13(10)
C1A	C2A	C6A	C7A	-68.94(14)
C11A	C6A	C7A	C8A	1.40(18)
C2A	C6A	C7A	C8A	-178.41(11)
C6A	C7A	C8A	C9A	-0.3(2)
C7A	C8A	C9A	C10A	-1.4(2)
C8A	C9A	C10A	C11A	1.95(19)
C9A	C10A	C11A	C6A	-0.80(19)
C7A	C6A	C11A	C10A	-0.87(17)
C2A	C6A	C11A	C10A	178.93(11)
C16A	C4A	C12A	C13A	54.56(13)

C1A C4A C12A C13A -175.89(10)
C3A C4A C12A C13A -76.74(13)
C4A C12A C13A C14A -54.76(14)
C12A C13A C14A C15A 55.64(15)
C13A C14A C15A C16A -56.18(15)
C14A C15A C16A C4A 56.58(14)
C12A C4A C16A C15A -55.87(13)
C1A C4A C16A C15A 173.82(10)
C3A C4A C16A C15A 74.52(14)
O1B C1B C2B C6B 21.75(15)
C4B C1B C2B C6B -104.78(10)
O1B C1B C2B C5B -105.21(12)
C4B C1B C2B C5B 128.25(10)
O1B C1B C2B C3B 140.20(11)
C4B C1B C2B C3B 13.67(8)
C6B C2B C3B C4B 103.70(11)
C5B C2B C3B C4B -129.76(10)
C1B C2B C3B C4B -13.63(8)
O1B C1B C4B C16B 102.21(12)
C2B C1B C4B C16B -130.32(10)
O1B C1B C4B C12B -26.70(15)
C2B C1B C4B C12B 100.77(11)
O1B C1B C4B C3B -141.15(11)
C2B C1B C4B C3B -13.67(8)
C2B C3B C4B C16B 130.30(10)
C2B C3B C4B C12B -101.53(10)
C2B C3B C4B C1B 13.80(8)
C6B C2B C5B O2B -175.11(9)
C3B C2B C5B O2B 53.81(13)
C1B C2B C5B O2B -44.34(13)
C5B C2B C6B C11B -104.70(13)
C3B C2B C6B C11B 24.51(16)
C1B C2B C6B C11B 124.82(12)
C5B C2B C6B C7B 71.81(13)
C3B C2B C6B C7B -158.97(11)
C1B C2B C6B C7B -58.66(15)
C11B C6B C7B C8B -1.58(19)
C2B C6B C7B C8B -178.29(12)

C6B C7B C8B C9B 0.9(2)

C7B C8B C9B C10B 0.5(2)

C8B C9B C10B C11B -1.1(2)

C9B C10B C11B C6B 0.4(2)

C7B C6B C11B C10B 0.97(19)

C2B C6B C11B C10B 177.55(12)

C16B C4B C12B C13B 55.38(14)

C1B C4B C12B C13B -173.53(11)

C3B C4B C12B C13B -75.12(14)

C4B C12B C13B C14B -54.23(15)

C12B C13B C14B C15B 53.83(15)

C13B C14B C15B C16B -54.93(16)

C12B C4B C16B C15B -57.11(13)

C1B C4B C16B C15B 172.20(10)

C3B C4B C16B C15B 72.39(14)

C14B C15B C16B C4B 57.03(15)

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9. Cartesian coordinates of the computed structures

SUBSTRATE 1

C	-1.040261	1.370652	-2.211633
H	-1.302576	0.606399	-2.940735
H	-0.156900	1.968011	-2.420129
C	-1.765987	1.559395	-1.111631
H	-1.465193	2.331420	-0.404957
C	-2.991622	0.763633	-0.762387
H	-3.048368	-0.121887	-1.406593
H	-2.902911	0.407393	0.273181
O	-6.158985	-0.056733	-1.033712
C	-5.374295	0.576124	-0.363981
H	-5.340445	0.439697	0.740029
C	-4.332527	1.546491	-0.899658
C	-4.346099	2.815280	-0.026002
C	-4.617426	1.928198	-2.356810
C	-5.596142	3.649628	-0.291863
H	-3.469225	3.425618	-0.263046
H	-4.288681	2.554326	1.038317
C	-5.828379	2.850991	-2.474394
H	-3.738136	2.439101	-2.763018
H	-4.787561	1.027284	-2.955224
H	-5.559732	4.585671	0.272231
H	-6.499586	3.101146	0.029231
H	-5.934721	3.211580	-3.501153
H	-6.747492	2.304463	-2.211663
O	-5.703062	4.001159	-1.656237

B_2pin_2

B	0.853406	-0.000189	0.000480
O	1.614312	1.136132	0.106838
O	1.613619	-1.137052	-0.105058
C	2.989450	0.723938	0.298242
C	2.989247	-0.725834	-0.295018
B	-0.853428	0.000404	-0.000414
O	-1.614440	-1.135451	0.110145
O	-1.613547	1.136775	-0.111813
C	-2.989778	-0.722425	0.298279
C	-2.988962	0.724680	-0.301442
C	-3.903538	1.710847	0.409029
H	-3.837260	2.690182	-0.073810
H	-4.943833	1.374621	0.353461
H	-3.630736	1.830772	1.459387
C	-3.253977	0.753743	-1.806902
H	-4.297302	0.516203	-2.033493
H	-3.039712	1.756897	-2.185998
H	-2.611459	0.045506	-2.338591
C	-3.256445	-0.751313	1.803449
H	-4.299835	-0.512986	2.028913
H	-3.043356	-1.754637	2.182759
H	-2.613967	-0.043576	2.335849
C	-3.904254	-1.707965	-0.413192
H	-3.839166	-2.687351	0.069705
H	-4.944380	-1.371033	-0.358743
H	-3.630397	-1.828059	-1.463255
C	3.903010	-1.708854	0.420851
H	3.837198	-2.690332	-0.057682
H	4.943383	-1.372935	0.364912
H	3.629060	-1.824072	1.471436
C	3.254555	0.759552	1.803543

H	4.297723	0.522292	2.031147
H	3.041015	1.764542	2.178157
H	2.611562	0.054154	2.338421
C	3.904660	1.706308	-0.416670
H	3.839012	2.687845	0.061763
H	4.944741	1.369673	-0.359604
H	3.631919	1.821684	-1.467553
C	3.255902	-0.761635	-1.800040
H	4.299457	-0.525031	-2.026557
H	3.042124	-1.766496	-2.174863
H	2.613911	-0.055842	-2.335601

I1

C	-0.863089	-2.380668	1.021249
C	-1.680605	-1.453601	1.668338
C	-2.247688	-1.664814	2.922832
C	-1.955645	-2.873182	3.555207
C	-1.147846	-3.825438	2.937117
C	-0.609018	-3.587098	1.676026
H	-2.364627	-3.083353	4.537596
H	-0.937917	-4.762047	3.443540
H	0.022546	-4.334183	1.206215
C	-3.189729	-0.588881	3.462770
C	-2.623567	0.765069	3.032311
C	-2.028052	0.849373	1.774155
C	-2.700125	1.939338	3.779128
C	-1.518944	2.032263	1.233625
C	-2.211044	3.140302	3.270475
H	-3.147305	1.926104	4.767109
C	-1.626306	3.189666	2.009412
H	-2.281564	4.045151	3.865380
H	-1.234754	4.129920	1.636915
O	-1.920874	-0.278974	0.998289
P	-0.123776	-1.868826	-0.584175
P	-0.603459	1.928062	-0.365989
Cu	1.048288	0.202596	-0.302933
B	3.047858	0.324321	0.153292
O	3.695243	-0.433073	1.140251
O	4.001020	1.130855	-0.481447
C	5.120290	-0.294881	0.993375
C	5.243935	1.067301	0.242663
C	-1.530768	-1.987081	-1.760919
C	-1.357346	-1.397748	-3.018173
C	-2.741348	-2.617898	-1.463081
C	-2.370012	-1.457018	-3.969308
H	-0.427165	-0.884764	-3.250719
C	-3.761624	-2.660921	-2.410838
H	-2.891513	-3.077977	-0.490754
C	-3.576047	-2.085782	-3.665163
H	-2.224655	-0.995608	-4.940847
H	-4.700849	-3.149125	-2.168420
H	-4.371981	-2.120560	-4.402984
C	-1.916862	1.871159	-1.660605
C	-1.552634	2.209660	-2.970815
C	-3.219594	1.433304	-1.412628
C	-2.480747	2.136324	-4.003885
H	-0.540969	2.545844	-3.183971
C	-4.144447	1.349871	-2.451235
H	-3.528118	1.163663	-0.408248
C	-3.781171	1.706470	-3.746352
H	-2.186122	2.412913	-5.011770
H	-5.153133	1.006607	-2.242546
H	-4.505082	1.643739	-4.553131

C	0.072878	3.626612	-0.577165
C	1.449623	3.814520	-0.422956
C	-0.740881	4.726333	-0.881045
C	2.002641	5.086980	-0.560119
H	2.091241	2.962307	-0.210626
C	-0.185962	5.993969	-1.017851
H	-1.810639	4.588760	-1.011475
C	1.187697	6.175618	-0.855479
H	3.073308	5.223538	-0.441852
H	-0.824017	6.840485	-1.252833
H	1.620377	7.165588	-0.965244
C	0.932877	-3.312122	-1.017179
C	2.265680	-3.286874	-0.587397
C	0.464535	-4.415742	-1.736890
C	3.112736	-4.354986	-0.870283
H	2.639673	-2.429266	-0.031973
C	1.317647	-5.478029	-2.025391
H	-0.566795	-4.447125	-2.075776
C	2.641687	-5.449693	-1.592081
H	4.144977	-4.325891	-0.533845
H	0.946685	-6.328935	-2.588858
H	3.305493	-6.278451	-1.819564
C	-4.569117	-0.774477	2.786255
H	-4.990378	-1.749314	3.052570
H	-5.260055	0.007311	3.117890
H	-4.490768	-0.723310	1.695924
C	-3.363234	-0.684099	4.980011
H	-2.411659	-0.558295	5.505308
H	-4.061637	0.077732	5.336335
H	-3.789255	-1.651913	5.257462
C	5.602428	-1.487919	0.162865
H	6.690777	-1.492243	0.046516
H	5.310534	-2.411151	0.673066
H	5.142774	-1.488554	-0.830121
C	6.403383	1.152463	-0.740821
H	6.411855	2.136192	-1.220523
H	7.360551	1.020092	-0.224786
H	6.322531	0.395954	-1.524378
C	5.274145	2.272839	1.186049
H	6.217150	2.336278	1.738119
H	5.162463	3.187075	0.595205
H	4.449178	2.231122	1.903556
C	5.773459	-0.328584	2.368562
H	5.633626	-1.315074	2.821421
H	6.850116	-0.141587	2.291658
H	5.337753	0.415075	3.039186

BpinO^{t}Bu

C	-0.018101	-2.039597	0.265671
C	-0.370245	-0.818350	-0.654492
C	-1.418824	0.126088	-0.088550
H	-1.602572	0.941279	-0.794632
H	-2.363192	-0.403844	0.070817
H	-1.098070	0.563014	0.859240
C	-0.743797	-1.231284	-2.078144
H	-1.726213	-1.710704	-2.111571
H	-0.775724	-0.339016	-2.709903
H	-0.005423	-1.920442	-2.499440
C	-0.108832	-1.706978	1.755286
H	-1.147504	-1.591081	2.077737
H	0.340395	-2.522713	2.328598
H	0.434003	-0.786559	1.991586
C	-0.802070	-3.307248	-0.037256

H	-0.502373	-4.101462	0.652800
H	-1.875116	-3.133184	0.091192
H	-0.623392	-3.657008	-1.056082
O	0.894243	-0.124589	-0.733250
O	1.374582	-2.262829	-0.038565
B	1.874245	-1.066409	-0.499399
O	3.205007	-0.905611	-0.678398
C	3.818635	0.263811	-1.256178
C	5.312544	-0.048146	-1.278563
H	5.872780	0.789365	-1.704831
H	5.680102	-0.231226	-0.264217
H	5.507921	-0.939719	-1.882219
C	3.295214	0.472819	-2.677602
H	3.466451	-0.425272	-3.279790
H	2.224424	0.691227	-2.670531
H	3.816697	1.309404	-3.152898
C	3.540801	1.481947	-0.375122
H	2.472969	1.712861	-0.352141
H	3.881306	1.294011	0.648170
H	4.075869	2.355847	-0.759666

I2

C	-0.863089	-2.380668	1.021249
C	-1.680605	-1.453601	1.668338
C	-2.247688	-1.664814	2.922832
C	-1.955645	-2.873182	3.555207
C	-1.147846	-3.825438	2.937117
C	-0.609018	-3.587098	1.676026
H	-2.364627	-3.083353	4.537596
H	-0.937917	-4.762047	3.443540
H	0.022546	-4.334183	1.206215
C	-3.189729	-0.588881	3.462770
C	-2.623567	0.765069	3.032311
C	-2.028052	0.849373	1.774155
C	-2.700125	1.939338	3.779128
C	-1.518944	2.032263	1.233625
C	-2.211044	3.140302	3.270475
H	-3.147305	1.926104	4.767109
C	-1.626306	3.189666	2.009412
H	-2.281564	4.045151	3.865380
H	-1.234754	4.129920	1.636915
O	-1.920874	-0.278974	0.998289
P	-0.123776	-1.868826	-0.584175
P	-0.603459	1.928062	-0.365989
Cu	1.048288	0.202596	-0.302933
B	3.047858	0.324321	0.153292
O	3.695243	-0.433073	1.140251
O	4.001020	1.130855	-0.481447
C	5.120290	-0.294881	0.993375
C	5.243935	1.067301	0.242663
C	-1.530768	-1.987081	-1.760919
C	-1.357346	-1.397748	-3.018173
C	-2.741348	-2.617898	-1.463081
C	-2.370012	-1.457018	-3.969308
H	-0.427165	-0.884764	-3.250719
C	-3.761624	-2.660921	-2.410838
H	-2.891513	-3.077977	-0.490754
C	-3.576047	-2.085782	-3.665163
H	-2.224655	-0.995608	-4.940847
H	-4.700849	-3.149125	-2.168420
H	-4.371981	-2.120560	-4.402984
C	-1.916862	1.871159	-1.660605
C	-1.552634	2.209660	-2.970815

C	-3.219594	1.433304	-1.412628
C	-2.480747	2.136324	-4.003885
H	-0.540969	2.545844	-3.183971
C	-4.144447	1.349871	-2.451235
H	-3.528118	1.163663	-0.408248
C	-3.781171	1.706470	-3.746352
H	-2.186122	2.412913	-5.011770
H	-5.153133	1.006607	-2.242546
H	-4.505082	1.643739	-4.553131
C	0.072878	3.626612	-0.577165
C	1.449623	3.814520	-0.422956
C	-0.740881	4.726333	-0.881045
C	2.002641	5.086980	-0.560119
H	2.091241	2.962307	-0.210626
C	-0.185962	5.993969	-1.017851
H	-1.810639	4.588760	-1.011475
C	1.187697	6.175618	-0.855479
H	3.073308	5.223538	-0.441852
H	-0.824017	6.840485	-1.252833
H	1.620377	7.165588	-0.965244
C	0.932877	-3.312122	-1.017179
C	2.265680	-3.286874	-0.587397
C	0.464535	-4.415742	-1.736890
C	3.112736	-4.354986	-0.870283
H	2.639673	-2.429266	-0.031973
C	1.317647	-5.478029	-2.025391
H	-0.566795	-4.447125	-2.075776
C	2.641687	-5.449693	-1.592081
H	4.144977	-4.325891	-0.533845
H	0.946685	-6.328935	-2.588858
H	3.305493	-6.278451	-1.819564
C	-4.569117	-0.774477	2.786255
H	-4.990378	-1.749314	3.052570
H	-5.260055	0.007311	3.117890
H	-4.490768	-0.723310	1.695924
C	-3.363234	-0.684099	4.980011
H	-2.411659	-0.558295	5.505308
H	-4.061637	0.077732	5.336335
H	-3.789255	-1.651913	5.257462
C	5.602428	-1.487919	0.162865
H	6.690777	-1.492243	0.046516
H	5.310534	-2.411151	0.673066
H	5.142774	-1.488554	-0.830121
C	6.403383	1.152463	-0.740821
H	6.411855	2.136192	-1.220523
H	7.360551	1.020092	-0.224786
H	6.322531	0.395954	-1.524378
C	5.274145	2.272839	1.186049
H	6.217150	2.336278	1.738119
H	5.162463	3.187075	0.595205
H	4.449178	2.231122	1.903556
C	5.773459	-0.328584	2.368562
H	5.633626	-1.315074	2.821421
H	6.850116	-0.141587	2.291658
H	5.337753	0.415075	3.039186

I3

Cu	-0.206117	0.067491	-1.031622
C	-1.849944	0.802737	-2.408581
H	-1.930525	0.065140	-3.202890
H	-1.365093	1.742432	-2.657757
C	-2.496398	0.630626	-1.227250
H	-2.505031	1.445968	-0.508153

P	0.571251	2.124180	0.113043
P	-0.414251	-1.603405	0.619574
B	1.428825	-0.499979	-2.159654
O	1.653630	-1.618235	-2.974061
O	2.645432	0.161558	-1.973535
C	3.072540	-1.845977	-3.086282
C	3.662324	-0.427819	-2.797440
C	-2.482547	-0.901784	4.712810
C	-2.005792	-0.225364	2.447925
C	-1.042406	-2.254775	3.326044
C	-1.676415	-2.027303	4.543542
C	-2.646298	-0.000463	3.664758
H	-0.414804	-3.132885	3.200666
H	-1.541222	-2.728386	5.361611
H	-2.975818	-0.725729	5.664054
C	-0.313743	2.783535	1.587949
C	-1.856228	3.540893	3.806925
C	0.202407	2.677171	2.881741
C	-1.617862	3.273125	1.421098
C	-2.380640	3.654813	2.519692
C	-0.565791	3.050494	3.982901
H	-2.035635	3.373179	0.422158
H	-3.384469	4.041180	2.369958
H	-2.451634	3.832786	4.666641
C	2.332166	2.032218	0.652124
C	5.038738	1.613562	1.244333
C	3.278438	3.020772	0.377535
C	2.782530	0.857068	1.254023
C	4.120579	0.613501	1.561693
C	4.621998	2.810729	0.668073
H	2.968695	3.949149	-0.090803
H	5.350656	3.582259	0.440768
H	6.092427	1.468991	1.456650
C	1.223564	-2.303830	1.080346
C	3.827451	-3.128540	1.692398
C	1.565565	-3.655322	1.024782
C	2.211180	-1.396570	1.468628
C	3.516933	-1.770573	1.781300
C	2.861941	-4.062777	1.326193
H	0.823283	-4.388171	0.725545
H	3.123587	-5.114476	1.271012
H	4.831168	-3.470192	1.920322
C	-1.289471	-3.051326	-0.104045
C	-2.688517	-5.063115	-1.457378
C	-0.899604	-3.441104	-1.393999
C	-2.381604	-3.680067	0.498509
C	-3.082439	-4.676346	-0.179707
C	-1.590656	-4.448848	-2.059156
H	-0.061866	-2.943865	-1.879922
H	-2.702791	-3.384461	1.492620
H	-3.938188	-5.148430	0.293544
H	-1.279112	-4.745228	-3.056405
H	-3.236567	-5.837866	-1.984944
C	0.624941	3.550154	-1.054052
C	0.800181	5.587691	-2.967516
C	0.342974	4.874368	-0.705142
C	1.005019	3.258102	-2.371229
C	1.096050	4.272241	-3.319924
C	0.424958	5.886189	-1.659728
H	0.061484	5.122940	0.313384
H	1.244107	2.232024	-2.639339
H	1.395274	4.032660	-4.335999
H	0.200354	6.910495	-1.377608
H	0.864548	6.378418	-3.709022

H	-2.115054	0.491335	1.639311
H	1.208967	2.302225	3.039430
H	-3.259004	0.886283	3.793032
H	-0.149941	2.958118	4.981644
O	1.829503	-0.083636	1.551670
C	4.474601	-0.688988	2.279597
C	-3.382073	-0.549534	-0.932985
H	-3.206463	-1.328740	-1.684135
H	-3.126681	-0.981157	0.039158
C	-1.208661	-1.358124	2.264022
O	-6.178850	-2.238649	-1.350893
C	-5.539091	-1.564258	-0.576105
H	-5.332961	-1.933555	0.453578
C	-4.901147	-0.217991	-0.885786
C	-5.216065	0.749727	0.272217
C	-5.420559	0.364865	-2.203084
C	-6.673932	1.198369	0.234233
H	-4.579011	1.636205	0.189407
H	-4.993698	0.277110	1.237693
C	-6.858009	0.862116	-2.070755
H	-4.780494	1.204491	-2.493949
H	-5.364039	-0.387788	-2.996216
H	-6.862996	1.954402	1.001501
H	-7.343118	0.343259	0.436410
H	-7.166980	1.385214	-2.979812
H	-7.540461	0.011185	-1.921110
O	-7.003347	1.787768	-1.006965
C	3.788437	0.444326	-4.048424
H	4.011452	1.470821	-3.741495
H	4.591188	0.101107	-4.708837
H	2.851201	0.456552	-4.613236
C	4.974804	-0.423793	-2.023764
H	5.764883	-0.934231	-2.585450
H	5.292922	0.607889	-1.844904
H	4.861789	-0.910711	-1.052365
C	3.383744	-2.402705	-4.468330
H	4.464701	-2.512533	-4.607750
H	2.926968	-3.390993	-4.580881
H	2.994395	-1.758591	-5.259860
C	3.440784	-2.870874	-2.012518
H	2.832677	-3.769627	-2.153004
H	4.495914	-3.158176	-2.063867
H	3.233311	-2.476386	-1.015200
C	5.939165	-1.080508	2.064374
H	6.176869	-2.000158	2.605202
H	6.165180	-1.230755	1.004046
H	6.607280	-0.309493	2.456462
C	4.222799	-0.488089	3.792901
H	4.437051	-1.412912	4.338577
H	4.870137	0.305173	4.180990
H	3.182999	-0.208634	3.988935

TS1

Cu	-0.503679	0.399259	-0.085091
C	-1.930359	1.017419	-1.449993
H	-2.277407	0.230738	-2.119949
H	-1.838636	1.980641	-1.954695
C	-2.498494	1.014860	-0.110598
H	-2.630857	1.994803	0.347392
P	0.979391	1.682613	1.112095
P	-0.187073	-1.878364	0.283867

B	0.066929	0.714762	-2.063394
O	0.144760	-0.221630	-3.084977
O	0.803940	1.842987	-2.387313
C	1.202345	0.180911	-3.981599
C	1.249686	1.726796	-3.754035
C	-0.216596	-3.238414	4.707379
C	-0.837199	-1.682266	2.973084
C	0.491033	-3.624900	2.432487
C	0.465278	-4.011796	3.769010
C	-0.870472	-2.075792	4.308204
H	1.021925	-4.232429	1.705043
H	0.977931	-4.917622	4.078426
H	-0.234058	-3.540960	5.750124
C	1.042037	1.351683	2.923017
C	0.940020	0.804346	5.666899
C	2.143945	0.794931	3.572189
C	-0.116289	1.628755	3.661412
C	-0.162609	1.369340	5.025599
C	2.088125	0.514198	4.937129
H	-0.986803	2.048565	3.162727
H	-1.063496	1.597855	5.587186
H	0.901090	0.589726	6.730534
C	2.729939	1.545359	0.552193
C	5.273345	1.163057	-0.568195
C	3.524814	2.640297	0.207656
C	3.255581	0.271234	0.328362
C	4.519066	0.043808	-0.217064
C	4.782819	2.448904	-0.354471
H	3.150067	3.647394	0.355794
H	5.385848	3.308193	-0.629598
H	6.257703	1.038151	-1.005865
C	1.363116	-2.584338	-0.409290
C	3.805685	-3.370966	-1.534125
C	1.432745	-3.713251	-1.227640
C	2.548408	-1.892912	-0.156015
C	3.778184	-2.249824	-0.705359
C	2.647036	-4.101973	-1.785594
H	0.532712	-4.279630	-1.443722
H	2.690414	-4.977494	-2.425415
H	4.738185	-3.685279	-1.989857
C	-1.508711	-2.881694	-0.508810
C	-3.693637	-4.093656	-1.769838
C	-1.752609	-2.660490	-1.872310
C	-2.364006	-3.717303	0.212239
C	-3.454719	-4.316611	-0.416650
C	-2.834858	-3.269750	-2.498209
H	-1.100155	-1.996892	-2.435999
H	-2.195068	-3.892113	1.270176
H	-4.119048	-4.956545	0.156167
H	-3.014688	-3.092562	-3.554517
H	-4.545425	-4.559284	-2.256396
C	0.664284	3.493137	1.054236
C	0.125246	6.229444	0.859814
C	1.095708	4.370660	2.055432
C	-0.036767	3.998395	-0.044649
C	-0.302260	5.362105	-0.142299
C	0.826082	5.732517	1.957803
H	1.641788	3.989433	2.913453
H	-0.352324	3.321628	-0.831640
H	-0.847100	5.744901	-1.000072
H	1.162762	6.406125	2.740029
H	-0.087091	7.291927	0.787136
H	-1.326121	-0.763920	2.657536
H	3.054920	0.580301	3.022402

H	-1.395284	-1.466075	5.036744
H	2.950044	0.073482	5.428894
O	2.462881	-0.798078	0.670507
C	4.995786	-1.404434	-0.334941
C	-3.509529	-0.038447	0.277292
H	-3.234596	-0.985808	-0.200271
H	-3.483911	-0.223777	1.359676
C	-0.160578	-2.455693	2.026925
C	-5.700114	-1.054900	0.266077
H	-5.517294	-1.873126	-0.467199
O	-6.340863	-1.272380	1.272623
C	-5.010663	0.246692	-0.083135
C	-5.575193	1.420964	0.721879
C	-5.194234	0.523603	-1.582395
C	-6.973266	1.809989	0.248708
H	-4.907850	2.281691	0.601732
H	-5.608540	1.166251	1.786378
C	-6.624849	0.950731	-1.896737
H	-4.513907	1.329181	-1.875281
H	-4.928387	-0.362211	-2.174452
H	-7.312350	2.720740	0.750689
H	-7.687959	1.006355	0.488940
H	-6.722809	1.230524	-2.949762
H	-7.324937	0.117286	-1.706406
O	-7.008615	2.083129	-1.141511
C	6.124628	-1.552835	-1.357578
H	6.991500	-0.954731	-1.064798
H	6.464495	-2.590567	-1.408407
H	5.806384	-1.240551	-2.357333
C	5.505603	-1.862040	1.051856
H	5.827740	-2.907502	1.008574
H	6.356193	-1.246903	1.362991
H	4.723704	-1.777172	1.812489
C	0.247097	2.491698	-4.618012
H	0.188229	3.524804	-4.262797
H	0.547512	2.506918	-5.669957
H	-0.752365	2.050958	-4.548116
C	2.633432	2.348411	-3.869321
H	2.569536	3.426169	-3.690973
H	3.323306	1.926935	-3.134699
H	3.045795	2.193780	-4.871961
C	2.475476	-0.528370	-3.519898
H	2.770507	-0.193144	-2.522227
H	2.286621	-1.604568	-3.473352
H	3.308484	-0.350577	-4.207157
C	0.843049	-0.250811	-5.394924
H	-0.144270	0.111758	-5.688923
H	1.581217	0.124638	-6.111188
H	0.837055	-1.343365	-5.456879

I4

Cu	0.767294	-0.076493	-0.742839
C	1.040417	-1.591023	-3.350102
H	0.840417	-0.712237	-3.980077
H	1.631541	-2.279968	-3.986926
C	1.837848	-1.197584	-2.082309
H	2.009404	-2.135292	-1.532748
P	0.287022	-0.924599	1.530712
P	-0.326993	2.028592	-0.789050
B	-0.314888	-2.274552	-2.984311
O	-1.549326	-1.863541	-3.429524
O	-0.404464	-3.362970	-2.142397
C	-2.546569	-2.551691	-2.643414

C	-1.772076	-3.821504	-2.147860
C	0.350929	4.920719	2.778322
C	1.163014	3.286971	1.195486
C	-1.150680	3.969749	1.145703
C	-0.921090	4.825683	2.219746
C	1.391688	4.154659	2.259758
H	-2.146477	3.909721	0.716928
H	-1.738462	5.419629	2.617852
H	0.529626	5.586826	3.617136
C	0.877477	0.165307	2.891139
C	1.911637	1.870869	4.855362
C	0.029447	0.755753	3.830391
C	2.247351	0.451687	2.934704
C	2.762619	1.288604	3.917660
C	0.545471	1.609941	4.803015
H	2.914384	0.032632	2.187454
H	3.828214	1.496116	3.940884
H	2.311132	2.533017	5.617655
C	-1.448535	-1.327191	2.009458
C	-4.171957	-1.894346	2.379531
C	-1.848991	-2.539667	2.577763
C	-2.448428	-0.412868	1.677788
C	-3.810852	-0.661148	1.839368
C	-3.199847	-2.819148	2.756965
H	-1.104390	-3.279311	2.852643
H	-3.499793	-3.769441	3.186640
H	-5.218923	-2.142484	2.516502
C	-2.159472	1.922516	-0.915043
C	-4.941576	1.571083	-0.908965
C	-2.930206	2.390848	-1.979528
C	-2.823538	1.274893	0.126280
C	-4.203867	1.102161	0.177901
C	-4.310450	2.202617	-1.978907
H	-2.452536	2.894543	-2.813727
H	-4.901329	2.560142	-2.815993
H	-6.018780	1.446449	-0.929495
C	0.135755	3.057730	-2.242613
C	0.895567	4.507402	-4.509367
C	0.776036	2.419573	-3.309175
C	-0.116530	4.432269	-2.318276
C	0.262264	5.152328	-3.446944
C	1.151833	3.140743	-4.440610
H	0.985829	1.354975	-3.242593
H	-0.606071	4.941453	-1.492835
H	0.064884	6.218842	-3.497501
H	1.648815	2.634464	-5.262608
H	1.192078	5.072928	-5.387663
C	1.149599	-2.519759	1.847377
C	2.439383	-4.986723	2.131754
C	1.805281	-2.839601	3.040028
C	1.138086	-3.450625	0.801119
C	1.773930	-4.680117	0.946602
C	2.452496	-4.065702	3.177124
H	1.818534	-2.132191	3.863280
H	0.633409	-3.217037	-0.133136
H	1.757363	-5.391869	0.126480
H	2.965843	-4.301479	4.104523
H	2.947082	-5.940373	2.241276
H	1.981312	2.675952	0.822158
H	-1.036232	0.549962	3.815881
H	2.384084	4.215321	2.695459
H	-0.125256	2.067009	5.524207
O	-2.037329	0.781463	1.139670
C	-4.782070	0.447939	1.433008

C	3.217683	-0.700831	-2.523107
H	3.742513	-1.476128	-3.112425
H	3.108205	0.156689	-3.208224
C	-0.110698	3.192087	0.626355
C	3.614119	1.015956	-0.810920
H	3.164151	1.700025	-1.562762
O	3.701934	1.371764	0.349917
C	4.160490	-0.269522	-1.388096
C	4.322397	-1.371566	-0.326712
C	5.556936	0.079599	-1.969925
C	5.497894	-1.147157	0.620362
H	4.473316	-2.322665	-0.852447
H	3.400626	-1.472009	0.256703
C	6.617969	0.237439	-0.887190
H	5.854553	-0.738321	-2.636179
H	5.505504	0.991502	-2.578878
H	5.658643	-2.037680	1.235472
H	5.290299	-0.300176	1.289174
H	7.602993	0.382667	-1.340547
H	6.403530	1.119781	-0.261590
O	6.710433	-0.918931	-0.078856
C	-6.199455	-0.080323	1.207221
H	-6.596383	-0.520678	2.125794
H	-6.873667	0.736205	0.934951
H	-6.230508	-0.835943	0.416063
C	-4.812819	1.507148	2.560666
H	-5.475415	2.333131	2.282603
H	-5.183851	1.059108	3.488085
H	-3.816986	1.917881	2.752677
C	-1.846201	-4.993583	-3.125585
H	-1.134575	-5.763069	-2.812811
H	-2.845882	-5.437197	-3.144497
H	-1.583799	-4.681177	-4.140948
C	-2.142134	-4.279148	-0.744932
H	-1.547627	-5.156097	-0.471008
H	-1.954586	-3.498204	-0.006011
H	-3.200235	-4.556425	-0.696670
C	-2.923988	-1.605186	-1.508892
H	-2.049114	-1.369910	-0.893923
H	-3.298079	-0.672010	-1.937233
H	-3.698758	-2.026713	-0.862463
C	-3.760155	-2.840850	-3.512886
H	-3.488856	-3.387109	-4.418678
H	-4.496951	-3.429252	-2.956529
H	-4.232843	-1.900095	-3.810477

TS2*anti*

Cu	-0.869287	0.579938	-0.246256
C	-0.531557	2.200485	-2.759546
H	-0.802457	2.599539	-3.757130
H	-0.338791	3.093097	-2.149759
C	-1.706210	1.397158	-2.196744
P	0.798621	1.650332	1.095701
P	-0.926964	-1.759729	0.089201
B	0.790923	1.404083	-3.012543
O	2.050866	1.885251	-2.745590
O	0.822985	0.174266	-3.628025
C	3.001894	1.037460	-3.429594
C	2.190968	-0.292908	-3.609754
C	-3.031573	-2.947148	4.041323
C	-2.692110	-1.417379	2.204629
C	-1.390482	-3.449218	2.342489
C	-2.046407	-3.785977	3.523543

C	-3.354848	-1.765565	3.378826
H	-0.629488	-4.113408	1.944196
H	-1.788603	-4.706567	4.038495
H	-3.542918	-3.213640	4.961587
C	0.441641	1.397523	2.891138
C	-0.202428	1.000944	5.584878
C	1.453575	1.291655	3.851950
C	-0.895530	1.315097	3.292365
C	-1.212872	1.120414	4.634987
C	1.131435	1.089533	5.190729
H	-1.678372	1.407790	2.543481
H	-2.254394	1.052179	4.934815
H	-0.451212	0.839273	6.629593
C	2.559015	1.105945	1.021927
C	5.153436	0.041964	0.984377
C	3.668954	1.949730	0.956099
C	2.796347	-0.268585	1.094484
C	4.070810	-0.832351	1.082813
C	4.955069	1.419139	0.928984
H	3.530158	3.024683	0.919562
H	5.810067	2.084466	0.867252
H	6.165546	-0.347201	0.966216
C	0.591797	-2.801525	0.044403
C	3.007398	-4.215937	-0.079284
C	0.649009	-4.053913	-0.572532
C	1.765484	-2.306168	0.613184
C	2.984676	-2.982576	0.570014
C	1.849786	-4.751859	-0.638524
H	-0.245137	-4.474489	-1.020818
H	1.885893	-5.718635	-1.129975
H	3.933885	-4.775469	-0.147269
C	-1.974509	-2.554312	-1.197560
C	-3.596010	-3.506677	-3.268057
C	-1.639976	-2.299567	-2.534913
C	-3.123102	-3.293532	-0.908349
C	-3.932970	-3.762522	-1.941929
C	-2.442958	-2.779859	-3.563255
H	-0.759761	-1.705636	-2.774189
H	-3.399297	-3.493534	0.122277
H	-4.829460	-4.328161	-1.706582
H	-2.175595	-2.573966	-4.595293
H	-4.231008	-3.869154	-4.070707
C	0.907205	3.481730	0.931441
C	0.935303	6.252567	0.518202
C	0.421245	4.348327	1.913706
C	1.406042	4.017214	-0.264358
C	1.426938	5.393930	-0.463768
C	0.431872	5.726385	1.704273
H	0.029301	3.953963	2.845861
H	1.786608	3.357120	-1.040074
H	1.822609	5.794914	-1.392167
H	0.048157	6.387946	2.475145
H	0.944549	7.326476	0.358187
H	-2.918197	-0.482534	1.695967
H	2.497151	1.361086	3.560965
H	-4.118553	-1.105460	3.779659
H	1.924880	1.001105	5.926904
O	1.691167	-1.075140	1.213910
C	4.181474	-2.344462	1.274358
C	-3.069265	1.955584	-2.622496
H	-2.994248	3.042687	-2.766378
H	-3.470507	1.532659	-3.553418
C	-1.710066	-2.261708	1.676438
C	-2.750171	1.914767	-0.403614

C	-3.904480	1.669652	-1.383446
C	-5.096010	2.612461	-1.161406
C	-4.400658	0.216317	-1.357810
C	-5.971968	2.169167	0.005605
H	-5.707725	2.629651	-2.073357
H	-4.739645	3.636507	-0.989493
C	-5.355564	-0.069227	-0.203386
H	-4.925192	0.013260	-2.301048
H	-3.554929	-0.474681	-1.301410
H	-6.859062	2.804470	0.092097
H	-5.404832	2.244849	0.948080
H	-5.794111	-1.066639	-0.308939
H	-4.811827	-0.028629	0.749585
O	-6.439906	0.845084	-0.170548
C	5.512915	-2.892919	0.756330
H	6.350092	-2.439852	1.293347
H	5.579637	-3.970037	0.930289
H	5.641008	-2.702742	-0.313916
C	4.068056	-2.643169	2.788528
H	4.103993	-3.723318	2.963411
H	4.897429	-2.173584	3.327313
H	3.130781	-2.259763	3.202935
C	2.317219	-1.223494	-2.410492
H	1.615890	-2.054659	-2.518247
H	3.325027	-1.636683	-2.316906
H	2.070607	-0.687546	-1.490780
C	2.473088	-1.046922	-4.899438
H	1.859325	-1.951889	-4.936884
H	2.244348	-0.444004	-5.780601
H	3.524491	-1.348424	-4.943506
C	3.335442	1.726688	-4.751906
H	2.447248	1.831370	-5.382501
H	3.723624	2.727716	-4.543625
H	4.095449	1.172560	-5.310104
C	4.248763	0.906794	-2.571047
H	4.009546	0.537347	-1.573535
H	4.964975	0.222251	-3.036912
H	4.730007	1.883620	-2.466306
H	-2.369964	2.952955	-0.489059
O	-2.687307	1.364642	0.754538
H	-1.650383	0.349368	-2.512928

TS2*$_{syn}$*

Cu	-0.879461	0.510979	-0.273229
C	-1.248924	-0.007836	-3.078809
H	-1.765056	-0.908515	-2.732261
H	-1.545692	0.064671	-4.145848
C	-1.721977	1.262584	-2.352132
H	-0.988241	2.059580	-2.503867
P	0.752524	1.940313	0.650285
P	-0.842032	-1.706470	0.548130
B	0.292299	-0.260783	-3.180844
O	0.829262	-1.478113	-3.527771
O	1.249024	0.724873	-3.100316
C	2.269838	-1.344805	-3.530256
C	2.465995	0.204169	-3.681248
C	-2.358557	-1.884410	4.933527
C	-2.385345	-0.889455	2.732230
C	-0.912197	-2.745080	3.202342
C	-1.382675	-2.785075	4.511750
C	-2.860786	-0.941710	4.040720
H	-0.155647	-3.456731	2.887294
H	-0.986276	-3.523193	5.202575

H	-2.723940	-1.917662	5.955645
C	0.441685	2.286726	2.432252
C	-0.154149	2.812634	5.111548
C	1.469404	2.548662	3.344685
C	-0.887538	2.292184	2.869290
C	-1.180258	2.558951	4.204899
C	1.170964	2.806816	4.679596
H	-1.682991	2.072027	2.157540
H	-2.213831	2.557712	4.538347
H	-0.384421	3.011663	6.154060
C	2.522334	1.433733	0.667950
C	5.156892	0.480649	0.731009
C	3.588306	2.277484	0.348158
C	2.822481	0.121537	1.038375
C	4.122182	-0.381407	1.092875
C	4.894420	1.799599	0.368203
H	3.394234	3.306707	0.065220
H	5.714390	2.459005	0.103027
H	6.183335	0.130759	0.746320
C	0.727262	-2.670315	0.626901
C	3.203683	-3.977693	0.763655
C	0.832909	-4.026287	0.307120
C	1.885436	-2.013660	1.046155
C	3.133415	-2.632608	1.121182
C	2.062838	-4.671965	0.368932
H	-0.048060	-4.577626	-0.002888
H	2.133450	-5.723157	0.109120
H	4.153554	-4.499563	0.799326
C	-1.984070	-2.848849	-0.335032
C	-3.783731	-4.361783	-1.856167
C	-1.672098	-3.210656	-1.653199
C	-3.201685	-3.257927	0.212817
C	-4.097775	-4.008310	-0.547319
C	-2.564519	-3.966912	-2.405335
H	-0.729780	-2.896670	-2.096826
H	-3.462998	-2.984815	1.230231
H	-5.043479	-4.315414	-0.110939
H	-2.309665	-4.240216	-3.424764
H	-4.484495	-4.943701	-2.447007
C	0.825678	3.604732	-0.128008
C	0.886670	6.061203	-1.464281
C	0.646928	4.795239	0.579575
C	1.033515	3.652051	-1.513631
C	1.071670	4.875477	-2.174471
C	0.672334	6.018292	-0.089445
H	0.485027	4.774061	1.652938
H	1.166713	2.728225	-2.072931
H	1.237945	4.901793	-3.247402
H	0.527434	6.938470	0.468606
H	0.907556	7.015259	-1.982416
H	-2.762375	-0.145842	2.035705
H	2.504883	2.549068	3.017365
H	-3.620974	-0.236061	4.362633
H	1.974785	3.003373	5.382784
O	1.763587	-0.685900	1.376937
C	4.312075	-1.801449	1.623988
C	-3.121121	1.702983	-2.832334
H	-3.152088	2.777800	-3.052448
H	-3.465696	1.177075	-3.732177
C	-1.407376	-1.793769	2.303591
C	-2.816963	1.716073	-0.616822
C	-3.953549	1.401048	-1.588952
C	-5.188896	2.286943	-1.379066
C	-4.378057	-0.074900	-1.523221

C	-6.013457	1.840260	-0.176003
H	-5.819391	2.238423	-2.277094
H	-4.884064	3.334136	-1.251707
C	-5.291503	-0.376114	-0.338511
H	-4.908547	-0.326765	-2.451259
H	-3.499353	-0.724626	-1.459231
H	-6.931161	2.430703	-0.089710
H	-5.429146	1.979097	0.748043
H	-5.690137	-1.392454	-0.413992
H	-4.718385	-0.293674	0.595375
O	-6.415760	0.488586	-0.295237
C	5.658120	-2.396794	1.205535
H	6.481807	-1.794035	1.596825
H	5.781533	-3.399976	1.621628
H	5.755731	-2.456200	0.117073
C	4.245218	-1.748872	3.169180
H	4.343406	-2.757320	3.583928
H	5.058775	-1.129224	3.560007
H	3.297071	-1.327077	3.515483
C	2.492586	0.671687	-5.135859
H	2.439649	1.763944	-5.159141
H	3.412897	0.361269	-5.638613
H	1.639482	0.278668	-5.697441
C	3.655237	0.770574	-2.922866
H	3.694593	1.856327	-3.052669
H	3.587771	0.559024	-1.855435
H	4.589875	0.348536	-3.306071
C	2.763650	-1.866740	-2.187184
H	2.370104	-1.252979	-1.375443
H	2.411323	-2.891420	-2.041664
H	3.855697	-1.862487	-2.127742
C	2.839925	-2.176275	-4.668231
H	2.381262	-1.920815	-5.625733
H	3.921403	-2.026001	-4.746099
H	2.658284	-3.237683	-4.475116
H	-2.488566	2.768891	-0.724406
O	-2.753951	1.221769	0.572251

I5$_{anti}$

Cu	0.530486	0.506671	-0.036654
C	2.599655	1.105738	3.220895
H	2.950078	0.080881	3.398882
H	2.938684	1.684771	4.097190
C	3.277020	1.659178	1.969921
H	2.890966	2.655919	1.724938
P	-1.235277	1.548598	-1.047067
P	0.517205	-1.853377	-0.002297
B	1.032130	1.146421	3.317362
O	0.310814	0.158804	3.949757
O	0.236272	2.206359	2.942078
C	-1.089895	0.510845	3.885750
C	-1.029340	2.055401	3.631253
C	1.812205	-2.803446	-4.337758
C	1.937489	-1.465387	-2.333600
C	0.409093	-3.338178	-2.445103
C	0.828121	-3.595062	-3.748941
C	2.370048	-1.742645	-3.626594
H	-0.346392	-3.969374	-1.985756
H	0.389444	-4.419968	-4.302348
H	2.140561	-3.011716	-5.351722
C	-1.103464	1.180052	-2.843675
C	-0.725964	0.642754	-5.559001
C	-2.191168	0.834493	-3.648815

C	0.176396	1.249803	-3.406078
C	0.361338	0.991322	-4.760078
C	-1.999721	0.562352	-5.001830
H	1.029908	1.494356	-2.776675
H	1.358062	1.046070	-5.186751
H	-0.579399	0.429378	-6.613493
C	-2.959973	1.076569	-0.623189
C	-5.495907	0.190401	0.172519
C	-3.978188	1.993420	-0.351793
C	-3.254668	-0.282863	-0.483394
C	-4.512569	-0.757056	-0.110856
C	-5.232134	1.552576	0.056477
H	-3.782377	3.057029	-0.438173
H	-6.011958	2.273971	0.277451
H	-6.485422	-0.130548	0.478494
C	-0.985871	-2.844717	0.364780
C	-3.377895	-4.087377	1.129135
C	-0.964973	-4.034820	1.096477
C	-2.232925	-2.324923	0.005820
C	-3.441065	-2.915613	0.375913
C	-2.152635	-4.649281	1.477413
H	-0.014656	-4.469228	1.388843
H	-2.124832	-5.568779	2.052978
H	-4.291830	-4.578723	1.443802
C	1.820660	-2.687208	0.992240
C	3.848181	-3.747805	2.602159
C	1.854426	-2.409397	2.364768
C	2.808115	-3.502684	0.435267
C	3.821272	-4.024886	1.238130
C	2.857310	-2.944598	3.165709
H	1.110273	-1.752196	2.808703
H	2.799652	-3.724395	-0.627301
H	4.589760	-4.649916	0.793382
H	2.874057	-2.719011	4.227815
H	4.640055	-4.153271	3.224647
C	-1.241211	3.383063	-0.993203
C	-1.163508	6.169333	-0.820515
C	-1.861543	4.167195	-1.972646
C	-0.571491	4.004105	0.065718
C	-0.538572	5.394381	0.152984
C	-1.823456	5.555085	-1.884591
H	-2.371004	3.692185	-2.806634
H	-0.083799	3.400415	0.827457
H	-0.017614	5.869358	0.978768
H	-2.305070	6.157951	-2.648415
H	-1.132002	7.252819	-0.755503
H	2.337627	-0.612582	-1.780646
H	-3.189395	0.774883	-3.224768
H	3.134663	-1.119174	-4.081173
H	-2.849118	0.288866	-5.620569
O	-2.236784	-1.168926	-0.737533
C	-4.733666	-2.268784	-0.117871
C	4.822943	1.645612	1.923177
H	5.338881	2.594078	2.111872
H	5.242932	0.885230	2.593625
C	0.962275	-2.271881	-1.733011
C	3.263412	0.800057	0.672373
H	3.227634	-0.269218	0.979351
O	2.358141	1.102360	-0.303065
C	4.783579	1.156369	0.455441
C	4.990161	2.267816	-0.574964
C	5.714384	-0.008467	0.118724
C	4.888817	1.714069	-1.994562
H	5.981666	2.721012	-0.432721

H	4.240253	3.056313	-0.448359
C	5.568880	-0.428465	-1.338875
H	6.758281	0.284627	0.301635
H	5.495895	-0.866563	0.768120
H	5.126769	2.484153	-2.735860
H	3.859029	1.367061	-2.157130
H	6.293555	-1.206286	-1.601002
H	4.560367	-0.840964	-1.504330
O	5.804964	0.652308	-2.223073
C	-5.942528	-2.678653	0.726624
H	-6.855571	-2.218056	0.340576
H	-6.097920	-3.759507	0.679003
H	-5.821909	-2.389210	1.775104
C	-4.969866	-2.712052	-1.581545
H	-5.097688	-3.798296	-1.629343
H	-5.872609	-2.236113	-1.978068
H	-4.127586	-2.438146	-2.224058
C	-0.923832	2.874161	4.918108
H	-0.689350	3.910648	4.659857
H	-1.864098	2.863319	5.476516
H	-0.128293	2.498183	5.568889
C	-2.154683	2.591033	2.763477
H	-2.049834	3.671588	2.631538
H	-2.154573	2.125598	1.778339
H	-3.122449	2.396766	3.237085
C	-1.705593	-0.265965	2.723863
H	-1.250617	0.019617	1.769376
H	-1.533728	-1.335660	2.875159
H	-2.784677	-0.098928	2.656517
C	-1.757705	0.106926	5.191618
H	-1.237347	0.520543	6.057835
H	-2.797335	0.449013	5.210133
H	-1.758141	-0.983263	5.282760

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Cu	-0.496877	0.318828	0.317364
C	-2.454525	0.379938	3.255001
H	-2.160257	1.396862	2.969596
H	-2.885496	0.457873	4.266833
C	-3.528315	-0.111783	2.289476
H	-3.727190	-1.178656	2.450745
P	-0.252940	-1.608352	-0.948362
P	1.065433	1.993214	0.120490
B	-1.166618	-0.505097	3.401421
O	0.018283	-0.037931	3.925671
O	-1.103910	-1.848588	3.116447
C	1.010529	-1.085038	3.830499
C	0.126899	-2.375292	3.660550
C	-0.137233	4.066749	-3.832939
C	-0.697360	3.044479	-1.719054
C	1.616367	3.207484	-2.411806
C	1.213327	3.825099	-3.594871
C	-1.090521	3.679945	-2.891752
H	2.672417	3.032512	-2.225994
H	1.957554	4.121826	-4.327775
H	-0.447782	4.550843	-4.754031
C	-0.512012	-0.957374	-2.648433
C	-1.093161	0.109872	-5.162907
C	0.272766	-1.297948	-3.751887
C	-1.583052	-0.070997	-2.809329
C	-1.879863	0.449871	-4.064008
C	-0.015450	-0.758713	-5.004150
H	-2.164639	0.230744	-1.939391

H	-2.716561	1.132948	-4.176736
H	-1.315781	0.525734	-6.140930
C	1.370704	-2.463103	-1.023003
C	3.928847	-3.603532	-0.939320
C	1.526705	-3.848324	-0.929456
C	2.527635	-1.680535	-1.075489
C	3.814062	-2.218740	-1.057029
C	2.796978	-4.411678	-0.874910
H	0.650426	-4.485955	-0.877789
H	2.906401	-5.487816	-0.788719
H	4.909916	-4.064389	-0.906764
C	2.869124	1.642616	0.061804
C	5.555269	0.844660	0.150527
C	3.828521	2.441959	0.689667
C	3.303674	0.452918	-0.530751
C	4.633277	0.029512	-0.504326
C	5.159623	2.043831	0.736422
H	3.527950	3.370100	1.164265
H	5.893099	2.669425	1.234602
H	6.597684	0.549741	0.201653
C	0.941995	3.357437	1.343833
C	0.723765	5.337996	3.302441
C	0.617995	3.013842	2.660446
C	1.148840	4.700593	1.012967
C	1.038610	5.686328	1.989896
C	0.515067	4.001998	3.636497
H	0.438340	1.974633	2.926084
H	1.393054	4.977564	-0.008732
H	1.196968	6.727501	1.725515
H	0.260911	3.725818	4.655442
H	0.634903	6.109053	4.061898
C	-1.465743	-2.987048	-0.865356
C	-3.359400	-5.030755	-0.650907
C	-1.800816	-3.758189	-1.984267
C	-2.087411	-3.245458	0.359794
C	-3.028777	-4.267457	0.465587
C	-2.743884	-4.775547	-1.876036
H	-1.329816	-3.559879	-2.942990
H	-1.838929	-2.646306	1.231439
H	-3.509032	-4.457938	1.420796
H	-3.002108	-5.366668	-2.749433
H	-4.099256	-5.821583	-0.570192
H	-1.442855	2.694650	-1.003468
H	1.108348	-1.983133	-3.639138
H	-2.145929	3.854620	-3.079574
H	0.601896	-1.021662	-5.857938
O	2.355313	-0.319619	-1.156930
C	4.985773	-1.258062	-1.246080
C	-4.840101	0.708738	2.230205
H	-5.741753	0.223447	2.623243
H	-4.739436	1.687522	2.715574
C	0.663337	2.816407	-1.470156
C	-3.286154	0.200166	0.762615
O	-2.274298	1.072312	0.480796
C	-4.740450	0.804233	0.688926
C	-5.712880	-0.111483	-0.057962
C	-4.819707	2.207518	0.097582
C	-5.486660	-0.017937	-1.563835
H	-6.749628	0.176188	0.165357
H	-5.585448	-1.153981	0.263504
C	-4.669790	2.171178	-1.419450
H	-5.783965	2.665412	0.359650
H	-4.018390	2.824215	0.516519
H	-6.222881	-0.613747	-2.112344

H	-4.485556	-0.408706	-1.814874
H	-4.827903	3.162208	-1.857657
H	-3.647604	1.843624	-1.664641
O	-5.616469	1.311595	-2.035276
C	6.309383	-1.857755	-0.766844
H	6.548370	-2.762572	-1.331867
H	7.131890	-1.158595	-0.938100
H	6.280452	-2.108169	0.298064
C	5.101238	-0.932113	-2.754702
H	5.909330	-0.212913	-2.922909
H	5.320869	-1.843312	-3.320448
H	4.173752	-0.502266	-3.144796
C	-0.237716	-3.041883	4.986582
H	-0.985981	-3.817136	4.799010
H	0.633284	-3.510675	5.452952
H	-0.666064	-2.322043	5.690473
C	0.692152	-3.405600	2.694754
H	0.004651	-4.252366	2.609771
H	0.838124	-2.986086	1.698399
H	1.654222	-3.781983	3.056539
C	1.887255	-0.780310	2.615512
H	1.305269	-0.778543	1.688607
H	2.331634	0.212469	2.733599
H	2.697810	-1.507988	2.513527
C	1.863943	-1.061983	5.090907
H	1.255310	-1.125175	5.995072
H	2.574624	-1.894405	5.087050
H	2.434735	-0.129499	5.129124
H	-3.216254	-0.733360	0.165205

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C	-1.428283	-2.995583	-0.443824
H	-1.235123	-3.145839	-1.513462
H	-1.920438	-3.912058	-0.088972
C	-0.104483	-2.810094	0.295023
H	-0.267505	-2.789492	1.377217
B	-2.402883	-1.775941	-0.256653
O	-3.104828	-1.197395	-1.284042
O	-2.617564	-1.162713	0.948526
C	-3.649241	0.046046	-0.785734
C	-3.671044	-0.191446	0.766579
C	1.088513	-3.730643	-0.059674
H	1.323837	-4.531977	0.647143
H	0.990428	-4.162173	-1.062046
C	0.765990	-1.601079	-0.082329
H	0.559943	-1.247541	-1.100741
O	0.697802	-0.525474	0.834173
C	2.038295	-2.505105	-0.048281
C	2.855144	-2.379785	1.242424
C	2.979475	-2.375686	-1.244708
C	3.785623	-1.166582	1.219217
H	3.463293	-3.287004	1.350250
H	2.200935	-2.315592	2.118555
C	3.840181	-1.125540	-1.121285
H	3.630704	-3.258246	-1.290513
H	2.405943	-2.340697	-2.179014
H	4.460892	-1.188404	2.079685
H	3.200284	-0.236947	1.281212
H	4.550124	-1.048148	-1.949974
H	3.194127	-0.233493	-1.144940
O	4.609752	-1.140488	0.067603
C	-4.964219	-0.840650	1.258608
H	-4.831185	-1.151881	2.298509

H	-5.804945	-0.142397	1.213944
H	-5.215364	-1.727292	0.668604
C	-3.346978	1.037186	1.602898
H	-3.412325	0.789008	2.666244
H	-2.335894	1.397193	1.404058
H	-4.057499	1.844196	1.397392
C	-2.679800	1.147147	-1.216582
H	-1.680914	0.986389	-0.801412
H	-2.590494	1.136186	-2.306634
H	-3.035521	2.135518	-0.910940
C	-5.014881	0.280152	-1.413613
H	-5.683843	-0.568232	-1.256482
H	-5.480502	1.176420	-0.991417
H	-4.904679	0.431397	-2.491377
C	1.034232	3.009105	0.664419
C	1.407694	2.572479	-0.802632
O	1.041051	1.755825	1.380754
O	0.955549	1.199211	-0.849740
B	0.886360	0.758580	0.451605
C	2.036562	3.949198	1.318330
H	2.119806	4.878957	0.746895
H	1.698894	4.200770	2.327917
H	3.026031	3.494156	1.394808
C	-0.373119	3.592131	0.779626
H	-0.634957	3.680215	1.837733
H	-0.431663	4.585891	0.326473
H	-1.113027	2.948490	0.298016
C	2.914441	2.559646	-1.057132
H	3.109268	2.087527	-2.024225
H	3.321189	3.574416	-1.083719
H	3.447298	1.991367	-0.288364
C	0.698856	3.354467	-1.897872
H	0.958046	4.416174	-1.839270
H	1.011947	2.982163	-2.877605
H	-0.386343	3.253877	-1.827250

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C	-0.540610	-0.618402	-0.151647
H	-0.018546	-1.327364	-0.808757
H	-0.077655	-0.729458	0.837154
B	-2.047886	-1.044707	-0.048943
O	-2.505623	-2.010515	0.811219
O	-3.047490	-0.490673	-0.808241
C	-3.885196	-2.275417	0.465031
C	-4.305005	-0.951764	-0.263137
C	-0.355047	0.800699	-0.666037
C	-0.920260	1.967579	0.175817
C	1.046939	1.464724	-0.588891
H	-0.719946	0.872503	-1.695449
H	-0.985728	1.705860	1.238305
H	-1.878359	2.389968	-0.140470
C	0.367164	2.782943	-0.138455
C	1.006909	3.540073	1.022056
C	0.174714	3.753975	-1.309324
C	0.195609	4.789909	1.344424
H	2.027781	3.836679	0.750596
H	1.074964	2.902189	1.908164
C	-0.574956	5.002288	-0.855188
H	1.157929	4.049318	-1.697564
H	-0.374595	3.278566	-2.130947
H	0.676724	5.377117	2.131883
H	-0.807534	4.502183	1.704730
H	-0.636641	5.735470	-1.664551

H	-1.605663	4.735438	-0.564827
O	0.076926	5.646734	0.222588
C	-3.886319	-3.493764	-0.458218
H	-3.395924	-4.327134	0.052695
H	-4.904380	-3.799596	-0.715523
H	-3.338372	-3.292914	-1.383914
C	-4.665202	-2.579244	1.734860
H	-5.730722	-2.692235	1.510848
H	-4.309530	-3.516812	2.172075
H	-4.546299	-1.790322	2.480219
C	-5.301445	-1.135567	-1.397173
H	-6.234517	-1.565738	-1.019645
H	-5.532900	-0.165501	-1.846746
H	-4.907173	-1.787478	-2.179315
C	-4.792144	0.134187	0.696478
H	-4.870686	1.079192	0.151572
H	-5.775540	-0.107217	1.109803
H	-4.090801	0.277719	1.524246
H	1.620024	1.511654	-1.522260
O	1.859433	0.937753	0.447594
C	3.413976	-2.049406	-0.738282
C	4.157810	-1.757087	0.614100
C	4.297531	-2.960152	1.533724
H	4.869948	-3.753004	1.041897
H	4.831923	-2.670250	2.443152
H	3.323733	-3.359538	1.824154
C	5.516868	-1.086459	0.413002
H	5.883379	-0.730805	1.379971
H	6.251399	-1.785131	0.002536
H	5.441727	-0.226099	-0.259122
C	2.334793	-3.123659	-0.603624
H	1.730078	-3.136741	-1.514984
H	2.775229	-4.115956	-0.471229
H	1.671887	-2.921187	0.242903
C	4.328056	-2.369158	-1.910757
H	4.921709	-3.263940	-1.698582
H	3.728580	-2.564125	-2.804854
H	5.006704	-1.542453	-2.129951
O	2.740939	-0.796101	-0.995076
O	3.291695	-0.785374	1.240503
B	2.595018	-0.178337	0.225050

I3’

Cu	0.526787	0.029192	-0.095128
C	3.343211	0.294147	-1.884654
H	3.782738	-0.095154	-2.824295
P	-0.520530	2.035095	0.620222
P	-0.860120	-0.992828	-1.746377
B	1.163405	-1.306949	1.330801
O	1.667394	-2.587856	1.044271
O	1.086155	-1.175695	2.724517
C	1.660184	-3.384978	2.240758
C	1.729941	-2.296613	3.355536
C	-3.698729	1.454211	-4.477915
C	-1.556429	1.097921	-3.429298
C	-3.346524	-0.478392	-3.074114
C	-4.178828	0.287689	-3.886681
C	-2.384084	1.855684	-4.252398
H	-3.728492	-1.388290	-2.619993
H	-5.203595	-0.028313	-4.058263
H	-4.349382	2.051928	-5.109252
C	-1.386043	3.222704	-0.487529
C	-2.610708	4.951460	-2.320585

C	-2.755143	3.485364	-0.406221
C	-0.638238	3.828073	-1.506649
C	-1.241803	4.700349	-2.405182
C	-3.365062	4.336742	-1.325922
H	0.424206	3.616029	-1.598907
H	-0.646344	5.171282	-3.181558
H	-3.086719	5.620311	-3.031186
C	-1.798209	1.561306	1.867412
C	-3.532377	0.516734	3.808025
C	-1.904375	2.163035	3.124189
C	-2.622554	0.463419	1.607351
C	-3.483113	-0.092173	2.555180
C	-2.764896	1.645053	4.085156
H	-1.291086	3.025544	3.362293
H	-2.830215	2.115743	5.060809
H	-4.182954	0.117881	4.578654
C	-1.981816	-2.066048	-0.759376
C	-3.598801	-3.504449	1.019150
C	-2.093725	-3.451357	-0.873956
C	-2.701921	-1.438811	0.258238
C	-3.529361	-2.116341	1.149580
C	-2.889654	-4.164895	0.018689
H	-1.544210	-3.974825	-1.649885
H	-2.962007	-5.244351	-0.068090
H	-4.218691	-4.082578	1.695651
C	-0.045120	-2.193812	-2.873542
C	1.309566	-4.044500	-4.472378
C	1.119364	-2.814317	-2.402535
C	-0.519945	-2.503089	-4.151067
C	0.158128	-3.422266	-4.948654
C	1.786026	-3.741798	-3.198026
H	1.488741	-2.576497	-1.406812
H	-1.419964	-2.026370	-4.528079
H	-0.216177	-3.653460	-5.941544
H	2.684415	-4.223529	-2.824740
H	1.836514	-4.762408	-5.094032
C	0.604300	3.089158	1.632908
C	2.453242	4.510780	3.181949
C	0.697542	4.477935	1.522007
C	1.439242	2.416968	2.537443
C	2.352749	3.125686	3.310033
C	1.623950	5.183807	2.288930
H	0.053346	5.016830	0.834416
H	1.372891	1.333896	2.628075
H	2.993716	2.593345	4.006680
H	1.692005	6.262946	2.188756
H	3.173895	5.062712	3.777983
H	-0.539312	1.426832	-3.233383
H	-3.353659	3.026490	0.374920
H	-2.006782	2.768382	-4.702682
H	-4.432325	4.524331	-1.256963
O	-2.562394	-0.074564	0.347215
C	-4.346960	-1.281766	2.134630
C	4.325783	0.513761	-0.749218
C	-2.027668	-0.078237	-2.837278
C	5.107711	-1.946117	-0.934866
H	6.042206	-1.737595	-1.456428
C	4.551109	-0.857660	-0.061596
C	3.161505	-1.866317	3.685962
H	3.125563	-0.968256	4.310383
H	3.706430	-2.642516	4.232495
H	3.718364	-1.622473	2.776085
C	0.984026	-2.645013	4.636386
H	1.393974	-3.553649	5.090802

H	1.086690	-1.829598	5.359219
H	-0.081245	-2.797190	4.449640
C	2.839371	-4.347382	2.210807
H	2.917172	-4.896901	3.155314
H	2.702618	-5.077831	1.406955
H	3.781226	-3.822829	2.033001
C	0.342786	-4.166242	2.245806
H	0.274337	-4.747628	1.321646
H	0.280010	-4.856878	3.093032
H	-0.515858	-3.488655	2.278237
C	-4.811736	-2.105987	3.337869
H	-5.442962	-2.937792	3.014064
H	-3.965146	-2.508988	3.902163
H	-5.422016	-1.497734	4.010601
C	-5.587784	-0.738452	1.386530
H	-6.214170	-1.568008	1.042446
H	-6.182348	-0.104684	2.052676
H	-5.299473	-0.143306	0.514627
O	2.144046	0.482341	-1.825890
C	4.534875	-3.141513	-1.065255
H	3.606028	-3.373103	-0.547064
H	4.979119	-3.920714	-1.679175
H	3.603030	-1.195418	0.368905
H	5.246080	-0.671740	0.769373
C	5.639199	1.085631	-1.326106
H	6.476384	0.811071	-0.674790
H	5.842273	0.645049	-2.309067
C	3.752548	1.504765	0.267342
H	2.837764	1.099942	0.707967
H	4.481050	1.618608	1.078356
C	3.459988	2.855370	-0.403338
H	2.409042	2.918490	-0.692046
H	3.674989	3.683400	0.289214
C	5.544543	2.617340	-1.436964
H	5.970561	3.097573	-0.542441
H	6.098361	2.985526	-2.304196
O	4.199749	3.023261	-1.606729

TS1’

Cu	-0.506872	0.072498	0.664313
C	-2.448631	1.011687	1.039699
P	1.171038	1.787512	0.883068
P	0.391892	-2.049656	0.526854
B	-1.596279	0.616519	-1.045144
O	-1.978317	-0.338931	-1.973595
O	-1.304676	1.807359	-1.679644
C	-1.649859	0.133132	-3.300628
C	-1.519604	1.689026	-3.101215
C	3.267276	-3.137434	3.985048
C	1.350102	-1.950879	3.129253
C	2.647146	-3.365564	1.663781
C	3.495449	-3.679314	2.721386
C	2.191898	-2.277078	4.188988
H	2.826000	-3.796778	0.683150
H	4.334194	-4.349441	2.558932
H	3.930512	-3.382722	4.809060
C	2.323005	1.458462	2.277979
C	3.917252	0.911889	4.511444
C	3.692158	1.236659	2.128055
C	1.755252	1.393608	3.557689
C	2.550527	1.140019	4.668696
C	4.482988	0.952966	3.240767
H	0.685618	1.546665	3.680292

H	2.100668	1.104764	5.656329
H	4.537062	0.698754	5.377084
C	2.248667	1.988265	-0.596015
C	3.687078	2.102886	-3.001377
C	2.510763	3.215691	-1.209068
C	2.739861	0.838826	-1.218402
C	3.472871	0.860552	-2.405190
C	3.213580	3.270008	-2.407668
H	2.145007	4.132165	-0.758980
H	3.397538	4.228788	-2.881478
H	4.238849	2.169530	-3.932569
C	1.354662	-2.390315	-1.007092
C	2.776317	-2.662282	-3.407485
C	1.172360	-3.514227	-1.816039
C	2.292749	-1.442584	-1.419331
C	3.016508	-1.546516	-2.607163
C	1.872436	-3.643743	-3.010583
H	0.465841	-4.282846	-1.523611
H	1.711584	-4.514791	-3.637385
H	3.304965	-2.780484	-4.346771
C	-0.830888	-3.422623	0.530442
C	-2.778113	-5.427537	0.450107
C	-1.820912	-3.408279	-0.461112
C	-0.828482	-4.443742	1.482375
C	-1.804755	-5.438499	1.444437
C	-2.781764	-4.412116	-0.505246
H	-1.837732	-2.604439	-1.194065
H	-0.067495	-4.469064	2.256211
H	-1.797513	-6.225728	2.192303
H	-3.540557	-4.396845	-1.281295
H	-3.535249	-6.205236	0.420247
C	0.634808	3.523696	1.203170
C	-0.259157	6.151477	1.583567
C	1.266975	4.360360	2.128347
C	-0.442456	4.022147	0.459563
C	-0.883644	5.328808	0.648694
C	0.817968	5.665117	2.320073
H	2.112194	3.998464	2.704837
H	-0.919438	3.390815	-0.284738
H	-1.720159	5.702007	0.065200
H	1.315180	6.302329	3.045278
H	-0.608519	7.168334	1.735813
H	0.522819	-1.262638	3.281171
H	4.152340	1.290446	1.146049
H	2.015527	-1.845340	5.168909
H	5.546138	0.774058	3.111276
O	2.479315	-0.359069	-0.597184
C	4.046099	-0.461238	-2.912903
C	1.569740	-2.496323	1.862065
C	-2.788357	2.469550	-3.440273
H	-2.668447	3.503665	-3.103802
H	-2.971455	2.479780	-4.518922
H	-3.666646	2.053344	-2.942723
C	-0.325296	2.324228	-3.804777
H	-0.404733	2.207663	-4.890469
H	-0.297463	3.394407	-3.578843
H	0.618991	1.888152	-3.471430
C	-2.753276	-0.302003	-4.254083
H	-2.566669	0.080509	-5.262648
H	-2.780325	-1.394640	-4.306044
H	-3.734809	0.046205	-3.925218
C	-0.332565	-0.537590	-3.688347
H	-0.448876	-1.623120	-3.625589
H	-0.033855	-0.280391	-4.709035

H	0.470619	-0.246715	-3.008074
C	4.396951	-0.402661	-4.401222
H	4.830327	-1.349748	-4.732941
H	3.517854	-0.185687	-5.016047
H	5.152000	0.365259	-4.587992
C	5.329544	-0.770874	-2.105708
H	5.751957	-1.729372	-2.424308
H	6.076285	0.012631	-2.270348
H	5.123512	-0.828474	-1.032627
O	-1.852631	0.624620	2.131907
H	-2.376249	2.086943	0.792930
C	-3.858602	-1.036872	0.809272
H	-3.424755	-1.330011	-0.150402
H	-3.143707	-1.328207	1.589908
C	-5.130214	-1.800940	1.026683
H	-5.547409	-1.778877	2.033651
C	-5.744325	-2.531613	0.096624
H	-6.648849	-3.093682	0.313692
H	-5.362215	-2.585700	-0.921199
C	-3.902574	0.506258	0.833684
C	-4.508879	1.114063	-0.444558
C	-4.662697	1.083794	2.059174
H	-4.198384	0.534685	-1.319347
H	-4.429224	0.495920	2.952552
C	-6.175104	1.182721	1.876462
H	-6.642384	0.187087	1.856970
H	-6.613296	1.737407	2.712191
C	-6.031146	1.206612	-0.438729
H	-6.477475	0.202002	-0.490008
H	-6.374500	1.771092	-1.311634
O	-6.518015	1.890385	0.699972
H	-4.110737	2.130797	-0.567087
H	-4.293279	2.100596	2.243908

I4’

Cu	0.445938	0.044097	-0.626695
C	3.229973	-0.627384	-0.311631
P	-0.767381	2.036901	-0.398425
P	-0.992433	-1.782782	-0.918308
B	2.641948	-0.743632	1.154813
O	2.931549	-1.713483	2.084575
O	1.644666	0.104990	1.601213
C	1.914934	-1.656688	3.114145
C	1.399509	-0.182870	2.995155
C	-3.814758	-0.839817	-4.469323
C	-1.651348	-0.755102	-3.407474
C	-3.503759	-1.817991	-2.284275
C	-4.329028	-1.512763	-3.364065
C	-2.472831	-0.466124	-4.492000
H	-3.913459	-2.347737	-1.429196
H	-5.374882	-1.803923	-3.340777
H	-4.459436	-0.600935	-5.309749
C	-1.764791	2.446315	-1.888515
C	-3.158510	2.964466	-4.259455
C	-3.159725	2.408910	-1.908649
C	-1.071522	2.729353	-3.073054
C	-1.764923	3.001781	-4.246794
C	-3.851684	2.658917	-3.092263
H	0.015769	2.746408	-3.074736
H	-1.215868	3.233452	-5.154459
H	-3.700574	3.166637	-5.178266
C	-1.943961	2.183985	1.016518
C	-3.541245	2.152092	3.324969

C	-1.967110	3.281777	1.882260
C	-2.760390	1.097853	1.337140
C	-3.567964	1.049114	2.474148
C	-2.755271	3.262573	3.027350
H	-1.348000	4.147422	1.674044
H	-2.754465	4.117547	3.695617
H	-4.142672	2.155123	4.227339
C	-2.104633	-2.241447	0.471015
C	-3.679200	-2.664389	2.750034
C	-2.186959	-3.511255	1.045803
C	-2.840769	-1.213767	1.061415
C	-3.641440	-1.388576	2.187947
C	-2.962716	-3.715971	2.182813
H	-1.624814	-4.335211	0.618772
H	-3.011105	-4.703324	2.630404
H	-4.277971	-2.848966	3.635315
C	-0.230699	-3.391733	-1.373342
C	1.034817	-5.813782	-1.961832
C	1.076328	-3.631540	-0.939557
C	-0.898878	-4.374839	-2.111121
C	-0.266933	-5.579764	-2.404053
C	1.706273	-4.839362	-1.228073
H	1.606597	-2.867566	-0.379965
H	-1.912814	-4.198542	-2.459064
H	-0.790356	-6.337090	-2.979724
H	2.722802	-5.011123	-0.887284
H	1.526111	-6.753696	-2.194835
C	0.291742	3.518650	-0.154903
C	1.992401	5.671694	0.374626
C	-0.011482	4.791716	-0.648016
C	1.449544	3.333049	0.607235
C	2.294483	4.407149	0.874485
C	0.839737	5.862272	-0.386171
H	-0.910020	4.949088	-1.237229
H	1.690560	2.339465	0.976647
H	3.199994	4.249201	1.452545
H	0.601893	6.847110	-0.776816
H	2.656343	6.507789	0.572777
H	-0.611229	-0.437934	-3.417909
H	-3.717172	2.190339	-1.003205
H	-2.068782	0.068185	-5.345664
H	-4.936755	2.620832	-3.096388
O	-2.735806	0.025998	0.478725
C	-4.447297	-0.185278	2.672672
C	-2.158113	-1.441535	-2.299026
C	-4.899996	-0.342306	4.125677
H	-5.496308	0.519058	4.437965
H	-5.540687	-1.221372	4.234807
H	-4.049293	-0.443363	4.806717
C	-5.695343	-0.044168	1.768970
H	-6.331597	-0.929860	1.865433
H	-6.275342	0.836555	2.062902
H	-5.417919	0.063862	0.716030
C	2.228494	0.816077	3.800962
H	1.944712	1.831157	3.507580
H	2.051570	0.707284	4.874826
H	3.298912	0.691706	3.609848
C	-0.081509	0.004163	3.279777
H	-0.350873	1.058350	3.166452
H	-0.692704	-0.581261	2.590378
H	-0.320615	-0.301649	4.303294
C	0.850540	-2.684878	2.734995
H	0.386759	-2.431130	1.778166
H	1.318924	-3.668038	2.634138

H	0.063165	-2.750582	3.491231
C	2.542126	-2.007093	4.453381
H	3.409754	-1.379942	4.668862
H	1.812093	-1.885054	5.259915
H	2.869136	-3.050950	4.446852
O	2.326869	-0.005922	-1.167290
H	3.425282	-1.675078	-0.631435
C	4.406004	1.528737	0.151695
H	4.102593	1.479292	1.209916
H	3.548231	1.914268	-0.406451
C	5.560877	2.479011	0.037950
H	6.468055	2.229145	0.590058
C	5.539579	3.606440	-0.672491
H	6.396873	4.273786	-0.714622
H	4.657375	3.900067	-1.238645
C	4.632303	0.082712	-0.344098
C	5.153904	0.094099	-1.792721
C	5.669474	-0.649599	0.529706
C	5.627170	-1.280039	-2.251726
H	5.994369	0.793577	-1.879047
H	4.350342	0.445836	-2.447829
C	6.114214	-1.980245	-0.072991
H	6.563576	-0.022235	0.634310
H	5.277145	-0.824256	1.539041
H	6.090679	-1.216082	-3.241266
H	4.777043	-1.977917	-2.330055
H	6.929341	-2.412942	0.515995
H	5.283493	-2.704829	-0.069755
O	6.613180	-1.822581	-1.387732

SUBSTRATE 3

C	-0.255973	0.232069	0.156069
H	-0.047527	-0.264907	-0.789699
H	-1.293716	0.261550	0.477219
C	0.715943	0.776048	0.884616
H	0.463037	1.269653	1.824202
C	2.171758	0.785231	0.512609
H	2.736466	0.260630	1.294168
H	2.309078	0.219940	-0.415262
C	2.693105	2.221022	0.357823
H	2.176655	2.688261	-0.488098
H	2.403769	2.802266	1.242062
C	4.495649	3.862459	-0.093953
H	5.553308	4.122509	-0.300884
O	3.661560	4.741656	-0.078620
C	4.210850	2.389477	0.158712
C	5.003662	1.961979	1.421751
C	4.739675	1.571747	-1.046442
C	6.509443	1.852597	1.186213
H	4.643607	0.976632	1.734765
H	4.807448	2.655973	2.247807
C	6.264692	1.498836	-1.106604
H	4.367070	0.546927	-0.954326
H	4.347714	1.977025	-1.987110
H	6.991690	1.418267	2.066281
H	6.960043	2.844403	1.020261
H	6.571787	0.808929	-1.897425
H	6.705172	2.481925	-1.338366
O	6.809015	0.999049	0.099241

$TS1_3$

Cu	-0.104040	0.577306	-0.557766

C	-1.214559	0.746614	-2.295800
H	-1.793687	-0.144728	-2.545251
H	-0.806691	1.236617	-3.181200
C	-1.772202	1.597315	-1.253883
H	-1.607803	2.667960	-1.386060
P	1.629107	1.899202	0.154535
P	-0.542728	-1.171510	0.924385
B	0.584649	-0.344525	-2.295910
O	0.394072	-1.672496	-2.655870
O	1.642560	0.198911	-3.010162
C	1.558391	-2.103704	-3.391636
C	2.070173	-0.758905	-4.000553
C	-1.255869	0.134197	5.308351
C	-1.313672	0.572844	2.937841
C	-0.500722	-1.549298	3.752203
C	-0.727206	-1.131494	5.060372
C	-1.552516	0.984301	4.246170
H	-0.093996	-2.539011	3.565178
H	-0.492088	-1.795260	5.886946
H	-1.431461	0.458552	6.329719
C	1.445129	2.572190	1.859332
C	0.971534	3.603176	4.418437
C	2.277945	2.226473	2.923586
C	0.368832	3.439461	2.088946
C	0.142494	3.963139	3.355795
C	2.033728	2.732030	4.200242
H	-0.295435	3.702612	1.269244
H	-0.689333	4.642142	3.517626
H	0.787385	4.000169	5.412109
C	3.287177	1.097199	0.148529
C	5.657743	-0.391434	-0.031607
C	4.408971	1.625949	-0.493340
C	3.401606	-0.179986	0.700132
C	4.566848	-0.943923	0.638698
C	5.581128	0.882806	-0.588885
H	4.358813	2.612512	-0.941813
H	6.442347	1.299237	-1.101334
H	6.582646	-0.951145	-0.117226
C	0.766223	-2.465367	1.031030
C	2.919460	-4.262478	1.006302
C	0.542603	-3.838058	0.903014
C	2.086423	-2.038331	1.177811
C	3.180483	-2.902084	1.163461
C	1.612305	-4.727927	0.888369
H	-0.469670	-4.213045	0.795951
H	1.426371	-5.791608	0.779576
H	3.739075	-4.972129	0.980122
C	-2.036239	-2.169561	0.516053
C	-4.254392	-3.695494	-0.247750
C	-2.138068	-2.666874	-0.791241
C	-3.066082	-2.421426	1.425473
C	-4.172713	-3.178034	1.041880
C	-3.236847	-3.434021	-1.164940
H	-1.344283	-2.465049	-1.507383
H	-3.009474	-2.032267	2.437279
H	-4.971235	-3.360238	1.754028
H	-3.300341	-3.825280	-2.176042
H	-5.112628	-4.292710	-0.541044
C	1.903978	3.418078	-0.844497
C	2.283704	5.665564	-2.463399
C	2.487207	4.576399	-0.318930
C	1.515418	3.394557	-2.187462
C	1.708144	4.513637	-2.993821
C	2.674497	5.695051	-1.125567

H	2.794894	4.605741	0.722247
H	1.084822	2.488807	-2.602290
H	1.404147	4.485414	-4.035908
H	3.125877	6.590417	-0.708971
H	2.428240	6.540257	-3.090489
H	-1.515987	1.241590	2.104881
H	3.123540	1.564190	2.766985
H	-1.955058	1.974442	4.434575
H	2.683144	2.447335	5.022554
O	2.289617	-0.687301	1.329177
C	4.568581	-2.293635	1.356005
C	-3.095872	1.220786	-0.623284
H	-3.102853	0.144163	-0.424025
H	-3.194900	1.708316	0.353749
C	-0.792536	-0.697770	2.681841
C	-4.319769	1.585332	-1.483547
H	-4.411897	2.679585	-1.518513
H	-4.136402	1.253014	-2.514649
C	-6.692815	1.599559	-1.947799
H	-6.624218	1.233683	-2.997356
O	-7.494019	2.460360	-1.655233
C	-5.671900	0.977266	-1.014298
C	-5.682712	-0.549482	-1.218419
C	-5.989329	1.289746	0.453994
C	-6.933918	-1.185728	-0.621766
H	-4.805616	-0.984326	-0.731955
H	-5.617684	-0.794894	-2.286374
C	-7.222223	0.529972	0.936949
H	-5.139980	0.987551	1.074470
H	-6.141541	2.365432	0.590706
H	-6.875197	-2.276056	-0.684946
H	-7.830224	-0.866060	-1.183448
H	-7.369516	0.682529	2.009846
H	-8.122087	0.893536	0.416857
O	-7.087107	-0.867705	0.746742
C	1.374261	-0.390718	-5.310696
H	1.620243	0.644726	-5.564195
H	1.698422	-1.032169	-6.135683
H	0.286641	-0.468615	-5.216056
C	1.140530	-3.153311	-4.409489
H	1.987368	-3.430440	-5.045867
H	0.797725	-4.054193	-3.891359
H	0.327588	-2.796720	-5.045693
C	2.531736	-2.707171	-2.377764
H	2.871212	-1.953904	-1.661240
H	2.020049	-3.496988	-1.820645
H	3.408506	-3.140912	-2.868531
C	3.580425	-0.661510	-4.155314
H	3.952298	-1.445514	-4.823377
H	3.845843	0.307592	-4.588692
H	4.087209	-0.749842	-3.191676
C	5.675151	-3.216962	0.841891
H	6.658773	-2.770804	1.010923
H	5.666460	-4.166070	1.384352
H	5.564359	-3.424778	-0.227005
C	4.785398	-2.040577	2.866808
H	4.760735	-2.988215	3.414498
H	5.757734	-1.565861	3.033817
H	4.009656	-1.388321	3.278843

$I4_3$

Cu	0.599215	0.022339	0.759960
C	3.824937	0.110798	3.004269

P	-0.772279	2.117258	0.645843
P	0.499412	-0.830368	-1.454146
C	0.929973	0.357589	-2.789736
C	1.807479	2.102108	-4.790060
C	2.136855	1.050872	-2.645104
C	0.154977	0.562374	-3.932244
C	0.588489	1.442628	-4.922525
C	2.582199	1.903057	-3.648753
H	-0.784010	0.032104	-4.060410
H	-0.024542	1.602532	-5.804394
H	2.147732	2.777692	-5.569144
C	-0.663445	3.224895	-0.822432
C	-0.334702	4.942818	-3.006649
C	-1.776093	3.695830	-1.525490
C	0.616122	3.620958	-1.225013
C	0.777084	4.484122	-2.304624
C	-1.610937	4.543863	-2.617426
H	1.492122	3.248236	-0.698881
H	1.775512	4.783164	-2.608135
H	-0.206616	5.606187	-3.856757
C	-2.566072	1.690123	0.695573
C	-5.223799	0.798824	0.638876
C	-3.476154	2.125973	1.659379
C	-3.033743	0.808187	-0.279040
C	-4.349525	0.358937	-0.355387
C	-4.791627	1.669733	1.636526
H	-3.154989	2.812810	2.435672
H	-5.490058	2.005133	2.396433
H	-6.257602	0.470838	0.636011
C	-1.096638	-1.568011	-2.005206
C	-3.632156	-2.660802	-2.475676
C	-1.223434	-2.822989	-2.604460
C	-2.269053	-0.871110	-1.709018
C	-3.546914	-1.390406	-1.905251
C	-2.484546	-3.360248	-2.842619
H	-0.336096	-3.393303	-2.858050
H	-2.574996	-4.340368	-3.299372
H	-4.603173	-3.111593	-2.649763
C	1.682750	-2.205983	-1.775353
C	3.472814	-4.328488	-2.108373
C	1.906002	-3.112342	-0.733702
C	2.355844	-2.376562	-2.989033
C	3.248937	-3.433150	-3.152495
C	2.795113	-4.169921	-0.900982
H	1.378102	-2.992534	0.208149
H	2.191179	-1.682469	-3.807449
H	3.772243	-3.554313	-4.096115
H	2.962730	-4.864752	-0.083506
H	4.175021	-5.146951	-2.235578
C	-0.640491	3.316030	2.042367
C	-0.439605	5.027146	4.251740
C	-0.780848	4.698517	1.882866
C	-0.400232	2.801878	3.321803
C	-0.305597	3.651020	4.420912
C	-0.676181	5.548091	2.981529
H	-0.970664	5.117414	0.899591
H	-0.287327	1.731022	3.457895
H	-0.119532	3.235683	5.406711
H	-0.783194	6.619855	2.843361
H	-0.358537	5.692072	5.106402
H	2.716999	0.945666	-1.732495
H	-2.777663	3.406805	-1.221599
H	3.524690	2.428880	-3.527942
H	-2.482655	4.897626	-3.159964

O	-2.108061	0.390467	-1.200973
C	-4.745166	-0.509232	-1.550891
C	4.089398	1.710710	1.168433
H	4.001178	-0.934212	3.287487
H	4.424748	0.714234	3.699717
C	2.349309	0.473818	3.246498
H	2.253783	0.471815	4.349240
H	2.186586	1.520815	2.949385
C	1.242360	-0.420216	2.647673
H	0.337072	-0.124272	3.202972
C	1.453298	-1.906566	3.034130
H	2.248041	-2.378906	2.441750
H	1.757431	-2.009847	4.095395
B	0.095236	-2.641778	2.799574
O	-1.049525	-2.344886	3.508472
O	-0.137903	-3.580231	1.818669
C	-2.162341	-2.864159	2.753736
C	-1.501376	-4.037414	1.953744
C	4.447902	0.307053	1.596672
C	5.987619	0.243022	1.750544
C	4.012863	-0.758833	0.584723
C	6.703203	0.175741	0.406425
H	6.354158	1.105724	2.321358
H	6.231223	-0.656116	2.328768
C	4.877131	-0.786512	-0.671538
H	2.965226	-0.613670	0.310392
H	4.079718	-1.739009	1.070551
H	6.558154	1.118952	-0.150147
H	7.778816	0.040774	0.553139
H	4.718916	0.123596	-1.270756
H	4.611736	-1.647556	-1.290851
O	6.256507	-0.915937	-0.369455
O	3.485418	2.032222	0.165789
H	4.427260	2.494585	1.881025
C	-3.268211	-3.284828	3.708601
H	-3.670730	-2.404553	4.218608
H	-4.086634	-3.762402	3.160151
H	-2.903072	-3.980488	4.467131
C	-2.646757	-1.732333	1.847158
H	-3.519762	-2.027674	1.258787
H	-2.920319	-0.868787	2.460287
H	-1.854111	-1.418199	1.159294
C	-2.082127	-4.258823	0.567462
H	-1.547353	-5.069368	0.063198
H	-3.139931	-4.534535	0.630589
H	-1.991092	-3.361649	-0.044632
C	-1.458241	-5.350494	2.733574
H	-2.453462	-5.795499	2.823973
H	-0.813145	-6.057626	2.204165
H	-1.049289	-5.202836	3.737675
C	-5.023975	0.428919	-2.749079
H	-5.281842	-0.158301	-3.636494
H	-5.858818	1.098493	-2.517805
H	-4.148707	1.041737	-2.986410
C	-5.996541	-1.342491	-1.262894
H	-6.282392	-1.926121	-2.141816
H	-5.840746	-2.028685	-0.424505
H	-6.845980	-0.695579	-1.029421

TS2*anti-3*

Cu	-0.021607	0.325467	-0.416839
C	-4.196345	2.881110	-1.649435
P	0.625241	-1.633752	-1.397287

P	1.463618	1.365233	1.070552
C	2.704658	2.056507	-0.097195
C	4.457683	3.149356	-1.974772
C	2.216665	2.540364	-1.316866
C	4.073938	2.117020	0.174466
C	4.947281	2.657945	-0.766211
C	3.092402	3.093621	-2.246267
H	4.461670	1.742774	1.117624
H	6.011292	2.697577	-0.552898
H	5.141205	3.571414	-2.705479
C	1.774664	-1.114246	-2.734848
C	3.406421	-0.178830	-4.798430
C	2.992958	-1.740442	-3.003135
C	1.378561	-0.010279	-3.501626
C	2.188075	0.446095	-4.535852
C	3.808600	-1.267866	-4.030032
H	0.443916	0.500107	-3.273082
H	1.874335	1.300729	-5.127474
H	4.043284	0.186339	-5.598460
C	1.533855	-2.952215	-0.492884
C	2.897460	-4.846907	1.060032
C	1.295427	-4.317941	-0.667617
C	2.475158	-2.575951	0.470672
C	3.176158	-3.494642	1.253126
C	1.967584	-5.256168	0.107846
H	0.569150	-4.648213	-1.402786
H	1.767406	-6.313580	-0.031238
H	3.413023	-5.596091	1.650877
C	2.481822	0.441078	2.289296
C	3.925850	-1.170110	4.069682
C	2.751609	0.885137	3.585530
C	2.968889	-0.814914	1.917404
C	3.696470	-1.637865	2.775931
C	3.461838	0.080267	4.470451
H	2.392077	1.857516	3.906762
H	3.657959	0.429784	5.478922
H	4.479102	-1.778861	4.776273
C	0.880254	2.831915	2.011961
C	-0.183913	5.017416	3.395932
C	-0.334545	2.714911	2.697350
C	1.558904	4.053713	2.029052
C	1.025921	5.141731	2.716848
C	-0.862759	3.800176	3.389670
H	-0.878070	1.774269	2.673631
H	2.499007	4.162512	1.496926
H	1.555641	6.089378	2.716457
H	-1.809140	3.698170	3.911832
H	-0.600616	5.869547	3.924264
C	-0.697488	-2.524103	-2.303705
C	-2.825048	-3.743131	-3.643202
C	-0.463677	-3.271007	-3.463934
C	-2.002979	-2.391146	-1.823811
C	-3.063537	-2.997102	-2.492108
C	-1.524112	-3.881319	-4.127187
H	0.546001	-3.368348	-3.853447
H	-2.205877	-1.804643	-0.932521
H	-4.070798	-2.864403	-2.111091
H	-1.336273	-4.457848	-5.027877
H	-3.651599	-4.210746	-4.169826
H	1.148962	2.466808	-1.530435
H	3.310059	-2.596190	-2.414007
H	2.706801	3.470069	-3.188977
H	4.757989	-1.755452	-4.230092
O	2.705743	-1.231547	0.633507

C	4.237494	-2.949020	2.208087
C	-2.044104	2.219430	-0.647927
H	-4.951835	3.667122	-1.768534
H	-4.142460	2.332225	-2.599864
C	-4.500376	1.897010	-0.518777
H	-4.773063	2.436591	0.398414
H	-5.325146	1.212765	-0.748137
C	-3.163800	1.171231	-0.341650
H	-3.076662	0.432006	-1.149355
C	-2.990556	0.462586	1.003956
H	-1.963646	0.053653	1.069643
H	-3.066024	1.192243	1.821425
B	-3.959234	-0.738942	1.276842
O	-4.453744	-1.047417	2.519471
O	-4.369074	-1.630459	0.311969
C	-5.425395	-2.104529	2.349572
C	-4.978011	-2.751322	0.994705
C	-2.802915	3.443496	-1.306596
C	-2.087509	3.994161	-2.543971
C	-2.939680	4.586176	-0.276572
C	-0.842380	4.796926	-2.185179
H	-1.794617	3.158685	-3.186997
H	-2.777419	4.639990	-3.105168
C	-1.623690	5.324470	-0.061205
H	-3.292904	4.200061	0.688149
H	-3.685305	5.311824	-0.629431
H	-0.094026	4.122395	-1.746708
H	-0.406694	5.264750	-3.074386
H	-0.876198	4.652256	0.392138
H	-1.759664	6.174138	0.615574
O	-1.121551	5.849396	-1.275944
O	-1.025127	1.683744	-1.406393
H	-1.661622	2.575606	0.331210
C	-5.363143	-3.035226	3.550649
H	-5.692795	-2.503672	4.448113
H	-6.025307	-3.894290	3.402801
H	-4.349283	-3.401222	3.725074
C	-6.798076	-1.436183	2.268681
H	-7.600806	-2.176022	2.202268
H	-6.955793	-0.838194	3.170622
H	-6.865160	-0.769712	1.403299
C	-6.117000	-3.298703	0.148538
H	-5.720467	-3.773238	-0.753838
H	-6.674508	-4.057194	0.707422
H	-6.807679	-2.509558	-0.155225
C	-3.890618	-3.812485	1.165642
H	-4.288140	-4.719436	1.630060
H	-3.492089	-4.076312	0.182144
H	-3.062962	-3.441380	1.778255
C	5.509515	-2.630559	1.385811
H	6.279726	-2.203266	2.036004
H	5.903405	-3.546057	0.932668
H	5.301515	-1.914033	0.585561
C	4.596463	-3.950998	3.307479
H	5.376562	-3.545322	3.957118
H	3.728668	-4.208265	3.922455
H	5.000304	-4.869359	2.873382

TS2$_{syn3}$

Cu	-0.899568	0.407635	-0.374034
C	-1.055053	-0.796447	-3.008710
H	-1.622141	-1.582812	-2.496897
H	-1.335566	-0.934712	-4.072605

C	-1.418937	0.625385	-2.541172
H	-0.528498	1.258992	-2.585702
P	0.603712	2.160157	0.225909
P	-0.677038	-1.556587	0.937903
B	0.475297	-1.139052	-2.991153
O	0.969535	-2.339430	-3.445965
O	1.478933	-0.262435	-2.645871
C	2.405096	-2.329481	-3.277314
C	2.721826	-0.796697	-3.152937
C	-2.014260	-0.838878	5.326738
C	-2.070979	-0.246796	2.985930
C	-0.728020	-2.111276	3.728847
C	-1.138228	-1.884589	5.038664
C	-2.481169	-0.024649	4.299382
H	-0.043796	-2.927454	3.517356
H	-0.771633	-2.524405	5.835767
H	-2.329701	-0.660915	6.350556
C	0.155571	3.041627	1.779025
C	-0.671099	4.374077	4.093516
C	1.094914	3.662381	2.608612
C	-1.202042	3.092617	2.116571
C	-1.611036	3.763113	3.267044
C	0.681856	4.320864	3.763614
H	-1.929543	2.588751	1.480960
H	-2.666219	3.797931	3.522136
H	-0.990310	4.888402	4.995161
C	2.405333	1.845517	0.448135
C	5.109665	1.204035	0.811090
C	3.407293	2.719406	0.016358
C	2.803390	0.668998	1.083579
C	4.140347	0.318952	1.279060
C	4.748336	2.397992	0.191811
H	3.135722	3.649641	-0.471255
H	5.517198	3.080809	-0.154897
H	6.161396	0.970508	0.934811
C	0.973400	-2.344390	1.180346
C	3.555308	-3.365335	1.564268
C	1.203790	-3.722027	1.150385
C	2.063271	-1.511693	1.443431
C	3.359401	-1.987198	1.644818
C	2.486964	-4.226572	1.329427
H	0.379623	-4.402961	0.968905
H	2.656041	-5.297635	1.288907
H	4.547104	-3.780633	1.703976
C	-1.709222	-2.980512	0.393654
C	-3.350237	-5.005024	-0.633578
C	-1.405663	-3.590837	-0.831784
C	-2.836315	-3.402885	1.100676
C	-3.653949	-4.408599	0.586149
C	-2.218040	-4.598440	-1.339002
H	-0.527596	-3.282770	-1.393750
H	-3.090653	-2.942372	2.050035
H	-4.531377	-4.722176	1.143689
H	-1.968865	-5.061700	-2.288818

I5$_{anti\text{-}3}$

Cu	-0.021607	0.325467	-0.416839
C	-4.196345	2.881110	-1.649435
P	0.625241	-1.633752	-1.397287
P	1.463618	1.365233	1.070552
C	2.704658	2.056507	-0.097195
C	4.457683	3.149356	-1.974772
C	2.216665	2.540364	-1.316866

C	4.073938	2.117020	0.174466
C	4.947281	2.657945	-0.766211
C	3.092402	3.093621	-2.246267
H	4.461670	1.742774	1.117624
H	6.011292	2.697577	-0.552898
H	5.141205	3.571414	-2.705479
C	1.774664	-1.114246	-2.734848
C	3.406421	-0.178830	-4.798430
C	2.992958	-1.740442	-3.003135
C	1.378561	-0.010279	-3.501626
C	2.188075	0.446095	-4.535852
C	3.808600	-1.267866	-4.030032
H	0.443916	0.500107	-3.273082
H	1.874335	1.300729	-5.127474
H	4.043284	0.186339	-5.598460
C	1.533855	-2.952215	-0.492884
C	2.897460	-4.846907	1.060032
C	1.295427	-4.317941	-0.667617
C	2.475158	-2.575951	0.470672
C	3.176158	-3.494642	1.253126
C	1.967584	-5.256168	0.107846
H	0.569150	-4.648213	-1.402786
H	1.767406	-6.313580	-0.031238
H	3.413023	-5.596091	1.650877
C	2.481822	0.441078	2.289296
C	3.925850	-1.170110	4.069682
C	2.751609	0.885137	3.585530
C	2.968889	-0.814914	1.917404
C	3.696470	-1.637865	2.775931
C	3.461838	0.080267	4.470451
H	2.392077	1.857516	3.906762
H	3.657959	0.429784	5.478922
H	4.479102	-1.778861	4.776273
C	0.880254	2.831915	2.011961
C	-0.183913	5.017416	3.395932
C	-0.334545	2.714911	2.697350
C	1.558904	4.053713	2.029052
C	1.025921	5.141731	2.716848
C	-0.862759	3.800176	3.389670
H	-0.878070	1.774269	2.673631
H	2.499007	4.162512	1.496926
H	1.555641	6.089378	2.716457
H	-1.809140	3.698170	3.911832
H	-0.600616	5.869547	3.924264
C	-0.697488	-2.524103	-2.303705
C	-2.825048	-3.743131	-3.643202
C	-0.463677	-3.271007	-3.463934
C	-2.002979	-2.391146	-1.823811
C	-3.063537	-2.997102	-2.492108
C	-1.524112	-3.881319	-4.127187
H	0.546001	-3.368348	-3.853447
H	-2.205877	-1.804643	-0.932521
H	-4.070798	-2.864403	-2.111091
H	-1.336273	-4.457848	-5.027877
H	-3.651599	-4.210746	-4.169826
H	1.148962	2.466808	-1.530435
H	3.310059	-2.596190	-2.414007
H	2.706801	3.470069	-3.188977
H	4.757989	-1.755452	-4.230092
O	2.705743	-1.231547	0.633507
C	4.237494	-2.949020	2.208087
C	-2.044104	2.219430	-0.647927
H	-4.951835	3.667122	-1.768534
H	-4.142460	2.332225	-2.599864

C	-4.500376	1.897010	-0.518777
H	-4.773063	2.436591	0.398414
H	-5.325146	1.212765	-0.748137
C	-3.163800	1.171231	-0.341650
H	-3.076662	0.432006	-1.149355
C	-2.990556	0.462586	1.003956
H	-1.963646	0.053653	1.069643
H	-3.066024	1.192243	1.821425
B	-3.959234	-0.738942	1.276842
O	-4.453744	-1.047417	2.519471
O	-4.369074	-1.630459	0.311969
C	-5.425395	-2.104529	2.349572
C	-4.978011	-2.751322	0.994705
C	-2.802915	3.443496	-1.306596
C	-2.087509	3.994161	-2.543971
C	-2.939680	4.586176	-0.276572
C	-0.842380	4.796926	-2.185179
H	-1.794617	3.158685	-3.186997
H	-2.777419	4.639990	-3.105168
C	-1.623690	5.324470	-0.061205
H	-3.292904	4.200061	0.688149
H	-3.685305	5.311824	-0.629431
H	-0.094026	4.122395	-1.746708
H	-0.406694	5.264750	-3.074386
H	-0.876198	4.652256	0.392138
H	-1.759664	6.174138	0.615574
O	-1.121551	5.849396	-1.275944
O	-1.025127	1.683744	-1.406393
H	-1.661622	2.575606	0.331210
C	-5.363143	-3.035226	3.550649
H	-5.692795	-2.503672	4.448113
H	-6.025307	-3.894290	3.402801
H	-4.349283	-3.401222	3.725074
C	-6.798076	-1.436183	2.268681
H	-7.600806	-2.176022	2.202268
H	-6.955793	-0.838194	3.170622
H	-6.865160	-0.769712	1.403299
C	-6.117000	-3.298703	0.148538
H	-5.720467	-3.773238	-0.753838
H	-6.674508	-4.057194	0.707422
H	-6.807679	-2.509558	-0.155225
C	-3.890618	-3.812485	1.165642
H	-4.288140	-4.719436	1.630060
H	-3.492089	-4.076312	0.182144
H	-3.062962	-3.441380	1.778255
C	5.509515	-2.630559	1.385811
H	6.279726	-2.203266	2.036004
H	5.903405	-3.546057	0.932668
H	5.301515	-1.914033	0.585561
C	4.596463	-3.950998	3.307479
H	5.376562	-3.545322	3.957118
H	3.728668	-4.208265	3.922455
H	5.000304	-4.869359	2.873382

I6$_{anti\text{-}3}$

C	-2.131406	-2.427580	-1.631091
C	-1.968719	-0.624344	-0.037375
H	-2.568330	-3.393579	-1.905613
H	-2.092328	-1.810264	-2.537941
C	-0.736341	-2.537414	-1.014472
H	-0.699058	-3.366894	-0.298251
H	0.047422	-2.719594	-1.756455
C	-0.540616	-1.191278	-0.288338

H	-0.078573	-0.498387	-1.000584
C	0.363917	-1.269070	0.949938
H	0.208791	-0.363866	1.551502
H	0.093981	-2.124814	1.580316
B	1.884758	-1.283499	0.567800
O	2.854157	-2.043691	1.168136
O	2.385524	-0.476392	-0.427209
C	4.062284	-1.903474	0.382545
C	3.827127	-0.539994	-0.357473
C	-2.961412	-1.692788	-0.562409
C	-4.265386	-1.120696	-1.129854
C	-3.325442	-2.646585	0.597646
C	-5.170916	-0.566550	-0.037415
H	-4.047574	-0.337446	-1.860772
H	-4.800029	-1.925723	-1.649999
C	-4.316393	-2.020492	1.576157
H	-2.431819	-2.954864	1.153530
H	-3.774572	-3.554323	0.176444
H	-4.691083	0.300681	0.446609
H	-6.124325	-0.230250	-0.455206
H	-3.840011	-1.194188	2.130341
H	-4.642651	-2.762071	2.311317
O	-5.483876	-1.551316	0.931887
H	-2.128364	-0.413604	1.025328
C	5.264489	-1.923938	1.313686
H	5.351193	-2.907860	1.783767
H	6.185086	-1.733695	0.752904
H	5.175849	-1.175993	2.104168
C	4.110795	-3.100576	-0.566868
H	5.029398	-3.103350	-1.160410
H	4.078891	-4.021919	0.021333
H	3.254846	-3.103864	-1.248750
C	4.391356	-0.471397	-1.768185
H	4.175651	0.509105	-2.203081
H	5.477614	-0.605231	-1.753577
H	3.953387	-1.233360	-2.415864
C	4.290379	0.671941	0.450406
H	5.381671	0.724259	0.501654
H	3.926540	1.581879	-0.035845
H	3.894769	0.648255	1.470409
O	-2.134972	0.598616	-0.767109
C	-0.028741	3.442275	-0.637844
C	-0.099059	3.036320	0.877223
B	-1.373449	1.655966	-0.389985
O	-0.712254	1.732089	0.812777
O	-1.163833	2.743488	-1.201618
C	1.252657	2.895025	1.559885
H	1.810003	3.836180	1.517757
H	1.109726	2.631817	2.612320
H	1.847162	2.109132	1.090137
C	1.221347	2.899771	-1.334886
H	1.104850	3.023030	-2.415374
H	2.116556	3.446350	-1.022985
H	1.374484	1.835872	-1.124255
C	-0.179129	4.930921	-0.905343
H	0.619856	5.490334	-0.408486
H	-0.109565	5.122476	-1.980152
H	-1.141592	5.308186	-0.553771
C	-1.025302	3.932345	1.696945
H	-1.186370	3.475124	2.677294
H	-0.590111	4.924332	1.847936
H	-1.998803	4.048905	1.211067

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C	-1.145100	1.477193	-1.901685
H	-1.451840	0.708138	-2.605457
H	-0.221281	2.005871	-2.119988
C	-1.866440	1.740493	-0.805962
C	-3.129565	0.960229	-0.511393
H	-3.083398	0.004514	-1.044414
H	-3.179936	0.722147	0.558097
O	-6.137046	-0.095046	-1.120292
C	-5.522048	0.687209	-0.431207
H	-5.673402	0.701638	0.672051
C	-4.462945	1.663540	-0.920615
C	-4.668750	3.000410	-0.182383
C	-4.546536	1.863685	-2.439596
C	-5.965473	3.694809	-0.607427
H	-3.825427	3.661530	-0.405880
H	-4.654029	2.831308	0.901935
C	-5.815749	2.603669	-2.875667
H	-3.667035	2.437952	-2.754607
H	-4.488878	0.889449	-2.936937
H	-6.063021	4.646721	-0.074389
H	-6.831938	3.082930	-0.317487
H	-5.776797	2.786671	-3.955213
H	-6.688062	1.964587	-2.694987
C	-1.436721	2.807769	0.142542
C	-1.500054	2.621870	1.529367
C	-0.953039	4.030813	-0.341821
C	-1.081081	3.621608	2.402701
H	-1.862764	1.682845	1.936491
C	-0.537769	5.032081	0.530548
H	-0.926220	4.203208	-1.413861
C	-0.599914	4.831323	1.907674
H	-1.130537	3.453052	3.474365
H	-0.174049	5.974898	0.132866
H	-0.280179	5.613200	2.589772
C	-5.990697	3.923032	-2.120360
H	-6.927666	4.407459	-2.416711
H	-5.176140	4.609205	-2.391083

$I3_{14}$

Cu	-0.017076	-0.195202	-0.660634
C	-2.177697	0.127410	-2.018383
H	-2.109771	-0.883800	-2.403016
H	-1.741785	0.904214	-2.636711
C	-2.864636	0.379854	-0.884440
P	0.987511	1.969846	-0.791000
P	0.039488	-0.932212	1.620352
B	0.959065	-1.660079	-1.739848
O	0.549118	-2.932997	-2.169292
O	2.341271	-1.562666	-1.917338
C	1.711467	-3.763164	-2.359389
C	2.828485	-2.707861	-2.631592
C	-0.606250	1.940265	5.210154
C	-1.466231	0.616124	3.388641
C	0.890781	0.589000	3.878357
C	0.677974	1.488733	4.921054
C	-1.681835	1.498339	4.440806
H	1.898332	0.238473	3.678589
H	1.521874	1.832120	5.511628
H	-0.769038	2.637271	6.026535
C	1.004650	3.190057	0.585871
C	0.909024	5.000008	2.715293
C	2.080831	4.050663	0.830273

C	-0.114140	3.241922	1.420215
C	-0.166465	4.149668	2.474599
C	2.034006	4.948064	1.892972
H	-0.946997	2.566963	1.247664
H	-1.044311	4.179053	3.111995
H	0.874323	5.700691	3.544330
C	2.781665	1.624564	-1.028571
C	5.451298	0.811002	-1.272946
C	3.564323	2.086224	-2.086484
C	3.379451	0.763015	-0.109995
C	4.706152	0.349940	-0.187880
C	4.887254	1.670366	-2.213110
H	3.136676	2.757834	-2.823947
H	5.486430	2.025407	-3.045612
H	6.486683	0.508561	-1.387439
C	1.721276	-1.653812	1.859504
C	4.313796	-2.715176	1.928948
C	1.953423	-2.920833	2.399452
C	2.824577	-0.937322	1.391930
C	4.128032	-1.432866	1.414304
C	3.239530	-3.449437	2.426810
H	1.122040	-3.507705	2.775440
H	3.406527	-4.440999	2.834877
H	5.308000	-3.147828	1.957201
C	-1.041118	-2.391035	1.939179
C	-2.710885	-4.623851	2.209401
C	-1.208466	-3.287571	0.873344
C	-1.703684	-2.636703	3.144345
C	-2.541281	-3.744000	3.274434
C	-2.034261	-4.397874	1.011723
H	-0.696569	-3.108433	-0.070174
H	-1.575121	-1.965037	3.987008
H	-3.057700	-3.918453	4.213721
H	-2.162234	-5.078854	0.175847
H	-3.369686	-5.480852	2.309366
C	0.572706	2.969903	-2.278053
C	-0.217004	4.323640	-4.598745
C	0.343533	4.347231	-2.248309
C	0.407042	2.276499	-3.485129
C	0.020814	2.950234	-4.639403
C	-0.053767	5.018934	-3.403404
H	0.460306	4.899097	-1.320919
H	0.577078	1.202404	-3.512266
H	-0.102138	2.401452	-5.568206
H	-0.235679	6.088941	-3.366571
H	-0.528272	4.849153	-5.496481
H	-2.306495	0.283605	2.786620
H	2.958289	4.017946	0.190545
H	-2.687923	1.846445	4.655156
H	2.875641	5.608700	2.078716
O	2.580769	0.323279	0.916218
C	5.253649	-0.508483	0.951365
C	-3.459504	-0.804859	-0.147079
H	-2.832824	-1.672689	-0.370210
H	-3.393699	-0.664843	0.937746
C	-0.180467	0.139654	3.102791
O	-5.361781	-3.537330	0.013566
C	-5.190314	-2.397895	0.383144
H	-5.188380	-2.157307	1.470853
C	-4.927146	-1.193922	-0.509959
C	-5.935282	-0.092293	-0.122817
C	-5.064832	-1.556573	-1.994909
C	-7.369495	-0.443414	-0.527423
H	-5.641329	0.838342	-0.620840

H	-5.879011	0.097994	0.956324
C	-6.505395	-1.864689	-2.417490
H	-4.697207	-0.709326	-2.585449
H	-4.413843	-2.408586	-2.220387
H	-8.037096	0.381373	-0.255223
H	-7.711085	-1.323534	0.035799
H	-6.535866	-2.028751	-3.500465
H	-6.831777	-2.797587	-1.945102
C	2.936587	-2.307904	-4.105183
H	3.579607	-1.425855	-4.182724
H	3.370384	-3.106033	-4.716257
H	1.955324	-2.047492	-4.513434
C	4.205723	-3.072707	-2.093294
H	4.577851	-3.992977	-2.557000
H	4.910853	-2.267049	-2.321668
H	4.186664	-3.206674	-1.009506
C	1.454206	-4.736650	-3.500833
H	2.353038	-5.323191	-3.720343
H	0.656701	-5.432805	-3.222495
H	1.146597	-4.217752	-4.411389
C	1.929217	-4.531706	-1.053953
H	1.023617	-5.098602	-0.816355
H	2.764019	-5.235980	-1.129237
H	2.124790	-3.844846	-0.225849
C	6.506403	-1.285944	0.540774
H	6.899069	-1.858702	1.385175
H	6.303307	-1.975059	-0.284152
H	7.301236	-0.600606	0.234572
C	5.612463	0.431918	2.127423
H	5.972553	-0.151087	2.981564
H	6.399000	1.130919	1.824548
H	4.744722	1.014805	2.451285
C	-3.058147	1.768792	-0.371464
C	-3.568716	2.015190	0.911339
C	-2.735931	2.887085	-1.159378
C	-3.730587	3.311079	1.394859
H	-3.853312	1.189340	1.551636
C	-2.888836	4.180611	-0.676700
H	-2.362067	2.756180	-2.168894
C	-3.384950	4.403232	0.606297
H	-4.126625	3.461857	2.394736
H	-2.618496	5.018850	-1.311758
H	-3.503314	5.414497	0.982741
C	-7.461379	-0.736488	-2.025776
H	-8.489522	-0.997441	-2.300348
H	-7.202277	0.173569	-2.584737

$TS1_{14}$

Cu	-0.315379	0.139097	-0.344412
C	-1.806397	0.185348	-1.787472
H	-2.135231	-0.749563	-2.236544
H	-1.674275	0.966981	-2.533155
C	-2.450837	0.524070	-0.527582
P	1.193395	1.934680	0.051931
P	0.104283	-1.643611	1.132854
B	0.168273	-0.568625	-2.225045
O	0.224968	-1.923885	-2.519824
O	0.866205	0.159092	-3.171781
C	1.272991	-2.117531	-3.495431
C	1.292257	-0.735933	-4.224065
C	-0.099559	-0.209021	5.523799
C	-0.718336	-0.005322	3.202918
C	0.791874	-1.757260	3.900334

C	0.707220	-1.302506	5.213319
C	-0.815853	0.436290	4.518830
H	1.415092	-2.615047	3.663394
H	1.269272	-1.804058	5.995363
H	-0.164512	0.143479	6.548828
C	1.189574	2.562894	1.780501
C	0.950860	3.438203	4.428672
C	2.206746	2.306742	2.701414
C	0.045035	3.251901	2.201538
C	-0.066776	3.699298	3.512395
C	2.081635	2.736226	4.021562
H	-0.757500	3.451913	1.498129
H	-0.956265	4.243012	3.816948
H	0.860350	3.776364	5.456521
C	2.962413	1.554020	-0.315524
C	5.565342	0.745600	-0.985506
C	3.770432	2.356319	-1.125771
C	3.508895	0.358404	0.150964
C	4.802910	-0.068953	-0.150150
C	5.055651	1.949210	-1.465342
H	3.388057	3.294936	-1.510705
H	5.667048	2.576636	-2.105715
H	6.572775	0.451859	-1.258977
C	1.705239	-2.538219	0.969379
C	4.211036	-3.698168	0.489472
C	1.838849	-3.926286	0.889717
C	2.861215	-1.770163	0.840078
C	4.122168	-2.310811	0.595101
C	3.083129	-4.499424	0.647203
H	0.966978	-4.561942	0.997841
H	3.174558	-5.578538	0.578040
H	5.168988	-4.166982	0.293152
C	-1.099213	-3.035196	1.065344
C	-2.974549	-5.093942	0.798435
C	-1.305292	-3.648822	-0.178934
C	-1.846415	-3.453489	2.167168
C	-2.784260	-4.476608	2.031006
C	-2.231091	-4.678519	-0.306863
H	-0.744350	-3.306534	-1.046016
H	-1.706840	-2.981270	3.134562
H	-3.366586	-4.788365	2.892549
H	-2.380064	-5.151173	-1.273235
H	-3.704690	-5.891039	0.695866
C	0.949061	3.452903	-0.963733
C	0.565873	5.666341	-2.634232
C	1.095192	4.749237	-0.463672
C	0.626252	3.274280	-2.313954
C	0.439980	4.375412	-3.144087
C	0.897303	5.849997	-1.294105
H	1.358525	4.908913	0.576593
H	0.529223	2.269566	-2.716762
H	0.188397	4.223637	-4.189644
H	1.005434	6.852427	-0.891085
H	0.410495	6.525604	-3.279768
H	-1.249735	0.515351	2.409147
H	3.104041	1.776670	2.399020
H	-1.435344	1.295833	4.753027
H	2.876964	2.525851	4.730186
O	2.706881	-0.411267	0.956728
C	5.306007	-1.350186	0.513601
C	-3.256467	-0.582988	0.131711
H	-2.752574	-1.528836	-0.081267
H	-3.251387	-0.493645	1.224805
C	0.077806	-1.110116	2.887751

C	-5.133568	-2.051712	0.424614
H	-4.703652	-2.979137	-0.016606
O	-5.785054	-2.111860	1.445385
C	-4.751063	-0.782447	-0.313340
C	-5.671169	0.382649	0.074297
C	-4.844303	-1.055293	-1.824940
C	-7.111684	0.192131	-0.413896
H	-5.265690	1.300946	-0.363095
H	-5.657259	0.512787	1.161010
C	-6.286293	-1.264965	-2.295836
H	-4.415886	-0.196880	-2.355210
H	-4.227347	-1.927418	-2.081025
H	-7.702079	1.080718	-0.163110
H	-7.568535	-0.651291	0.117831
H	-6.301464	-1.426689	-3.379578
H	-6.698315	-2.175910	-1.837625
C	6.489684	-1.961431	-0.239723
H	7.333584	-1.267057	-0.260694
H	6.843216	-2.863635	0.265963
H	6.223333	-2.219893	-1.269336
C	5.749734	-1.004541	1.954935
H	6.089832	-1.908166	2.471097
H	6.572864	-0.283027	1.933444
H	4.928006	-0.570733	2.532821
C	0.258785	-0.631711	-5.344375
H	0.184749	0.411893	-5.663917
H	0.541558	-1.236202	-6.211281
H	-0.729655	-0.953626	-5.002144
C	2.660828	-0.292370	-4.717257
H	2.578394	0.679503	-5.213155
H	3.370090	-0.192122	-3.892710
H	3.060454	-1.009980	-5.441299
C	2.559954	-2.400238	-2.717792
H	2.847310	-1.541080	-2.104584
H	2.393326	-3.250912	-2.050838
H	3.390517	-2.642699	-3.387624
C	0.916309	-3.304525	-4.375624
H	-0.077269	-3.195782	-4.815727
H	1.646882	-3.417408	-5.183245
H	0.926736	-4.222117	-3.779378
C	-2.670841	1.918945	-0.117045
C	-3.204756	2.242101	1.155045
C	-2.380018	3.019977	-0.952944
C	-3.411616	3.554529	1.558442
H	-3.465015	1.445778	1.844324
C	-2.566085	4.333763	-0.539383
H	-1.987144	2.850310	-1.948232
C	-3.083535	4.623057	0.722550
H	-3.825083	3.743836	2.546116
H	-2.303329	5.139846	-1.220114
H	-3.234955	5.649319	1.042390
C	-7.165361	-0.070483	-1.920239
H	-8.199222	-0.242034	-2.241003
H	-6.807750	0.819439	-2.456865

$I4_{14}$

Cu	-0.531238	-0.274470	0.672983
C	0.816819	-2.222175	2.647716
H	0.865143	-1.401787	3.376547
H	0.701321	-3.144053	3.250891
C	-0.452066	-2.054486	1.745254
P	-1.091629	-0.191441	-1.769563
P	0.082943	1.977752	1.196719

B	2.244218	-2.306853	1.993315
O	2.984051	-1.220599	1.586123
O	2.946351	-3.482764	1.874810
C	4.203825	-1.700781	0.983022
C	4.312676	-3.162545	1.551271
C	-2.251554	5.761001	-0.166001
C	-2.034500	3.797880	1.220206
C	-0.351573	4.292684	-0.432389
C	-1.065343	5.427763	-0.812202
C	-2.737359	4.938307	0.848390
H	0.581732	4.065457	-0.936208
H	-0.685154	6.054606	-1.613150
H	-2.800307	6.651649	-0.457065
C	-1.835243	1.410110	-2.285683
C	-3.199786	3.730584	-3.033813
C	-2.945830	1.841822	-1.553889
C	-1.401364	2.159865	-3.381726
C	-2.078568	3.319421	-3.750123
C	-3.631492	2.990829	-1.935362
H	-0.540413	1.835112	-3.959012
H	-1.732789	3.897919	-4.601705
H	-3.728981	4.633815	-3.322368
C	0.480474	-0.274570	-2.725067
C	3.020846	-0.361899	-3.909728
C	0.787106	-1.259974	-3.665032
C	1.479268	0.646005	-2.407525
C	2.743551	0.651604	-2.992419
C	2.053808	-1.308898	-4.240385
H	0.040800	-2.000808	-3.932514
H	2.287295	-2.087040	-4.959961
H	3.996239	-0.416792	-4.380548
C	1.824467	2.308252	0.675319
C	4.455603	2.560611	-0.267311
C	2.840789	2.755428	1.521883
C	2.174203	2.004824	-0.641272
C	3.469132	2.114005	-1.145447
C	4.143543	2.881927	1.051490
H	2.621192	2.989657	2.557536
H	4.925481	3.226148	1.720576
H	5.480200	2.661963	-0.607831
C	0.126477	2.323701	3.005757
C	0.178019	2.723967	5.775628
C	-0.014172	1.246914	3.881539
C	0.287603	3.612224	3.532455
C	0.315732	3.808893	4.908828
C	0.012188	1.441979	5.261204
H	-0.154261	0.252213	3.472763
H	0.389699	4.462841	2.864851
H	0.442831	4.810887	5.307248
H	-0.101369	0.592715	5.928338
H	0.196349	2.882340	6.849701
C	-2.166282	-1.374494	-2.705132
C	-3.769841	-3.218362	-4.081520
C	-2.810378	-1.010056	-3.894569
C	-2.334546	-2.674140	-2.219855
C	-3.130236	-3.590932	-2.903394
C	-3.606400	-1.925254	-4.576231
H	-2.696636	-0.006331	-4.291711
H	-1.847398	-2.974986	-1.301404
H	-3.245861	-4.594968	-2.506340
H	-4.101618	-1.626354	-5.495258
H	-4.394546	-3.929975	-4.613229
H	-2.431245	3.151382	1.997008
H	-3.263886	1.285543	-0.674448

H	-3.669118	5.181553	1.350379
H	-4.491351	3.319489	-1.360137
O	1.155807	1.587428	-1.461908
C	3.693002	1.791955	-2.623305
C	-1.650695	-2.204084	2.710583
H	-1.798990	-3.255298	3.013421
H	-1.371446	-1.702601	3.648772
C	-0.822128	3.475069	0.596900
C	-2.961558	-0.134149	2.526297
H	-2.630916	0.160279	3.546405
O	-3.234056	0.731933	1.717638
C	-3.048511	-1.633012	2.330652
C	-3.517254	-1.998195	0.918244
C	-4.073951	-2.136763	3.379149
C	-4.968987	-1.616024	0.614428
H	-3.404365	-3.080125	0.789810
H	-2.848260	-1.526159	0.194846
C	-5.512711	-1.714544	3.071565
H	-4.016497	-3.232988	3.391246
H	-3.776890	-1.797284	4.380220
H	-5.235618	-1.994326	-0.379387
H	-5.060000	-0.525414	0.575599
H	-6.186175	-2.135227	3.826678
H	-5.605686	-0.621902	3.143213
C	5.153575	1.440256	-2.914799
H	5.295057	1.233891	-3.978906
H	5.808502	2.280812	-2.671047
H	5.480012	0.566258	-2.342413
C	3.295006	3.034330	-3.454902
H	3.928878	3.886200	-3.188131
H	3.417102	2.828206	-4.523211
H	2.251841	3.314754	-3.278244
C	5.103988	-3.245363	2.857606
H	4.986222	-4.247280	3.280202
H	6.170505	-3.063691	2.696062
H	4.734062	-2.523659	3.592076
C	4.838023	-4.190821	0.559244
H	4.881499	-5.174470	1.036154
H	4.191048	-4.269086	-0.316875
H	5.848503	-3.928433	0.229557
C	4.018961	-1.642613	-0.532746
H	3.228559	-2.313247	-0.877026
H	3.740183	-0.622382	-0.804917
H	4.943413	-1.900810	-1.058188
C	5.344938	-0.776814	1.384862
H	5.405530	-0.655196	2.468335
H	6.301267	-1.166611	1.021143
H	5.187432	0.210015	0.941269
C	-0.357364	-3.154712	0.706722
C	0.571288	-3.018357	-0.346309
C	-1.081508	-4.357959	0.727537
C	0.772094	-4.000417	-1.305078
H	1.130005	-2.087878	-0.416294
C	-0.902105	-5.346077	-0.244659
H	-1.811868	-4.540177	1.508858
C	0.025113	-5.179631	-1.267123
H	1.496018	-3.833732	-2.098935
H	-1.496097	-6.255362	-0.194125
H	0.159428	-5.946211	-2.024427
C	-5.929987	-2.165995	1.669993
H	-6.956150	-1.845842	1.456640
H	-5.924541	-3.264643	1.632457

TS2*anti*-14

Cu	-0.259138	0.597176	0.505308
C	3.124166	0.805456	1.121014
H	3.399035	1.447360	1.967512
H	2.764867	-0.122638	1.565451
C	2.038485	1.512881	0.283271
P	-0.298356	-1.447927	1.770975
P	-2.166698	0.882168	-0.964142
B	4.395415	0.506295	0.245081
O	4.936214	-0.745366	0.074720
O	5.043474	1.460634	-0.506042
C	6.116382	-0.611711	-0.744130
C	5.877059	0.765537	-1.456381
C	-5.841446	-0.149117	1.658405
C	-3.680745	0.883031	1.357799
C	-4.710723	-0.319074	-0.467230
C	-5.802499	-0.612648	0.344447
C	-4.784034	0.604274	2.160669
H	-4.692118	-0.673391	-1.493718
H	-6.625421	-1.200516	-0.051013
H	-6.694425	-0.377752	2.290315
C	-1.591080	-1.423641	3.082771
C	-3.468617	-1.251725	5.148508
C	-2.400769	-2.519475	3.391182
C	-1.749433	-0.228560	3.797365
C	-2.668839	-0.153622	4.839771
C	-3.342364	-2.428246	4.413705
H	-1.172956	0.648934	3.506251
H	-2.776927	0.773737	5.394646
H	-4.196229	-1.187793	5.952159
C	-0.539109	-3.052719	0.895350
C	-0.673070	-5.365115	-0.665118
C	-0.135316	-4.283816	1.417465
C	-1.079257	-3.038485	-0.397242
C	-1.111103	-4.162321	-1.222150
C	-0.215862	-5.438023	0.646414
H	0.263205	-4.335287	2.425424
H	0.096022	-6.390927	1.060721
H	-0.701710	-6.269821	-1.265327
C	-2.254871	-0.296960	-2.379617
C	-2.273140	-2.277492	-4.346904
C	-2.610258	0.019426	-3.687298
C	-1.914593	-1.624832	-2.095311
C	-1.922277	-2.640240	-3.042870
C	-2.608587	-0.968728	-4.670189
H	-2.888349	1.035302	-3.945526
H	-2.883884	-0.716940	-5.689117
H	-2.299438	-3.037025	-5.122406
C	-2.693927	2.472061	-1.740654
C	-3.353889	4.945424	-2.887231
C	-1.848565	3.072025	-2.683670
C	-3.873933	3.128537	-1.381269
C	-4.199531	4.358483	-1.950816
C	-2.176421	4.296087	-3.255417
H	-0.926836	2.575744	-2.970225
H	-4.545802	2.688103	-0.652195
H	-5.119029	4.856497	-1.658600
H	-1.509099	4.744492	-3.985077
H	-3.609235	5.903907	-3.328772
C	1.260189	-1.760188	2.722427
C	3.763032	-1.907947	3.990439
C	1.486168	-1.101324	3.935654
C	2.309700	-2.495007	2.155820
C	3.547883	-2.571650	2.786463

C	2.726566	-1.175342	4.563159
H	0.698217	-0.517977	4.400129
H	2.173227	-3.003472	1.207010
H	4.348858	-3.137077	2.321633
H	2.881033	-0.654643	5.503443
H	4.731413	-1.959372	4.478483
H	-2.841922	1.451250	1.753830
H	-2.304352	-3.446374	2.834630
H	-4.806468	0.960165	3.185449
H	-3.972652	-3.282853	4.640615
O	-1.601150	-1.849055	-0.789855
C	-1.610368	-4.087266	-2.665974
C	2.321290	3.023708	0.180313
H	3.263516	3.257689	0.688849
H	2.435489	3.404702	-0.840482
C	-3.640975	0.426044	0.037005
C	0.722553	2.434911	1.743006
C	1.132686	3.662067	0.913472
C	1.507955	4.848871	1.815746
C	0.043555	4.080052	-0.079555
C	0.291440	5.496478	2.482735
H	2.025364	5.599877	1.200697
H	2.230272	4.515026	2.572883
C	-1.163564	4.775464	0.553146
H	0.502715	4.757620	-0.815330
H	-0.284258	3.196680	-0.632362
H	0.609149	6.346103	3.098699
H	-0.179853	4.770072	3.157650
H	-1.839433	5.123327	-0.237253
H	-1.708638	4.043449	1.156806
C	-0.523739	-4.642601	-3.607795
H	-0.284528	-5.680888	-3.361429
H	-0.861957	-4.626319	-4.647620
H	0.393163	-4.050172	-3.534293
C	-2.898233	-4.924861	-2.803818
H	-3.272035	-4.887919	-3.832050
H	-2.707949	-5.972482	-2.549712
H	-3.680874	-4.546143	-2.139395
C	5.067900	0.642280	-2.749192
H	4.758309	1.641666	-3.067709
H	5.660774	0.192193	-3.551140
H	4.164561	0.043688	-2.600612
C	7.136212	1.582332	-1.704744
H	6.874632	2.521347	-2.201542
H	7.651866	1.823514	-0.772882
H	7.826116	1.035495	-2.355595
C	7.317091	-0.600916	0.201687
H	7.278481	0.255188	0.881945
H	7.302030	-1.513480	0.804714
H	8.262180	-0.567746	-0.348221
C	6.196225	-1.806873	-1.682690
H	5.270397	-1.931497	-2.248318
H	7.026339	-1.690154	-2.386852
H	6.367603	-2.720224	-1.104933
H	1.490198	2.165267	2.491414
O	-0.488377	2.148521	2.038393
C	1.749058	0.786801	-0.990081
C	1.866701	-0.625424	-1.068204
C	1.376793	1.433148	-2.191208
C	1.598406	-1.329605	-2.235145
H	2.181376	-1.180412	-0.192693
C	1.118089	0.725553	-3.360821
H	1.279516	2.513057	-2.210059
C	1.220014	-0.663467	-3.399792

H	1.693854	-2.412933	-2.231011
H	0.831354	1.271587	-4.256459
H	1.001568	-1.211963	-4.310749
C	-0.732763	5.947196	1.438141
H	-1.605206	6.395341	1.928183
H	-0.282846	6.732114	0.812585

I5$_{anti\text{-}14}$

Cu	0.453681	-0.123602	-0.045691
C	-3.023196	-0.797938	-1.469265
H	-2.183767	-0.085945	-1.486545
H	-2.816343	-1.539391	-2.252542
C	-3.008294	-1.511488	-0.096194
P	0.824849	2.045243	0.607500
P	2.170210	-1.494700	-0.822744
B	-4.348395	-0.015301	-1.775710
O	-4.391462	1.340276	-1.997814
O	-5.589024	-0.598642	-1.824338
C	-5.776713	1.743312	-1.922381
C	-6.530534	0.407701	-2.257421
C	4.113184	-2.925511	3.135030
C	2.190441	-2.208326	1.862367
C	4.357793	-2.363162	0.798798
C	4.914329	-2.787967	2.002803
C	2.752441	-2.636403	3.062347
H	4.990928	-2.255633	-0.077332
H	5.976067	-3.009415	2.056381
H	4.551552	-3.253166	4.073045
C	1.252225	1.856243	2.386327
C	1.799617	1.446006	5.093016
C	2.202738	2.646554	3.037608
C	0.578066	0.851240	3.095518
C	0.851035	0.655866	4.446158
C	2.475945	2.438748	4.387913
H	-0.141843	0.207182	2.588402
H	0.327993	-0.125411	4.989571
H	2.016087	1.284392	6.144808
C	2.184111	3.075835	-0.091462
C	4.248653	4.544961	-1.296211
C	2.092636	4.465799	-0.217206
C	3.344275	2.458328	-0.570798
C	4.388617	3.164144	-1.172688
C	3.113569	5.192827	-0.817432
H	1.208428	4.981821	0.141255
H	3.023385	6.269689	-0.915810
H	5.032783	5.128766	-1.765510
C	3.581083	-0.837538	-1.798505
C	5.715249	0.329370	-3.187598
C	4.199703	-1.520346	-2.847906
C	4.064012	0.432459	-1.472003
C	5.134912	1.033280	-2.132723
C	5.251994	-0.934509	-3.544094
H	3.850962	-2.510012	-3.125556
H	5.720679	-1.468769	-4.364157
H	6.544716	0.761168	-3.736704
C	1.697210	-3.029556	-1.712229
C	0.807716	-5.293640	-3.090670
C	0.686258	-2.922642	-2.674449
C	2.259467	-4.280978	-1.447431
C	1.811454	-5.408704	-2.131377
C	0.248550	-4.047329	-3.367004
H	0.229821	-1.955416	-2.870820
H	3.035876	-4.381071	-0.694897

H	2.245684	-6.379055	-1.910977
H	-0.538299	-3.952856	-4.108945
H	0.457859	-6.175328	-3.618929
C	-0.605985	3.196940	0.600998
C	-2.835084	4.876752	0.463751
C	-0.851581	4.124537	1.618614
C	-1.492045	3.111240	-0.477187
C	-2.599653	3.949762	-0.548863
C	-1.961808	4.962472	1.547033
H	-0.178323	4.190962	2.468399
H	-1.327133	2.369795	-1.254836
H	-3.287327	3.853072	-1.382444
H	-2.147749	5.678776	2.341429
H	-3.704818	5.525104	0.415296
H	1.126047	-1.977653	1.793121
H	2.733236	3.422676	2.493259
H	2.123438	-2.733600	3.942569
H	3.218825	3.053059	4.887746
O	3.442601	1.094369	-0.438074
C	5.626793	2.376091	-1.597112
C	-3.458601	-2.996515	-0.039632
H	-4.427517	-3.231953	0.409170
H	-3.432865	-3.451086	-1.036168
C	2.991729	-2.074094	0.721748
C	-1.565720	-2.037711	0.280423
H	-1.116613	-2.299195	-0.702912
O	-0.728382	-1.285053	1.040878
C	-2.201596	-3.375045	0.788800
C	-2.457056	-3.410660	2.300784
C	-1.483094	-4.653699	0.353531
C	-1.174646	-3.655152	3.104361
H	-3.181942	-4.212679	2.512481
H	-2.917581	-2.475055	2.630728
C	-0.181728	-4.871504	1.127408
H	-2.149600	-5.516744	0.509787
H	-1.273019	-4.606817	-0.723335
H	-1.413472	-3.735430	4.172359
H	-0.531148	-2.779559	2.974394
H	0.309399	-5.794569	0.796251
H	0.504780	-4.049090	0.895805
C	6.473381	3.135035	-2.621056
H	6.831339	4.078039	-2.199525
H	7.361989	2.556840	-2.887676
H	5.911031	3.352130	-3.534369
C	6.487930	2.107930	-0.339220
H	7.366963	1.512522	-0.606222
H	6.825990	3.055162	0.093201
H	5.925703	1.563730	0.425246
C	-6.746991	0.198954	-3.756114
H	-7.094805	-0.823929	-3.926304
H	-7.498348	0.887826	-4.152918
H	-5.816489	0.338029	-4.314886
C	-7.837675	0.210779	-1.504218
H	-8.293415	-0.739759	-1.797058
H	-7.677080	0.192484	-0.424280
H	-8.543380	1.013290	-1.741800
C	-6.019218	2.224499	-0.492372
H	-5.858822	1.419353	0.228718
H	-5.311839	3.024766	-0.259467
H	-7.034860	2.612166	-0.368391
C	-6.017572	2.877406	-2.906863
H	-5.691752	2.615034	-3.915586
H	-7.080406	3.137828	-2.938505
H	-5.463009	3.766056	-2.589600

C	-3.632460	-0.607607	0.954139
C	-2.973129	0.576889	1.306720
C	-4.872581	-0.856829	1.553095
C	-3.511799	1.464390	2.231854
H	-2.013231	0.788360	0.857110
C	-5.417224	0.025060	2.486381
H	-5.431750	-1.749298	1.293580
C	-4.737812	1.189740	2.834515
H	-2.968667	2.372828	2.478104
H	-6.380248	-0.199810	2.936833
H	-5.162408	1.878503	3.559261
C	-0.432868	-4.909282	2.636005
H	0.517225	-5.011170	3.175136
H	-1.032149	-5.799434	2.878409

I6$_{anti\text{-}15}$

C	0.803487	-2.771506	-1.085345
H	0.906673	-3.000951	-2.151173
H	1.124757	-3.674185	-0.551529
C	1.745010	-1.582504	-0.727304
B	-0.728064	-2.530230	-0.810303
O	-1.681016	-2.654410	-1.787321
O	-1.259101	-2.171005	0.402159
C	-2.929417	-2.154809	-1.252999
C	-2.699317	-2.260969	0.295866
C	2.650772	-1.111705	-1.904315
H	3.726426	-1.281730	-1.822654
H	2.318146	-1.536822	-2.855669
C	1.071081	-0.165719	-0.786316
H	0.108423	-0.207519	-1.312028
O	0.921039	0.482133	0.452362
C	2.189122	0.354241	-1.734669
C	3.235492	1.245765	-1.053564
C	1.683449	1.007929	-3.021744
C	2.775551	2.697215	-0.863461
H	4.133227	1.236780	-1.688274
H	3.525141	0.817089	-0.088697
C	1.155635	2.421231	-2.780773
H	2.511591	1.041552	-3.744626
H	0.903072	0.377055	-3.466431
H	3.611986	3.295434	-0.484136
H	1.996927	2.737179	-0.093624
H	0.795190	2.857503	-3.719402
H	0.294152	2.364626	-2.104051
C	-3.101169	-3.614503	0.879111
H	-2.738808	-3.678800	1.908946
H	-4.187810	-3.738132	0.888535
H	-2.661034	-4.440756	0.312634
C	-3.310370	-1.128783	1.102990
H	-3.111568	-1.283075	2.167736
H	-2.876121	-0.173862	0.804685
H	-4.394934	-1.089758	0.960310
C	-3.079432	-0.714505	-1.744718
H	-2.292209	-0.063773	-1.353525
H	-3.023409	-0.708087	-2.837202
H	-4.047065	-0.296637	-1.450316
C	-4.069992	-3.009089	-1.785657
H	-3.908069	-4.070729	-1.588527
H	-5.017986	-2.708426	-1.328454
H	-4.157913	-2.873207	-2.867541
C	-1.241627	2.892796	1.907768
C	-1.755984	2.851722	0.420876
O	0.004993	2.171058	1.829120

O	-1.151727	1.635863	-0.084007
B	-0.054906	1.381198	0.709489
C	-0.963290	4.291420	2.438854
H	-1.876159	4.895214	2.425813
H	-0.612986	4.228453	3.473111
H	-0.196644	4.800637	1.851606
C	-2.142723	2.136608	2.882692
H	-1.632678	2.059274	3.846882
H	-3.091993	2.657551	3.036633
H	-2.352996	1.123476	2.530760
C	-1.221089	4.006310	-0.425577
H	-1.474440	3.829938	-1.474551
H	-1.665015	4.958358	-0.122077
H	-0.132739	4.089393	-0.346300
C	-3.265645	2.754246	0.268182
H	-3.745569	3.645886	0.683781
H	-3.524628	2.692722	-0.792896
H	-3.673162	1.875788	0.771532
C	2.451349	-1.841191	0.598974
C	1.672771	-2.038764	1.750018
C	3.838490	-1.924882	0.730666
C	2.261296	-2.303930	2.980295
H	0.591901	-1.980432	1.673785
C	4.433309	-2.193970	1.964785
H	4.482776	-1.782741	-0.129768
C	3.649117	-2.382966	3.096077
H	1.633241	-2.448113	3.855075
H	5.515762	-2.254950	2.033806
H	4.110446	-2.589956	4.057261
C	2.237583	3.307188	-2.160131
H	1.845004	4.312886	-1.968776
H	3.061687	3.420623	-2.878579

I3'$_{14}$

Cu	-0.060453	-0.081567	-0.086374
C	-3.104363	-0.069234	-1.344744
H	-3.839462	0.693783	-1.670664
P	1.489772	-1.792124	-0.761737
P	0.773541	1.999028	-0.940421
B	-0.444556	-0.235265	1.928583
O	-0.348915	0.776778	2.893938
O	-0.638226	-1.452550	2.603267
C	-0.160185	0.186393	4.191132
C	-0.808509	-1.221458	4.012046
C	3.443884	2.351639	-4.718143
C	1.469838	1.545748	-3.590479
C	3.074439	2.889172	-2.393793
C	3.859023	2.970614	-3.541890
C	2.244518	1.643130	-4.741710
H	3.402210	3.384652	-1.484618
H	4.793893	3.522668	-3.516787
H	4.056006	2.414897	-5.612826
C	2.429416	-1.751574	-2.345145
C	3.717344	-1.602069	-4.829009
C	3.801862	-1.505012	-2.416995
C	1.704951	-1.905559	-3.535167
C	2.347008	-1.851362	-4.766966
C	4.439186	-1.420296	-3.653579
H	0.631715	-2.077849	-3.496645
H	1.774454	-1.987801	-5.679509
H	4.217827	-1.543501	-5.790767
C	2.794507	-1.770122	0.548709
C	4.532861	-1.542330	2.739586

C	3.199901	-2.904409	1.256479
C	3.317993	-0.539111	0.953526
C	4.180941	-0.389017	2.039831
C	4.057003	-2.789907	2.345365
H	2.825342	-3.881236	0.971099
H	4.354014	-3.678568	2.892925
H	5.193076	-1.476017	3.597179
C	1.830714	2.615443	0.432777
C	3.406687	3.223046	2.666363
C	1.661899	3.825714	1.104159
C	2.808478	1.740260	0.907697
C	3.620042	2.012295	2.005076
C	2.439900	4.120550	2.220703
H	0.908248	4.530452	0.767778
H	2.294650	5.059142	2.746020
H	4.003510	3.479745	3.534639
C	-0.441547	3.362547	-1.158413
C	-2.386088	5.363256	-1.363336
C	-1.656022	3.243453	-0.473785
C	-0.212011	4.490490	-1.951993
C	-1.183116	5.483833	-2.056367
C	-2.620050	4.242570	-0.568752
H	-1.840298	2.360772	0.132026
H	0.725060	4.595656	-2.491132
H	-0.997615	6.354888	-2.677730
H	-3.553981	4.141607	-0.023470
H	-3.140251	6.140398	-1.444813
C	0.887247	-3.533178	-0.647682
C	-0.191847	-6.102826	-0.361184
C	1.151425	-4.521337	-1.599118
C	0.088499	-3.849075	0.460727
C	-0.441270	-5.127329	0.603109
C	0.607289	-5.797260	-1.459492
H	1.779186	-4.303183	-2.456853
H	-0.121160	-3.090964	1.213375
H	-1.058379	-5.357919	1.466689
H	0.815216	-6.553790	-2.210312
H	-0.614464	-7.097464	-0.254224
H	0.549059	0.968466	-3.606597
H	4.383923	-1.383098	-1.508613
H	1.921574	1.147755	-5.651931
H	5.505524	-1.219534	-3.694110
O	2.949378	0.558916	0.220052
C	4.719796	1.008319	2.347274
C	-3.687150	-1.267374	-0.619921
C	1.872211	2.175849	-2.408397
C	-4.488235	0.543719	1.093657
C	-3.904512	-0.834341	0.864993
C	-2.311291	-1.236138	4.301155
H	-2.730821	-2.183210	3.947893
H	-2.519103	-1.147617	5.372321
H	-2.825748	-0.423596	3.779165
C	-0.121841	-2.344531	4.778315
H	-0.142909	-2.153309	5.856741
H	-0.640954	-3.290463	4.593050
H	0.917324	-2.463724	4.463091
C	-0.817849	1.067510	5.243790
H	-0.758302	0.602221	6.233754
H	-0.302278	2.031758	5.291870
H	-1.868074	1.257840	5.010973
C	1.351494	0.125320	4.431485
H	1.762078	1.133961	4.327166
H	1.593907	-0.247765	5.432045
H	1.840744	-0.512096	3.689293

C	5.181648	1.136041	3.801481
H	5.580225	2.135619	3.993599
H	4.363421	0.945233	4.502824
H	5.992866	0.434568	4.012792
C	5.921741	1.277493	1.410739
H	6.315523	2.284820	1.581444
H	6.719937	0.552790	1.602334
H	5.631909	1.197658	0.358367
O	-1.924624	0.108963	-1.578221
C	-3.778313	1.494680	1.712671
H	-2.761353	1.311489	2.053571
H	-4.200572	2.477515	1.907528
H	-2.933653	-0.880497	1.365692
H	-4.544109	-1.597090	1.327148
C	-5.012034	-1.685381	-1.316601
H	-5.722281	-2.026757	-0.558109
H	-5.474253	-0.807170	-1.784929
C	-2.689094	-2.432813	-0.631345
H	-1.787717	-2.131845	-0.092230
H	-3.139000	-3.251709	-0.056423
C	-2.322546	-2.913679	-2.047067
H	-1.416370	-2.400554	-2.383754
H	-2.079150	-3.981185	-2.001624
C	-4.816916	-2.794697	-2.367660
H	-4.881039	-3.778063	-1.884833
H	-5.632168	-2.752936	-3.097302
C	-3.458939	-2.676279	-3.057013
H	-3.381630	-3.383090	-3.889653
H	-3.370748	-1.673221	-3.497479
C	-5.867594	0.825805	0.605886
C	-6.938450	-0.013033	0.938014
C	-6.115944	1.939374	-0.204900
C	-8.222874	0.259434	0.478370
H	-6.765560	-0.881027	1.568074
C	-7.400437	2.209806	-0.670674
H	-5.288221	2.584923	-0.485757
C	-8.458043	1.370395	-0.330326
H	-9.043220	-0.397534	0.751800
H	-7.572679	3.074405	-1.304851
H	-9.459658	1.578042	-0.694486

TS1'$_{14}$

Cu	0.186718	-0.264668	0.309661
C	1.792158	-1.669408	0.863407
P	-1.634377	-0.609961	1.807133
P	0.030091	1.697482	-0.921534
B	0.320976	-1.995103	-0.871259
O	0.464760	-1.837789	-2.243920
O	-0.448530	-3.112139	-0.602970
C	-0.534029	-2.651838	-2.899869
C	-0.819991	-3.766344	-1.834736
C	-0.371445	5.498045	1.683886
C	0.377796	3.228206	1.364037
C	-0.856330	4.349759	-0.383116
C	-0.950955	5.485049	0.416044
C	0.294742	4.370450	2.156021
H	-1.300910	4.348439	-1.374210
H	-1.474685	6.361892	0.047496
H	-0.444525	6.385626	2.305077
C	-1.824070	0.834352	2.927535
C	-1.912844	3.015117	4.675288
C	-2.948119	1.659124	2.964717
C	-0.735629	1.117276	3.764297

C	-0.788297	2.190201	4.645661
C	-2.985661	2.753061	3.828793
H	0.153192	0.492366	3.716067
H	0.055648	2.393181	5.298162
H	-1.949059	3.862168	5.353701
C	-3.283201	-0.840656	1.025548
C	-5.628781	-1.231577	-0.458159
C	-4.163822	-1.874859	1.351372
C	-3.624860	-0.013372	-0.046165
C	-4.789265	-0.171095	-0.797440
C	-5.322087	-2.073443	0.607793
H	-3.932065	-2.540180	2.176178
H	-5.992655	-2.887945	0.861729
H	-6.539907	-1.403603	-1.020259
C	-1.379864	1.762523	-2.107393
C	-3.583231	1.631821	-3.835466
C	-1.258596	2.151314	-3.443809
C	-2.638341	1.348324	-1.666759
C	-3.755037	1.272518	-2.499590
C	-2.350133	2.077735	-4.302125
H	-0.302598	2.495111	-3.822089
H	-2.239537	2.370944	-5.341007
H	-4.420457	1.580032	-4.522566
C	1.460769	2.101659	-2.006259
C	3.667703	2.559665	-3.661234
C	1.831097	1.154109	-2.970954
C	2.210737	3.270975	-1.871871
C	3.315099	3.494046	-2.693441
C	2.920752	1.389844	-3.800631
H	1.278121	0.220537	-3.048088
H	1.946597	4.009610	-1.121894
H	3.897697	4.402170	-2.572867
H	3.199977	0.649696	-4.544500
H	4.528084	2.735161	-4.299859
C	-1.569540	-2.020238	2.992660
C	-1.466856	-4.238414	4.698519
C	-2.017454	-1.919079	4.314219
C	-1.080455	-3.247489	2.530199
C	-1.032112	-4.349717	3.380046
C	-1.962148	-3.021913	5.162612
H	-2.410530	-0.978707	4.687439
H	-0.756199	-3.343487	1.497916
H	-0.649595	-5.296253	3.009596
H	-2.309151	-2.929207	6.187370
H	-1.422347	-5.096677	5.362368
H	0.875395	2.337737	1.740090
H	-3.803182	1.450635	2.328467
H	0.735895	4.371125	3.147613
H	-3.862179	3.393793	3.845182
O	-2.746458	1.000603	-0.343268
C	-5.089203	0.866819	-1.876621
C	-0.189625	3.214224	0.087421
C	0.060475	-5.006153	-1.984309
H	-0.058412	-5.634069	-1.096422
H	-0.228356	-5.594133	-2.860750
H	1.117516	-4.746084	-2.073933
C	-2.281197	-4.184825	-1.727593
H	-2.634917	-4.604006	-2.675190
H	-2.386448	-4.954042	-0.956498
H	-2.922874	-3.344619	-1.453299
C	0.030544	-3.153393	-4.219733
H	-0.677356	-3.829567	-4.709914
H	0.208033	-2.306037	-4.889051
H	0.977040	-3.680087	-4.079911

C	-1.739706	-1.744063	-3.153024
H	-1.420662	-0.876966	-3.738630
H	-2.528673	-2.263160	-3.705493
H	-2.158101	-1.377932	-2.211483
C	-6.076069	0.341004	-2.921913
H	-6.290942	1.108667	-3.669618
H	-5.689194	-0.545988	-3.433121
H	-7.031668	0.086985	-2.455866
C	-5.699030	2.112529	-1.190560
H	-5.898248	2.891837	-1.933265
H	-6.640825	1.848974	-0.698412
H	-5.021893	2.525144	-0.436473
O	1.732877	-0.618242	1.630765
H	1.382302	-2.607535	1.279956
C	3.404371	-0.733784	-0.847572
H	3.291730	-1.111424	-1.867434
H	2.583919	-0.025852	-0.717320
C	4.686841	0.063217	-0.794596
C	5.559999	0.019690	-1.809158
H	6.443431	0.651554	-1.840382
H	5.401002	-0.641890	-2.656735
C	3.138767	-1.911944	0.138196
C	3.110380	-3.246016	-0.630364
C	4.157576	-2.046175	1.302578
H	2.462225	-3.142699	-1.505233
H	4.243302	-1.088096	1.819077
C	5.537225	-2.573708	0.897862
H	6.054850	-1.833019	0.279618
H	6.144671	-2.712331	1.800181
C	4.495046	-3.720759	-1.075461
H	4.925692	-2.992177	-1.775923
H	4.400575	-4.665630	-1.623555
H	2.662299	-4.017748	0.012770
H	3.726138	-2.750514	2.029294
C	5.434081	-3.885283	0.119166
H	6.426241	-4.212893	-0.212603
H	5.041435	-4.672787	0.778211
C	4.918790	0.989277	0.350581
C	3.856806	1.677106	0.953859
C	6.213522	1.213840	0.837846
C	4.088743	2.584593	1.982040
H	2.839158	1.485491	0.636071
C	6.445139	2.114980	1.873094
H	7.046308	0.661999	0.411183
C	5.382998	2.810902	2.445680
H	3.249941	3.115851	2.423525
H	7.457051	2.267337	2.237336
H	5.561044	3.515028	3.253127

I4'$_{14}$

Cu	0.263292	0.253315	-0.753528
C	-2.291655	1.597373	-0.705522
P	0.887223	-2.006365	-0.682374
P	2.129748	1.661201	-0.567639
B	-1.915827	1.387811	0.818772
O	-2.083180	2.292101	1.838560
O	-1.261413	0.247598	1.255912
C	-1.319784	1.830139	2.978005
C	-1.191967	0.294073	2.697334
C	5.158285	0.516634	-3.881763
C	2.901022	0.879259	-3.113429
C	4.754811	1.197041	-1.601171
C	5.639937	0.842122	-2.616676

C	3.787495	0.540333	-4.130000
H	5.140719	1.455220	-0.619301
H	6.707236	0.822853	-2.417487
H	5.848666	0.238701	-4.672416
C	1.975586	-2.440156	-2.099710
C	3.558321	-2.932754	-4.354147
C	3.329748	-2.746270	-1.956650
C	1.423340	-2.365609	-3.385612
C	2.206882	-2.625256	-4.504224
C	4.117911	-2.983431	-3.081167
H	0.373631	-2.110842	-3.511474
H	1.763845	-2.576751	-5.494323
H	4.173527	-3.124837	-5.227932
C	1.767746	-2.637114	0.811815
C	2.956047	-3.320133	3.260638
C	1.399861	-3.809385	1.479083
C	2.758848	-1.848475	1.398855
C	3.370632	-2.157277	2.614357
C	1.986611	-4.144064	2.694187
H	0.634359	-4.452500	1.058756
H	1.684489	-5.051857	3.206215
H	3.395870	-3.597950	4.212189
C	3.092111	1.629558	0.998212
C	4.353463	1.335320	3.482908
C	3.403927	2.751509	1.768685
C	3.443558	0.377510	1.504610
C	4.079936	0.193440	2.730221
C	4.022135	2.601574	3.006237
H	3.141608	3.741890	1.411506
H	4.250163	3.478268	3.603724
H	4.837992	1.243783	4.448759
C	1.855002	3.458665	-0.834396
C	1.323963	6.185209	-1.149186
C	0.594252	3.975197	-0.521113
C	2.848041	4.319616	-1.314512
C	2.581794	5.676543	-1.471576
C	0.330388	5.333987	-0.672781
H	-0.186671	3.311798	-0.163489
H	3.829931	3.929233	-1.567114
H	3.356439	6.338114	-1.847364
H	-0.653652	5.721426	-0.426894
H	1.118604	7.244025	-1.275134
C	-0.512107	-3.191706	-0.808184
C	-2.736295	-4.883652	-0.840053
C	-0.468540	-4.395569	-1.517405
C	-1.673634	-2.847023	-0.109479
C	-2.780803	-3.690379	-0.122902
C	-1.580314	-5.234621	-1.535414
H	0.429122	-4.679131	-2.058484
H	-1.707134	-1.904141	0.429554
H	-3.683245	-3.405996	0.410284
H	-1.543010	-6.164893	-2.094220
H	-3.602938	-5.537441	-0.861989
H	1.830675	0.872781	-3.305054
H	3.778890	-2.806899	-0.970317
H	3.405457	0.276031	-5.110778
H	5.171621	-3.214145	-2.957441
O	3.121525	-0.707729	0.726611
C	4.478009	-1.230084	3.114410
C	3.378975	1.219205	-1.843162
C	4.712869	-1.374239	4.619633
H	5.016889	-2.394679	4.866395
H	5.524919	-0.719363	4.946353
H	3.814249	-1.129645	5.194451

C	5.783224	-1.585429	2.363316
H	6.591881	-0.917035	2.676218
H	6.076338	-2.616670	2.585029
H	5.660271	-1.489288	1.280163
C	-2.379075	-0.516112	3.218084
H	-2.318115	-1.533142	2.818614
H	-2.373572	-0.577696	4.310032
H	-3.329911	-0.077784	2.898552
C	0.117893	-0.334590	3.143764
H	0.120955	-1.401113	2.899705
H	0.969625	0.132093	2.645296
H	0.247906	-0.231288	4.225745
C	0.025224	2.552025	2.928930
H	0.573989	2.291545	2.020737
H	-0.145368	3.632279	2.923602
H	0.649966	2.302520	3.791319
C	-2.068424	2.185197	4.252405
H	-3.094631	1.812311	4.234188
H	-1.557529	1.766174	5.125213
H	-2.103510	3.272244	4.369170
O	-1.388814	0.947934	-1.543666
H	-2.262677	2.695364	-0.873309
C	-3.814478	-0.364595	-0.782764
H	-3.546619	-0.550919	0.264169
H	-2.996601	-0.770915	-1.382001
C	-5.091654	-1.104137	-1.094874
C	-5.240311	-1.784582	-2.238450
H	-6.140220	-2.353184	-2.459277
H	-4.449098	-1.801692	-2.983383
C	-3.776546	1.167573	-1.007986
C	-4.102681	1.492063	-2.477210
C	-4.779935	1.898050	-0.093730
C	-4.204763	2.993925	-2.763010
H	-5.057410	1.019626	-2.745814
H	-3.325544	1.039777	-3.102314
C	-4.867548	3.404893	-0.358016
H	-5.778210	1.471394	-0.255614
H	-4.536932	1.713397	0.960788
H	-4.501687	3.149651	-3.807315
H	-3.219183	3.462943	-2.649180
H	-5.632289	3.846857	0.292133
H	-3.919264	3.890653	-0.097881
C	-5.202463	3.680380	-1.826230
H	-5.227890	4.759861	-2.017767
H	-6.211670	3.297368	-2.036601
C	-6.184882	-1.105098	-0.080283
C	-7.521504	-0.938857	-0.466320
C	-5.907108	-1.279150	1.282459
C	-8.546573	-0.954382	0.475197
H	-7.752169	-0.772983	-1.514756
C	-6.931436	-1.300731	2.224452
H	-4.880944	-1.410825	1.613125
C	-8.256072	-1.136371	1.825496
H	-9.574473	-0.814702	0.153322
H	-6.692587	-1.445354	3.274158
H	-9.054686	-1.144555	2.561170

SUBSTRATE 24

C	-1.105619	1.304894	-1.800448
H	-1.421646	0.527516	-2.490883
H	-0.152163	1.786143	-1.999804
C	-1.853091	1.636634	-0.741491
C	-3.156374	0.918462	-0.463803

H	-3.146195	-0.035978	-1.001001
H	-3.230979	0.677721	0.603914
O	-6.178316	-0.002466	-1.213489
C	-5.558351	0.725337	-0.471224
H	-5.744222	0.696020	0.626481
C	-4.451283	1.684280	-0.884014
C	-4.638886	2.994398	-0.094143
C	-4.477790	1.951792	-2.394770
C	-5.897619	3.749346	-0.530065
H	-3.768105	3.636008	-0.259823
H	-4.667685	2.777694	0.981497
C	-5.706793	2.752634	-2.838372
H	-3.570397	2.509247	-2.656333
H	-4.434397	0.998527	-2.932622
H	-5.983017	4.679971	0.041165
H	-6.792335	3.154261	-0.296455
H	-5.625394	2.980545	-3.906944
H	-6.605172	2.136678	-2.714444
C	-1.414289	2.721525	0.180492
C	-1.516708	2.565130	1.592202
C	-0.904962	3.901561	-0.317997
C	-1.109065	3.556218	2.444835
H	-1.908586	1.639095	2.001499
C	-0.477911	4.948600	0.538598
H	-0.849864	4.053110	-1.392955
C	-0.580831	4.777004	1.947163
H	-1.184334	3.417171	3.520062
C	-5.863690	4.043408	-2.031381
H	-6.773419	4.572298	-2.336492
H	-5.018347	4.712443	-2.244642
C	0.041172	6.170096	0.030617
H	0.116522	6.299755	-1.045793
C	-0.158744	5.827192	2.804582
H	-0.238628	5.689753	3.879749
C	0.340977	6.994676	2.285160
H	0.661661	7.792884	2.947627
C	0.441313	7.167581	0.883031
H	0.837944	8.096775	0.485230

$I3_{24}$

Cu	0.319155	0.461694	0.690896
C	-1.657730	0.979609	2.265365
H	-1.274892	1.969264	2.486696
H	-1.410631	0.203065	2.980198
C	-2.473020	0.787484	1.206450
P	0.728170	-1.857725	1.114568
P	0.364033	0.829926	-1.684829
B	1.767167	1.726451	1.450575
O	1.771132	3.114276	1.667413
O	3.077566	1.259897	1.579490
C	3.131625	3.589419	1.660931
C	3.929528	2.309350	2.061336
C	-1.353244	-2.255539	-4.701068
C	-1.661687	-0.447248	-3.134789
C	0.559837	-1.217415	-3.653792
C	0.023125	-2.171976	-4.514913
C	-2.195831	-1.386241	-4.010108
H	1.636635	-1.160259	-3.533607
H	0.687170	-2.848408	-5.044348
H	-1.769636	-2.996877	-5.376149
C	0.243782	-3.211005	-0.032992
C	-0.634822	-5.203079	-1.786903
C	0.972901	-4.397135	-0.174992

C	-0.917221	-3.029176	-0.787010
C	-1.363610	-4.025014	-1.651748
C	0.536532	-5.386026	-1.051847
H	-1.473149	-2.101170	-0.699824
H	-2.275481	-3.870811	-2.220481
H	-0.975692	-5.978611	-2.466473
C	2.562275	-2.021492	1.174960
C	5.362652	-1.979116	1.127069
C	3.292909	-2.550052	2.239108
C	3.275412	-1.493788	0.099747
C	4.665364	-1.469066	0.032208
C	4.684637	-2.516280	2.218931
H	2.775253	-2.970560	3.095222
H	5.245788	-2.918474	3.056466
H	6.447353	-1.971242	1.130444
C	2.147576	1.003963	-2.129763
C	4.909945	1.262065	-2.524307
C	2.659465	2.061883	-2.884498
C	3.056112	0.077217	-1.615323
C	4.436096	0.172891	-1.794327
C	4.030931	2.192574	-3.073940
H	1.985996	2.801471	-3.304250
H	4.418770	3.026450	-3.649983
H	5.975823	1.384984	-2.682926
C	-0.295642	2.476597	-2.187095
C	-1.266425	5.043562	-2.749533
C	-0.103063	3.525834	-1.276299
C	-0.961610	2.733090	-3.388105
C	-1.451678	4.009558	-3.662812
C	-0.581555	4.800258	-1.559986
H	0.419717	3.340443	-0.340003
H	-1.103483	1.940776	-4.115978
H	-1.974746	4.193741	-4.596544
H	-0.433251	5.601071	-0.842088
H	-1.654677	6.034936	-2.961561
C	0.227846	-2.470590	2.775674
C	-0.631928	-3.188010	5.342545
C	-0.369579	-3.712949	2.998548
C	0.396841	-1.591575	3.854470
C	-0.025167	-1.950495	5.130718
C	-0.800678	-4.067227	4.275974
H	-0.514682	-4.403085	2.173382
H	0.855530	-0.619671	3.685872
H	0.112548	-1.260427	5.957675
H	-1.270216	-5.033424	4.435443
H	-0.970897	-3.465298	6.336144
H	-2.326031	0.220510	-2.593620
H	1.882053	-4.547969	0.400619
H	-3.270982	-1.446616	-4.145544
H	1.109026	-6.302607	-1.159139
O	2.526183	-0.983183	-0.930335
C	5.309911	-0.959353	-1.255659
C	-2.762894	1.983049	0.319165
H	-1.898015	2.648808	0.387588
H	-2.819593	1.683685	-0.733320
C	-0.275934	-0.341063	-2.956623
O	-3.823878	5.125273	-0.148576
C	-3.980185	3.946333	-0.372218
H	-4.082196	3.585429	-1.421269
C	-4.025370	2.832922	0.664438
C	-5.335078	2.046353	0.447230
C	-3.959339	3.392082	2.092336
C	-6.575876	2.852683	0.839592
H	-5.295305	1.133119	1.051153

H	-5.403951	1.726484	-0.600266
C	-5.217724	4.162143	2.507198
H	-3.818809	2.549302	2.779127
H	-3.075139	4.032129	2.188948
H	-7.470526	2.237489	0.694036
H	-6.681067	3.722543	0.175870
H	-5.131448	4.452506	3.560263
H	-5.284948	5.087726	1.925432
C	4.058730	2.125980	3.575517
H	4.437454	1.119047	3.775954
H	4.750868	2.849209	4.018789
H	3.085860	2.224882	4.066578
C	5.297314	2.170709	1.405857
H	5.953114	3.002838	1.684907
H	5.767771	1.239834	1.738290
H	5.214977	2.136353	0.317318
C	3.261315	4.757277	2.628407
H	4.303772	5.085818	2.702328
H	2.665588	5.603117	2.270991
H	2.907920	4.493660	3.627732
C	3.435398	4.053705	0.234860
H	2.705963	4.815484	-0.057609
H	4.436683	4.488469	0.151637
H	3.355963	3.221857	-0.470173
C	6.759540	-0.517289	-1.041327
H	7.206291	-0.188960	-1.983539
H	6.831133	0.300263	-0.318105
H	7.367284	-1.352985	-0.684429
C	5.286830	-2.111484	-2.289167
H	5.706399	-1.773062	-3.242343
H	5.881084	-2.956229	-1.925552
H	4.267049	-2.465238	-2.469572
C	-3.081946	-0.540333	0.910753
C	-3.749654	-0.788411	-0.271309
C	-2.981124	-1.614280	1.847444
C	-4.288129	-2.063065	-0.584085
C	-3.486119	-2.854817	1.574288
H	-2.490727	-1.457704	2.800998
C	-4.144781	-3.126350	0.346081
H	-3.377629	-3.653991	2.302358
C	-6.483960	3.331961	2.289204
H	-7.371787	3.917124	2.553643
H	-6.467677	2.457402	2.954568
C	-4.940825	-2.314678	-1.819986
C	-4.640182	-4.412082	0.011826
C	-5.408630	-3.569774	-2.121073
H	-5.902168	-3.753573	-3.070650
C	-5.253629	-4.631018	-1.196862
H	-5.624754	-5.619712	-1.448954
H	-5.062359	-1.496401	-2.525012
H	-4.519127	-5.222367	0.725755
H	-3.874887	-0.006432	-1.010614

$TS1_{24}$

Cu	0.022402	-0.243602	0.464830
C	1.253586	-0.987452	1.968850
H	1.195941	-2.041030	2.234888
H	1.278453	-0.349900	2.849745
C	2.136267	-0.682369	0.855087
P	-0.744077	2.013148	0.402829
P	-0.724323	-1.429225	-1.430337
B	-0.912844	-1.107565	2.090992
O	-1.456722	-2.382838	2.031309

O	-1.449183	-0.403680	3.152738
C	-2.638433	-2.393675	2.862811
C	-2.299922	-1.290089	3.915521
C	0.656939	0.715201	-5.284545
C	0.895107	0.224677	-2.937023
C	-0.936542	-0.730887	-4.190043
C	-0.489901	-0.076027	-5.334312
C	1.351988	0.861554	-4.086663
H	-1.824704	-1.355180	-4.234365
H	-1.035195	-0.186263	-6.266799
H	1.004231	1.223314	-6.179200
C	-0.299648	2.941055	-1.122568
C	0.571231	4.210312	-3.461532
C	-1.204023	3.228954	-2.146509
C	1.047990	3.283756	-1.288638
C	1.478988	3.927611	-2.442221
C	-0.766223	3.853648	-3.313028
H	1.763063	3.060227	-0.504473
H	2.527284	4.193270	-2.544322
H	0.906059	4.702324	-4.369737
C	-2.573338	2.201177	0.559303
C	-5.364269	2.226104	0.846106
C	-3.184911	3.047488	1.487914
C	-3.403562	1.392532	-0.216506
C	-4.795059	1.389840	-0.112780
C	-4.567245	3.050085	1.636491
H	-2.578483	3.694011	2.112183
H	-5.027992	3.702890	2.370756
H	-6.440641	2.250218	0.975584
C	-2.536167	-1.711742	-1.609072
C	-5.325336	-1.995567	-1.593832
C	-3.124173	-2.947917	-1.888155
C	-3.386703	-0.634415	-1.365840
C	-4.776599	-0.738606	-1.344156
C	-4.508221	-3.087274	-1.875538
H	-2.500677	-3.810128	-2.096746
H	-4.953820	-4.054472	-2.084335
H	-6.401292	-2.130241	-1.581326
C	-0.076065	-3.141720	-1.624089
C	0.925411	-5.750982	-1.748805
C	-0.282868	-4.031678	-0.559856
C	0.645418	-3.565721	-2.740612
C	1.147782	-4.865507	-2.798866
C	0.207622	-5.330985	-0.628358
H	-0.820530	-3.695610	0.324213
H	0.824785	-2.886276	-3.567850
H	1.714973	-5.182451	-3.668522
H	0.037374	-6.014776	0.197989
H	1.316051	-6.762849	-1.798224
C	-0.165002	3.108519	1.766534
C	0.707367	4.648404	3.935248
C	0.175118	4.451864	1.587783
C	-0.086438	2.548707	3.046890
C	0.343472	3.316542	4.125001
C	0.617434	5.214735	2.666031
H	0.106938	4.908625	0.606119
H	-0.369859	1.510792	3.200060
H	0.402809	2.870100	5.113232
H	0.889586	6.254479	2.511673
H	1.054300	5.244087	4.774288
H	1.414313	0.365410	-1.991690
H	-2.253915	2.975147	-2.043863
H	2.236777	1.488021	-4.038050
H	-1.478244	4.067212	-4.104478

O	-2.784539	0.575545	-1.129677
C	-5.584445	0.534205	-1.102343
C	2.582549	-1.859856	0.006241
H	1.766354	-2.586073	-0.007471
H	2.729775	-1.569894	-1.041247
C	-0.243610	-0.584415	-2.984959
C	3.874424	-3.812640	-0.527716
H	3.101145	-4.588301	-0.328455
O	4.591345	-3.907546	-1.500686
C	3.858592	-2.657656	0.456926
C	5.157540	-1.844772	0.378577
C	3.673254	-3.232733	1.872458
C	6.379764	-2.625053	0.875590
H	5.036931	-0.944414	0.989868
H	5.318614	-1.511680	-0.651547
C	4.892473	-4.028102	2.347412
H	3.500115	-2.397479	2.561028
H	2.771782	-3.860063	1.900263
H	7.260424	-1.973131	0.855614
H	6.585948	-3.455799	0.190057
H	4.722786	-4.391073	3.367381
H	5.024201	-4.918825	1.715977
C	-6.997755	0.231062	-0.599350
H	-7.562552	1.156296	-0.458459
H	-7.549714	-0.360759	-1.334044
H	-6.980734	-0.316262	0.348284
C	-5.680441	1.308407	-2.438481
H	-6.218664	0.711266	-3.181714
H	-6.217753	2.250751	-2.290663
H	-4.688568	1.538279	-2.839442
C	-1.467951	-1.810168	5.086539
H	-1.097455	-0.959088	5.665372
H	-2.061528	-2.444547	5.751456
H	-0.604933	-2.384202	4.735286
C	-3.497394	-0.500263	4.420852
H	-3.167788	0.244451	5.151595
H	-4.002501	0.024831	3.607158
H	-4.216390	-1.163457	4.912858
C	-3.819153	-2.021005	1.963417
H	-3.711476	-1.005724	1.570198
H	-3.851225	-2.710250	1.114558
H	-4.770601	-2.087064	2.499807
C	-2.829529	-3.790029	3.432398
H	-1.931505	-4.143702	3.943345
H	-3.664589	-3.805532	4.140287
H	-3.059309	-4.489690	2.622918
C	2.837545	0.597297	0.730736
C	3.590038	0.934008	-0.396583
C	2.811582	1.577202	1.779729
C	4.254801	2.173011	-0.533148
C	3.441232	2.785779	1.675633
H	2.270463	1.361168	2.692645
C	4.177261	3.138652	0.511795
H	3.376076	3.497653	2.495366
C	6.161291	-3.175430	2.286346
H	7.030407	-3.761712	2.605828
H	6.063750	-2.338319	2.991720
C	4.983388	2.511766	-1.709355
H	5.050260	1.779385	-2.510572
C	5.588078	3.738000	-1.836935
H	6.138229	3.978981	-2.742305
C	5.501511	4.696031	-0.796993
H	5.982410	5.662701	-0.912252
C	4.810618	4.395715	0.352573

H	3.676748	0.233813	-1.221294
H	4.736207	5.123124	1.157703

$I4_{24}$

Cu	0.264813	0.348700	-0.352489
C	2.418850	-0.633435	-2.246806
H	1.844194	-1.532527	-2.015409
H	2.702863	-0.735160	-3.311443
C	1.567040	0.632796	-2.050587
P	0.176246	-2.007195	0.459788
P	-1.433051	1.713962	0.673234
B	3.731082	-0.801441	-1.397981
O	4.986485	-0.847146	-1.955494
O	3.772379	-1.003934	-0.034585
C	5.898357	-1.365906	-0.963401
C	5.154967	-1.053837	0.384298
C	-1.526298	1.004950	5.253883
C	-0.317867	1.346341	3.192189
C	-2.729407	1.242696	3.175242
C	-2.729292	1.038088	4.551964
C	-0.322924	1.168150	4.573172
H	-3.673779	1.287424	2.641112
H	-3.671538	0.913586	5.077251
H	-1.527229	0.851659	6.328927
C	0.549812	-1.924123	2.257605
C	1.330148	-1.798193	4.937821
C	-0.252881	-2.489041	3.248544
C	1.735946	-1.270958	2.619427
C	2.132370	-1.225483	3.951490
C	0.133026	-2.415503	4.586011
H	2.363292	-0.832317	1.846302
H	3.060931	-0.730507	4.221072
H	1.632895	-1.753184	5.979641
C	-1.421469	-2.937800	0.340885
C	-3.881237	-4.195874	-0.141569
C	-1.491464	-4.321643	0.146407
C	-2.627411	-2.231219	0.348853
C	-3.866576	-2.823246	0.096288
C	-2.708789	-4.943528	-0.099035
H	-0.587291	-4.918049	0.167030
H	-2.744141	-6.016295	-0.258407
H	-4.820550	-4.700182	-0.339554
C	-3.142915	1.289392	0.115285
C	-5.705963	0.406085	-0.593659
C	-4.110729	2.195825	-0.318636
C	-3.506172	-0.058287	0.178441
C	-4.779975	-0.528571	-0.131010
C	-5.374698	1.752452	-0.693124
H	-3.887231	3.254632	-0.361760
H	-6.113576	2.466501	-1.042119
H	-6.708027	0.088971	-0.859490
C	-1.475956	3.564399	0.622658
C	-1.571687	6.367328	0.473242
C	-1.670661	4.212063	-0.604716
C	-1.312268	4.344626	1.770220
C	-1.354293	5.735724	1.693313
C	-1.729233	5.599331	-0.678806
H	-1.781373	3.624089	-1.509456
H	-1.152794	3.875752	2.734932
H	-1.222657	6.323764	2.596497
H	-1.890044	6.078836	-1.639585
H	-1.611952	7.450881	0.417517
C	1.330022	-3.349687	-0.104005

C	2.992107	-5.406202	-1.058577
C	2.281740	-3.940122	0.728379
C	1.216022	-3.816837	-1.421039
C	2.040668	-4.828868	-1.897675
C	3.103499	-4.962659	0.255013
H	2.393529	-3.611940	1.755397
H	0.453472	-3.408975	-2.077639
H	1.933057	-5.170886	-2.922305
H	3.833890	-5.411260	0.921942
H	3.636517	-6.199108	-1.425553
H	0.623934	1.471802	2.663611
H	-1.176515	-2.994173	2.981464
H	0.617390	1.142743	5.113806
H	-0.500824	-2.851254	5.352336
O	-2.539642	-0.903229	0.652540
C	-5.131686	-1.975613	0.202665
C	2.434863	1.880776	-2.304626
H	3.431960	1.519657	-2.589729
H	2.092821	2.446075	-3.182790
C	-1.523173	1.391723	2.485144
C	2.595070	2.167846	0.158328
C	2.650550	2.913094	-1.158970
C	4.083179	3.494848	-1.289779
C	1.629328	4.056137	-1.220167
C	4.373055	4.644879	-0.325581
H	4.190883	3.852620	-2.323195
H	4.819296	2.689860	-1.167194
C	1.925738	5.245263	-0.300716
H	1.599438	4.414966	-2.259339
H	0.641681	3.653120	-0.995210
H	5.388256	5.020373	-0.497656
H	4.342504	4.277745	0.708910
H	1.199666	6.041057	-0.500358
H	1.786216	4.935906	0.738699
C	-6.255188	-2.508995	-0.693172
H	-6.520299	-3.533254	-0.420351
H	-7.163952	-1.914813	-0.568938
H	-5.966134	-2.489206	-1.747295
C	-5.600884	-2.012631	1.677257
H	-6.492096	-1.389694	1.806895
H	-5.845161	-3.038948	1.970920
H	-4.821890	-1.640286	2.350461
C	5.513434	0.309182	0.975275
H	4.822351	0.540834	1.791679
H	6.529971	0.306970	1.378812
H	5.439540	1.107218	0.232399
C	5.306758	-2.122180	1.457493
H	4.735010	-1.837103	2.345908
H	4.941944	-3.091589	1.117855
H	6.357539	-2.222116	1.747778
C	6.035621	-2.863425	-1.238385
H	5.073170	-3.374264	-1.138238
H	6.389280	-3.004428	-2.263625
H	6.753283	-3.332663	-0.559225
C	7.246064	-0.678376	-1.122259
H	7.151804	0.409027	-1.087319
H	7.934228	-0.996322	-0.332634
H	7.686742	-0.950188	-2.085837
H	3.118999	1.198759	0.154416
O	2.105639	2.580276	1.197304
C	3.349617	5.769492	-0.493993
H	3.555389	6.581561	0.212854
H	3.450421	6.193489	-1.503523
C	0.237126	0.579630	-2.669085

C	-0.464163	-0.622017	-2.878582
C	-0.501645	1.777914	-3.002789
C	-1.837654	-0.669134	-3.215785
H	0.038327	-1.569292	-2.732314
C	-1.812136	1.755385	-3.386174
H	-0.001835	2.736809	-2.919940
C	-2.547299	0.538241	-3.468987
H	-2.321770	2.688172	-3.620839
C	-2.553533	-1.896689	-3.290194
H	-2.025361	-2.825282	-3.084619
C	-3.892778	-1.915551	-3.596190
H	-4.421424	-2.863919	-3.641315
C	-4.592393	-0.712131	-3.846306
C	-3.924605	0.489413	-3.783602
H	-4.452583	1.422548	-3.966458
H	-5.652495	-0.740394	-4.079940

TS2*anti*-24

Cu	-0.246447	0.825590	0.413654
C	3.118527	1.353286	1.033148
H	3.397223	2.210150	1.659314
H	2.755794	0.593209	1.726346
C	2.035315	1.793462	0.030404
P	-0.230772	-0.887452	2.101891
P	-2.188155	0.786908	-1.014826
B	4.388494	0.813709	0.276499
O	4.939222	-0.428321	0.479097
O	5.026508	1.510762	-0.723794
C	6.112211	-0.538045	-0.353223
C	5.867977	0.576689	-1.431688
C	-5.842359	0.541077	1.822091
C	-3.666454	1.412068	1.245335
C	-4.744391	-0.197826	-0.196499
C	-5.829855	-0.247635	0.672635
C	-4.764047	1.375078	2.102267
H	-4.749837	-0.805159	-1.096850
H	-6.669296	-0.899152	0.448881
H	-6.691134	0.503199	2.498349
C	-1.528487	-0.608872	3.378224
C	-3.401551	-0.050794	5.377096
C	-2.279759	-1.640776	3.946362
C	-1.738626	0.709877	3.801084
C	-2.655901	0.981329	4.812517
C	-3.221076	-1.358891	4.933311
H	-1.198792	1.521092	3.314010
H	-2.804007	2.005480	5.142282
H	-4.128130	0.163684	6.155133
C	-0.460374	-2.648664	1.602316
C	-0.712061	-5.260697	0.617888
C	0.118406	-3.726367	2.281442
C	-1.222363	-2.939510	0.466512
C	-1.356058	-4.226943	-0.057811
C	0.002500	-5.019412	1.788158
H	0.678118	-3.550673	3.193144
H	0.468281	-5.843801	2.317993
H	-0.786139	-6.276833	0.246842
C	-2.326774	-0.710709	-2.080766
C	-2.536512	-3.130325	-3.473620
C	-2.616059	-0.716185	-3.444757
C	-2.140248	-1.944807	-1.453045
C	-2.272067	-3.167872	-2.104451
C	-2.698229	-1.919454	-4.139237
H	-2.780262	0.217778	-3.970365

H	-2.912283	-1.913371	-5.203094
H	-2.636320	-4.055155	-4.030952
C	-2.721017	2.142283	-2.153998
C	-3.405896	4.258037	-3.866537
C	-1.883864	2.503338	-3.217765
C	-3.906800	2.857121	-1.962057
C	-4.244608	3.908350	-2.812714
C	-2.223230	3.548801	-4.069204
H	-0.958573	1.961275	-3.379119
H	-4.574406	2.603395	-1.145884
H	-5.168526	4.453872	-2.646393
H	-1.560695	3.811621	-4.888187
H	-3.670516	5.078538	-4.526459
C	1.322839	-0.944710	3.110843
C	3.798354	-0.739346	4.426976
C	1.480073	-0.092918	4.209757
C	2.428277	-1.693749	2.686673
C	3.652575	-1.595142	3.339631
C	2.706735	0.008346	4.860392
H	0.647921	0.504697	4.565939
H	2.346178	-2.354453	1.830493
H	4.496118	-2.173497	2.978638
H	2.806036	0.677723	5.709621
H	4.755575	-0.653491	4.931940
H	-2.812451	2.046184	1.471857
H	-2.135738	-2.666508	3.620857
H	-4.765709	1.985867	2.999310
H	-3.807080	-2.165902	5.362755
O	-1.877292	-1.889623	-0.110387
C	-2.268625	-4.442627	-1.263860
C	2.252235	3.242095	-0.437759
H	3.193441	3.625456	-0.026886
H	2.331918	3.371265	-1.522759
C	-3.652868	0.628136	0.088682
C	0.657234	2.995113	1.235543
C	1.048992	4.003694	0.143161
C	1.402643	5.371050	0.751463
C	-0.050191	4.164325	-0.911706
C	0.175587	6.133786	1.257880
H	1.906984	5.970124	-0.020793
H	2.130981	5.230749	1.561501
C	-1.268011	4.967127	-0.449995
H	0.395145	4.661076	-1.786776
H	-0.365432	3.172410	-1.243280
H	0.479789	7.106822	1.661225
H	-0.283282	5.575361	2.084442
H	-1.949164	5.114442	-1.296530
H	-1.803139	4.384466	0.306172
C	-1.852832	-5.666887	-2.085527
H	-1.887611	-6.574918	-1.478412
H	-2.544840	-5.826469	-2.916139
H	-0.842995	-5.552158	-2.488745
C	-3.707804	-4.654917	-0.734456
H	-4.403176	-4.782811	-1.570606
H	-3.750275	-5.549042	-0.103666
H	-4.042207	-3.799654	-0.138567
C	5.066942	0.083541	-2.638349
H	4.759752	0.947421	-3.234630
H	5.664395	-0.578667	-3.272029
H	4.163179	-0.447165	-2.326888
C	7.124171	1.296462	-1.899588
H	6.859218	2.054498	-2.642676
H	7.635841	1.795140	-1.073757
H	7.818791	0.591474	-2.367525

C	7.319751	-0.258676	0.541134
H	7.283724	0.755535	0.950049
H	7.310899	-0.961732	1.379190
H	8.261082	-0.383214	-0.002058
C	6.183280	-1.953627	-0.907507
H	5.254381	-2.233579	-1.409119
H	7.009920	-2.048922	-1.618920
H	6.355540	-2.661622	-0.091031
H	1.419777	2.920172	2.032082
O	-0.543138	2.727453	1.560462
C	-0.856503	6.316821	0.142269
H	-1.736266	6.850540	0.520627
H	-0.420117	6.945351	-0.647766
C	1.747966	0.762123	-0.993186
C	1.920958	-0.601899	-0.729166
C	1.309921	1.085828	-2.325319
C	1.634786	-1.614691	-1.673099
H	2.306497	-0.916611	0.231605
C	1.046947	0.127409	-3.264536
H	1.182962	2.127486	-2.597953
C	1.185184	-1.257909	-2.974671
H	0.722810	0.421580	-4.260666
C	1.799633	-2.993854	-1.366056
H	2.133092	-3.273737	-0.369324
C	1.532503	-3.959010	-2.305026
H	1.660424	-5.008125	-2.053594
C	1.082966	-3.599347	-3.597749
C	0.910648	-2.274423	-3.920555
H	0.559586	-1.988859	-4.909069
H	0.869165	-4.373330	-4.328845

TS2$_{syn24}$

Cu	0.398096	0.175168	-0.768594
C	-1.486479	1.727579	0.714329
H	-0.746139	1.102068	1.228332
H	-0.979611	2.662682	0.469932
C	-2.005947	1.109875	-0.616095
P	0.763239	-2.129912	-0.602379
P	2.183380	1.517765	0.132735
B	-2.699916	1.993300	1.677428
O	-2.959949	1.242086	2.799127
O	-3.666901	2.943244	1.447657
C	-4.327316	1.509450	3.182074
C	-4.565282	2.935798	2.578369
C	5.760935	1.058139	-2.761969
C	3.404184	1.358483	-2.342514
C	4.935855	1.081921	-0.491946
C	5.991354	0.953509	-1.392364
C	4.466490	1.263741	-3.235694
H	5.127515	1.021178	0.575323
H	6.996980	0.782061	-1.020559
H	6.588122	0.969432	-3.459916
C	2.477611	-2.496915	-1.176213
C	5.024766	-2.991205	-2.218580
C	3.373085	-3.320492	-0.488959
C	2.867899	-1.923013	-2.389485
C	4.132273	-2.177917	-2.912224
C	4.643684	-3.560228	-1.005718
H	2.181571	-1.266981	-2.919924
H	4.425488	-1.724447	-3.853583
H	6.015728	-3.178593	-2.620870
C	0.754392	-2.762389	1.122061
C	0.886856	-3.511282	3.816749

C	-0.037916	-3.805748	1.601146
C	1.583508	-2.106024	2.033141
C	1.709395	-2.476561	3.369272
C	0.014394	-4.160498	2.946447
H	-0.703155	-4.333865	0.926473
H	-0.615131	-4.963621	3.315622
H	0.933092	-3.830366	4.852214
C	2.807719	1.208334	1.842647
C	3.411049	0.673501	4.528552
C	3.310026	2.214737	2.674315
C	2.695912	-0.075061	2.384651
C	2.957577	-0.370015	3.723785
C	3.610181	1.948168	4.004437
H	3.443918	3.218503	2.286778
H	3.990966	2.740359	4.640641
H	3.630980	0.493397	5.575148
C	1.950927	3.352379	0.153381
C	1.328571	6.088686	0.114330
C	1.097164	3.907415	1.117981
C	2.503422	4.192526	-0.815638
C	2.192048	5.551504	-0.834330
C	0.787955	5.262193	1.098260
H	0.674680	3.278942	1.896434
H	3.171860	3.795634	-1.571897
H	2.628154	6.187994	-1.598317
H	0.120807	5.670922	1.851043
H	1.082231	7.145772	0.093338
C	-0.195843	-3.388793	-1.535771
C	-1.692103	-5.250499	-2.985816
C	-1.342517	-2.990642	-2.221203
C	0.208741	-4.729333	-1.593972
C	-0.538436	-5.655089	-2.312364
C	-2.091161	-3.919288	-2.942663
H	-1.665470	-1.955951	-2.174887
H	1.108543	-5.049278	-1.075653
H	-0.221404	-6.692921	-2.348742
H	-2.993121	-3.599675	-3.454941
H	-2.277273	-5.975717	-3.543278
H	2.384728	1.472569	-2.705893
H	3.085074	-3.778121	0.453034
H	4.279114	1.329927	-4.303294
H	5.334781	-4.195731	-0.459931
O	2.320017	-1.068555	1.524006
C	2.813789	-1.817316	4.194387
C	-2.665374	2.203854	-1.481039
H	-3.665678	1.923393	-1.827864
H	-2.798052	3.134186	-0.919448
C	3.638675	1.291000	-0.962745
C	-1.018335	1.012493	-2.560958
C	-1.697901	2.381773	-2.659044
C	-2.401947	2.564273	-4.014337
C	-0.716909	3.537652	-2.407223
C	-1.429334	2.800070	-5.171541
H	-3.081579	3.425267	-3.933676
H	-3.032821	1.687517	-4.214067
C	0.226549	3.830371	-3.578036
H	-1.311537	4.437998	-2.195077
H	-0.132457	3.327771	-1.506072
H	-1.984978	2.940851	-6.106118
H	-0.800052	1.910183	-5.305169
H	0.815543	4.727800	-3.354860
H	0.927680	2.996447	-3.680969
C	2.535883	-1.905847	5.697667
H	2.457710	-2.949525	6.012912

H	3.358655	-1.470245	6.270149
H	1.609942	-1.389292	5.967859
C	4.137301	-2.555676	3.880325
H	4.964357	-2.097816	4.432692
H	4.061258	-3.608266	4.172043
H	4.374007	-2.511604	2.812465
C	-4.120055	4.064177	3.508740
H	-4.122322	5.005375	2.951582
H	-4.794717	4.169148	4.363340
H	-3.106123	3.893595	3.883401
C	-5.981358	3.189916	2.084519
H	-6.056979	4.204935	1.683286
H	-6.261780	2.490516	1.294410
H	-6.697350	3.095866	2.907338
C	-5.191136	0.430762	2.526131
H	-5.125277	0.474273	1.434728
H	-4.833431	-0.552633	2.842604
H	-6.240695	0.527799	2.819000
C	-4.445634	1.428510	4.696078
H	-3.722297	2.078128	5.193366
H	-5.452364	1.714858	5.017042
H	-4.264313	0.401356	5.026164
H	-1.718814	0.187955	-2.797648
O	0.220599	0.817311	-2.793973
C	-2.758858	-0.150059	-0.463602
C	-2.458756	-1.060225	0.609640
C	-3.732525	-0.570643	-1.365460
C	-3.076850	-2.270006	0.741166
C	-4.383907	-1.827992	-1.263080
H	-4.017619	0.060936	-2.201182
C	-4.053794	-2.707124	-0.196158
H	-2.815166	-2.922529	1.570516
H	-1.717088	-0.779494	1.348783
C	-5.349858	-2.253843	-2.214889
C	-4.675159	-3.976571	-0.118549
C	-5.596302	-4.367983	-1.061396
C	-5.938144	-3.492224	-2.118043
H	-6.670352	-3.804263	-2.857399
H	-5.610934	-1.584079	-3.030872
H	-4.405509	-4.641781	0.698467
H	-6.064487	-5.345675	-0.997683
C	-0.535818	4.010260	-4.891999
H	0.165711	4.167091	-5.719868
H	-1.163043	4.911628	-4.832366

I3'$_{24}$

Cu	-0.970899	0.275383	0.694909
C	2.183153	0.135344	-0.926278
H	1.293648	0.017798	-0.263879
P	-2.231409	1.424779	-0.975870
P	-1.220394	-2.078586	0.294573
B	-0.185156	1.181783	2.367675
O	0.947947	0.750794	3.073793
O	-0.626607	2.377397	2.946766
C	1.134490	1.560939	4.249626
C	0.365738	2.865216	3.869899
C	-1.132304	-3.855397	-3.991225
C	-0.034599	-2.822705	-2.105890
C	-2.387824	-3.341260	-1.992490
C	-2.334993	-3.844372	-3.291415
C	0.019406	-3.346333	-3.392702
H	-3.329672	-3.362941	-1.453323
H	-3.237258	-4.236785	-3.750753

H	-1.092417	-4.254009	-5.000479
C	-2.376652	0.781145	-2.691067
C	-2.452802	-0.211442	-5.304149
C	-3.547318	0.879832	-3.450134
C	-1.250862	0.168467	-3.248744
C	-1.284779	-0.315092	-4.553426
C	-3.585229	0.381674	-4.749553
H	-0.346122	0.054124	-2.657275
H	-0.404010	-0.789243	-4.973851
H	-2.483439	-0.599176	-6.317896
C	-3.981273	1.472018	-0.402702
C	-6.576269	1.333672	0.647752
C	-4.735056	2.634135	-0.228795
C	-4.572401	0.258399	-0.048915
C	-5.859967	0.149827	0.472025
C	-6.021740	2.562422	0.297118
H	-4.310412	3.597625	-0.491437
H	-6.597578	3.471738	0.436015
H	-7.580671	1.303946	1.055964
C	-2.830146	-2.599878	1.029159
C	-5.324305	-3.110687	2.207442
C	-2.973304	-3.623271	1.969070
C	-3.970265	-1.864831	0.698819
C	-5.226487	-2.093150	1.259546
C	-4.210210	-3.871466	2.555018
H	-2.111746	-4.216835	2.256289
H	-4.307853	-4.663402	3.290579
H	-6.277364	-3.322373	2.679980
C	-0.008411	-3.135315	1.189742
C	1.818579	-4.658763	2.660916
C	0.668857	-2.571009	2.275048
C	0.238170	-4.469910	0.845718
C	1.149314	-5.225851	1.576883
C	1.575031	-3.333391	3.009604
H	0.496867	-1.530758	2.540948
H	-0.281629	-4.919486	0.004797
H	1.336381	-6.259206	1.300788
H	2.097923	-2.882902	3.848235
H	2.530702	-5.249912	3.229004
C	-1.841768	3.209362	-1.198132
C	-1.157212	5.912596	-1.410565
C	-2.049309	3.897471	-2.397223
C	-1.293693	3.887519	-0.101993
C	-0.956435	5.233948	-0.210137
C	-1.706009	5.243066	-2.502507
H	-2.468996	3.383075	-3.256311
H	-1.118980	3.359250	0.833497
H	-0.527645	5.750779	0.643412
H	-1.864698	5.767286	-3.440065
H	-0.885546	6.960495	-1.496024
H	0.865391	-2.396296	-1.668605
H	-4.432213	1.345634	-3.025820
H	0.961131	-3.342747	-3.933585
H	-4.500015	0.458199	-5.329508
O	-3.814666	-0.871972	-0.237806
C	-6.397309	-1.254783	0.745594
C	-1.238657	-2.826646	-1.389672
C	4.273583	0.180064	1.137289
C	3.460196	1.395440	0.745280
C	1.227721	3.874019	3.105865
H	0.580754	4.663311	2.710940
H	1.979140	4.339457	3.751241
H	1.736235	3.401899	2.259891
C	-0.328886	3.558742	5.033569

H	0.399603	3.868638	5.790493
H	-0.846055	4.454307	4.675603
H	-1.067972	2.908533	5.506246
C	2.625187	1.744177	4.500383
H	2.792664	2.415891	5.349247
H	3.083983	0.779138	4.736288
H	3.136686	2.153729	3.626928
C	0.500177	0.802772	5.417490
H	0.961284	-0.187176	5.487241
H	0.652333	1.319951	6.369900
H	-0.573550	0.664247	5.260336
C	-7.570781	-1.241845	1.727457
H	-7.952873	-2.254292	1.882663
H	-7.283438	-0.824407	2.697255
H	-8.400253	-0.653458	1.326530
C	-6.872100	-1.859562	-0.597406
H	-7.226804	-2.884052	-0.444904
H	-7.692747	-1.263367	-1.009360
H	-6.063689	-1.882498	-1.334539
O	2.484521	-0.744054	-1.705736
C	3.750943	-0.736599	1.960523
H	2.748609	-0.610347	2.359352
H	4.317743	-1.610700	2.270955
H	2.590366	1.439481	1.407574
H	4.034102	2.317343	0.901478
C	2.942836	1.431806	-0.723729
C	1.937257	2.602806	-0.813869
C	4.070754	1.595177	-1.754651
C	1.456666	2.894971	-2.235098
H	2.430397	3.497153	-0.409302
H	1.081270	2.394957	-0.158392
C	3.563583	1.891913	-3.169460
H	4.712532	2.421945	-1.422318
H	4.692675	0.696844	-1.767734
C	2.629339	3.100747	-3.193263
H	0.810929	3.778422	-2.221743
H	0.835882	2.063109	-2.595581
H	4.420961	2.056963	-3.831618
H	3.030826	1.014026	-3.553392
H	2.260425	3.279539	-4.209506
H	3.186986	3.999380	-2.893343
C	5.648686	0.016993	0.592559
C	6.064091	-1.192664	0.080401
C	6.560909	1.110575	0.590553
C	7.373417	-1.369723	-0.437336
C	7.832179	0.970004	0.102050
H	6.245519	2.067870	0.994528
C	8.276926	-0.270607	-0.428568
H	8.520165	1.811289	0.115408
H	5.369826	-2.028141	0.044634
C	7.807296	-2.612079	-0.973611
C	9.078061	-2.753702	-1.470982
H	9.400406	-3.707698	-1.877252
C	9.977382	-1.659781	-1.459608
H	10.979986	-1.785883	-1.856965
C	9.585334	-0.447073	-0.951065
H	10.271362	0.395911	-0.941206
H	7.113853	-3.448849	-0.981934

TS1'$_{24}$

Cu	-0.637968	0.328836	-0.799563
C	0.939413	1.742981	-1.355326
P	-2.656221	1.542742	-0.390499

P	-0.931050	-1.968624	-0.841130
B	0.663803	0.927036	0.739255
O	1.402013	-0.034518	1.412873
O	0.316346	1.948852	1.598661
C	1.321369	0.207995	2.836055
C	0.847652	1.709396	2.918534
C	-4.158903	-3.392106	-3.836770
C	-2.503601	-1.790455	-3.122641
C	-2.940888	-3.752710	-1.784583
C	-3.902528	-4.161862	-2.703002
C	-3.455902	-2.209497	-4.048220
H	-2.740317	-4.360507	-0.907032
H	-4.450461	-5.084123	-2.534992
H	-4.909406	-3.713649	-4.552584
C	-4.030568	1.072602	-1.520179
C	-5.988066	0.329443	-3.378686
C	-5.198596	0.436730	-1.097961
C	-3.848337	1.327592	-2.886385
C	-4.828354	0.974827	-3.806482
C	-6.166900	0.056529	-2.026146
H	-2.936290	1.809872	-3.229159
H	-4.679285	1.189730	-4.860365
H	-6.747472	0.039222	-4.098326
C	-3.339452	1.297907	1.300369
C	-4.147772	0.764791	3.930780
C	-3.724120	2.338717	2.147884
C	-3.384084	-0.001571	1.809964
C	-3.796610	-0.304800	3.107189
C	-4.114146	2.073298	3.456095
H	-3.701338	3.362447	1.790123
H	-4.399017	2.891232	4.109833
H	-4.465686	0.581022	4.951076
C	-1.414443	-2.732110	0.765450
C	-2.146786	-3.653066	3.309647
C	-0.821333	-3.876375	1.304403
C	-2.409517	-2.105074	1.518450
C	-2.792001	-2.531934	2.790176
C	-1.181134	-4.328665	2.569091
H	-0.060975	-4.406886	0.742500
H	-0.704587	-5.212088	2.981318
H	-2.405175	-4.017682	4.297597
C	0.554409	-2.939344	-1.328173
C	2.922959	-4.230615	-2.074766
C	1.678604	-2.902389	-0.491446
C	0.631935	-3.624285	-2.542245
C	1.814626	-4.262448	-2.914549
C	2.850698	-3.552362	-0.858834
H	1.637465	-2.343778	0.440768
H	-0.226215	-3.661372	-3.206046
H	1.864122	-4.786759	-3.864064
H	3.716014	-3.511039	-0.204430
H	3.843801	-4.725855	-2.367044
C	-2.611216	3.381491	-0.531346
C	-2.417364	6.172627	-0.679765
C	-3.623489	4.130679	-1.139027
C	-1.508032	4.047652	0.017622
C	-1.413825	5.434306	-0.056276
C	-3.523284	5.518161	-1.216155
H	-4.494744	3.636988	-1.557102
H	-0.734953	3.479091	0.526214
H	-0.551461	5.936432	0.372445
H	-4.314467	6.086876	-1.695429
H	-2.339988	7.253847	-0.744445
H	-1.967417	-0.857470	-3.274701

H	-5.365986	0.239482	-0.043661
H	-3.657533	-1.603057	-4.925263
H	-7.067534	-0.445392	-1.685601
O	-3.013829	-1.009905	0.953522
C	-3.916418	-1.777273	3.496487
C	-2.236867	-2.561401	-1.988708
C	1.977980	2.711390	3.147144
H	1.584857	3.724136	3.018970
H	2.382444	2.627218	4.160292
H	2.794985	2.574840	2.436257
C	-0.270897	1.969914	3.922090
H	0.062903	1.754927	4.942346
H	-0.561653	3.023609	3.874652
H	-1.157497	1.369607	3.707777
C	2.688156	-0.067031	3.447018
H	2.684838	0.151572	4.519662
H	2.935755	-1.125645	3.319041
H	3.471464	0.525827	2.970293
C	0.297055	-0.782211	3.387132
H	0.606472	-1.800152	3.133223
H	0.208327	-0.708848	4.475268
H	-0.687196	-0.612954	2.946722
C	-3.870736	-1.972451	5.014210
H	-3.986434	-3.028204	5.271920
H	-2.929254	-1.610309	5.438935
H	-4.697141	-1.444067	5.496222
C	-5.266775	-2.307397	2.958726
H	-5.374851	-3.370969	3.194974
H	-6.096623	-1.760638	3.418131
H	-5.337415	-2.190185	1.873003
O	0.198527	1.374933	-2.369394
H	0.696379	2.722992	-0.920651
C	2.679517	0.001588	-1.688808
H	2.326649	-0.474582	-0.772266
H	1.998836	-0.323054	-2.480866
C	4.066296	-0.501909	-2.005443
C	4.355905	-0.983267	-3.221101
H	5.323202	-1.419067	-3.456576
H	3.613400	-0.974914	-4.014482
C	5.095075	-0.528090	-0.926863
C	4.729322	-0.810261	0.422810
C	6.422951	-0.284301	-1.207396
C	5.673385	-0.879182	1.412345
H	3.684260	-0.957962	0.676242
C	7.423454	-0.342652	-0.203152
C	7.047410	-0.653124	1.133010
H	5.376297	-1.101364	2.434124
C	2.467677	1.520250	-1.518060
C	3.289169	2.113704	-0.358480
C	2.877519	2.265097	-2.811442
C	3.135729	3.631032	-0.209453
H	4.347877	1.904727	-0.552719
H	3.051962	1.600006	0.576769
C	2.726713	3.786112	-2.703160
H	3.928077	2.024862	-3.024909
H	2.279022	1.880767	-3.642849
C	3.508122	4.346139	-1.511057
H	3.777812	3.981534	0.607519
H	2.108352	3.885774	0.078377
H	3.072461	4.255926	-3.631454
H	1.665506	4.046231	-2.599463
H	3.340332	5.425451	-1.417244
H	4.583096	4.206517	-1.694057
C	8.792762	-0.094386	-0.491200

C	9.739385	-0.159374	0.499839
C	9.363867	-0.472147	1.829040
H	10.123434	-0.519832	2.603535
C	8.048458	-0.712165	2.137883
H	7.754426	-0.950063	3.156896
H	6.721459	-0.020204	-2.218582
H	9.077625	0.145830	-1.512193
H	10.783338	0.030010	0.268753

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Cu	-0.982609	0.207275	-0.977306
C	1.749874	1.125719	-1.266664
P	-2.525002	1.793786	-0.310049
P	-1.861358	-1.995963	-0.827134
B	1.765200	1.006233	0.310289
O	2.050695	-0.132312	1.031871
O	1.380522	2.043815	1.131535
C	1.587051	0.073704	2.382791
C	1.579768	1.636466	2.501085
C	-5.922979	-2.731352	-2.934708
C	-3.720522	-1.750365	-2.870487
C	-4.500386	-3.081281	-1.015464
C	-5.710969	-3.283854	-1.674435
C	-4.923958	-1.966560	-3.533496
H	-4.342416	-3.522530	-0.035745
H	-6.487510	-3.877875	-1.201856
H	-6.866723	-2.890855	-3.447467
C	-4.059399	1.566950	-1.297282
C	-6.288544	1.207156	-2.946671
C	-5.287697	1.197747	-0.748465
C	-3.952507	1.743458	-2.683270
C	-5.064185	1.578469	-3.500754
C	-6.395480	1.010295	-1.573519
H	-2.996802	2.019766	-3.122987
H	-4.972013	1.728525	-4.572141
H	-7.154640	1.065995	-3.585971
C	-3.056473	1.756968	1.452459
C	-3.536524	1.514933	4.203518
C	-3.087014	2.890642	2.269032
C	-3.305368	0.520280	2.052747
C	-3.544750	0.363215	3.417581
C	-3.322622	2.767656	3.633895
H	-2.897847	3.869340	1.841541
H	-3.331672	3.653420	4.260548
H	-3.709481	1.442966	5.271682
C	-2.108111	-2.581021	0.899077
C	-2.424475	-3.186297	3.617793
C	-1.566661	-3.753082	1.429762
C	-2.806780	-1.740836	1.767564
C	-2.996416	-2.015487	3.120249
C	-1.717645	-4.046717	2.781737
H	-1.006757	-4.427603	0.790839
H	-1.282662	-4.954455	3.187149
H	-2.531606	-3.439366	4.666902
C	-0.764198	-3.272190	-1.558798
C	1.045371	-5.125475	-2.593080
C	0.563980	-2.897577	-1.792047
C	-1.187973	-4.570790	-1.864404
C	-0.283754	-5.493791	-2.380366
C	1.466209	-3.830260	-2.303095
H	0.869603	-1.864465	-1.607856
H	-2.222620	-4.859479	-1.698443
H	-0.614322	-6.500760	-2.616969

H	2.498125	-3.538529	-2.480557
H	1.749173	-5.849046	-2.994036
C	-2.124689	3.569323	-0.571105
C	-1.388781	6.244114	-0.910472
C	-3.082476	4.522897	-0.932191
C	-0.798766	3.966861	-0.372586
C	-0.434199	5.300586	-0.538704
C	-2.712911	5.853996	-1.104643
H	-4.116832	4.228274	-1.082316
H	-0.053288	3.237766	-0.068544
H	0.598513	5.597943	-0.382638
H	-3.460730	6.587400	-1.390594
H	-1.103198	7.282600	-1.048958
H	-2.952921	-1.133760	-3.331970
H	-5.391939	1.061332	0.323416
H	-5.087155	-1.523336	-4.510790
H	-7.345089	0.716169	-1.137123
O	-3.305120	-0.578151	1.229147
C	-3.854431	-1.043438	3.929022
C	-3.495148	-2.313848	-1.610108
C	2.924308	2.213718	2.941370
H	2.908795	3.298182	2.800286
H	3.124329	2.006393	3.996679
H	3.745906	1.805781	2.344024
C	0.449204	2.203793	3.345862
H	0.523346	1.851535	4.379744
H	0.504870	3.296581	3.352864
H	-0.526370	1.918178	2.948013
C	2.530576	-0.637178	3.339982
H	2.244069	-0.442800	4.378555
H	2.481693	-1.717113	3.170593
H	3.564125	-0.315160	3.195974
C	0.189162	-0.533026	2.463205
H	0.241749	-1.592303	2.199594
H	-0.237755	-0.446013	3.466121
H	-0.486403	-0.042169	1.753962
C	-3.611377	-1.173989	5.434162
H	-3.864584	-2.180062	5.778509
H	-2.569183	-0.966858	5.696390
H	-4.253860	-0.485222	5.988843
C	-5.341527	-1.349846	3.630988
H	-5.588867	-2.365737	3.955495
H	-5.985945	-0.645069	4.166352
H	-5.560237	-1.270200	2.561761
O	0.771310	0.251982	-1.767835
H	1.481318	2.175693	-1.491822
C	3.406976	-0.660168	-1.830086
H	3.008152	-1.025776	-0.881462
H	2.794771	-1.127484	-2.604567
C	4.831123	-1.138612	-1.986407
C	5.253379	-1.673836	-3.140428
H	6.254942	-2.077901	-3.262332
H	4.589388	-1.739187	-3.998507
C	5.752172	-1.047234	-0.814219
C	5.260010	-1.201199	0.515323
C	7.097914	-0.797418	-0.986554
C	6.100209	-1.131499	1.595103
H	4.200821	-1.362583	0.684265
C	7.992618	-0.717845	0.110870
C	7.489524	-0.891160	1.430168
H	5.705427	-1.260369	2.599925
C	3.144647	0.871693	-1.913683
C	4.224681	1.695537	-1.181788
C	3.131041	1.286985	-3.398732

C	4.055721	3.208295	-1.354937
H	5.211110	1.425082	-1.579533
H	4.249229	1.432174	-0.115958
C	3.009934	2.799182	-3.620862
H	4.058149	0.930936	-3.871899
H	2.298395	0.770828	-3.890532
C	4.069382	3.581007	-2.839542
H	4.865461	3.728069	-0.829007
H	3.118583	3.542999	-0.893087
H	3.092637	3.020792	-4.691742
H	2.012994	3.139301	-3.312320
H	3.918307	4.659453	-2.967564
H	5.062429	3.348903	-3.250743
C	9.379362	-0.460578	-0.066936
C	10.221696	-0.386582	1.013286
C	9.719684	-0.562819	2.326089
H	10.397808	-0.501499	3.171946
C	8.384979	-0.808004	2.529010
H	7.994142	-0.941896	3.534384
H	7.492376	-0.628293	-1.985130
H	9.761589	-0.325666	-1.075409
H	11.279771	-0.191695	0.866172

SUBSTRATE 28

C	-0.936534	1.314348	-1.567031
H	-1.195538	0.438498	-2.156901
H	-0.058977	1.875596	-1.879333
C	-1.661063	1.684686	-0.508197
C	-2.857125	0.862825	-0.078320
H	-2.831415	-0.077141	-0.641657
O	-5.793281	-0.234530	-1.039687
C	-5.207455	0.322572	-0.138674
H	-5.297074	-0.056020	0.904789
C	-1.300291	2.908683	0.293419
H	-0.282626	3.240487	0.069737
H	-1.975046	3.742524	0.068417
H	-1.375170	2.716438	1.369394
H	-2.753470	0.600329	0.983458
C	-4.266491	1.509682	-0.283789
C	-4.618373	2.512418	0.834546
C	-4.395385	2.157323	-1.668938
C	-5.983028	3.169747	0.607899
H	-3.853611	3.293001	0.876143
H	-4.595132	1.998637	1.804258
C	-5.742654	2.855174	-1.882190
H	-3.590838	2.894674	-1.777029
H	-4.232688	1.397782	-2.441220
C	-6.043952	3.851757	-0.760633
H	-6.179572	3.892900	1.406848
H	-6.776611	2.411253	0.669546
H	-5.737403	3.365394	-2.851779
H	-6.539554	2.103952	-1.923902
H	-7.027989	4.308465	-0.913780
H	-5.306481	4.666317	-0.788061

$I3_{28}$

Cu	-0.010696	0.047788	-0.862025
C	-2.198075	0.524761	-2.389890
H	-2.142195	-0.479926	-2.798418
H	-1.720743	1.317354	-2.960015
C	-2.903003	0.789628	-1.276229
P	0.966123	2.187434	-0.442504

P	-0.398241	-1.039076	1.217301
B	1.115209	-1.246849	-2.009312
O	0.772518	-2.440027	-2.666186
O	2.509509	-1.158124	-1.961438
C	1.944767	-3.268030	-2.781446
C	3.098480	-2.217802	-2.727838
C	-1.542130	1.278740	5.062529
C	-1.554451	1.022972	2.666075
C	-0.451959	-0.619974	4.045627
C	-0.805149	0.101577	5.182387
C	-1.918476	1.738304	3.803230
H	0.122850	-1.536487	4.144749
H	-0.503113	-0.254217	6.162857
H	-1.813961	1.841916	5.950275
C	0.625231	3.248578	1.030857
C	-0.130359	4.716262	3.306325
C	1.401530	3.214548	2.191927
C	-0.536121	4.027322	1.027583
C	-0.906408	4.764135	2.149775
C	1.022589	3.937367	3.321944
H	-1.162274	4.085636	0.143347
H	-1.806047	5.372094	2.120216
H	-0.423188	5.281068	4.186191
C	2.774296	1.833160	-0.319754
C	5.446105	0.999261	-0.176936
C	3.754243	2.473131	-1.077771
C	3.180703	0.785134	0.506447
C	4.499965	0.352569	0.617241
C	5.078760	2.050419	-1.013940
H	3.478931	3.291521	-1.735613
H	5.832754	2.545759	-1.617435
H	6.486131	0.693453	-0.139916
C	1.177983	-1.892209	1.640269
C	3.702542	-3.039120	2.024516
C	1.293971	-3.240548	1.979315
C	2.351798	-1.145406	1.532426
C	3.624683	-1.680689	1.714439
C	2.550608	-3.809717	2.166438
H	0.401472	-3.851804	2.071936
H	2.634030	-4.861720	2.419493
H	4.671041	-3.505022	2.171309
C	-1.572736	-2.453666	1.150373
C	-3.322670	-4.619505	0.867306
C	-1.566735	-3.221706	-0.023797
C	-2.462333	-2.779689	2.176317
C	-3.337474	-3.856456	2.031614
C	-2.434528	-4.300418	-0.159248
H	-0.886720	-2.964451	-0.834341
H	-2.484400	-2.190010	3.087678
H	-4.030035	-4.097793	2.832525
H	-2.425465	-4.886660	-1.073146
H	-4.004794	-5.456684	0.756233
C	0.909655	3.370475	-1.853682
C	0.842711	5.007772	-4.126146
C	1.055578	4.756785	-1.733169
C	0.738253	2.814204	-3.127676
C	0.708127	3.627305	-4.257026
C	1.017444	5.569755	-2.863689
H	1.203322	5.207232	-0.757141
H	0.633460	1.736489	-3.227701
H	0.576111	3.181279	-5.238077
H	1.130962	6.644402	-2.757026
H	0.813907	5.644160	-5.005524
H	-1.813000	1.397194	1.679189

H	2.311645	2.627585	2.228498
H	-2.477504	2.662921	3.703231
H	1.637871	3.891017	4.215263
O	2.196883	0.184639	1.250025
C	4.818187	-0.727761	1.651649
C	-3.604239	-0.318240	-0.534388
H	-3.170299	-1.282171	-0.856295
H	-3.381299	-0.220456	0.539204
C	-0.831135	-0.167113	2.777423
O	-5.860062	-2.679145	-1.010076
C	-5.495793	-1.777832	-0.271168
H	-5.258705	-2.005364	0.803394
C	3.454581	-1.640956	-4.099970
H	4.114437	-0.779325	-3.959077
H	3.971697	-2.371697	-4.730269
H	2.558155	-1.297170	-4.624795
C	4.362873	-2.688049	-2.020031
H	4.803067	-3.551349	-2.531202
H	5.101660	-1.880126	-2.017713
H	4.157725	-2.959461	-0.982036
C	1.867571	-4.073703	-4.070667
H	2.785650	-4.651802	-4.222842
H	1.030693	-4.777312	-4.018834
H	1.713885	-3.429782	-4.939400
C	1.944978	-4.208999	-1.574518
H	1.009926	-4.777885	-1.563035
H	2.777443	-4.919211	-1.608846
H	2.006532	-3.642277	-0.641758
C	6.125645	-1.460544	1.340177
H	6.342033	-2.205864	2.110050
H	6.088126	-1.962294	0.369216
H	6.967180	-0.762652	1.339567
C	4.948299	-0.039825	3.032059
H	5.148748	-0.785167	3.808826
H	5.771641	0.681874	3.018442
H	4.030044	0.492408	3.299752
C	-3.105215	2.201841	-0.796193
H	-4.090714	2.559987	-1.120112
H	-3.084078	2.279187	0.296580
H	-2.348777	2.879225	-1.198947
C	-5.163140	-0.346637	-0.674096
C	-5.822517	0.606566	0.349486
C	-5.648400	-0.050228	-2.102785
C	-7.349949	0.637541	0.218298
H	-5.430868	1.617304	0.206296
H	-5.528392	0.299645	1.358375
C	-7.177717	0.021432	-2.222844
H	-5.224023	0.903444	-2.423433
H	-5.256089	-0.813951	-2.777305
C	-7.770015	1.006740	-1.209207
H	-7.768550	1.342024	0.938910
H	-7.761179	-0.347494	0.469826
H	-7.449066	0.315959	-3.238830
H	-7.602868	-0.970695	-2.058558
H	-8.858328	1.032518	-1.294930
H	-7.409890	2.017138	-1.433831

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Cu	-0.450538	0.461490	-0.148175
C	-1.894823	0.899264	-1.561764
H	-2.288687	0.029385	-2.086990
H	-1.802969	1.769393	-2.216512
C	-2.436362	1.147235	-0.226814

P	1.148504	1.817056	0.816904
P	-0.219633	-1.772038	0.537145
B	0.029217	0.414098	-2.181442
O	0.045522	-0.719069	-2.985810
O	0.775991	1.424658	-2.771758
C	1.080743	-0.549892	-3.976404
C	1.157110	1.005250	-4.098603
C	-0.217318	-2.390699	5.126003
C	-0.845059	-1.136156	3.164588
C	0.473107	-3.145889	2.939969
C	0.456439	-3.308786	4.322022
C	-0.870879	-1.306737	4.546035
H	0.995581	-3.867569	2.318528
H	0.968587	-4.154044	4.771875
H	-0.228679	-2.519072	6.204226
C	1.172494	1.754252	2.655937
C	1.016373	1.650760	5.447802
C	2.254803	1.292659	3.404716
C	0.005884	2.158832	3.318397
C	-0.065840	2.123667	4.705426
C	2.170918	1.230703	4.795392
H	-0.848981	2.504138	2.741488
H	-0.971573	2.450710	5.207203
H	0.956395	1.607795	6.531075
C	2.891921	1.483271	0.314803
C	5.422319	0.793734	-0.682332
C	3.760935	2.468692	-0.159877
C	3.342006	0.162178	0.290418
C	4.595398	-0.215901	-0.191999
C	5.011832	2.124280	-0.660901
H	3.450929	3.507995	-0.159937
H	5.672302	2.898261	-1.038301
H	6.401687	0.547873	-1.077981
C	1.287739	-2.654862	-0.043205
C	3.683616	-3.734962	-1.017772
C	1.294714	-3.894431	-0.685618
C	2.510130	-2.002625	0.116222
C	3.719039	-2.505695	-0.360439
C	2.485074	-4.427490	-1.171160
H	0.365742	-4.437818	-0.821987
H	2.478781	-5.388319	-1.675677
H	4.597524	-4.165849	-1.411536
C	-1.577599	-2.868816	-0.049419
C	-3.741693	-4.335896	-1.049129
C	-1.856004	-2.874280	-1.424049
C	-2.394504	-3.599335	0.816077
C	-3.474061	-4.326623	0.316733
C	-2.927451	-3.610230	-1.919042
H	-1.231835	-2.296159	-2.101841
H	-2.200118	-3.597260	1.883935
H	-4.107480	-4.883647	1.000253
H	-3.132057	-3.610896	-2.985671
H	-4.584158	-4.901942	-1.435008
C	0.998996	3.619313	0.466193
C	0.764380	6.325901	-0.204302
C	1.286911	4.608719	1.411144
C	0.599687	3.997556	-0.821555
C	0.487961	5.344771	-1.154067
C	1.165074	5.955539	1.077325
H	1.607087	4.332990	2.411056
H	0.395383	3.233660	-1.566932
H	0.178842	5.627021	-2.156151
H	1.386466	6.715573	1.820513
H	0.669205	7.376480	-0.462021

H	-1.332559	-0.278960	2.706983
H	3.171108	0.982495	2.912022
H	-1.389071	-0.583943	5.168116
H	3.016092	0.859784	5.367240
O	2.484249	-0.795520	0.773229
C	4.983260	-1.691249	-0.092518
C	-3.432783	0.138984	0.319810
H	-3.104646	-0.855114	-0.000233
H	-3.408113	0.122026	1.418589
C	-0.177263	-2.055973	2.352424
C	-5.469692	-1.134068	0.169651
H	-5.194571	-1.859762	-0.629570
O	-6.063628	-1.514934	1.156163
C	6.112158	-2.052643	-1.060585
H	7.012743	-1.475181	-0.835830
H	6.384337	-3.106440	-0.958731
H	5.827313	-1.865059	-2.100622
C	5.448877	-1.974665	1.355227
H	5.705307	-3.033093	1.467671
H	6.333038	-1.373825	1.591761
H	4.666294	-1.734253	2.081073
C	0.123723	1.582262	-5.065603
H	0.088762	2.668691	-4.941428
H	0.378133	1.364057	-6.107096
H	-0.875059	1.184269	-4.860650
C	2.540963	1.556222	-4.406789
H	2.498009	2.647613	-4.474011
H	3.257936	1.294374	-3.625517
H	2.905968	1.171265	-5.364730
C	2.357306	-1.165566	-3.401923
H	2.684207	-0.629686	-2.506279
H	2.155498	-2.202848	-3.120523
H	3.173527	-1.156154	-4.130860
C	0.671010	-1.276048	-5.247980
H	-0.318429	-0.963847	-5.589091
H	1.393236	-1.086981	-6.048913
H	0.643787	-2.354539	-5.064530
C	-2.650106	2.601349	0.152089
H	-1.777952	3.212757	-0.099136
H	-3.513012	3.060760	-0.360764
H	-2.826720	2.716186	1.229264
C	-4.954142	0.270211	-0.074209
C	-5.701799	1.280282	0.809702
C	-5.122038	0.596038	-1.566836
C	-7.159791	1.481735	0.383566
H	-5.182137	2.242122	0.766732
H	-5.659351	0.938185	1.849156
C	-6.588363	0.781403	-1.967166
H	-4.566139	1.514020	-1.788399
H	-4.659946	-0.198219	-2.167921
C	-7.266580	1.843402	-1.099505
H	-7.619272	2.262997	0.999878
H	-7.723835	0.559617	0.570610
H	-6.651315	1.054013	-3.026756
H	-7.126753	-0.171176	-1.856038
H	-8.317470	1.957794	-1.388865
H	-6.780015	2.813615	-1.273852

$I4_{28}$

Cu	-0.616055	-0.428346	0.624975
C	-0.233511	-1.961967	3.164851
H	-0.247526	-1.031099	3.751962
H	-0.549852	-2.754079	3.875097

C	-1.206984	-1.884553	1.960206
P	-0.301633	-0.876996	-1.759987
P	-0.069874	1.907328	0.872740
B	1.257734	-2.239763	2.770389
O	1.964786	-1.518045	1.831945
O	2.021076	-3.239524	3.330399
C	3.195455	-2.227247	1.574305
C	3.382003	-3.049659	2.892242
C	-1.831176	5.123043	-2.003934
C	-2.015041	3.685450	-0.073335
C	0.017944	3.706267	-1.362393
C	-0.541348	4.648743	-2.222388
C	-2.565566	4.637887	-0.924455
H	1.029739	3.367865	-1.549988
H	0.040691	5.015357	-3.062579
H	-2.262923	5.861544	-2.672746
C	-1.086009	0.391067	-2.835505
C	-2.405627	2.290543	-4.402843
C	-2.254704	1.000884	-2.368650
C	-0.581905	0.740835	-4.091536
C	-1.234934	1.694124	-4.867397
C	-2.917523	1.937561	-3.157171
H	0.324101	0.272098	-4.464781
H	-0.831296	1.968200	-5.837602
H	-2.914372	3.034168	-5.009091
C	1.430172	-0.942203	-2.391522
C	4.171624	-0.942047	-2.985496
C	1.982549	-1.950364	-3.184545
C	2.282981	0.077693	-1.963621
C	3.649720	0.110050	-2.232941
C	3.344619	-1.952395	-3.469797
H	1.354167	-2.748819	-3.563102
H	3.765723	-2.748570	-4.075076
H	5.230688	-0.969815	-3.217075
C	1.759339	2.173010	0.831008
C	4.550355	2.378495	0.610713
C	2.510323	2.753635	1.854795
C	2.456852	1.687092	-0.275709
C	3.836386	1.795346	-0.435357
C	3.895067	2.844693	1.747324
H	2.016598	3.127474	2.745062
H	4.467730	3.292459	2.553133
H	5.628539	2.474284	0.545251
C	-0.539706	2.619923	2.504935
C	-1.278240	3.581485	5.027781
C	-1.006671	1.747036	3.488342
C	-0.450979	3.987929	2.795766
C	-0.816253	4.463941	4.050241
C	-1.374029	2.222414	4.746148
H	-1.091746	0.690447	3.256308
H	-0.096783	4.681351	2.038419
H	-0.742766	5.525464	4.266396
H	-1.738971	1.529862	5.498775
H	-1.566106	3.957084	6.005135
C	-1.045559	-2.447865	-2.380454
C	-2.276208	-4.875385	-3.062162
C	-2.243893	-2.459943	-3.100523
C	-0.475312	-3.670401	-2.001342
C	-1.078654	-4.873970	-2.349001
C	-2.857170	-3.666501	-3.433395
H	-2.711660	-1.527193	-3.399065
H	0.442632	-3.682729	-1.420387
H	-0.618874	-5.811149	-2.050340
H	-3.790426	-3.656793	-3.988458

H	-2.754023	-5.814438	-3.324308
H	-2.610980	3.293577	0.743535
H	-2.645141	0.757602	-1.382836
H	-3.575517	4.994988	-0.745709
H	-3.822409	2.406926	-2.784320
O	1.698450	1.090114	-1.251725
C	4.448808	1.322929	-1.754710
C	-2.632103	-1.764958	2.540984
H	-2.971401	-2.755948	2.904004
H	-2.597191	-1.135110	3.444254
C	-0.711568	3.214080	-0.276314
C	-3.594181	0.304230	1.644497
H	-3.521734	0.752170	2.659458
O	-3.555104	1.031782	0.672105
C	-3.782843	-1.193950	1.664564
C	-3.854344	-1.796733	0.254898
C	-5.125981	-1.430228	2.405244
C	-5.092946	-1.384568	-0.546949
H	-3.855200	-2.889173	0.359779
H	-2.944721	-1.534840	-0.295091
C	-6.349528	-0.983507	1.600941
H	-5.201378	-2.506380	2.607803
H	-5.102614	-0.929222	3.381962
H	-5.098099	-1.929161	-1.498616
H	-5.034339	-0.318059	-0.788769
H	-7.261065	-1.214092	2.163749
H	-6.331814	0.106967	1.467096
C	5.939161	1.003671	-1.609875
H	6.361104	0.686051	-2.566742
H	6.496286	1.893326	-1.304983
H	6.113111	0.213331	-0.872977
C	4.271843	2.451667	-2.797808
H	4.795664	3.355280	-2.469749
H	4.681751	2.140085	-3.764055
H	3.215364	2.699969	-2.940652
C	4.099598	-2.261559	3.989165
H	4.013468	-2.807148	4.933188
H	5.161916	-2.132976	3.762458
H	3.650927	-1.272883	4.125482
C	4.041553	-4.407686	2.705615
H	4.137451	-4.909856	3.672923
H	3.456867	-5.051636	2.045399
H	5.044922	-4.291546	2.283174
C	2.957776	-3.101803	0.342966
H	2.191901	-3.860169	0.532761
H	2.613664	-2.463517	-0.475039
H	3.875289	-3.605144	0.023822
C	4.306079	-1.229888	1.289691
H	4.350701	-0.445029	2.047417
H	5.274679	-1.739504	1.248544
H	4.131964	-0.758646	0.320759
C	-6.382931	-1.660092	0.228421
H	-7.253318	-1.318588	-0.343416
H	-6.498949	-2.744211	0.368218
C	-1.084070	-3.247505	1.257807
H	-0.064599	-3.419570	0.888532
H	-1.316489	-4.084599	1.949639
H	-1.743757	-3.357463	0.394828

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Cu	0.090056	-0.032369	-0.577883
C	2.792026	0.451348	1.325897
H	2.291913	0.713803	0.369140

P	-1.024476	-1.872870	0.428926
P	-0.877153	1.968505	0.267773
B	1.334881	-0.131403	-2.210023
O	2.605347	0.467082	-2.246256
O	1.145042	-0.827154	-3.408635
C	3.179902	0.319079	-3.557193
C	2.392459	-0.904662	-4.123749
C	-2.626909	2.237356	4.553405
C	-0.852665	1.651776	3.024047
C	-2.882185	2.658523	2.190021
C	-3.388325	2.708871	3.486678
C	-1.356959	1.714807	4.319809
H	-3.483797	3.032031	1.366584
H	-4.378704	3.118617	3.661765
H	-3.023532	2.274486	5.563674
C	-1.375431	-1.890024	2.233082
C	-1.774752	-1.810006	5.002227
C	-2.666590	-1.942246	2.761216
C	-0.284801	-1.783909	3.106758
C	-0.481999	-1.760549	4.482199
C	-2.864017	-1.892458	4.140067
H	0.724627	-1.711889	2.711084
H	0.373173	-1.686646	5.147254
H	-1.931476	-1.777732	6.076139
C	-2.661226	-2.149409	-0.375227
C	-5.024921	-2.352713	-1.870998
C	-3.095099	-3.390115	-0.850002
C	-3.467658	-1.040457	-0.640305
C	-4.639546	-1.100749	-1.394487
C	-4.269144	-3.488796	-1.588535
H	-2.500351	-4.277603	-0.660320
H	-4.593395	-4.456261	-1.958018
H	-5.927578	-2.452650	-2.464014
C	-2.326148	2.283846	-0.822933
C	-4.572769	2.477748	-2.487536
C	-2.524566	3.420545	-1.607084
C	-3.279950	1.267977	-0.903216
C	-4.417380	1.334381	-1.703185
C	-3.636420	3.508508	-2.441072
H	-1.805968	4.233339	-1.572799
H	-3.779279	4.391708	-3.055404
H	-5.435547	2.576081	-3.137438
C	0.133870	3.492569	0.076405
C	1.723915	5.757791	-0.323370
C	1.214204	3.448840	-0.812791
C	-0.138500	4.677421	0.768405
C	0.655331	5.803510	0.570634
C	2.000311	4.581375	-1.015612
H	1.448166	2.524422	-1.336753
H	-0.970459	4.720372	1.465494
H	0.439221	6.717702	1.115288
H	2.839638	4.537193	-1.703157
H	2.343012	6.636883	-0.475336
C	-0.167858	-3.471604	0.112787
C	1.230266	-5.814731	-0.504210
C	-0.075759	-4.504214	1.048816
C	0.445594	-3.621678	-1.138197
C	1.130238	-4.792584	-1.447138
C	0.629243	-5.667255	0.743356
H	-0.545739	-4.402713	2.022199
H	0.404974	-2.811515	-1.862906
H	1.601899	-4.898719	-2.419547
H	0.703647	-6.460130	1.481541
H	1.777653	-6.722299	-0.740512

H	0.135003	1.233693	2.843928
H	-3.524528	-2.024587	2.100587
H	-0.760391	1.340757	5.146113
H	-3.873453	-1.925512	4.538543
O	-3.057153	0.160497	-0.121392
C	-5.429954	0.194052	-1.590304
C	-1.611786	2.126409	1.949463
C	5.404045	2.045915	1.138890
C	5.025007	0.791227	0.377972
C	3.028833	-2.250840	-3.765274
H	2.332307	-3.050787	-4.034273
H	3.965163	-2.417025	-4.307100
H	3.227019	-2.323226	-2.691347
C	2.117900	-0.848649	-5.620400
H	3.055455	-0.825269	-6.186337
H	1.559765	-1.738300	-5.928030
H	1.526825	0.029595	-5.888491
C	4.681921	0.105526	-3.423194
H	5.131517	-0.107228	-4.399170
H	5.152553	1.010386	-3.026094
H	4.912152	-0.720006	-2.745922
C	2.904485	1.619914	-4.314196
H	3.329631	2.454057	-3.747752
H	3.358386	1.616917	-5.310112
H	1.829494	1.794574	-4.418203
C	-6.354052	0.124461	-2.808149
H	-6.918841	1.054426	-2.914854
H	-5.793807	-0.051136	-3.731498
H	-7.089838	-0.675184	-2.689308
C	-6.283230	0.437470	-0.322379
H	-6.837965	1.376689	-0.416614
H	-6.999616	-0.379485	-0.187691
H	-5.659222	0.497511	0.574676
O	2.266352	0.714931	2.388522
C	4.582928	3.096767	1.197785
H	3.620288	3.099064	0.692674
H	4.843062	3.992928	1.756122
H	4.482311	1.056320	-0.537271
H	5.932201	0.258394	0.067871
C	6.751423	2.048129	1.810640
H	6.851246	1.206532	2.504974
H	7.549062	1.935186	1.065672
H	6.927934	2.974433	2.364520
C	4.139648	-0.223440	1.158119
C	3.942489	-1.462580	0.254534
C	4.739325	-0.638809	2.508436
C	3.144940	-2.570062	0.939279
H	4.939806	-1.839677	-0.011231
H	3.454458	-1.152219	-0.674452
C	3.963570	-1.773290	3.190681
H	5.773194	-0.965281	2.330924
H	4.783977	0.229711	3.173645
C	3.777944	-2.980314	2.268692
H	3.060404	-3.434367	0.272246
H	2.118369	-2.220943	1.108233
H	4.489065	-2.072569	4.104708
H	2.982354	-1.395056	3.498073
H	3.160983	-3.741715	2.760018
H	4.755962	-3.441712	2.071167

TS1'$_{28}$

Cu	0.496832	0.056609	-0.583191
C	2.460942	0.975986	-0.855190

P	-1.178419	1.704059	-1.010485
P	-0.347749	-2.090189	-0.379530
B	1.455977	0.704110	1.169870
O	1.696616	-0.206767	2.186604
O	1.186604	1.949934	1.701957
C	1.278839	0.367967	3.445755
C	1.257041	1.912831	3.142260
C	-2.846602	-3.500818	-4.009621
C	-1.095848	-2.147787	-3.050966
C	-2.415019	-3.594253	-1.636733
C	-3.146558	-4.007380	-2.745921
C	-1.817957	-2.575217	-4.162056
H	-2.647826	-3.998982	-0.656037
H	-3.949569	-4.728079	-2.624271
H	-3.417974	-3.825202	-4.874167
C	-2.230675	1.268504	-2.454479
C	-3.665848	0.529134	-4.739790
C	-3.600475	1.016193	-2.374553
C	-1.582574	1.142651	-3.690650
C	-2.299303	0.792545	-4.828625
C	-4.311399	0.635298	-3.511824
H	-0.511865	1.320736	-3.757305
H	-1.787501	0.708946	-5.782637
H	-4.223596	0.240025	-5.625384
C	-2.359649	1.967567	0.374659
C	-3.980406	2.178359	2.652226
C	-2.689092	3.220369	0.896304
C	-2.875763	0.842054	1.020364
C	-3.699340	0.910435	2.143749
C	-3.483199	3.322682	2.033479
H	-2.306152	4.118698	0.423949
H	-3.720612	4.300840	2.438922
H	-4.604253	2.282830	3.533049
C	-1.432470	-2.372215	1.083623
C	-3.048721	-2.555636	3.366980
C	-1.309499	-3.456938	1.955352
C	-2.412508	-1.420176	1.371939
C	-3.230516	-1.479148	2.500397
C	-2.106727	-3.542920	3.091472
H	-0.573560	-4.228183	1.757284
H	-1.992569	-4.383820	3.767754
H	-3.653675	-2.638092	4.263140
C	0.919884	-3.413226	-0.210922
C	2.994820	-5.272662	0.050528
C	1.771502	-3.374387	0.901420
C	1.118962	-4.389248	-1.189417
C	2.157278	-5.310966	-1.060293
C	2.795533	-4.305266	1.034797
H	1.644482	-2.595788	1.649947
H	0.470876	-4.433626	-2.059034
H	2.306277	-6.061685	-1.830523
H	3.452482	-4.261422	1.897852
H	3.803586	-5.990372	0.148788
C	-0.636038	3.422534	-1.402446
C	0.289755	6.016870	-1.912613
C	-1.218971	4.197287	-2.410180
C	0.405234	3.967823	-0.640866
C	0.863382	5.257336	-0.895343
C	-0.754605	5.485730	-2.665384
H	-2.035969	3.798505	-3.002916
H	0.841497	3.387649	0.167121
H	1.673462	5.665973	-0.298333
H	-1.213063	6.074541	-3.454218
H	0.652577	7.019901	-2.116375

H	-0.305708	-1.410028	-3.163351
H	-4.123278	1.119330	-1.428510
H	-1.586602	-2.171201	-5.142384
H	-5.375351	0.431927	-3.435905
O	-2.544551	-0.379704	0.486234
C	-4.290941	-0.393882	2.675168
C	-1.385367	-2.659276	-1.783643
C	2.527663	2.649946	3.561638
H	2.498996	3.665610	3.156403
H	2.603697	2.718321	4.651036
H	3.427066	2.160909	3.182356
C	0.038405	2.651275	3.685301
H	0.008632	2.603455	4.778650
H	0.091872	3.704248	3.392569
H	-0.893184	2.241746	3.288881
C	2.264807	-0.061579	4.522460
H	2.012613	0.396811	5.484069
H	2.221694	-1.148219	4.643536
H	3.290648	0.209993	4.264104
C	-0.105119	-0.205867	3.746841
H	-0.048444	-1.298069	3.757923
H	-0.481111	0.131544	4.717440
H	-0.822916	0.084566	2.977038
C	-4.748036	-0.265556	4.130077
H	-5.193527	-1.200902	4.478392
H	-3.917198	-0.005564	4.793393
H	-5.522504	0.500097	4.223516
C	-5.509808	-0.761864	1.795708
H	-5.943220	-1.709574	2.131365
H	-6.275134	0.017761	1.867302
H	-5.226958	-0.869542	0.744221
O	1.931878	0.561942	-1.977627
H	2.366545	2.052170	-0.652012
C	3.755969	-1.107382	-0.387550
H	3.246247	-1.288864	0.561311
H	3.085928	-1.452448	-1.182827
C	5.029529	-1.919319	-0.427701
C	5.759929	-2.142528	0.669637
H	6.669103	-2.739127	0.640268
H	5.463726	-1.744376	1.637407
C	5.389819	-2.537294	-1.752199
H	5.422599	-1.787558	-2.549969
H	6.353391	-3.054311	-1.718418
H	4.618210	-3.264160	-2.037467
C	3.875570	0.426721	-0.532932
C	4.497987	1.048302	0.729836
C	4.767833	0.820522	-1.735725
C	4.704850	2.563688	0.640317
H	5.477660	0.575830	0.880380
H	3.899333	0.787576	1.607651
C	4.968545	2.334332	-1.865837
H	5.751929	0.351660	-1.598729
H	4.329316	0.413318	-2.651502
C	5.549836	2.932492	-0.581799
H	5.192744	2.920320	1.555485
H	3.735175	3.074590	0.592220
H	5.634714	2.542997	-2.711182
H	4.011956	2.820123	-2.096697
H	5.637373	4.021519	-0.672241
H	6.567756	2.542763	-0.438440

I4'$_{28}$

Cu	-0.391747	-0.138124	-0.527112

C	-3.131284	-1.157012	-0.085832
P	1.293766	-1.793807	-0.831284
P	0.525863	1.990339	-0.476433
B	-2.500580	-1.061993	1.360914
O	-1.567941	-0.092567	1.698031
O	-2.661874	-1.978866	2.370551
C	-1.231638	-0.267415	3.092650
C	-1.590148	-1.772259	3.319659
C	3.042159	2.785705	-4.278351
C	1.208985	1.697634	-3.151510
C	2.654229	3.199570	-1.932614
C	3.396713	3.419608	-3.089327
C	1.945483	1.927963	-4.309686
H	2.932839	3.699879	-1.009620
H	4.252515	4.087319	-3.061668
H	3.623708	2.956277	-5.179332
C	2.364609	-1.518956	-2.310144
C	3.812090	-1.030739	-4.659586
C	3.666272	-1.018200	-2.247555
C	1.791472	-1.764554	-3.565042
C	2.513158	-1.531207	-4.730187
C	4.382442	-0.771494	-3.417290
H	0.776678	-2.148756	-3.633003
H	2.057241	-1.735546	-5.694324
H	4.374274	-0.840847	-5.568859
C	2.468937	-1.989553	0.574705
C	4.090604	-2.036874	2.868899
C	2.710580	-3.188222	1.252692
C	3.051965	-0.832414	1.096473
C	3.881623	-0.823060	2.217726
C	3.506348	-3.208002	2.392803
H	2.252871	-4.107943	0.907221
H	3.674543	-4.145023	2.913664
H	4.714796	-2.076933	3.754870
C	1.657029	2.385177	0.926157
C	3.293606	2.714669	3.181602
C	1.534797	3.518966	1.733748
C	2.640562	1.455643	1.267449
C	3.469454	1.587295	2.380895
C	2.342453	3.677435	2.855207
H	0.790679	4.272260	1.499929
H	2.228721	4.557106	3.480367
H	3.906910	2.854089	4.065055
C	-0.660655	3.391716	-0.389480
C	-2.538832	5.439672	-0.089201
C	-1.637781	3.316641	0.610821
C	-0.636588	4.495647	-1.243714
C	-1.579709	5.512246	-1.096370
C	-2.564434	4.340982	0.768824
H	-1.676654	2.440218	1.253024
H	0.114647	4.567464	-2.024481
H	-1.560383	6.364272	-1.769193
H	-3.321382	4.268843	1.543273
H	-3.271414	6.233224	0.022338
C	0.661380	-3.488033	-1.152052
C	-0.428283	-6.008555	-1.652507
C	1.498511	-4.568853	-1.463020
C	-0.725074	-3.668036	-1.129251
C	-1.264175	-4.931189	-1.377100
C	0.955011	-5.825043	-1.704319
H	2.574207	-4.424148	-1.519801
H	-1.367415	-2.795681	-0.982810
H	-2.341803	-5.066440	-1.361826
H	1.607184	-6.660817	-1.939305

H	-0.850613	-6.990969	-1.842622
H	0.368238	1.008414	-3.171536
H	4.138141	-0.823796	-1.290661
H	1.671876	1.423809	-5.230706
H	5.393292	-0.380381	-3.352113
O	2.760998	0.351310	0.458593
C	4.524141	0.506517	2.608048
C	1.554964	2.335726	-1.956491
C	-2.085002	-2.106737	4.716766
H	-2.308822	-3.175367	4.784453
H	-1.315905	-1.873386	5.460056
H	-2.992326	-1.552312	4.965675
C	-0.457376	-2.713651	2.909014
H	0.388726	-2.657339	3.599663
H	-0.830793	-3.741461	2.899650
H	-0.098691	-2.475761	1.902979
C	-2.117777	0.691773	3.885859
H	-1.883947	0.659496	4.953939
H	-1.946064	1.712297	3.530387
H	-3.178587	0.457639	3.754090
C	0.234570	0.073809	3.295738
H	0.394993	1.144724	3.142957
H	0.551508	-0.176164	4.313421
H	0.864817	-0.472531	2.591719
C	5.042550	0.495658	4.047086
H	5.521571	1.447717	4.290354
H	4.238471	0.315060	4.767236
H	5.804162	-0.278551	4.173325
C	5.709631	0.773339	1.650096
H	6.174030	1.736193	1.886167
H	6.463441	-0.013502	1.755533
H	5.384316	0.799515	0.605728
O	-2.145306	-0.881080	-1.037047
H	-3.456401	-2.213474	-0.187997
C	-4.003723	1.177644	-0.062148
H	-3.843977	1.308493	1.015583
H	-3.027693	1.296282	-0.542329
C	-4.924908	2.267791	-0.557335
C	-5.929289	2.747420	0.183764
H	-6.579542	3.540700	-0.178711
H	-6.127568	2.369193	1.184099
C	-4.603162	2.843720	-1.911315
H	-4.571030	2.064108	-2.679750
H	-5.324795	3.606814	-2.217889
H	-3.605174	3.300159	-1.888871
C	-4.422291	-0.296640	-0.295594
C	-5.528642	-0.693597	0.701219
C	-4.939252	-0.509654	-1.730712
C	-6.111813	-2.092049	0.467949
H	-6.344340	0.038077	0.618062
H	-5.146863	-0.616183	1.729020
C	-5.497316	-1.914589	-1.975764
H	-5.742039	0.213262	-1.931623
H	-4.118526	-0.300723	-2.424255
C	-6.602318	-2.254880	-0.972796
H	-6.936813	-2.266513	1.169228
H	-5.354620	-2.855635	0.683894
H	-5.884718	-1.981853	-2.999605
H	-4.692159	-2.656308	-1.899631
H	-6.972100	-3.274069	-1.137136
H	-7.453281	-1.578291	-1.138218

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