

Discovering Enantioselective Protodeauration in Gold

Catalysis: Asymmetric Synthesis of Cyclobutenes

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1. General Methods

¹H-NMR spectra were recorded on a Bruker 600 spectrometer (600 MHz). Chemical shifts are reported in ppm from TMS with the solvent resonance as the internal standard. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = double doublet, t = triplet, td = triple doublet, dt = double triplet, q = quartet, b = broad, m = multiplet), coupling constants (Hz). ¹³C-NMR spectra were recorded on a Bruker 600 spectrometer (150 MHz) with complete proton decoupling. Chemical shifts are reported in ppm from TMS with the solvent as the internal standard.

HRMS spectra were obtained with a G2XS QToF mass spectrometer using ESI ionization techniques, as specified case by case.

Chromatographic purification was done with 240-400 mesh silica gel.

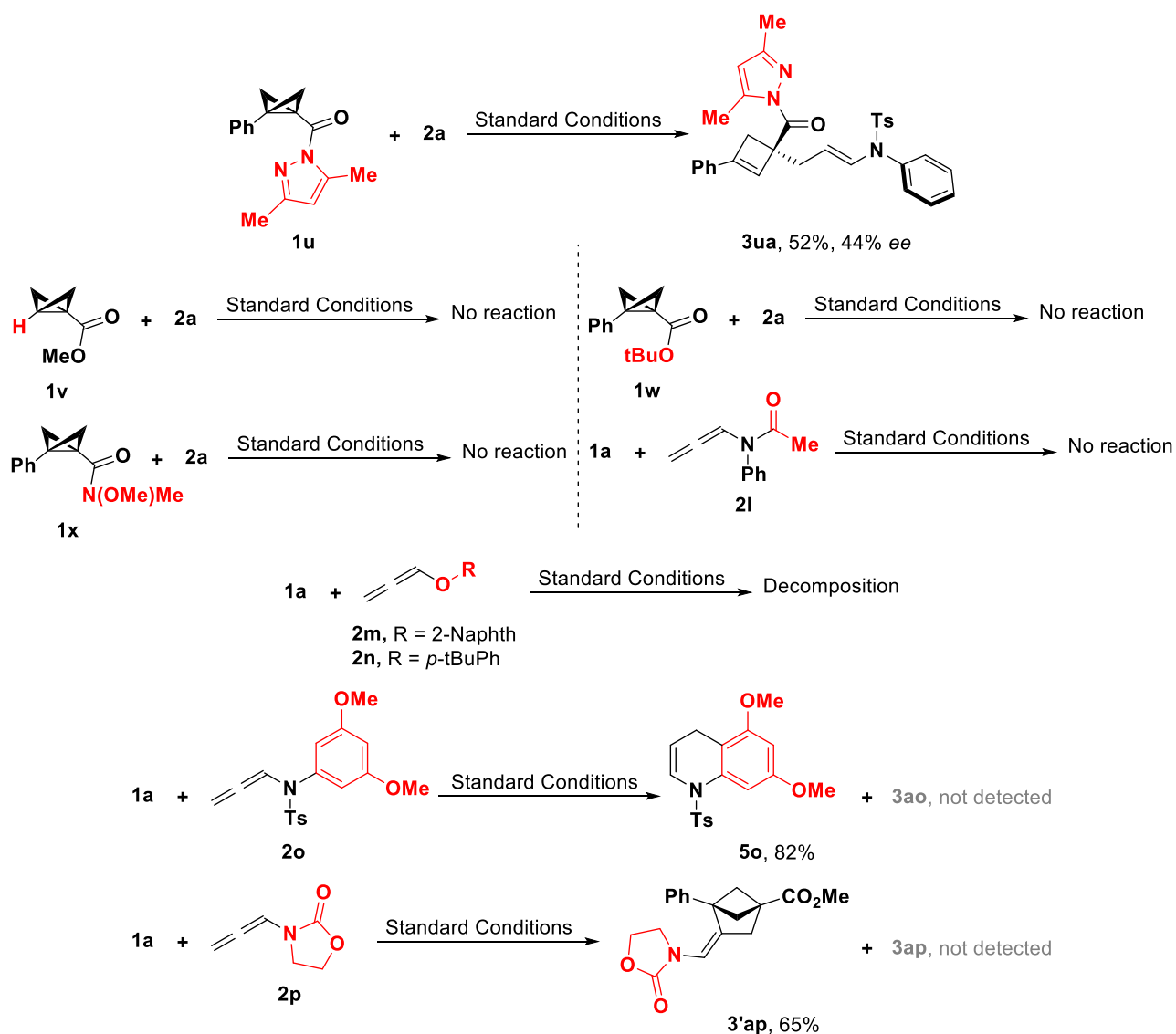
Anhydrous solvents, including DCM for the catalytic processes, were supplied by Merck in Sureseal® bottles and used without any further purification.

Bicyclobutanes **1**¹ and allenamides **2**² are known compounds and were prepared following literature procedures. Gold catalysts have always been used as pre-cationized complexes, procedures for phosphine complexation of AuCl•DMS and subsequent cationization with AgNTf₂, are reported in the literature.³

Computational Methods

All the calculations reported in this work were carried out with the Orca 6.0 code.⁴ The molecular system was simulated at the B97-3C level, which implies the use of a modified def2-TVP basis set (def2-mTZVP), its associated auxiliary basis set and electron core potentials.⁵ The effect of solvation was included in the calculations via the polarizable continuum dielectric model (PCM) and solved in its conductor approach (CPCM).⁶ The solvent parameters used to this end were those associated to acetonitrile. After successful geometry optimization a second derivatives calculation was issued to verify the nature of the stationary points located through the diagonalization of the Hessian.

2. Unproductive substrates



All reactions were run under the optimized conditions reported in Table 1, entry of the Main Text. Acyl-pyrazole derivative **1u** furnished the desired product in moderate yield and very low enantiomeric excess. No reactivity was observed for *t*-Bu ester **1w** and Weinreb amide **1x**, probably due to an unfavourable interaction of the Au cation with the carboxyl moiety of these substrates. Unsubstituted BCB **1v** also showed no reactivity, underlying the importance of the formation of a stable carbocation during the reaction machinery. *N*-Acetyl protected allenamide **2l** did not afford any product, probably due to scarce nucleophilicity of the cumulene undergoing a difficult Au-activation. Allenyl ethers **2m** and **2n** led to the formation of complex reaction mixtures evidencing decomposition of both reaction partners. Allenamide **2o** did not engage in the desired reaction but afforded a cyclization by-product (**5o**) as the sole reaction outcome, in high yield. Oxazolidinone **2p** underwent exclusive $[2\sigma+2\pi]$ -cycloaddition with no formation of the desired cyclobutene.

3. Preparation and characterization of compounds 3.

3.1 General Procedures

General procedure A for the preparation of racemic products **rac-3**:

In a heat-gun dried 10 mL two-necked round bottomed flask covered with an aluminum foil, under inert atmosphere (Ar), the appropriate bicyclo[1.1.0]butane **1** (0.1 mmol, 1 equiv) the appropriate allenamide **2** (0.15 mmol, 1.5 equiv) and [PedroPhosAu]NTf₂ Errore. L'argomento parametro è sconosciuto. (0.005 mmol, 4.6 mg, 5 mol%) were stirred in dry DCM (1.0 mL) at room temperature, in the dark, for 1 h. The solvent was then evaporated, and the crude mixture was directly purified by FC on silica gel.

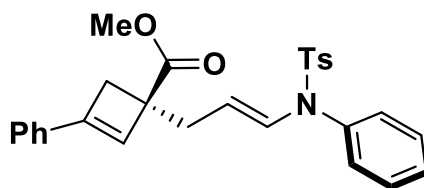
Alternatively, the reaction leading to products **rac-3** can be run under the same conditions reported in General procedure **B** using racemic **Cat1** (obtained mixing equal amounts of pre-formed (**R**)-**Cat1** and (**S**)-**Cat1**).

General procedure B for the preparation of enantioenriched products **3**:

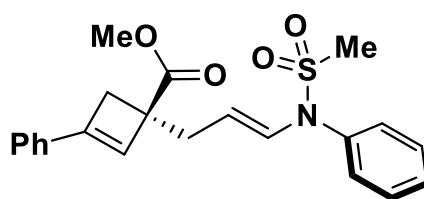
In a heat-gun dried 10 mL two-necked round bottomed flask covered with an aluminium foil, under inert atmosphere (Ar), the appropriate bicyclo[1.1.0]butane **1** (0.1 mmol, 1 equiv) the appropriate allenamide **2** (0.15 mmol, 1.5 equiv) and **Cat1** (0.00125 mmol, 2.7 mg, 1.25 mol%) were stirred in dry DCM (1.0 mL) at room temperature, in the dark, for 1 h. The solvent was then evaporated, and the crude mixture was directly purified by FC on silica gel.

*Note: The reactions leading to products **3ea**, **3fa**, **3ga**, **3ha** and **3ia** were run in toluene for 16 h, instead of DCM for 1 h. In these cases, an increase in the enantiomeric excess was observed by switching solvent, although accompanied by a slower reaction.*

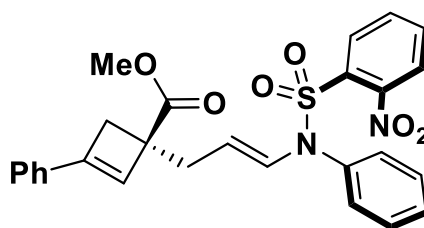
3.2 Characterization data of compounds 3



3aa. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 78%, (0.078 mmol, 36.4 mg). **ee** = 94%. $[\alpha]_D = -1.7$ ($c = 0.52$, CHCl₃). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 80:20, flow 0.8 mL/min, $t_{(R)} = 9.6$ min, $t_{(S)} = 9.0$ min. **¹H NMR** (600 MHz, CDCl₃) $\delta = 7.53 - 7.51$ (m, 2H), 7.34 – 7.30 (m, 2H), 7.29 – 7.27 (m, 2H), 7.26 – 7.23 (m, 4H) overlapped with the residual solvent peak, 7.21 – 7.17 (m, 2H), 7.01 (dt, $J = 13.9, 1.1$ Hz, 1H), 6.88 – 6.82 (m, 2H), 6.20 (s, 1H), 4.39 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 3.62 (s, 3H), 3.04 (d, $J = 12.9$ Hz, 1H), 2.58 – 2.52 (m, 2H), 2.46 (dd, $J = 13.6, 7.9$ Hz, 1H) partially overlapped with 2.45 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃) $\delta = 174.9, 146.2, 143.8, 136.7, 135.8, 133.6, 131.2, 130.1$ (2C), 129.5 (2C), 129.3 (2C), 128.8, 128.4, 128.3 (2C), 128.2, 127.5 (2C), 124.7 (2C), 107.2, 51.8, 51.0, 37.0, 36.4, 21.6; **HRMS (ESI)** m/z : $[M + Na]^+$ calcd. for C₂₈H₂₇NO₄SNa⁺: 496.1553; found 496.1550.

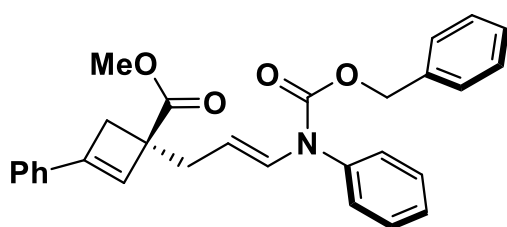


3ab. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 51%, (0.051 mmol, 20.2 mg). **ee** = 96%. $[\alpha]_D = -2.3$ ($c = 0.60$, CHCl₃). **HPLC analysis:** ID column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8 mL/min, $t_{(R)} = 24.6$ min, $t_{(S)} = 23.6$ min. **¹H NMR** (600 MHz, CDCl₃) $\delta = 7.38 - 7.29$ (m, 7H), 7.24 – 7.20 (m, 3H), 6.87 (dt, $J = 13.9, 1.1$ Hz, 1H), 6.27 (s, 1H), 4.53 (ddd, $J = 13.9, 8.0, 7.3$ Hz, 1H), 3.66 (s, 3H), 3.10 (d, $J = 13.0$ Hz, 1H), 2.96 (s, 3H), 2.61 – 2.55 (m, 2H), 2.49 (ddd, $J = 13.9, 8.1, 1.1$ Hz, 1H); **¹³C NMR** (151 MHz, CDCl₃) $\delta = 174.9, 146.4, 136.7, 133.6, 130.6, 129.8$ (2C), 129.8 (2C), 129.1, 128.4 (2C), 128.2, 124.8 (2C), 120.8, 107.5, 51.9, 51.1, 38.7, 37.2, 36.4; **HRMS (ESI)** m/z : $[M + Na]^+$ calcd. for C₂₂H₂₃NO₄SNa⁺: 420.1240; found 420.1248.



3ac. Colourless oil. FC eluent: *n*-hexane/DCM: 1:1. Yield = 40%, (0.040 mmol, 20.2 mg). **ee** = 95%. $[\alpha]_D = -7.3$ ($c = 0.22$, CHCl₃). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 96:4, flow 1.0 mL/min, $t_{(R)} = 49.1$ min, $t_{(S)} = 45.7$ min. **¹H NMR** (600 MHz, CDCl₃) $\delta = 7.70 - 7.64$ (m, 2H), 7.51 (dt, $J = 8.0, 1.0$ Hz, 1H), 7.46 (ddd, $J = 8.0, 4.9, 3.9$ Hz, 1H), 7.33 – 7.27 (m, 6H), 7.24 – 7.18 (m, 2H), 7.07 – 7.00 (m, 3H), 6.29 (s, 1H), 4.41 (ddd, $J = 13.9, 8.2, 7.3$ Hz, 1H), 3.65 (s, 3H), 3.08 (d, $J = 13.0$ Hz, 1H), 2.65 (d, $J = 13.0$ Hz, 1H), 2.61 (ddd, $J = 13.9, 7.4, 1.3$ Hz, 1H), 2.54 (ddd, $J = 13.9, 8.2, 1.1$ Hz, 1H); **¹³C NMR** (151 MHz, CDCl₃) $\delta = 174.9,$

147.9, 146.3, 135.5, 134.0, 133.7, 132.1, 131.5, 131.2, 131.2, 130.5 (2C), 129.6 (2C), 129.3, 128.4, 128.3 (2C), 128.3, 124.8 (2C), 124.1, 106.8, 51.9, 51.0, 37.1, 36.2; **HRMS (ESI)** m/z : $[M + Na]^+$ calcd. for $C_{27}H_{24}N_2O_6SNa^+$: 527.1247; found 527.1251.



3ad. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1.

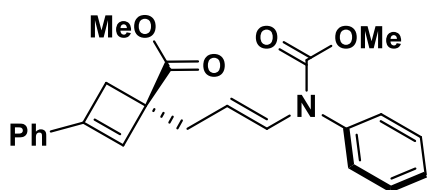
Yield = 49%, (0.049 mmol, 22.2 mg). **ee** = 89%. $[\alpha]_D =$

+ 3.9 ($c = 0.18$, $CHCl_3$). **HPLC analysis:** OD-H column

(254 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.7

mL/min, $t_{(R)} = 16.8$ min, $t_{(S)} = 15.6$ min. **1H NMR** (600

MHz, $CDCl_3$) $\delta = 7.36 - 7.26$ (m, 11H) overlapped with the residual solvent peak, 7.25 – 7.14 (bm, 3H), 7.09 – 7.04 (bm, 2H), 6.25 (s, 1H), 5.16 (s, 2H), 4.44 (dt, $J = 14.8, 7.7$ Hz, 1H), 3.63 (s, 3H), 3.07 (d, $J = 12.9$ Hz, 1H), 2.61 – 2.54 (m, 2H), 2.48 (dd, $J = 13.8, 8.1$ Hz, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) $\delta = 175.0, 153.4, 146.2, 138.4$ (b), 136.2, 133.7, 131.6 (b), 129.3 (2C), 128.6 (2C), 128.5 (b, 2C), 128.4 (2C), 128.4, 128.3, 128.0 (b, 2C), 127.8, 124.8 (2C), 107.7, 67.6 (b), 51.9, 51.0, 37.1, 36.6; **HRMS (ESI)** m/z : $[M + Na]^+$ calcd. for $C_{29}H_{27}NO_4Na^+$: 476.1832; found 476.1828.



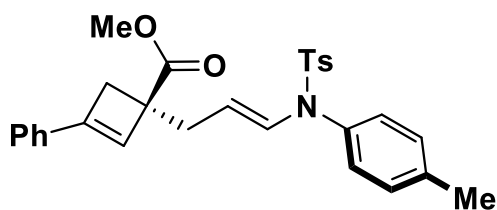
3ae. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield

= 60%, (0.060 mmol, 22.6 mg). **ee** = 95%. $[\alpha]_D = - 3.3$ ($c =$

0.46, $CHCl_3$). **HPLC analysis:** ID column (254 nm), 30 °C,

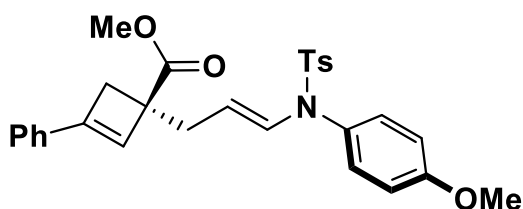
method: *n*-Hex:IPA = 85:15, flow 0.7 mL/min, $t_{(R)} = 14.2$ min,

$t_{(S)} = 13.7$ min. **1H NMR** (600 MHz, $CDCl_3$) $\delta = 7.36 - 7.27$ (m, 8H), 7.21 – 7.13 (bm, 1H), 7.07 – 7.03 (m, 2H), 6.26 (s, 1H), 4.46 – 4.37 (m, 1H), 3.70 (bs, 3H), 3.64 (s, 3H), 3.07 (d, $J = 12.9$ Hz, 1H), 2.62 – 2.54 (m, 2H), 2.48 (ddd, $J = 13.9, 8.1, 1.1$ Hz, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) $\delta = 175.0, 154.2, 146.2, 138.4, 133.7, 131.7, 129.3$ (2C), 128.6 (2C), 128.4 (2C), 128.4, 128.3, 127.8, 124.8 (2C), 107.4, 53.4, 51.9, 51.1, 37.1, 36.6; **HRMS (ESI)** m/z : $[M + Na]^+$ calcd. for $C_{23}H_{23}NO_4Na^+$: 400.1519; found 400.1521.

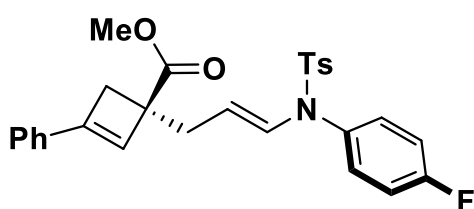


3af. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 51%, (0.051 mmol, 24.8 mg). **ee** = 95%. $[\alpha]_D = -13.2$ ($c = 0.46$, CHCl_3). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.7 mL/min, $t_{(R)} = 14.1$ min, $t_{(S)} = 12.9$ min. **^1H NMR** (600

MHz, CDCl_3) $\delta = 7.55 - 7.50$ (m, 2H), 7.34 – 7.30 (m, 2H), 7.30 – 7.26 (m, 1H), 7.26 – 7.22 (m, 4H) overlapped with the residual solvent peak, 7.03 – 6.96 (m, 3H), 6.74 – 6.69 (m, 2H), 6.20 (s, 1H), 4.39 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 3.62 (s, 3H), 3.04 (d, $J = 12.9$ Hz, 1H), 2.58 – 2.52 (m, 2H), 2.48 – 2.43 (m, 4H), 2.30 (s, 3H); **^{13}C NMR** (151 MHz, CDCl_3) $\delta = 174.9, 146.2, 143.7, 138.8, 135.9, 133.9, 133.6, 131.3, 130.0$ (2C), 129.7 (2C), 129.5 (2C), 128.4, 128.3 (2C), 128.2, 127.5 (2C), 124.7 (2C), 106.9, 51.8, 51.0, 37.1, 36.4, 21.6, 21.2; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{29}\text{H}_{29}\text{NO}_4\text{SNa}^+$: 510.1710; found 510.1707.

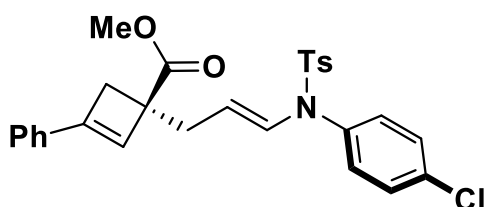


3ag. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 66%, (0.066 mmol, 33.2 mg). **ee** = 92%. $[\alpha]_D = -9.8$ ($c = 0.27$, CHCl_3). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.6 mL/min, $t_{(R)} = 23.1$ min, $t_{(S)} = 21.4$ min. **^1H NMR** (600 MHz, CDCl_3) $\delta = 7.53 - 7.50$ (m, 2H), 7.32 (ddt, $J = 8.1, 6.6, 1.2$ Hz, 2H), 7.29 – 7.26 (m, 1H), 7.26 – 7.23 (m, 4H) overlapped with the residual solvent peak, 7.01 (dt, $J = 13.9, 1.1$ Hz, 1H), 6.75 – 6.71 (m, 2H), 6.68 – 6.65 (m, 2H), 6.20 (s, 1H), 4.38 (ddd, $J = 13.9, 8.2, 7.2$ Hz, 1H), 3.76 (s, 3H), 3.63 (s, 3H), 3.04 (d, $J = 12.9$ Hz, 1H), 2.58 – 2.51 (m, 2H), 2.48 – 2.41 (m, 4H); **^{13}C NMR** (151 MHz, CDCl_3) $\delta = 174.9, 159.6, 146.1, 143.7, 135.8, 133.6, 131.5, 131.2$ (2C), 129.5 (2C), 128.9, 128.4, 128.3 (2C), 128.3, 127.5 (2C), 124.7 (2C), 114.5, 106.6, 55.4, 51.9, 51.0, 37.0, 36.3, 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{29}\text{H}_{29}\text{NO}_5\text{SNa}^+$: 526.1659; found 526.1652.

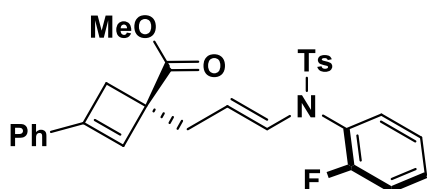


3ah. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 60%, (0.060 mmol, 29.5 mg). **ee** = 96%. $[\alpha]_D = +5.1$ ($c = 0.36$, CHCl_3). **HPLC analysis:** ID column (254 nm), 30 °C, method: *n*-Hex:IPA = 88:12, flow 0.9 mL/min, $t_{(R)} = 28.9$ min, $t_{(S)} = 31.1$ min. **^1H NMR** (600 MHz, CDCl_3) $\delta = 7.53 - 7.49$ (m, 2H), 7.34 – 7.31 (m, 2H), 7.30 – 7.26 (m, 3H), 7.25 – 7.22 (m, 2H), 7.00 (dt, $J = 13.9, 1.1$ Hz, 1H), 6.88 – 6.83 (m, 2H), 6.82 – 6.78 (m, 2H), 6.20 (s, 1H), 4.37 (ddd, $J = 13.9, 8.2, 7.2$ Hz, 1H), 3.63 (s, 3H), 3.04 (d, $J = 12.9$ Hz, 1H), 2.56 (ddd, $J = 13.8, 7.2,$

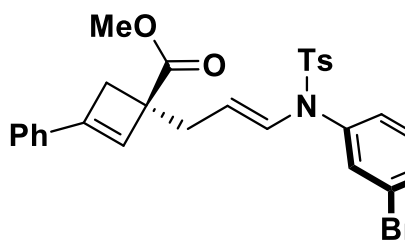
1.2 Hz, 1H), 2.52 (d, J = 12.9 Hz, 1H), 2.49 – 2.44 (m, 4H); ^{13}C NMR (151 MHz, CDCl_3) δ = 174.8, 162.4 (d, J = 249.2 Hz), 146.2, 144.0, 135.4, 133.5, 132.5 (d, J = 3.2 Hz), 131.9 (d, J = 8.7 Hz), 131.2, 129.6, 128.5, 128.4, 128.1, 127.5, 124.7, 116.3 (d, J = 22.6 Hz), 107.1, 51.9, 50.9, 36.9, 36.2, 21.7; ^{19}F NMR (565 MHz, CDCl_3) δ = -111.7 (m, 1F); **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{28}\text{H}_{26}\text{FNO}_4\text{SNa}^+$: 514.1459; found 514.1465.



3ai. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 60%, (0.060 mmol, 30.4 mg). **ee** = 96%. $[\alpha]_{\text{D}}^{25}$ = +2.5 (c = 0.59, CHCl_3). **HPLC analysis:** OD-H column (280 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.5 mL/min, t_{R} = 21.7 min, t_{S} = 20.2 min. ^1H NMR (600 MHz, CDCl_3) δ = 7.52 – 7.49 (m, 2H), 7.34 – 7.31 (m, 2H), 7.31 – 7.28 (m, 1H), 7.28 – 7.26 (m, 2H), 7.25 – 7.22 (m, 2H), 7.15 – 7.12 (m, 2H), 6.98 (d, J = 14.0 Hz, 1H), 6.79 – 6.74 (m, 2H), 6.20 (s, 1H), 4.40 (ddd, J = 14.0, 8.1, 7.2 Hz, 1H), 3.63 (s, 3H), 3.04 (d, J = 13.0 Hz, 1H), 2.56 (ddd, J = 13.9, 7.2, 1.2 Hz, 1H), 2.52 (d, J = 12.9 Hz, 1H), 2.49 – 2.44 (m, 4H); ^{13}C NMR (151 MHz, CDCl_3) δ = 174.8, 146.2, 144.1, 135.4, 135.2, 134.8, 133.5, 131.4 (2C), 131.0, 129.7 (2C), 129.6 (2C), 128.5, 128.4 (2C), 128.1, 127.5 (2C), 124.7 (2C), 107.5, 51.9, 50.9, 36.9, 36.2, 21.7; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{28}\text{H}_{26}\text{ClNO}_4\text{SNa}^+$: 530.1163; found 530.1155.

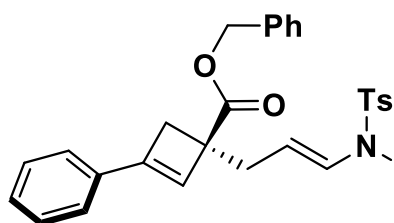


3aj. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 45%, (0.045 mmol, 22.1 mg). **ee** = 93%. $[\alpha]_{\text{D}}^{25}$ = -2.0 (c = 0.56, CHCl_3). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.6 mL/min, t_{R} = 37.3 min, t_{S} = 34.9 min. ^1H NMR (600 MHz, CDCl_3) δ = 7.61 – 7.55 (m, 2H), 7.34 – 7.27 (m, 4H), 7.27 – 7.24 (m, 4H) overlapped with the residual solvent peak, 7.05 – 6.98 (m, 2H), 6.97 – 6.92 (m, 2H), 6.21 (s, 1H), 4.39 (dddd, J = 13.8, 8.2, 7.1, 1.1 Hz, 1H), 3.60 (s, 3H), 3.04 (d, J = 13.0 Hz, 1H), 2.60 – 2.53 (m, 2H), 2.50 – 2.43 (m, 4H); ^{13}C NMR (151 MHz, CDCl_3) δ = 174.9, 159.2 (d, J = 255.7 Hz), 146.4, 144.0, 135.9, 133.6, 132.4, 130.9 (d, J = 8.0 Hz), 129.7 (d, J = 23.2 Hz) partially overlapped with 129.6 (2C), 128.4, 128.3 (2C), 128.1, 127.4 (2C), 124.8 (2C), 124.7 (d, J = 3.7 Hz), 123.9 (d, J = 12.4 Hz), 116.9 (d, J = 19.7 Hz), 106.9, 51.8, 50.9, 37.2, 36.4, 21.7; ^{19}F NMR (565 MHz, CDCl_3) δ = -117.06 – -117.37 (m, 1F); **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{28}\text{H}_{26}\text{FNO}_4\text{SNa}^+$: 514.1459; found 514.1451.



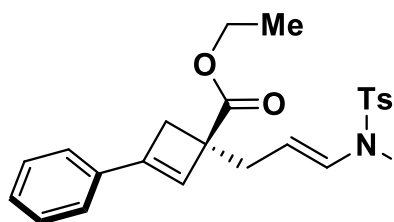
3ak. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 53%, (0.053 mmol, 29.2 mg). **ee** = 90%. $[\alpha]_D^{25} = +5.5$ ($c = 0.37$, CHCl_3). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.6 mL/min, $t_{(R)} = 17.0$ min, $t_{(S)} = 15.7$ min. **$^1\text{H NMR}$** (600 MHz, CDCl_3) $\delta = 7.53 -$

7.50 (m, 2H), 7.44 (ddd, $J = 8.0, 2.0, 1.0$ Hz, 1H), 7.34 – 7.30 (m, 2H), 7.30 – 7.25 (m, 5H) overlapped with the residual solvent peak, 7.07 (t, $J = 1.9$ Hz, 1H), 7.04 (t, $J = 8.0$ Hz, 1H), 6.95 (dt, $J = 14.0, 1.1$ Hz, 1H), 6.77 (ddd, $J = 8.0, 2.0, 1.0$ Hz, 1H), 6.22 (s, 1H), 4.43 (ddd, $J = 14.0, 8.1, 7.3$ Hz, 1H), 3.63 (s, 3H), 3.06 (d, $J = 12.9$ Hz, 1H), 2.59 – 2.52 (m, 2H), 2.46 (d, $J = 9.9$ Hz, 4H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3) $\delta = 174.8, 146.4, 144.2, 138.1, 135.4, 133.5, 133.2, 132.0, 130.9, 130.5, 129.7$ (2C), 128.7, 128.5, 128.4 (2C), 128.1, 127.5 (2C), 124.8 (2C), 122.4, 108.1, 51.9, 50.9, 37.2, 36.4, 21.7; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{28}\text{H}_{26}\text{BrNO}_4\text{SNa}^+$: 574.0658; found 574.0666.



3ba. Colourless oil. FC eluent: *n*-hexane/DCM: 2:1. Yield = 52%, (0.052 mmol, 29.2 mg). **ee** = 87%. $[\alpha]_D^{25} = +14.5$ ($c = 0.20$, CHCl_3). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.8 mL/min, $t_{(R)} = 17.3$ min, $t_{(S)} = 15.1$ min. **$^1\text{H NMR}$** (600 MHz, CDCl_3) $\delta = 7.53 -$

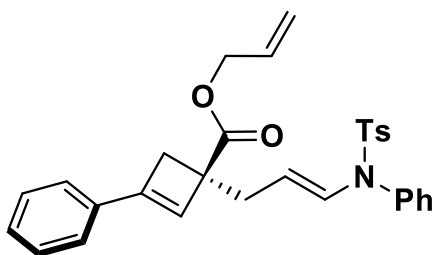
7.50 (m, 2H), 7.36 – 7.30 (m, 6H), 7.29 – 7.27 (m, 3H), 7.25 – 7.22 (m, 3H), 7.17 – 7.14 (m, 2H), 7.02 (dt, $J = 13.9, 1.1$ Hz, 1H), 6.84 – 6.79 (m, 2H), 6.22 (s, 1H), 5.05 (s, 2H), 4.39 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 3.07 (d, $J = 12.9$ Hz, 1H), 2.58 (ddd, $J = 13.8, 7.3, 1.2$ Hz, 1H), 2.54 (d, $J = 12.9$ Hz, 1H), 2.49 (ddd, $J = 13.8, 8.1, 1.0$ Hz, 1H), 2.43 (s, 3H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3) $\delta = 174.2, 146.3, 143.8, 136.7, 136.0, 135.8, 133.6, 131.3, 130.0$ (2C), 129.5 (2C), 129.3 (2C), 128.8, 128.6 (2C), 128.4, 128.3 (2C), 128.2, 128.1, 127.9 (2C), 127.5 (2C), 124.8 (2C), 107.1, 66.3, 51.1, 37.0, 36.5, 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{34}\text{H}_{31}\text{NO}_4\text{SNa}^+$: 572.1866; found 572.1859.



3ca. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 68%, (0.068 mmol, 33.1 mg). **ee** = 94%. $[\alpha]_D^{25} = -1.3$ ($c = 0.16$, CHCl_3). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8 mL/min, $t_{(R)} = 17.3$ min, $t_{(S)} = 18.8$ min. **$^1\text{H NMR}$** (600 MHz, CDCl_3) $\delta = 7.54 -$

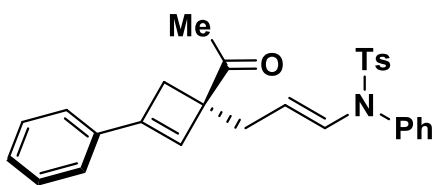
7.50 (m, 2H), 7.34 – 7.30 (m, 2H), 7.30 – 7.27 (m, 2H), 7.26 – 7.23 (m, 4H) overlapped with the residual solvent peak, 7.22 – 7.17 (m, 2H), 7.01 (dt, $J = 13.8, 1.1$ Hz, 1H), 6.88 – 6.81

(m, 2H), 6.21 (s, 1H), 4.39 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 4.07 (q, $J = 7.1$ Hz, 2H), 3.04 (d, $J = 12.9$ Hz, 1H), 2.58 – 2.51 (m, 2H), 2.48 – 2.43 (m, 4H), 1.18 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 174.4, 146.1, 143.8, 136.7, 135.8, 133.7, 131.2, 130.1$ (2C), 129.5 (2C), 129.3 (2C), 128.8, 128.4, 128.3 (2C + 1C overlapped), 127.5 (2C), 124.7 (2C), 107.2, 60.6, 51.0, 37.0, 36.5, 21.6, 14.3; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{29}\text{H}_{29}\text{NO}_4\text{SNa}^+$: 510.1710; found 510.1705.



3da. Colourless oil. FC eluent: *n*-hexane/acetone: 15:1. Yield = 82%, (0.082 mmol, 40.9 mg). **ee** = 91%. $[\alpha]_{\text{D}} = -3.6$ ($c = 0.28$, CHCl_3). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8 mL/min, $t_{\text{R}} = 19.8$ min, $t_{\text{S}} = 21.1$ min. ^1H NMR (600 MHz, CDCl_3) $\delta = 7.54$

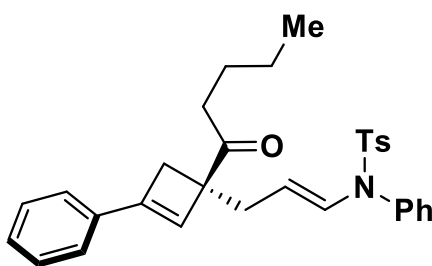
– 7.50 (m, 2H), 7.34 – 7.30 (m, 2H), 7.30 – 7.27 (m, 2H), 7.26 – 7.23 (m, 4H) overlapped with the residual solvent peak, 7.21 – 7.17 (m, 2H), 7.02 (dt, $J = 13.9, 1.1$ Hz, 1H), 6.87 – 6.84 (m, 2H), 6.22 (s, 1H), 5.83 (ddt, $J = 17.2, 10.4, 5.7$ Hz, 1H), 5.25 (dq, $J = 17.2, 1.6$ Hz, 1H), 5.18 (dq, $J = 10.4, 1.3$ Hz, 1H), 4.51 (dt, $J = 5.7, 1.4$ Hz, 2H), 4.39 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 3.07 (d, $J = 12.9$ Hz, 1H), 2.61 – 2.52 (m, 2H), 2.48 (ddd, $J = 13.8, 8.1, 1.0$ Hz, 1H), 2.44 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 174.0, 146.3, 143.8, 136.7, 135.8, 133.6, 132.2, 131.3, 130.1$ (2C), 129.5 (2C), 129.3 (2C), 128.8, 128.4, 128.3 (2C), 128.2, 127.5 (2C), 124.7 (2C), 118.1, 107.1, 65.2, 51.1, 37.1, 36.6, 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{30}\text{H}_{29}\text{NO}_4\text{SNa}^+$: 522.1710; found 522.1714. *Note: Product 3da was isolated along with 10% inseparable [2+2] cycloadduct 3'da (characteristic signal: 4.61 ppm).*



3ea. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 46%, (0.046 mmol, 21.0 mg). **ee** = 84%. $[\alpha]_{\text{D}} = -5.9$ ($c = 0.09$, CHCl_3). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8 mL/min, $t_{\text{R}} = 19.3$

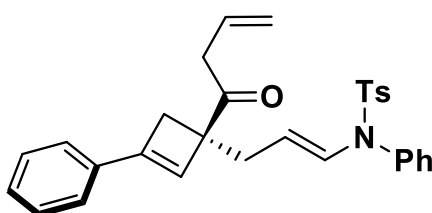
min, $t_{\text{S}} = 17.3$ min. ^1H NMR (600 MHz, CDCl_3) $\delta = 7.53$ – 7.49 (m, 2H), 7.36 – 7.32 (m, 2H), 7.32 – 7.28 (m, 1H), 7.28 – 7.23 (m, 5H) overlapped with the residual solvent peak, 7.19 – 7.15 (m, 2H), 6.99 (dt, $J = 13.9, 1.1$ Hz, 1H), 6.84 – 6.80 (m, 2H), 6.27 (s, 1H), 4.37 (ddd, $J = 13.9, 8.2, 7.1$ Hz, 1H), 2.91 (d, $J = 13.2$ Hz, 1H), 2.55 (ddd, $J = 14.0, 7.1, 1.3$ Hz, 1H), 2.52 (d, $J = 13.2$ Hz, 1H), 2.45 (s, 3H), 2.40 (ddd, $J = 14.0, 8.3, 1.0$ Hz, 1H), 2.11 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 210.2, 147.0, 143.8, 136.7, 135.8, 133.5, 131.2, 130.0$ (2C), 129.5 (2C), 129.3 (2C), 128.9, 128.8, 128.5, 128.4 (2C), 127.5 (2C), 124.7 (2C), 107.5, 57.5,

36.3, 34.9, 26.3, 21.6; **HRMS (ESI)** m/z : $[M + Na]^+$ calcd. for $C_{28}H_{27}NO_3SNa^+$: 480.1604; found 480.1611.



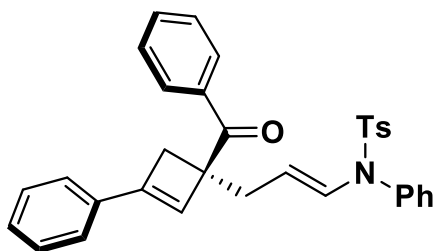
3fa. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 42%, (0.042 mmol, 20.9 mg). **ee** = 82%. $[\alpha]_D = -6.7$ ($c = 0.64$, $CHCl_3$). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8 mL/min, $t_{(R)} = 19.7$ min, $t_{(S)} = 17.6$ min. **1H NMR** (600 MHz, $CDCl_3$) $\delta = 7.54 - 7.49$ (m, 2H), 7.36 – 7.32 (m, 2H), 7.32 – 7.28 (m, 1H), 7.28

– 7.23 (m, 5H) overlapped with the residual solvent peak, 7.19 – 7.15 (m, 2H), 6.98 (dt, $J = 14.0, 1.1$ Hz, 1H), 6.85 – 6.79 (m, 2H), 6.28 (s, 1H), 4.34 (ddd, $J = 13.9, 8.3, 7.1$ Hz, 1H), 2.87 (d, $J = 13.2$ Hz, 1H), 2.56 (ddd, $J = 13.9, 7.1, 1.3$ Hz, 1H), 2.51 (d, $J = 13.2$ Hz, 1H), 2.44 (s, 3H), 2.40 – 2.35 (m, 2H), 1.49 – 1.42 (m, 2H), 1.25 – 1.19 (m, 2H), 0.86 (t, $J = 7.3$ Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) $\delta = 212.3, 146.8, 143.8, 136.7, 135.8, 133.6, 131.1, 130.0$ (2C), 129.6 (2C), 129.3 (2C), 128.9, 128.8, 128.5, 128.4 (2C), 127.5 (2C), 124.7 (2C), 107.6, 57.2, 38.5, 36.4, 35.3, 25.9, 22.4, 21.6, 14.0; **HRMS (ESI)** m/z : $[M + Na]^+$ calcd. for $C_{31}H_{33}NO_3SNa^+$: 522.2073; found 522.2067.

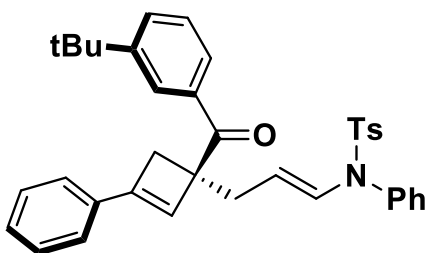


3ga. Colourless oil. FC eluent: *n*-hexane/acetone: 15:1. Yield = 38%, (0.038 mmol, 18.4 mg). **ee** = 77%. $[\alpha]_D = -1.1$ ($c = 0.17$, $CHCl_3$). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.7 mL/min, $t_{(R)} = 26.8$ min, $t_{(S)} = 23.9$ min. **1H NMR** (600 MHz, $CDCl_3$) $\delta = 7.51$

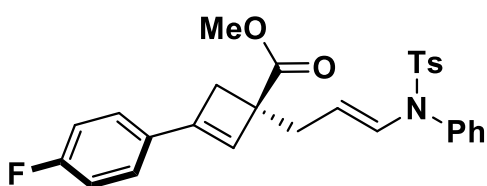
– 7.47 (m, 2H), 7.36 – 7.28 (m, 3H), 7.28 – 7.21 (m, 5H) overlapped with the residual solvent peak, 7.19 – 7.13 (m, 2H), 6.97 (dd, $J = 14.0, 1.2$ Hz, 1H), 6.83 – 6.77 (m, 2H), 6.27 (s, 1H), 5.81 (ddt, $J = 17.1, 10.2, 6.8$ Hz, 1H), 5.09 (dq, $J = 10.2, 1.4$ Hz, 1H), 5.01 (dq, $J = 17.2, 1.6$ Hz, 1H), 4.34 (ddd, $J = 13.9, 8.3, 7.1$ Hz, 1H), 3.23 (ddt, $J = 16.9, 6.7, 1.5$ Hz, 1H), 3.16 (ddt, $J = 16.9, 6.9, 1.4$ Hz, 1H), 2.88 (d, $J = 13.4$ Hz, 1H), 2.60 – 2.48 (m, 2H), 2.43 (s, 3H), 2.38 (ddd, $J = 13.9, 8.3, 1.0$ Hz, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) $\delta = 209.8, 147.0, 143.8, 136.7, 135.7, 133.5, 131.2, 131.0, 130.0$ (2C), 129.6 (2C), 129.3 (2C), 128.8, 128.6, 128.6, 128.5 (2C), 127.5 (2C), 124.7 (2C), 118.4, 107.4, 57.2, 43.4, 36.4, 35.0, 21.6; **HRMS (ESI)** m/z : $[M + Na]^+$ calcd. for $C_{30}H_{29}NO_3SNa^+$: 506.1760; found 506.1765.



3ha. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 32%, (0.032 mmol, 16.6 mg). **ee** = 80%. $[\alpha]_D = -19.6$ ($c = 0.29$, CHCl_3). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 92:8, flow 0.5 mL/min, $t_{(R)} = 21.2$ min, $t_{(S)} = 19.7$ min. **$^1\text{H NMR}$** (600 MHz, CDCl_3) $\delta = 7.89 - 7.84$ (m, 2H), 7.58 – 7.54 (m, 1H), 7.48 – 7.43 (m, 4H), 7.33 – 7.27 (m, 4H), 7.26 – 7.22 (m, 4H), 7.19 – 7.13 (m, 2H), 6.92 (dt, $J = 14.0$, 1.1 Hz, 1H), 6.84 – 6.78 (m, 2H), 6.48 (s, 1H), 4.38 (dt, $J = 13.9$, 7.7 Hz, 1H), 3.27 (d, $J = 12.8$ Hz, 1H), 2.81 (d, $J = 12.8$ Hz, 1H), 2.78 (ddd, $J = 13.9$, 7.4, 1.2 Hz, 1H), 2.65 (ddd, $J = 14.0$, 8.1, 1.1 Hz, 1H), 2.45 (s, 3H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3) $\delta = 201.8$, 145.3, 143.8, 136.5, 135.6, 135.6, 133.6, 132.7, 131.2, 130.1 (2C), 129.5 (2C), 129.5, 129.3 (2C), 128.9 (2C), 128.8, 128.5 (2C), 128.3 (2C + 1C overlapped), 127.4 (2C), 124.7 (2C), 106.6, 56.7, 38.2, 38.0, 21.7; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{33}\text{H}_{29}\text{NO}_3\text{SNa}^+$: 542.1760; found 542.1764.



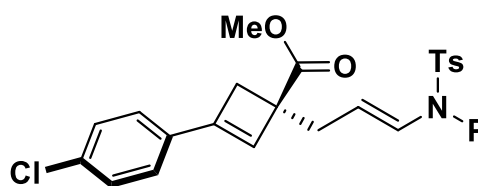
3ia. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 43%, (0.043 mmol, 24.8 mg). **ee** = 60%. $[\alpha]_D = -3.8$ ($c = 0.13$, CHCl_3). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 92:8, flow 0.5 mL/min, $t_{(R)} = 24.4$ min, $t_{(S)} = 30.2$ min. **$^1\text{H NMR}$** (600 MHz, CDCl_3) $\delta = 7.93$ (t, $J = 1.9$ Hz, 1H), 7.65 (d, $J = 7.6$ Hz, 1H), 7.58 (d, $J = 7.9$ Hz, 1H), 7.50 – 7.44 (m, 2H), 7.37 (t, $J = 7.7$ Hz, 1H), 7.33 – 7.21 (m, 8H) overlapped with the residual solvent peak, 7.16 – 7.11 (m, 2H), 6.95 (d, $J = 13.9$ Hz, 1H), 6.83 – 6.78 (m, 2H), 6.47 (s, 1H), 4.40 (dt, $J = 13.9$, 7.7 Hz, 1H), 3.26 (d, $J = 12.8$ Hz, 1H), 2.83 – 2.75 (m, 2H), 2.65 (dd, $J = 13.9$, 8.2 Hz, 1H), 2.45 (s, 3H), 1.35 (s, 9H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3) $\delta = 202.1$, 151.6, 145.2, 143.8, 136.5, 135.7, 135.4, 133.6, 131.2, 130.1 (2C), 129.8, 129.6, 129.5 (2C), 129.3 (2C), 128.8, 128.3 (2C), 128.3, 128.1, 127.5 (2C), 126.2, 125.8, 124.7 (2C), 106.8, 56.7, 38.1, 37.9, 34.9, 31.3 (3C), 29.7, 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{37}\text{H}_{37}\text{NO}_3\text{SNa}^+$: 598.2386; found 598.2393.



3ja. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 62%, (0.062 mmol, 30.4 mg). **ee** = 93%. $[\alpha]_D = -7.0$ ($c = 0.46$, CHCl_3). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 92:8, flow 0.7 mL/min, $t_{(R)} = 41.7$ min, $t_{(S)} = 45.9$ min.

$^1\text{H NMR}$ (600 MHz, CDCl_3) $\delta = 7.54 - 7.50$ (m, 2H), 7.32 – 7.28 (m, 1H), 7.27 – 7.24 (m, 2H) overlapped with the residual solvent peak, 7.23 –

7.19 (m, 4H), 7.03 – 6.98 (m, 3H), 6.86 – 6.83 (m, 2H), 6.14 (s, 1H), 4.37 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 3.62 (s, 3H), 3.02 (d, $J = 12.9$ Hz, 1H), 2.55 (ddd, $J = 13.9, 7.3, 1.2$ Hz, 1H), 2.51 (d, $J = 12.9$ Hz, 1H), 2.48 – 2.43 (m, 4H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 174.8, 162.7$ (d, $J = 248.1$ Hz), 145.2, 143.8, 136.7, 135.8, 131.3, 130.1 (2C), 130.0 (d, $J = 2.8$ Hz), 129.5 (2C), 129.3 (2C), 128.8, 127.7 (d, $J = 2.3$ Hz), 127.5 (2C), 126.6 (d, $J = 8.2$ Hz, 2C), 115.4 (d, $J = 21.8$ Hz, 2C), 107.0, 51.9, 50.9, 37.1, 36.4, 21.6; ^{19}F NMR (565 MHz, CDCl_3) $\delta = -112.31$ – -112.58 (m, 1F); **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{28}\text{H}_{26}\text{FNO}_4\text{SNa}^+$: 514.1459; found 514.1452.

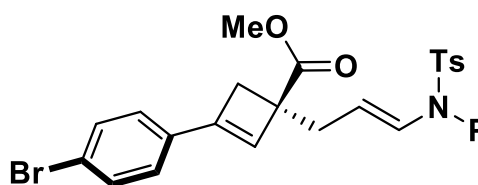


3ka. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1.

Yield = 71%, (0.071 mmol, 36.0 mg). **ee** = 92%. $[\alpha]_{\text{D}} =$

-6.4 ($c = 0.68$, CHCl_3). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8

mL/min, $t_{\text{R}} = 21.7$ min, $t_{\text{S}} = 24.1$ min. ^1H NMR (600 MHz, CDCl_3) $\delta = 7.53$ – 7.50 (m, 2H), 7.32 – 7.27 (m, 3H), 7.26 – 7.23 (m, 2H) overlapped with the residual solvent peak, 7.23 – 7.19 (m, 2H), 7.19 – 7.16 (m, 2H), 7.01 (dt, $J = 14.0, 1.1$ Hz, 1H), 6.87 – 6.83 (m, 2H), 6.20 (s, 1H), 4.36 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 3.62 (s, 3H), 3.02 (d, $J = 12.9$ Hz, 1H), 2.55 (ddd, $J = 13.8, 7.3, 1.2$ Hz, 1H), 2.51 (d, $J = 13.0$ Hz, 1H), 2.48 – 2.43 (m, 4H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 174.6, 145.1, 143.9, 136.7, 135.8, 134.1, 132.1, 131.3, 130.0$ (2C), 129.6 (2C), 129.3 (2C), 129.0, 128.9, 128.6 (2C), 127.5 (2C), 126.1 (2C), 106.9, 51.9, 51.1, 37.0, 36.3, 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{28}\text{H}_{26}\text{ClNO}_4\text{SNa}^+$: 530.1163; found 530.1170.

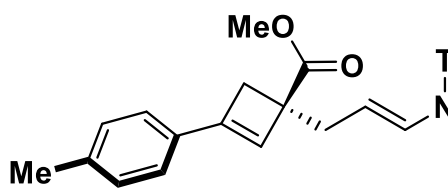


3la. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1.

Yield = 64%, (0.064 mmol, 35.3 mg). **ee** = 92%. $[\alpha]_{\text{D}} =$

-2.1 ($c = 0.63$, CHCl_3). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8

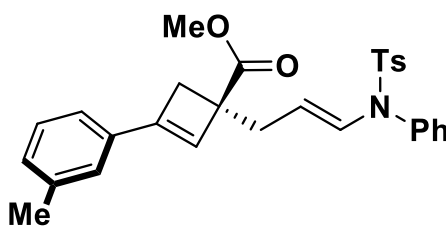
mL/min, $t_{\text{R}} = 23.4$ min, $t_{\text{S}} = 25.7$ min. ^1H NMR (600 MHz, CDCl_3) $\delta = 7.53$ – 7.50 (m, 2H), 7.48 – 7.42 (m, 2H), 7.32 – 7.28 (m, 1H), 7.26 – 7.23 (m, 2H), 7.23 – 7.20 (m, 2H), 7.13 – 7.09 (m, 2H), 7.01 (dt, $J = 13.9, 1.1$ Hz, 1H), 6.87 – 6.83 (m, 2H), 6.22 (s, 1H), 4.36 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 3.62 (s, 3H), 3.02 (d, $J = 12.9$ Hz, 1H), 2.55 (ddd, $J = 13.8, 7.3, 1.2$ Hz, 1H), 2.51 (d, $J = 13.0$ Hz, 1H), 2.48 – 2.43 (m, 4H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 174.6, 145.2, 143.9, 136.6, 135.8, 132.5, 131.5$ (2C), 131.3, 130.0 (2C), 129.6 (2C), 129.3 (2C), 129.2, 128.9, 127.5 (2C), 126.3 (2C), 122.3, 106.9, 51.9, 51.1, 37.0, 36.3, 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{28}\text{H}_{26}\text{BrNO}_4\text{SNa}^+$: 574.0658; found 574.0662.



3ma. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1.

Yield = 52%, (0.052 mmol, 25.3 mg). **ee** = 95%. $[\alpha]_D^{25}$ =

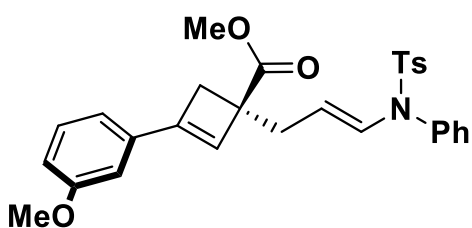
- 11.3 (*c* = 0.43, CHCl₃). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8 mL/min, *t*_(R) = 23.1 min, *t*_(S) = 27.6 min. **¹H NMR** (600 MHz, CDCl₃) δ = 7.54 – 7.49 (m, 2H), 7.31 – 7.28 (m, 1H), 7.26 – 7.23 (m, 2H), 7.20 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.16 – 7.13 (m, 2H), 7.13 – 7.11 (m, 2H), 7.00 (dt, *J* = 13.9, 1.1 Hz, 1H), 6.88 – 6.83 (m, 2H), 6.13 (s, 1H), 4.39 (ddd, *J* = 13.9, 8.1, 7.3 Hz, 1H), 3.61 (s, 3H), 3.02 (d, *J* = 12.9 Hz, 1H), 2.54 (ddd, *J* = 13.8, 7.3, 1.2 Hz, 1H), 2.51 (d, *J* = 12.9 Hz, 1H), 2.47 – 2.42 (m, 4H), 2.35 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃) δ = 175.0, 146.2, 143.8, 138.3, 136.7, 135.8, 131.2, 131.0, 130.1 (2C), 129.5 (2C), 129.3 (2C), 129.0 (2C), 128.8, 127.5 (2C), 127.0, 124.7 (2C), 107.3, 51.8, 51.0, 37.1, 36.5, 21.6, 21.4; **HRMS (ESI)** *m/z*: [M + Na]⁺ calcd. for C₂₉H₂₉NO₄SN⁺: 510.1710; found 510.1714.



3na. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1.

Yield = 69%, (0.052 mmol, 33.6 mg). **ee** = 93%. $[\alpha]_D^{25}$ = - 9.7

(*c* = 0.19, CHCl₃). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 95:5, flow 0.6 mL/min, *t*_(R) = 21.5 min, *t*_(S) = 19.7 min. **¹H NMR** (600 MHz, CDCl₃) δ = 7.55 – 7.50 (m, 2H), 7.31 – 7.27 (m, 1H), 7.26 – 7.23 (m, 2H), 7.21 (td, *J* = 7.7, 2.3 Hz, 3H), 7.12 – 7.07 (m, 2H), 7.05 (d, *J* = 7.6 Hz, 1H), 7.01 (dt, *J* = 14.0, 1.1 Hz, 1H), 6.89 – 6.84 (m, 2H), 6.19 (s, 1H), 4.40 (ddd, *J* = 13.9, 8.1, 7.3 Hz, 1H), 3.61 (s, 3H), 3.03 (d, *J* = 12.9 Hz, 1H), 2.58 – 2.51 (m, 2H), 2.48 – 2.43 (m, 4H), 2.34 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃) δ = 174.9, 146.4, 143.8, 137.9, 136.7, 135.9, 133.6, 131.2, 130.1 (2C), 129.5 (2C), 129.3 (2C), 129.2, 128.8, 128.3, 128.0, 127.5 (2C), 125.4, 121.9, 107.3, 51.8, 51.0, 37.2, 36.5, 21.6, 21.4; **HRMS (ESI)** *m/z*: [M + Na]⁺ calcd. for C₂₉H₂₉NO₄SN⁺: 510.1710; found 510.1704.

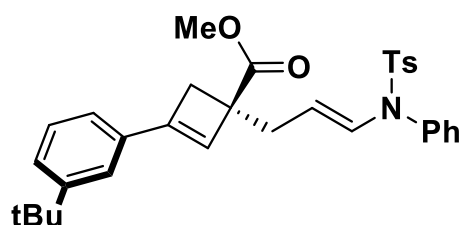


3oa. Colourless oil. FC eluent: *n*-hexane/acetone: 15:1.

Yield = 65%, (0.065 mmol, 32.7 mg). **ee** = 94%. $[\alpha]_D^{25}$ = -

11.8 (*c* = 0.11, CHCl₃). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8 mL/min, *t*_(R) = 17.8 min, *t*_(S) = 20.1 min. **¹H NMR** (600 MHz, CDCl₃) δ = 7.54 – 7.50 (m, 2H), 7.32 – 7.27 (m, 1H), 7.25 – 7.19 (m, 5H), 7.01 (dt, *J* = 13.9, 1.1 Hz, 1H), 6.88 – 6.82 (m, 4H), 6.78 (dd, *J* = 2.6, 1.5 Hz, 1H), 6.21 (s, 1H), 4.39 (ddd, *J* =

13.9, 8.1, 7.3 Hz, 1H), 3.81 (s, 3H), 3.61 (s, 3H), 3.03 (d, $J = 12.9$ Hz, 1H), 2.59 – 2.50 (m, 2H), 2.48 – 2.42 (m, 4H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 174.8, 159.7, 146.2, 143.8, 136.7, 135.8, 135.0, 131.2, 130.1$ (2C), 129.5 (2C), 129.4, 129.3 (2C), 128.8, 128.6, 127.5 (2C), 117.4, 114.1, 110.0, 107.2, 55.3, 51.8, 51.0, 37.2, 36.5, 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{29}\text{H}_{29}\text{NO}_5\text{SNa}^+$: 526.1659; found 526.1651.



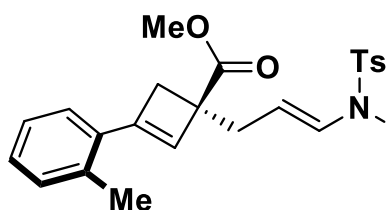
3pa. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1.

Yield = 41%, (0.041 mmol, 21.7 mg). **ee** = 94%. $[\alpha]_{\text{D}} = -$

1.6 ($c = 0.54$, CHCl_3). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 92:8, flow 0.5 mL/min,

$t_{\text{R}} = 19.3$ min, $t_{\text{S}} = 18.1$ min. ^1H NMR (600 MHz, CDCl_3)

$\delta = 7.54 - 7.51$ (m, 2H), 7.35 – 7.30 (m, 2H), 7.30 – 7.27 (m, 1H), 7.26 – 7.22 (m, 3H), 7.20 – 7.16 (m, 2H), 7.06 (dt, $J = 7.5, 1.4$ Hz, 1H), 7.02 (dt, $J = 14.0, 1.1$ Hz, 1H), 6.90 – 6.84 (m, 2H), 6.21 (s, 1H), 4.40 (ddd, $J = 13.9, 8.1, 7.3$ Hz, 1H), 3.61 (s, 3H), 3.06 (d, $J = 12.9$ Hz, 1H), 2.59 – 2.52 (m, 2H), 2.50 – 2.42 (m, 4H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 174.9, 151.3, 146.7, 143.8, 136.7, 135.8, 133.3, 131.2, 130.1$ (2C), 129.5 (2C), 129.3 (2C), 128.8, 128.1, 127.8, 127.5 (2C), 125.6, 122.0, 121.5, 107.4, 51.8, 51.0, 37.3, 36.6, 34.7, 31.3 (3C), 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{32}\text{H}_{35}\text{NO}_4\text{SNa}^+$: 522.2179; found 522.2186.

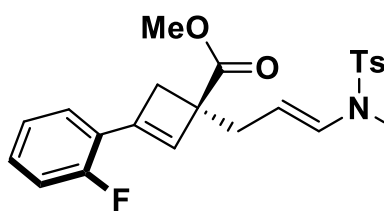


3qa. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield

= 32%, (0.032 mmol, 15.6 mg). **ee** = 88%. $[\alpha]_{\text{D}} = -7.6$ ($c =$

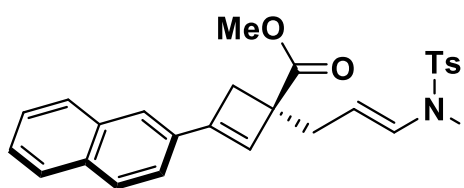
0.38, CHCl_3). **HPLC analysis:** OD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.6 mL/min, $t_{\text{R}} = 23.2$

min, $t_{\text{S}} = 18.2$ min. ^1H NMR (600 MHz, CDCl_3) $\delta = 7.54 - 7.49$ (m, 2H), 7.30 – 7.27 (m, 1H), 7.25 – 7.22 (m, 2H), 7.22 – 7.14 (m, 5H), 7.07 (dd, $J = 7.3, 1.7$ Hz, 1H), 7.01 (dd, $J = 14.0, 1.1$ Hz, 1H), 6.86 – 6.81 (m, 2H), 6.07 (s, 1H), 4.41 (ddd, $J = 13.9, 8.3, 7.1$ Hz, 1H), 3.62 (s, 3H), 3.13 (d, $J = 12.8$ Hz, 1H), 2.59 (d, $J = 12.8$ Hz, 1H), 2.55 (ddd, $J = 13.8, 7.1, 1.3$ Hz, 1H), 2.48 (ddd, $J = 13.8, 8.3, 1.0$ Hz, 1H), 2.44 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3) $\delta = 175.0, 146.0, 143.8, 137.2, 136.7, 135.8, 132.2, 131.8, 131.2, 130.6, 130.0$ (2C), 129.5 (2C), 129.3 (2C), 128.8, 128.2, 127.5 (2C), 126.6, 125.8, 107.2, 51.9, 51.2, 38.4, 36.4, 21.8, 21.6; **HRMS (ESI)** m/z : $[\text{M} + \text{Na}]^+$ calcd. for $\text{C}_{29}\text{H}_{29}\text{NO}_4\text{SNa}^+$: 510.1710; found 510.1711.



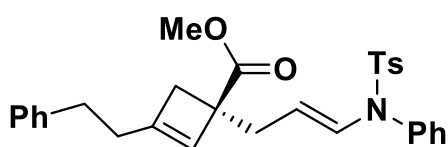
3ra. Colourless oil. FC eluent: *n*-hexane/acetone: 15:1. Yield = 51%, (0.051 mmol, 25.0 mg). **ee** = 86%. $[\alpha]_D = -10.0$ (*c* = 0.15, CHCl₃). **HPLC analysis:** AD-H column (254 nm), 30 °C, method: *n*-Hex:IPA = 90:10, flow 0.6 mL/min, *t*_(R) = 26.8

min, *t*_(S) = 24.4 min. **¹H NMR** (600 MHz, CDCl₃) δ = 7.54 – 7.51 (m, 2H), 7.31 – 7.27 (m, 1H), 7.25 – 7.23 (m, 3H), 7.23 – 7.18 (m, 2H), 7.14 – 7.07 (m, 2H), 7.06 – 7.00 (m, 2H), 6.88 – 6.83 (m, 2H), 6.28 (d, *J* = 3.0 Hz, 1H), 4.40 (ddd, *J* = 13.9, 8.1, 7.2 Hz, 1H), 3.62 (s, 3H), 3.10 (d, *J* = 13.0 Hz, 1H), 2.57 (dd, *J* = 13.4, 7.5 Hz, 2H), 2.50 – 2.45 (m, 1H), 2.44 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃) δ = 174.6, 161.2 (d, *J* = 252.2 Hz), 143.8, 140.8, 136.7, 135.8, 133.6 (d, *J* = 7.4 Hz), 131.3, 130.0 (2C), 129.7 (d, *J* = 7.6 Hz), 129.5 (2C), 129.4 (d, *J* = 4 Hz), 129.3, 129.3 (2C), 128.8, 127.5 (2C), 127.3 (d, *J* = 4.5 Hz), 115.56 (d, *J* = 21.0 Hz), 107.1, 52.4, 51.9, 38.1, 36.4, 21.6; **¹⁹F NMR** (565 MHz, CDCl₃) δ = -113.43 – -114.19 (m, 1F); **HRMS (ESI)** *m/z*: [M + Na]⁺ calcd. for C₂₈H₂₆FNO₄SN⁺: 514.1459; found 514.1452.



3sa. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1. Yield = 57%, (0.057 mmol, 29.8 mg). **ee** = 94%. $[\alpha]_D = -4.5$ (*c* = 0.11, CHCl₃). **HPLC analysis:** AD-H column (280 nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.8

mL/min, *t*_(R) = 28.1 min, *t*_(S) = 23.6 min. **¹H NMR** (600 MHz, CDCl₃) δ = 7.83 – 7.79 (m, 2H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.60 (s, 1H), 7.53 – 7.50 (m, 2H), 7.50 – 7.47 (m, 2H), 7.45 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.23 – 7.20 (m, 2H), 7.19 – 7.16 (m, 2H), 7.06 – 7.02 (m, 2H), 6.87 – 6.84 (m, 2H), 6.32 (s, 1H), 4.42 (ddd, *J* = 13.9, 8.1, 7.2 Hz, 1H), 3.64 (s, 3H), 3.16 (d, *J* = 12.8 Hz, 1H), 2.65 (d, *J* = 12.8 Hz, 1H), 2.60 (ddd, *J* = 13.9, 7.3, 1.2 Hz, 1H), 2.50 (ddd, *J* = 13.8, 8.2, 1.0 Hz, 1H), 2.40 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃) δ = 174.9, 146.3, 143.8, 136.7, 135.8, 133.2, 131.3, 130.1 (2C), 129.5 (2C), 129.3 (2C), 128.9, 128.8, 128.2, 128.0, 127.8, 127.5, 127.3 (2C), 126.5, 126.3, 123.9, 122.5, 121.8, 107.1, 51.9, 51.2, 37.1, 36.5, 21.6; **HRMS (ESI)** *m/z*: [M + Na]⁺ calcd. for C₃₂H₂₉NO₄SN⁺: 546.1710; found 546.1703.



3ta. Colourless oil. FC eluent: *n*-hexane/EtOAc: 10:1.

Yield = 38%, (0.038 mmol, 19.0 mg). **ee** = 81%. $[\alpha]_D^{25} = -$

3.5 (*c* = 0.13, CHCl₃). **HPLC analysis:** AD-H column (230

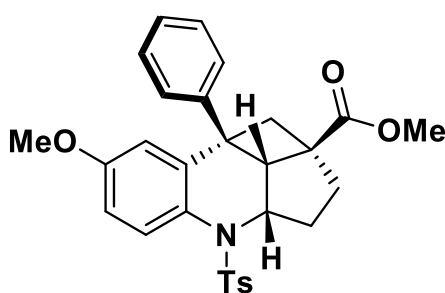
nm), 30 °C, method: *n*-Hex:IPA = 85:15, flow 0.7 mL/min,

$t_{(R)} = 11.2$ min, $t_{(S)} = 12.6$ min. **¹H NMR** (600 MHz, CDCl₃)

$\delta = 7.55 - 7.51$ (m, 2H), 7.36 – 7.30 (m, 3H), 7.30 – 7.23 (m, 4H) partially overlapped with the residual solvent peak, 7.21 – 7.17 (m, 1H), 7.16 – 7.13 (m, 2H), 6.97 (dt, *J* = 13.9, 1.1 Hz, 1H), 6.95 – 6.91 (m, 2H), 5.69 (t, *J* = 1.6 Hz, 1H), 4.34 (dt, *J* = 13.9, 7.7 Hz, 1H), 3.58 (s, 3H), 2.72 – 2.63 (m, 3H), 2.44 (ddd, *J* = 13.8, 7.2, 1.2 Hz, 1H), 2.41 (s, 3H), 2.33 (dd, *J* = 13.8, 8.1 Hz, 1H), 2.30 – 2.21 (m, 2H), 2.16 (d, *J* = 13.0 Hz, 1H); **¹³C NMR** (151 MHz, CDCl₃) $\delta = 175.2, 150.5, 143.8, 141.5, 136.8, 135.9, 130.9, 130.1$ (2C), 129.7, 129.5 (2C), 129.4 (2C), 128.9, 128.4 (2C), 128.2 (2C), 127.5 (2C), 126.0, 107.7, 51.7, 51.5, 39.8, 36.6, 32.7, 32.5, 21.6; **HRMS (ESI)** *m/z*: [M + Na]⁺ calcd. for C₃₀H₃₁NO₄SN⁺: 524.1866; found 524.1873.

4. Preparation of Compound 4ag

In flame-dried small round bottom flask, compound **3ag** (50.3 mg, 0.1 mmol) was dissolved in dry DCM (0.5 mL) and HCl (4 M in 1,4-dioxane, 0.1 mL, 0.4 mmol) was added. The resulting mixture was stirred at room temperature for 3 h, after which it was directly purified by FC on silica gel to afford pure product **4ag**. For the assignment of the relative and absolute configuration see section 6.

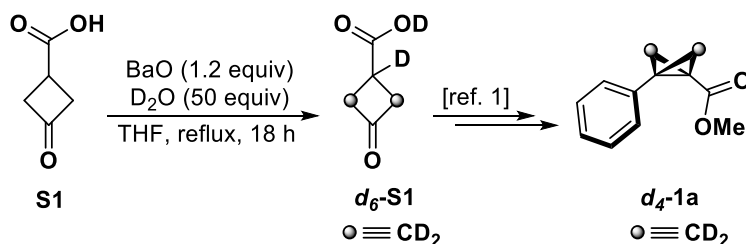


4ag. White foam. FC eluent: *n*-hexane/EtOAc: 8:1. Yield = 82%, (0.082 mmol, 41.2 mg). **ee** = 92%. $[\alpha]_D^{25} = -32.3$ (*c* = 0.30, CHCl₃). **HPLC analysis**: ID column (254 nm), 30 °C, method: *n*-Hex:IPA = 92:8, flow 0.9 mL/min, $t_{(major)}$ = 66.9 min, $t_{(minor)}$ = 54.7 min. **¹H NMR** (600 MHz, CDCl₃) δ = 7.76 (d, *J* = 9.0 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.11 – 7.06 (m, 2H),

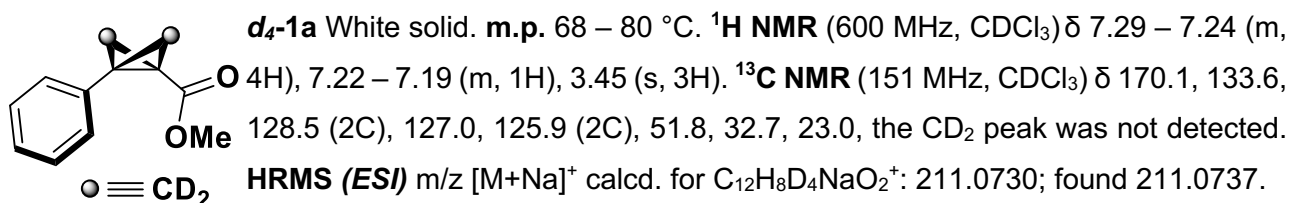
7.06 – 7.01 (m, 1H), 7.01 – 6.96 (m, 2H), 6.78 (dd, *J* = 9.1, 3.0 Hz, 1H), 6.57 – 6.51 (m, 2H), 6.29 (d, *J* = 3.0 Hz, 1H), 5.11 (ddd, *J* = 10.8, 8.7, 7.2 Hz, 1H), 3.67 (s, 3H), 3.67 (s, 3H), 3.54 (dd, *J* = 13.6, 2.3 Hz, 1H), 3.00 (dd, *J* = 8.8, 2.2 Hz, 1H), 2.34 (s, 3H), 2.25 (dt, *J* = 13.1, 6.7 Hz, 1H), 2.17 (d, *J* = 13.3 Hz, 1H), 2.03 – 1.94 (m, 1H), 1.90 (td, *J* = 12.7, 6.6 Hz, 1H), 1.75 (dd, *J* = 12.6, 6.7 Hz, 1H); **¹³C NMR** (151 MHz, CDCl₃) δ = 176.0, 157.7, 147.2, 143.5, 139.2, 136.5, 129.8 (2C), 128.7, 128.0 (2C), 127.4 (2C), 126.4 (2C), 126.1 (2C), 125.5, 113.3, 113.0, 58.5, 55.3, 52.2, 51.0, 47.8, 43.2, 39.0, 33.8, 30.2, 21.6; **HRMS (ESI)** *m/z*: [M + Na]⁺ calcd. for C₂₉H₂₉NO₅SNa⁺: 526.1659; found 526.1663.

5. Deuteration Experiments

5.1 Preparation and Characterization of **d₄-1a**

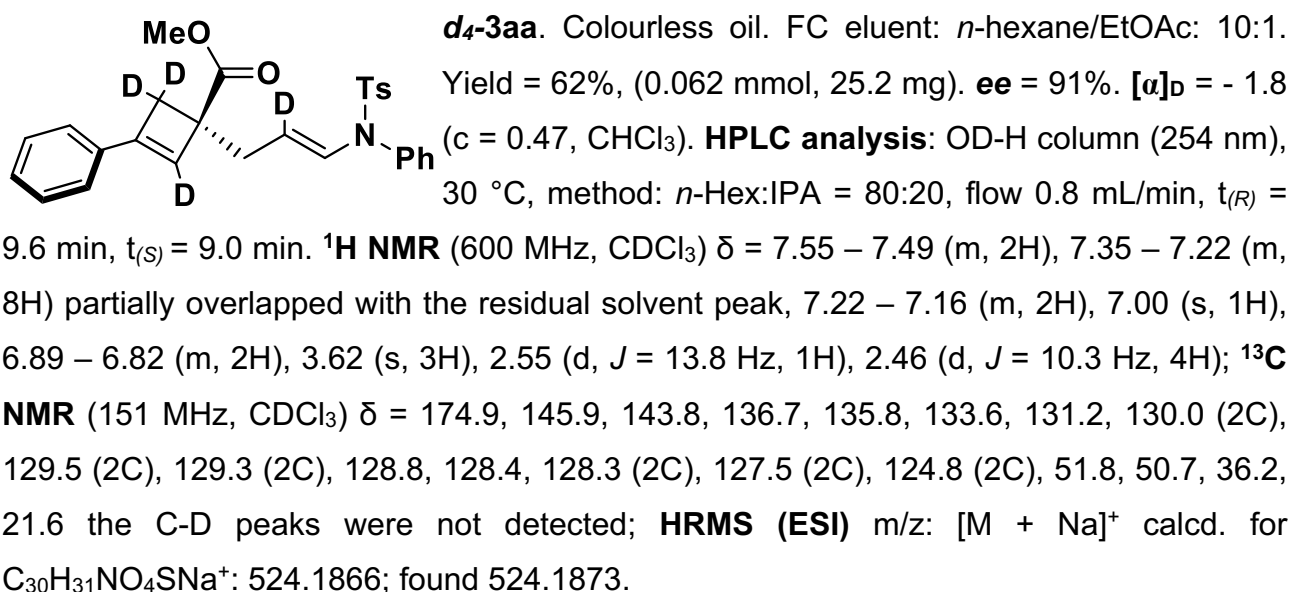


Product **d₄-1a** was obtained following the same literature procedure employed for all other compounds **1**,^{Error. L'argomento parametro è sconosciuto.} starting from **d₆-12**. This was obtained by deuteration of **12** following an unmodified reported procedure.⁷



5.1 Preparation and Characterization of **d₄-3aa**

Product **d₄-3aa** was obtained following general procedure **B** starting from **d₄-1a**.

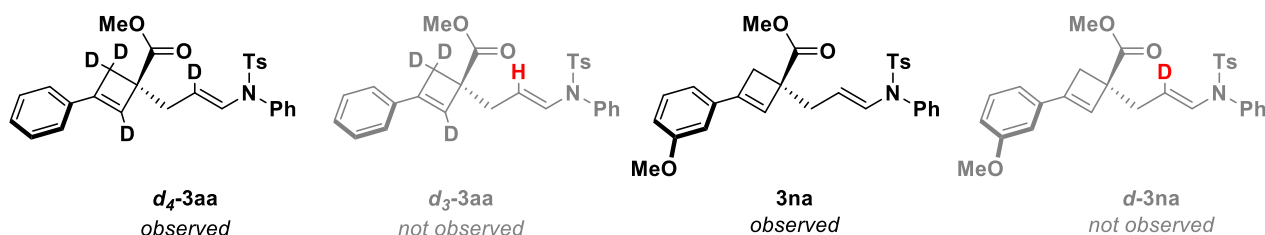


5.2 Determination of KIE

The KIE was calculated by employing the competition method, subjecting an excess of **1a** (2.5 equiv, 0.25 mmol, 47.0 mg), an excess of **d₄-1a** (2.5 equiv, 0.25 mmol 48.0 mg) and allenamide **2a** (1.0 equiv, 0.1 mmol, 28.5 mg) to general procedure B. After column chromatography, the product was isolated as a 1.7:1 mixture of **3aa** and **d₄-3aa** in 59% yield (0.059 mmol, 27.9 mg).

5.3 Crossover Experiment

In this experiment, **1a** (1.5 equiv, 0.15 mmol, 28.2 mg), **1n** (1.5 equiv, 0.15 mmol 32.7 mg) and allenamide **2a** (1.0 equiv, 0.1 mmol, 28.5 mg) were subjected to general procedure B. After column chromatography, only products **d₄-3aa** and **3na** (56% isolated yield) were isolated. Putative products **d₃-3aa** and **d-3na** were not observed, indicating no crossover and an intramolecular mechanism for the protodeauration step.



6. Determination of the Absolute Configuration

6.1 Assignment of the relative configuration

Since we were not able to obtain single crystals from compounds **3** or **4ag**, we turned on a widely adopted approach, involving the comparison of experimental and theoretical electronic circular dichroism (ECD) spectra, which has proven to be a reliable method for absolute configuration assignment.⁸

Compound **4ag** was selected as the prototype for the assignment of the relative and absolute configuration. Its chemical structure and ¹H/¹³C assignment were confirmed by 2D-NMR investigation, while the relative configuration of the four stereogenic carbons was then assigned by NOE experiments. Hereafter the atom numbering is reported in Table S1.

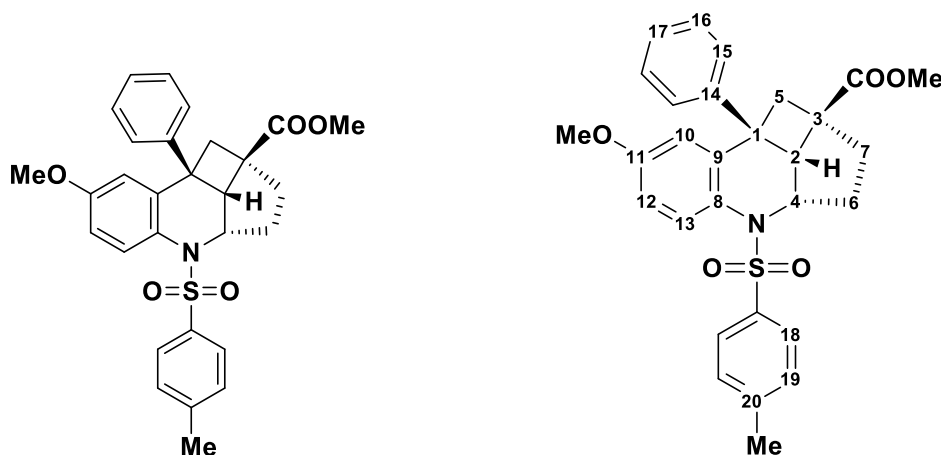


Table S1. Atom numbering and full assignment of the NMR signals of **4ag**

Label	¹³ C	¹ H	note
1	38.9	-	HMBC with H _{5'} , H _{5''} , H ₄ , H ₁₅
2	50.1	3.06	HMBC with COOMe and C ₁₄
3	47.6	-	HMBC with H ₇ , H ₆ , H _{5'} , H _{5''}
4	58.2	5.03	
5	42.8	3.50 and 2.21	² J = 13.5 Hz, ⁴ J with 3.06 ppm = 2.2 Hz
6	29.9	2.15 and 1.90	m, coupled with H ₄ at 5.03 by COSY
7	33.0	1.89 and 1.74	m, assigned by HMBC with COOMe
8	125.7	-	HMBC with H ₁₀ , H ₁₂ , H ₁₃ and H ₄
9	139.8	-	HMBC with H ₁₃ , H _{5'} and H _{5''}
10	113.1	6.35	d, ⁴ J = 2.9 Hz
11	157.9		HMBC from 3.64 ppm (Ar-OMe)
12	112.7	6.81	dd, J = 9.0; 2.9 Hz

13	128.2	7.64	d, $J = 9.0$ Hz
14	147.5	-	HMBC with H ₁₅ , H ₂ , H _{5'} and H _{5''}
15	126.4	6.62 (2H)	COSY with H ₁₆ and H ₁₇
16	128.1	7.06 (2H)	Overlapped with H ₁₇ , HMBC with 147.5
17	125.7	7.07	Overlapped with H ₁₆
18	127.3	7.61 (2H)	AA'BB', 2H
19	130.1	7.26 (2H)	AA'BB', 2H, HMBC from Ar-Me
20	144.3	-	HMBC from 2.40 ppm (Ar-Me)
Ar-Me	20.5	2.40	
Ar-OMe	55.0	3.64	
COOMe	175.4 (CO) 51.44 (OMe)	3.58 (Me)	

Backbone assignment

HSQC spectra showed the presence of three CH₂ and 6 diastereotopic hydrogens, with an isolated CH₂ (3.50 and 2.21 ppm for ¹H, 42.75 ppm for ¹³C), developing a simple AB signal. The diastereotopic hydrogen at 3.50 ppm shows a very small coupling constant with the signal at 3.06 ppm (⁴J; 2.2 Hz). Two CHs were observed at 3.06 ppm (50.20 ppm for ¹³C) and 5.03 (58.27 for the ¹³C) ppm. The latter corresponds to the CH bound to the nitrogen. This was confirmed by HMBC showing J coupling with the quaternary aromatic carbon (C₈), that was unambiguously identified by HMBC correlation with H₁₀, H₁₂ and H₁₃. The CH at 3.06 ppm shows a ¹J_{CH} of 148.2 Hz, compatible with the known values for cyclobutane rings.⁹ Similar ¹J_{CH} were observed for the two hydrogens at 3.50 and 2.21 ppm (142.0 Hz). COSY spectra allowed to connect the hydrogen at 5.03 ppm with that at 3.06, and to the two diastereotopic hydrogens at 2.15 and 1.90 ppm (H_{6'} and H_{6''}). Weak ⁴J couplings were also observed with H_{7'} and H_{7''} at 1.89 and 1.74 ppm, respectively. Finally, HMBC allowed to observe the ³J relationship of the hydrogen at 3.06 with the aromatic C₁₄ quaternary carbon and to the carbonyl at 175.0 ppm.

Relative configuration

The relative configuration of the four stereocarbons was assigned by NOE analysis, using the DPGFSE-NOE 1D sequence.¹⁰

On saturation of the H₂ hydrogen at 3.06 ppm (Figure S1), strong NOE was observed on H₄, on the ortho hydrogens of the 1-phenyl ring (H₁₅), and on the hydrogens of the tosyl moiety

(H₁₈). This implies that H₂ is *syn* to the phenyl ring on C₁, and H₄ is *syn* to H₂ too. Weak and similar NOEs were observed on H_{5'} and H_{7'}, thus H_{7'} must be *anti* with respect to H₂.

On saturation of H₄ (Figure S2), in addition to the expected NOE on H₂, strong NOEs were observed on H_{6'} and H_{7'}, and again on H₁₈ on the tosyl moiety. This further confirms that the aromatic ring of tosyl moiety is close to H₂ and H₄.

Finally, saturation of the ortho hydrogens of the 1-phenyl ring (H₁₅, Figure S3) yielded NOE on H₁₀, H_{5'} and H₂. These confirms the *syn* relationship of the 1-phenyl with respect to H₂ and assigns the signal of H_{5'} at 3.50 ppm. Weaker NOEs were observed on the hydrogens of the tosyl moiety (H₁₈ and H₁₉), further confirming that the main conformations place the phenyl ring of the tosyl moiety on the same side of the 1-phenyl of H₂ and H₄.

All NOEs data are in very good agreement with the 1*R**,2*R**,3*R**,4*S** relative configuration (numbering as from Table S1).

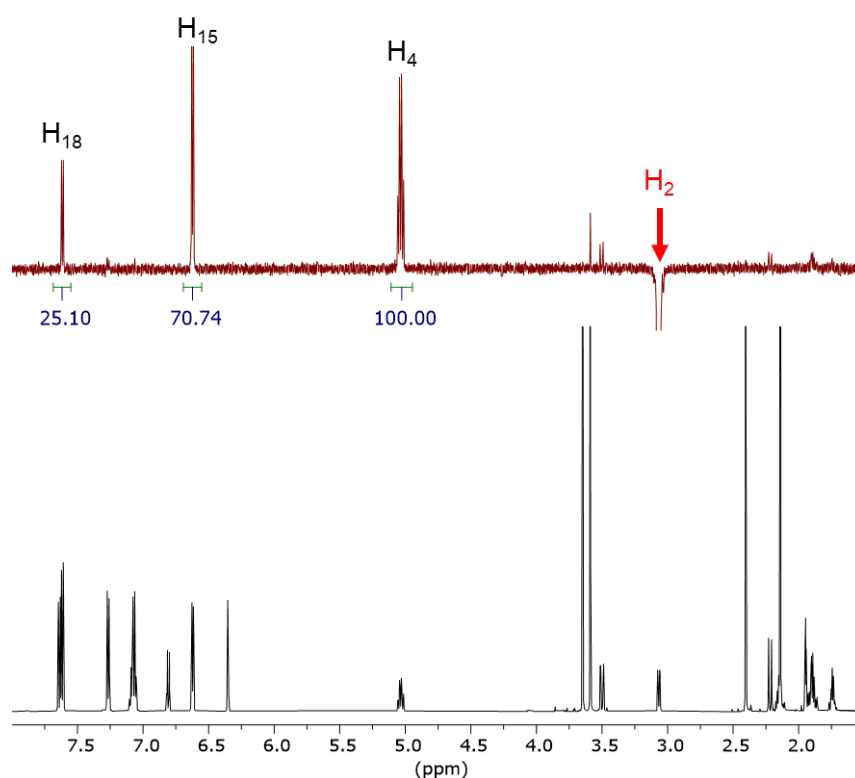


Figure S1. DPGSE-NOE of compound **4ag** (600 MHz in CD₃CN). Bottom: ¹H control spectrum. Top: NOE spectrum with saturation of H₂ at 3.06 ppm (50 Hz-wide R-SNOB shaped pulse). Key integrations, relative to the NOE intensity of H₄, are reported.

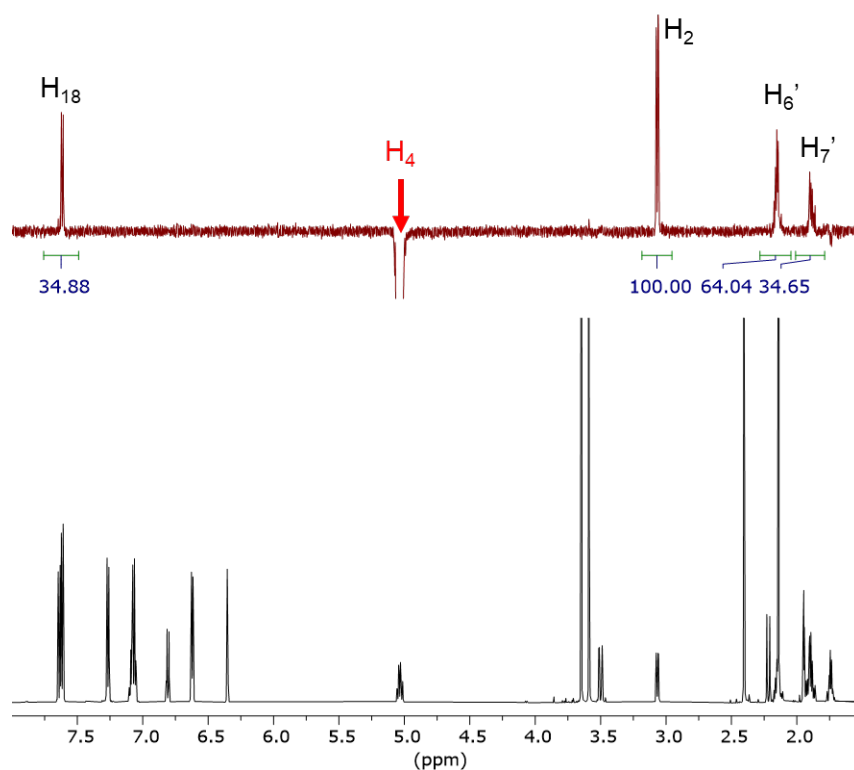


Figure S2. DPGSE-NOE of compound **4ag** (600 MHz in CD₃CN). Bottom: ¹H control spectrum. Top: NOE spectrum with saturation of H₄ at 5.03 ppm (50 Hz-wide R-SNOB shaped pulse). Key integrations, relative to the NOE intensity of H₂, are reported.

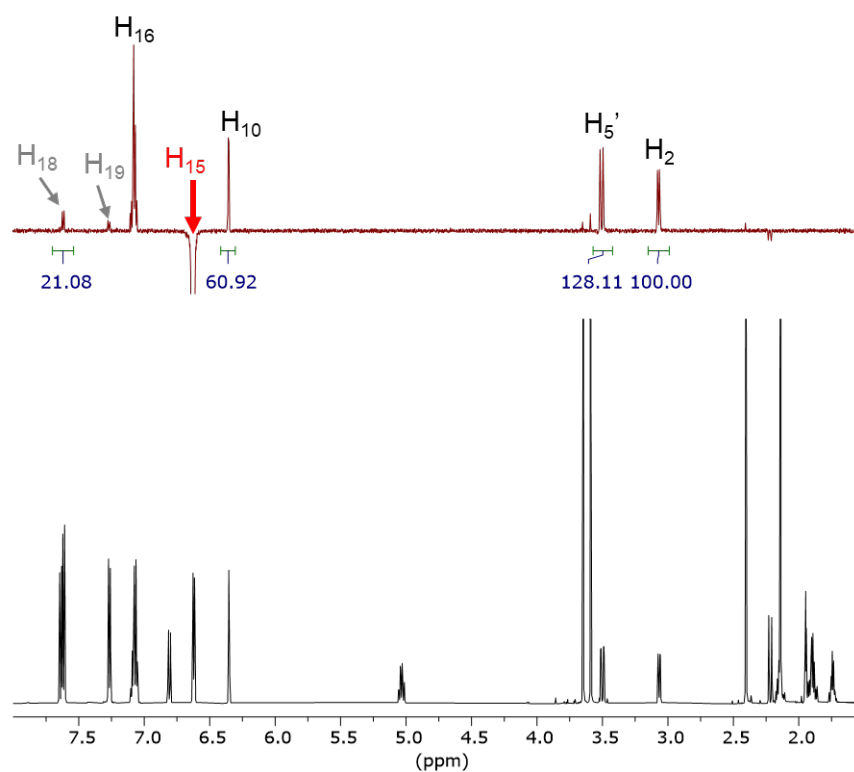


Figure S3. DPGSE-NOE of compound **4ag** (600 MHz in CD₃CN). Bottom: ¹H control spectrum. Top: NOE spectrum with saturation of H₁₅ at 6.62 ppm (50 Hz-wide R-SNOB shaped pulse). Key integrations, relative to the NOE intensity of H₂, are reported.

Two additional NOE experiments were acquired by saturation of the COOMe signal at 3.58 ppm and by saturation of the aromatic OMe at 3.64 ppm, to further investigate the conformational preferences of the two moieties (Figure S4). When the aromatic OMe group is saturated (Figure S4, top), nearly equivalent NOEs were observed on H₁₀ and H₁₂, suggesting that the two different conformations available for OMe are $\approx$ 1:1 populated. When the COOMe signal was saturated (Figure S4, middle trace), weak NOEs (due to the larger distance) were observed on H₁₅ and H₂ with similar intensity. This means that both conformations corresponding to 180° rotation of the COOMe moiety are populated in a $\approx$ 1:1 ratio.

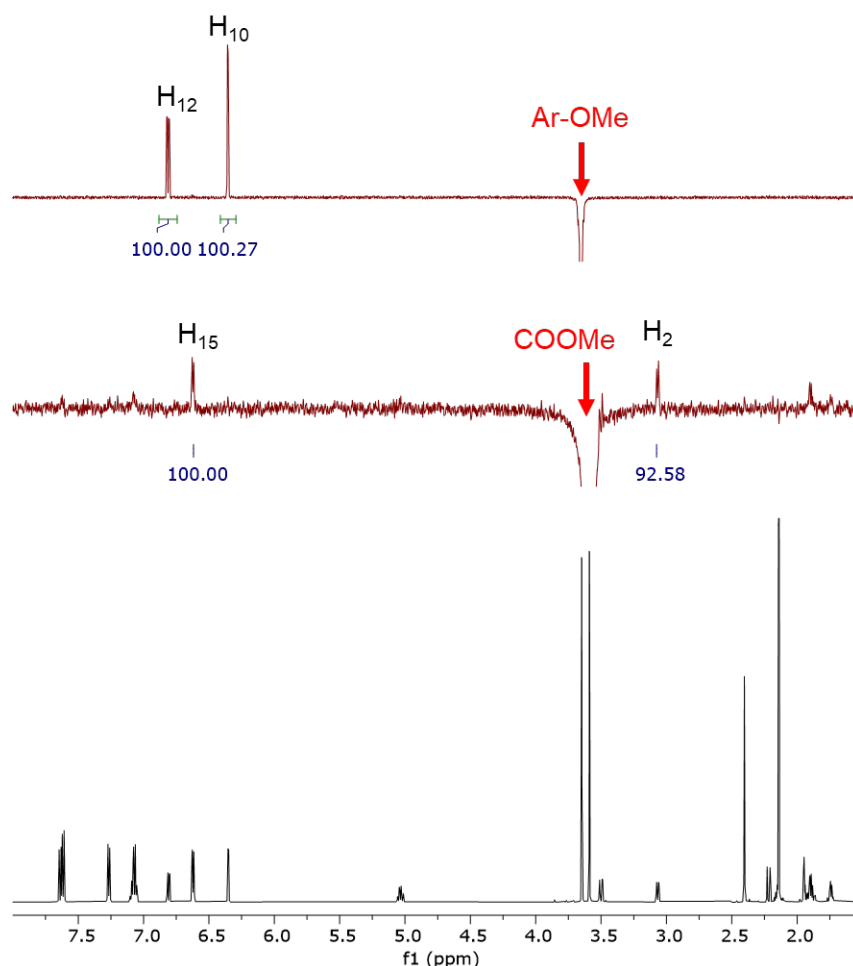


Figure S4. DPGSE-NOE of compound **4ag** (600 MHz in CD₃CN). Bottom: ¹H control spectrum. Middle trace: saturation of COOMe signal at 3.58 ppm. Top trace: saturation of Ar-OMe signal at 3.64 ppm. Both NOE spectra were recorded using a 25 Hz-wide R-SNOB shaped pulse. Integrations are relative within each spectrum.

6.2 Assignment of the Absolute Configuration

Conformational analysis

Taking into consideration the relative configuration determined by NMR analysis, the conformational space of compound **4ag** was sampled using CREST (version 2.12),¹¹ using a meta-dynamic calculation at the tight-binding GFN2-xTB¹² level, and considering acetonitrile as an implicit solvation thanks to the ALPB theory.¹³ The resulting ensemble was then partitioned into 30 clusters based on Principal Component Analysis (PCA) on dihedral angles (geometries were named as **c1-c30**). The 30 unique conformers from the output (geometries) were further optimized, sorted and pruned using ORCA (release 6.1.0)¹⁴ at the B3LYP-D4/def2-SVP [CPCM(acetonitrile)].

After this step, only 8 conformations were found within a 2 kcal/mol range with respect to the global minimum (**c4**, **c8**, **c10**, **c11**, **c12**, **c13**, **c14**, **c15** in the CREST output file).

Final optimization was obtained with Gaussian 16¹⁵ using full optimization at the B3LYP-GD3BJ/6-311G(d,p) and M06-2X/6-311G(d,p) level of theory. After this step, conformation **c12** was found to be superimposable to **c8** and it was therefore removed from the ensemble. Frequency analysis confirmed that all the optimized structures corresponded to energy minima (no imaginary frequency). For thermochemistry evaluation and Boltzmann distribution, calculated frequencies were then dumped using mRRHO¹⁶ theory (with cut-off set at 100 cm⁻¹, using 298K as temperature, 1M as concentration and 1 bar as pressure).¹⁷ Table S2 summarizes the relative calculated energies, and the populations derived from dumped energies at 298K.

Table S2. Summary of relative energies among conformations of **4ag** (energies in kcal/mol).

Opt. meth.	B3LYP-D3BJ/6-311G(d,p) IEF-PCM(acetonitrile)				M06-2x/6-311G(d,p) IEF-PCM(acetonitrile)			
Conf.	ΔH°	ΔG°	d- ΔG° (100 cm ⁻¹)	Pop %	ΔH°	ΔG°	d- ΔG° (100 cm ⁻¹)	Pop %
c8	0.47	0.40	0.34	18	0.32	0.46	0.20	21
c10	0.79	0.41	0.47	14	0.53	0.83	0.45	14
c4	0.00	0.00	0.00	31	0.00	0.22	0.01	29
c11	0.37	0.06	0.20	22	0.22	0.00	0.00	29
c13	1.28	0.86	1.04	6	1.71	1.12	1.28	3
c13b	1.97	1.22	1.32	3	1.96	1.84	2.08	1
c15b	1.62	1.10	1.16	4	1.09	2.71	1.56	2
c15	1.61	0.77	1.56	2	1.92	1.57	1.76	1
c14	4.73	1.91	3.34	0	4.83	2.22	3.92	0
c14b	4.37	1.58	2.99	0	4.05	3.22	3.46	0

Since the main scaffold is relatively rigid, conformational flexibility mainly arises from rotation of the phenyl ring at C1 and from rotation of the COOMe and OMe substituents. In addition, nitrogen inversion can position the tosyl ring either above or below the mean plane of the six-membered heterocycle.

When the tosyl and phenyl rings are oriented on the same side of the ring, stacking interactions may occur, either in a face-to-face or an edge-to-face arrangement, the latter corresponding to a 90° rotation of the C1 phenyl ring.

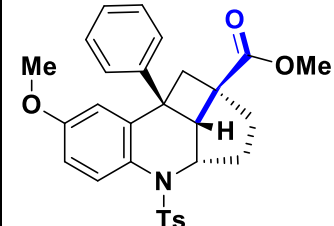
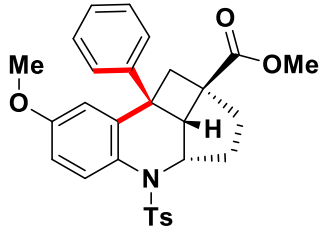
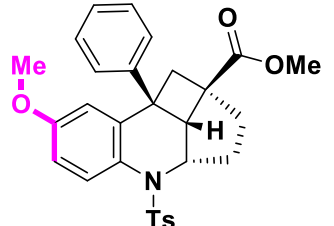
Within the conformational set examined here, all geometries except **c14** place the tosyl and phenyl rings on the same side of the six-membered ring, whereas in **c14** the tosyl ring is oriented outward. Notably, this conformation is the highest in energy among the eight considered, in agreement with NOE experiments indicating that the tosyl and phenyl rings remain in close spatial proximity. Indeed, strong NOEs were observed for H₁₅ and H₁₈ upon saturation of H₂ (see Figure S1).

Conformations **c8**, **c4**, **c10**, and **c11** arise from the four possible combinations generated by 180° rotation of the COOMe and Ar-OMe groups, with the phenyl ring arranged in a face-to-face orientation with the tosyl ring. Conformations **c13** and **c15** differ from these four in that the phenyl ring adopts an edge-to-face arrangement relative to the tosyl ring. In analogy with

the previous observations, two additional geometries (**c13b** and **c15b**) were generated by rotating the OMe group, mirroring the situation in conformations **c8**, **c4**, **c10**, and **c11**. Full optimization was obtained with the same above-mentioned DFT levels of theory.

In summary, the primary conformational distinction concerns the relative orientation of the two aromatic rings, which may engage in either face-to-face stacking or face-to-edge interactions. The remaining six stacked conformations of Table S2 are produced from the various combinations of COOMe and Ar-OMe rotations. Table S3 summarizes the geometrical parameters of the optimized geometries, and Figure S5 shows the 3D-structure of the ten conformations.

Table S3. Geometrical parameters of the best conformations of compound **4ag** with B3LYP-D3BJ/6-311g(d,p) optimization. Geometric parameters from M06-2x optimizations are reported in parenthesis. Except for **c14** and **c14b**, the tosyl ring is stacked with the 1-phenyl group.

Conf.			
c8	13 (14)	0 (0)	0 (-1)
c10	13 (14)	0 (-1)	180 (179)
c4	-121 (-122)	17 (12)	0 (-1)
c11	-121 (-122)	17 (13)	180 (180)
c13	-117 (-113)	85 (84)	0 (-1)
c13b	-118 (-114)	86 (85)	180 (179)
c15b	113 (125)	85 (84)	0 (-1)
c15	110 (125)	85 (85)	180 (179)
c14 (N-inv.)	-118 (-119)	31 (30)	180 (180)
c14b (N-inv.)	-117 (-112)	79 (80)	180 (180)

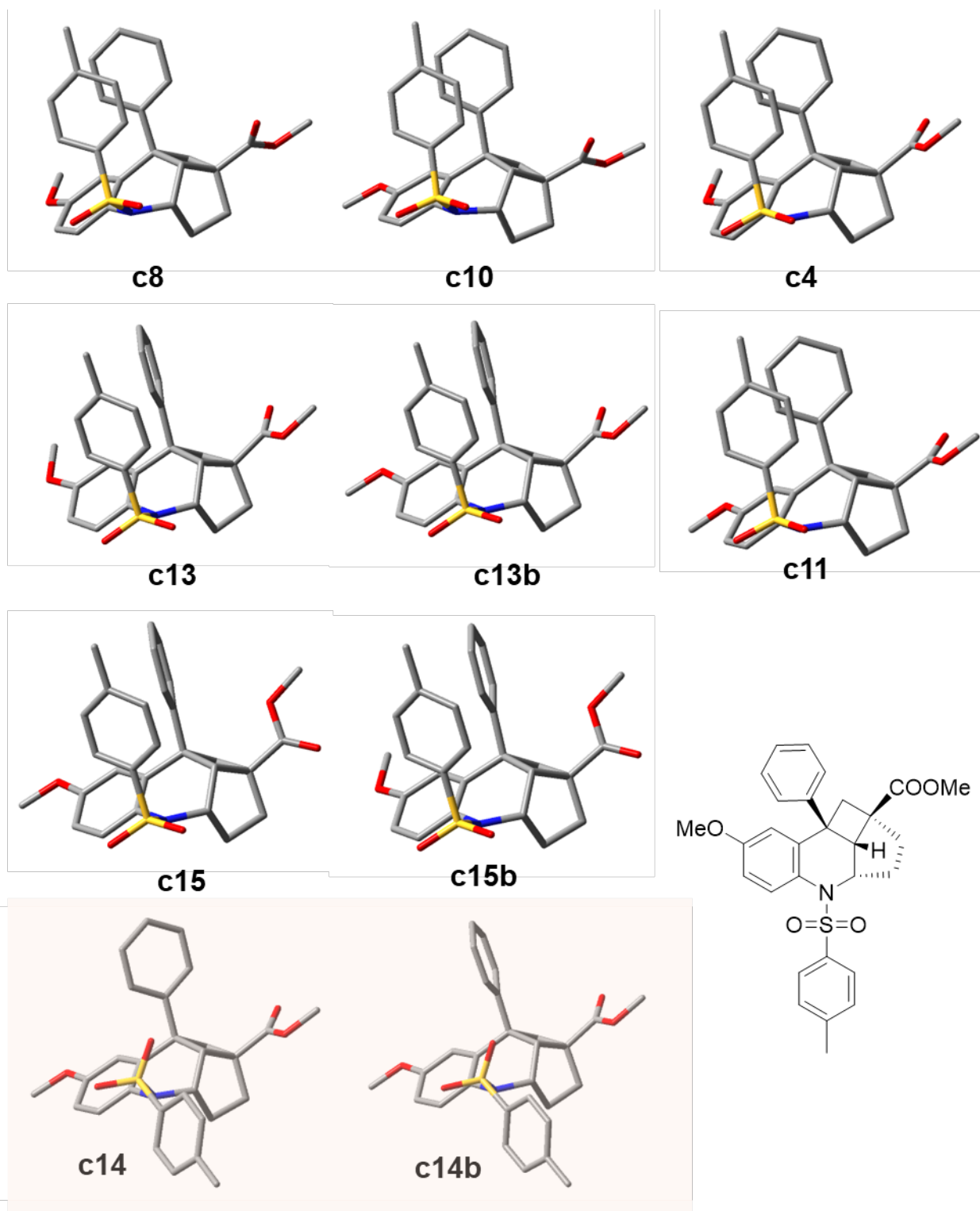


Figure S5. 3D structures of the 8 stacked conformations and the first 2 "open" conformations.

Absolute Configuration

Given the presence of strong UV chromophores, the absolute configuration was determined by TD-DFT simulation of the Electron Circular Dichroism (ECD) spectra.¹⁸

The UV and ECD spectra of **4ag** were recorded on a sample with 92% ee using a JASCO J-810 spectropolarimeter. The acquisition was carried out with a cell path of 0.1 cm in the 185-400 nm range, using hypergrade LC-MS acetonitrile (Merck), at a concentration of $\approx 1 \cdot 10^{-4}$ M, in order to obtain a maximum absorbance between 0.7 and 0.9 in the UV/vis spectrum. The acquisition is an average of 8 scans at a scan rate of $50 \text{ nm} \cdot \text{min}^{-1}$ (Figure S6)

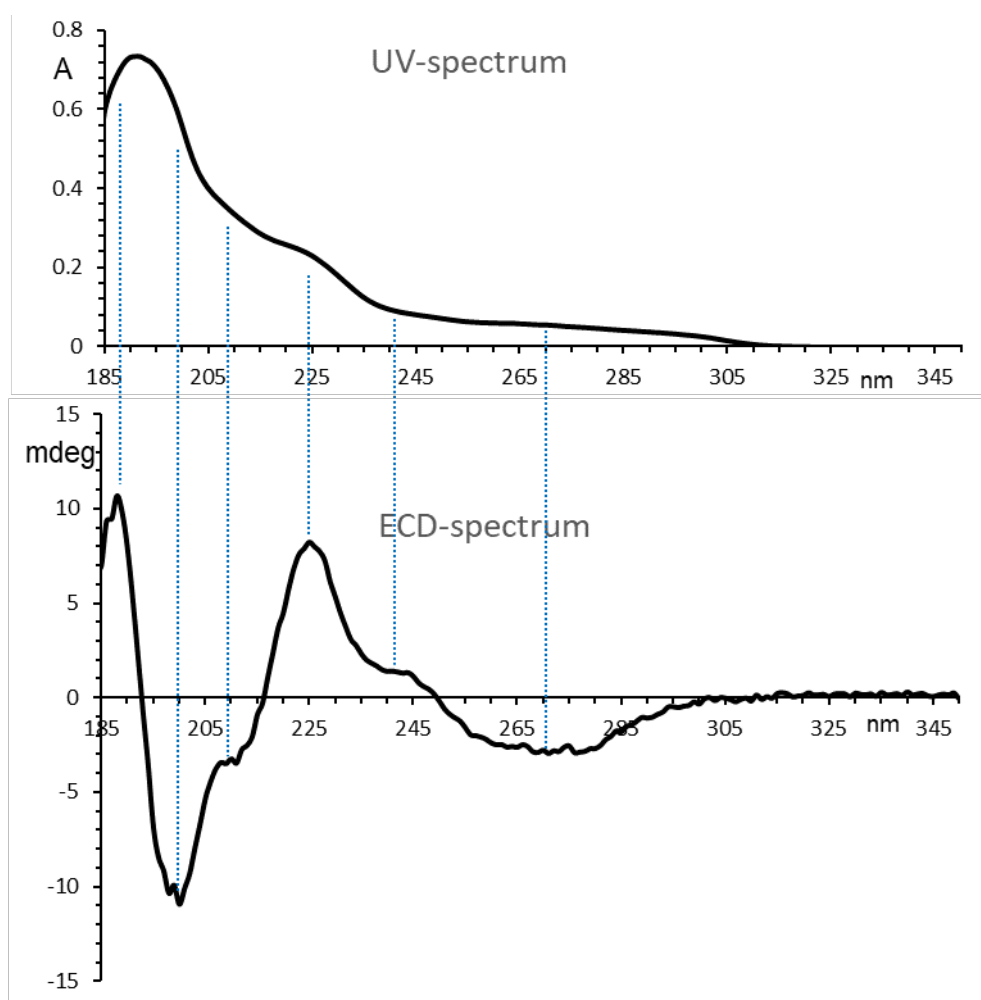


Figure S6. UV and ECD spectrum of **4ag** in acetonitrile ($\approx 1 \cdot 10^{-4}$ M, 0.1 path length).

The ECD spectrum shows two broad bands: one negative centered at 270 nm, another positive at 241 nm. A stronger positive band is centered at 225 nm, followed by two negative bands at 210 and 200 nm, and a positive band at 187 nm. Albeit very close to the lowest attainable wavelength, the latter and the negative band at 200 nm seem to define a negative

exciton coupling, given that the absorbance maximum in the UV spectrum corresponds to a null value in the ECD spectrum (192 nm).

The TD-DFT simulations of the UV and ECD spectra of **4ag** were performed using the geometries of the conformations reported in Table S1 (both B3LYP-D3BJ and M06-2X geometries were used for the TD-DFT simulations). To ensure data redundancy, calculations were carried out with the ω B97X-D functional which includes empirical dispersion,¹⁹ and with CAM-B3LYP, which incorporates long-range corrections.²⁰ All calculations employed the 6-311++G(2d,p) basis set, known to provide good performance at a reasonable computational cost.²¹ The solvent (acetonitrile) was included using the IEF-PCM formalism. For each conformation, 60 transitions were computed in order to cover the 3.0–8.0 eV energy range ($\approx$ 413–155 nm). Each transition was convoluted with a Gaussian function (0.25 eV half-width) to obtain the simulated spectra. The 1*R*, 2*R*, 3*R*, 4*S* absolute configuration was used in all calculations. Being very high the energy of conformations **c14** and **c14b**, they were excluded from the ensemble used for the final simulation. The UV/ECD spectra of the eight stacked conformations were then weighted and summed using Boltzmann populations at 298 K, based on the relative energies reported in Table S2 (damped ΔG° energies). The resulting simulated spectra were eventually converted into the nm scale, and compared with the experimental spectrum. In all the cases (Figures S7-S10), the agreement with the experimental spectrum was very good and reliably assigns the 1*R*, 2*R*, 3*R*, 4*S* absolute configuration to **4ag**.

It is worth noting that in all TD-DFT calculations the broad band at 270 nm is simulated to be negative. The nature of this transition was investigated by molecular orbital (MO) visualization, performed for conformers **c4**, **c13**, and **c14**, i.e. the most populated structures within the conformational families (Figure S11). For **c4** and **c13** this negative band arises mainly from the $S_0 \rightarrow S_2$ transition, while the $S_0 \rightarrow S_1$ transition is at lower energy (very weak and positive). In both **c4** and **c13**, the $S_0 \rightarrow S_2$ transition is mainly described by the HOMO $\rightarrow$ LUMO excitation (58% in **c4** and 60% in **c13**). The HOMO is localized on the dihydroquinoline ring, whereas the LUMO is predominantly localized on the tosyl ring. Therefore, this transition has a significant charge-transfer (CT) character. Since the tosyl ring adopts the same spatial arrangement in all eight conformations, this feature further supports its conformational preference.

Consistently, when the ECD spectrum of conformer **c14** was calculated, the low energy band was much weaker and generated by the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$, both very weak. In this more open structure, the two chromophores are farther apart, reducing the intensity of the

charge-transfer interaction corresponding to $S_0 \rightarrow S_2$, whereas the $S_0 \rightarrow S_1$ has much less CT character.

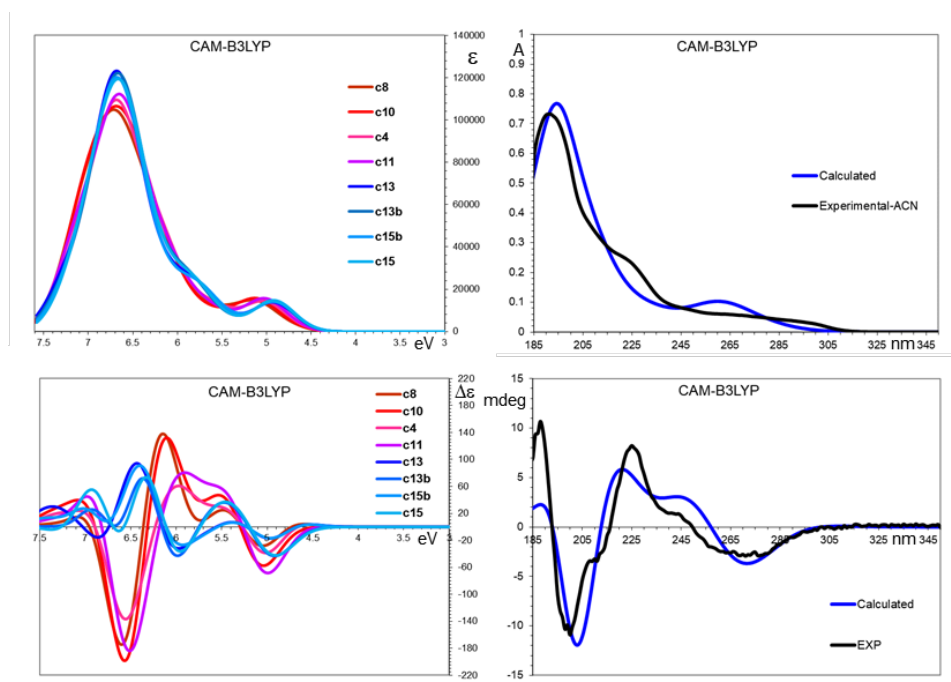


Figure S7. Left: TD-DFT simulation of the UV and ECD spectrum of the eight stacked conformations of **4ag**, at the TD-DFT CAM-B3LYP/6-311++G(2d,p)//B3LYP-D3BJ/6-311G(d,p) level. For each graph, the four reddish lines are related to the face-to-face arrangement of the phenyl and tosyl group, whereas the bluish lines are those of the four edge-to-face conformations. Right: comparison between the Boltzmann-averaged simulated spectra and the experimental ones. The simulated spectra were red-shifted by 0.45 eV and vertically scaled to match the experimental ones.

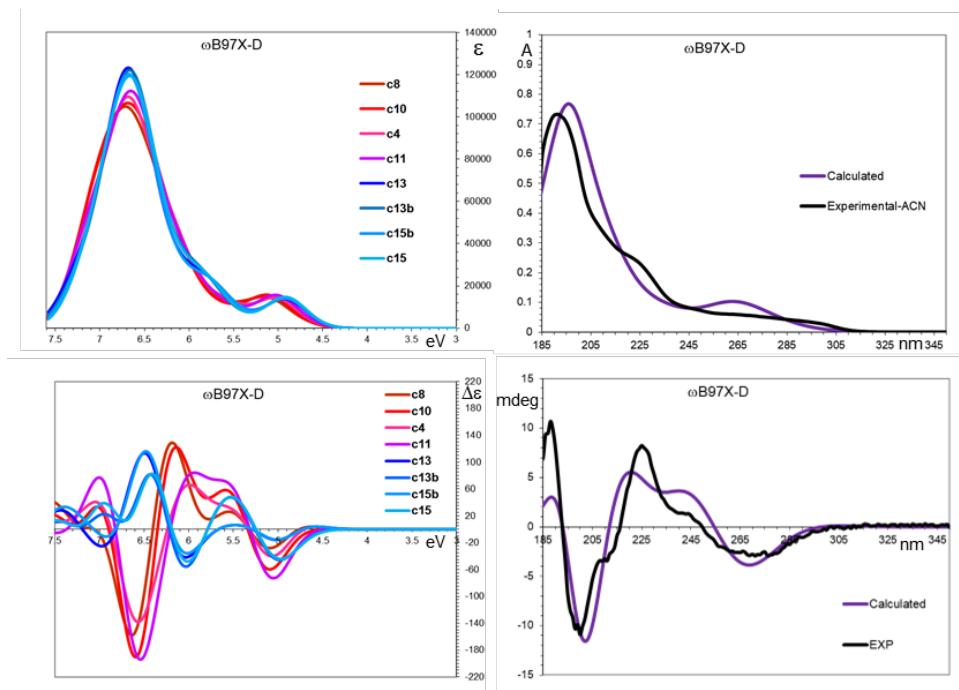


Figure S8. Left: TD-DFT simulation of the UV and ECD spectrum of the eight stacked conformations of **4ag**, at the TD-DFT ω B97X-D/6-311++G(2d,p)//B3LYP-D3BJ/6-311G(d,p) level. For each graph, the four reddish lines are related to the face-to-face arrangement of the phenyl and tosyl group, whereas the bluish lines are those of the four edge-to-face conformations. Right: comparison between the Boltzmann-averaged simulated spectra and the experimental ones. The simulated spectra were red-shifted by 0.45 eV and vertically scaled to match the experimental ones.

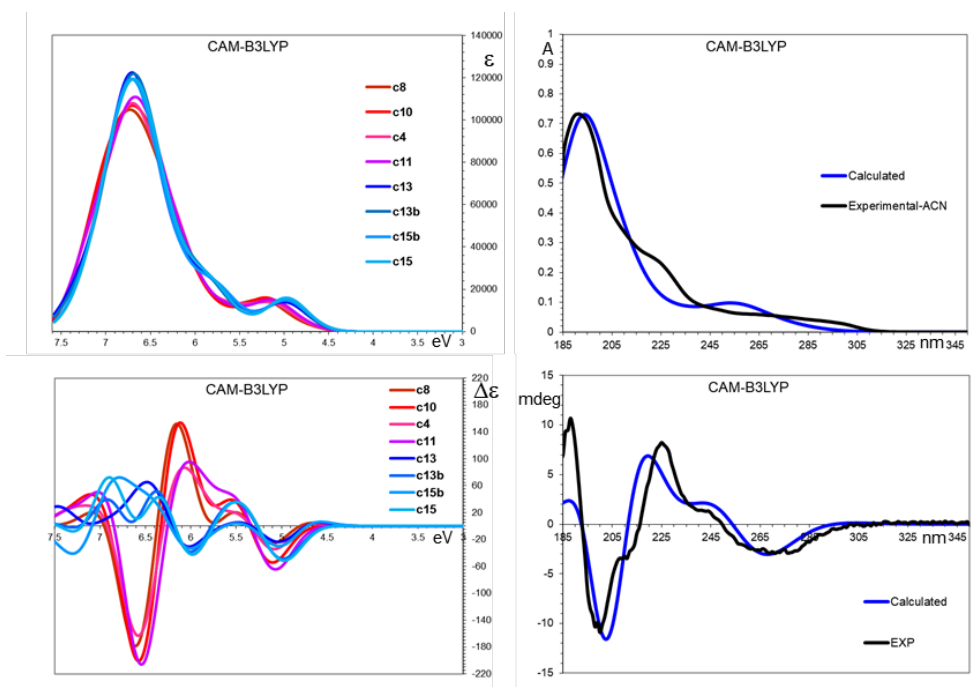


Figure S9. Left: TD-DFT simulation of the UV and ECD spectrum of the eight stacked conformations of **4ag**, at the TD-DFT CAM-B3LYP/6-311++G(2d,p)//M06-2x/6-311G(d,p) level. For each graph, the four reddish lines are related to the face-to-face arrangement of the phenyl and tosyl group, whereas the bluish lines are those of the four edge-to-face conformations. Right: comparison between the Boltzmann-averaged simulated spectra and the experimental ones. The simulated spectra were red-shifted by 0.45 eV and vertically scaled to match the experimental ones.

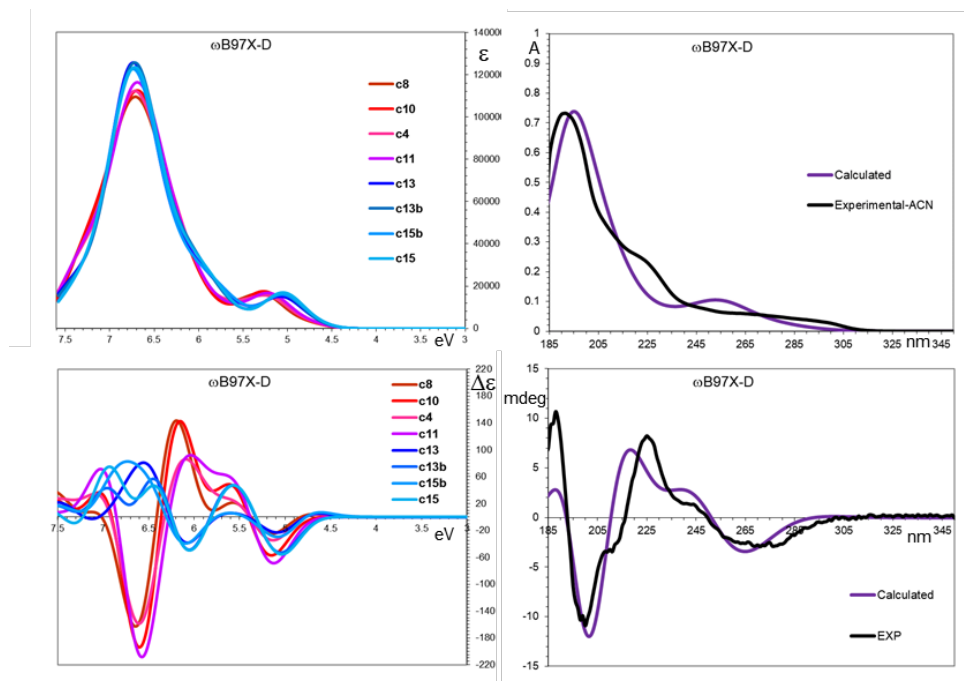


Figure S10. Left: TD-DFT simulation of the UV and ECD spectrum of the eight stacked conformations of **4ag**, at the TD-DFT ω B97x-D/6-311++G(2d,p)//M06-2x/6-311G(d,p) level. For each graph, the four reddish lines are related to the face-to-face arrangement of the phenyl and tosyl group, whereas the bluish lines are those of the four edge-to-face conformations. Right: comparison between the Boltzmann-averaged simulated spectra and the experimental ones. The simulated spectra were red-shifted by 0.45 eV and vertically scaled to match the experimental ones.

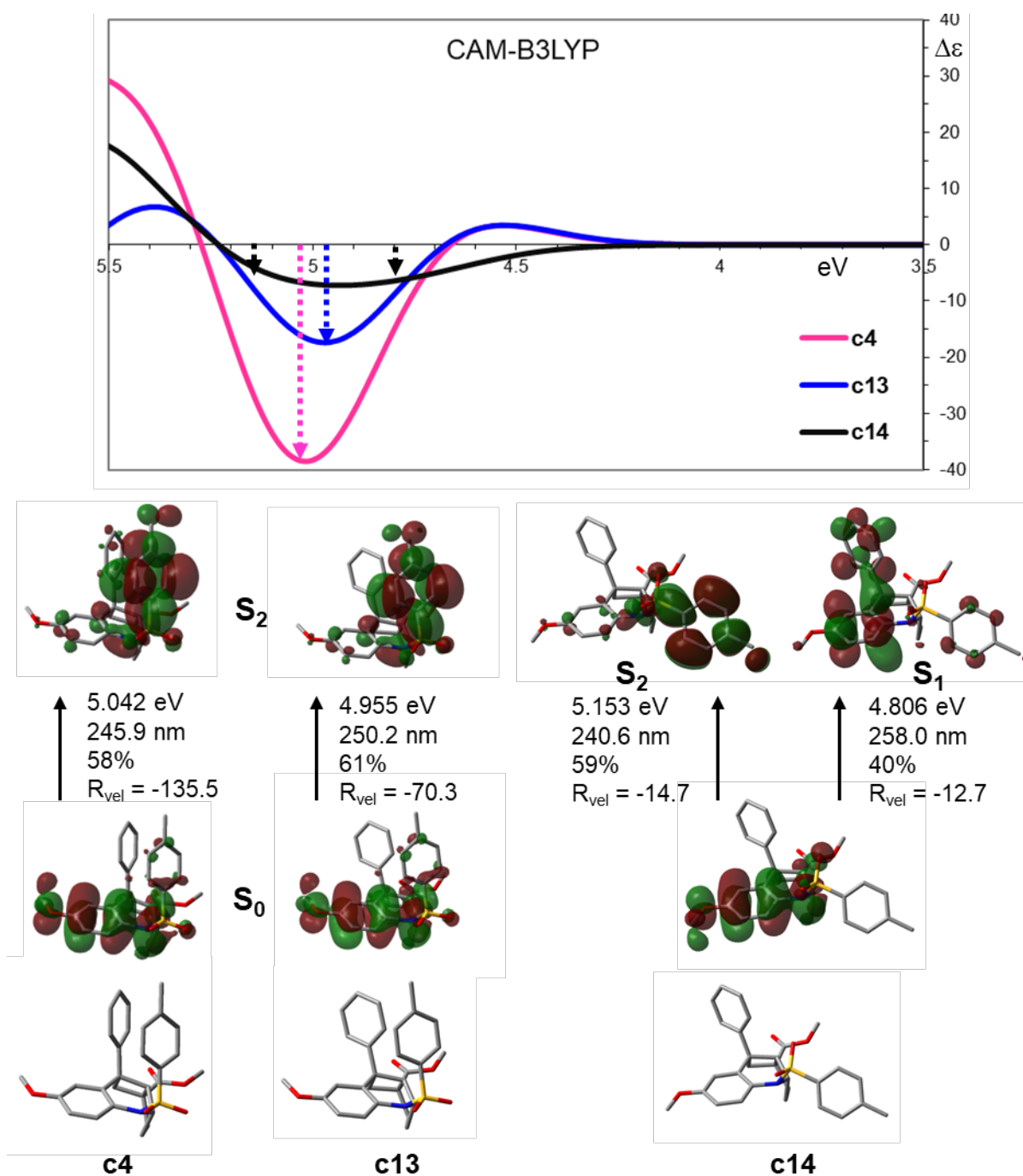


Figure S11. Top: calculated ECD spectra for conformation **c4**, **c13**, **c14** of **4ag** (TDDFT-CAM-B3LYP/6-311++G(2d,p)//B3LYP-D3BJ/6-311G(d,p)). Bottom: MO involved in the S_0 - S_x transition yielding the low energy ECD band.

7. Additional Computational Details

7.1 Non-covalent interactions

Non-covalent interactions at key transition states were computed through the analysis of the electron densities and their reduced gradient using the NCIPLOT code.²² This analysis helps identify some key interactions that help explain the enantioselection process in the bimetallic gold complex.

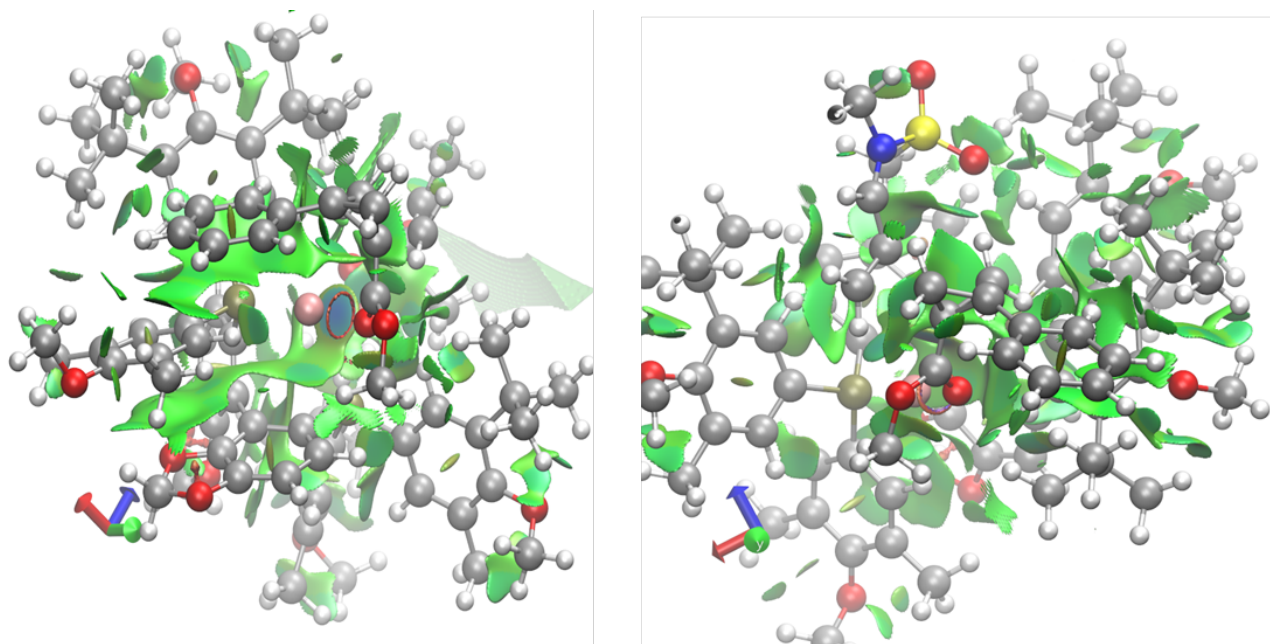


Figure S12. Map of non-covalent interactions in **Int1** (left) and **Int1'** (right).

The BCB phenyl ring on the left structure (**Int1**) is oriented such that it can elude most of the steric clashes with the bulky SEGPHOS ligand surrounding the bimetallic core of the catalyst. This is however not the case for the substrate pose ultimately producing the minor enantiomer (**Int1'**), where the phenyl ring cannot be so easily accommodated due to the geometrical restrictions of the rest of the substrate and the chelation mode onto the gold atoms. As a consequence of these and other interactions, this last mode of binding on the catalyst is energetically disfavored along the entire reaction path towards the cyclobutene derivative **ent-3aa**.

7.2 Int2 ↔ Int2' interconversion

Given the covalent nature of the Au-C bond between the substrate and the catalytic system and the large steric demands of the surrounding ligands we deemed implausible that the intermediates formed after BCB coupling to the allenamide would have the flexibility to interconvert inside the groove formed by the catalytic complex. Furthermore, the evolution of both intermediates towards protodeauration products requires only about 4 kcal/mol, which is sub-conformational activation energies for most organic substrates. However, in order to confirm that this hypothesis is valid, we performed a mono-dimensional scan starting at **Int2** and exploring decreasing values of the relevant CCCC dihedral angle shown in the plot below. Despite this motion being described by a just a single C-C bond rotation, it implies a long-range motion for the phenyl unit of the BCB, which sweeps a vast area in the entire process, creating some steric contacts. Additionally, the methylene group linking the BCB unit and the residue derived from the allenamide needs to rotate inwards, closer to the Au-Au bond region, which causes this interaction to be temporarily severed and imposing a large energy demand on this conformational motion. As a result, the **Int2** ↔ **Int2'** direct interconversion inside the catalytic complex requires more than 25 kcal/mol, which renders this motion non-competitive, even with respect to reaction reversion via C-C breaking of the BCB unit decoupling from the allenamide.

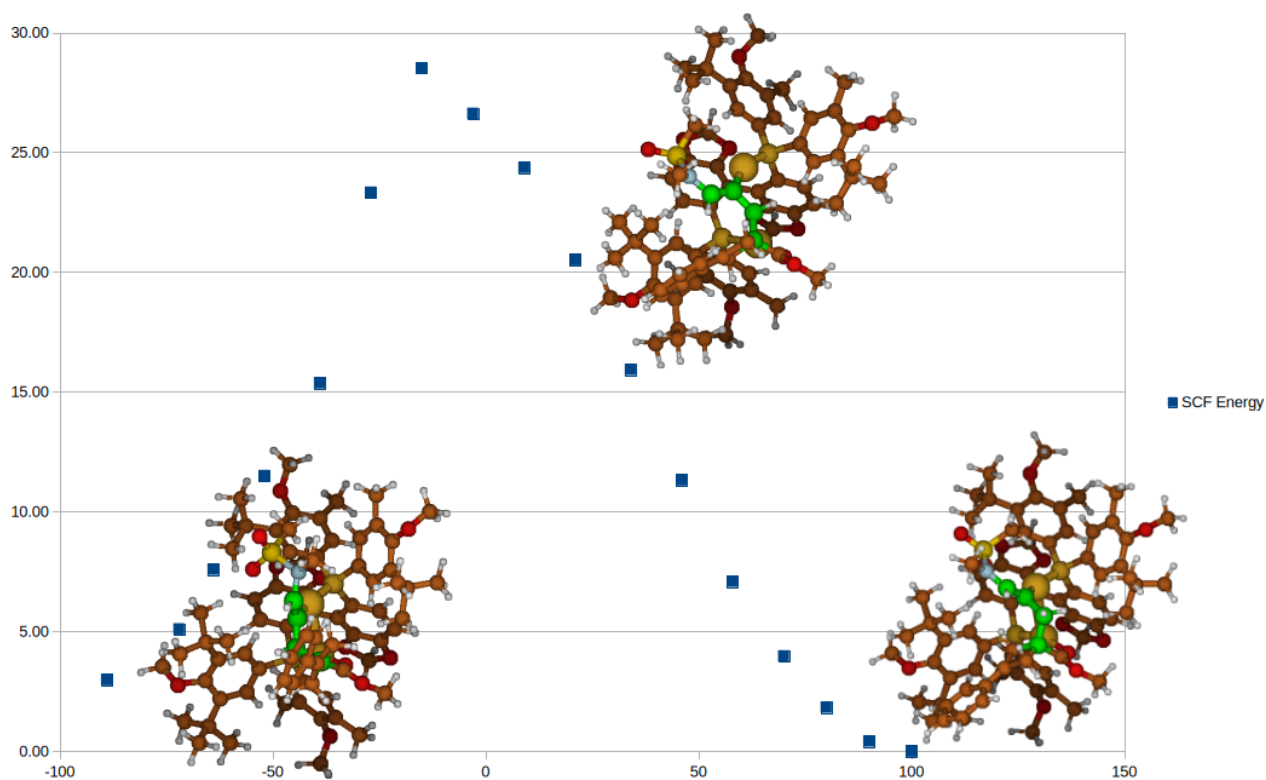


Figure S13. Mono-dimensional energy scan for the **Int2-Int2'** interconversion via direct single C-C bond rotation. The scanned dihedral bond is highlighted using green carbon atoms.

10. DFT-Calculation Coordinates for Chapters 6 and 7.2

10.1 DFT-Calculation Coordinates for Chapter 6

B3LYP-GD3BJ Optimization

b3lyp/6-311g(d,p) opt freq scrf(solvent=acetonitrile) EmpiricalDispersion=GD3BJ

CONFORMER 4

	0	1	
C	2.57793400	-1.97558600	-1.24780100
C	1.33300300	-1.39616600	-0.96127600
C	0.80983300	-1.47895100	0.33076600
C	1.54094700	-2.14519100	1.32281600
C	2.79179800	-2.68802200	1.04492000
C	3.31254300	-2.59236300	-0.25447800
H	2.95737100	-1.92615200	-2.25794500
H	1.11834900	-2.20756800	2.31584900
H	4.27888800	-3.03299100	-0.46489500
C	-0.53613900	-0.89668600	0.70258400
C	-1.43417000	-0.49636400	-0.52026700
H	-1.72332500	0.55004200	-0.53308000
N	0.54771000	-0.83491500	-2.02303700
C	-0.91010500	-0.99104500	-1.87401300
H	-1.38156300	-0.43052900	-2.67745600
C	-1.60352600	-1.99136600	1.07503900
H	-2.03859500	-1.89420200	2.06701100
H	-1.23164400	-3.00775100	0.94831300
C	-2.52448500	-1.52524400	-0.07760800
C	-1.32811600	-2.47014600	-1.97481600
H	-1.38620900	-2.80107000	-3.01190900
H	-0.59492000	-3.09957200	-1.46584500
C	-2.67778600	-2.51859500	-1.25182600
H	-2.93990300	-3.51833900	-0.90009700
H	-3.47154500	-2.17166600	-1.91625400
C	-3.84574400	-0.94577300	0.35426600
O	-4.36933800	-1.10608300	1.43527100
C	-0.40975000	0.23852100	1.71459400
C	0.80739400	0.89033000	1.93027100
C	-1.53354100	0.69881700	2.41598500
C	0.90692700	1.95256700	2.82551900
H	1.68904400	0.57238400	1.39320600
C	-1.43826500	1.76671400	3.30385900
H	-2.49665800	0.22428000	2.28459100
C	-0.21390600	2.39716100	3.51877300
H	1.86461600	2.43785200	2.97068400
H	-2.32315200	2.10020400	3.83387500
H	-0.13684400	3.22364800	4.21539900
O	3.57270400	-3.33062700	1.95363400
C	3.08991700	-3.44500100	3.29259600
H	2.15712300	-4.01544700	3.32929200
H	3.86323500	-3.97715400	3.84189800
H	2.93440700	-2.45945500	3.74134400
O	-4.38922800	-0.20435500	-0.62460900
C	-5.66026500	0.41257300	-0.33132800
H	-5.93380300	0.95446200	-1.23243200
H	-6.40527000	-0.34844900	-0.09946400
H	-5.56053400	1.09610300	0.51203400
S	1.11087800	0.55679500	-2.79803000
O	2.49370300	0.28885800	-3.19161400
O	0.11283200	0.87400000	-3.82284800

C	1.14090600	1.88635800	-1.61088700
C	2.33064900	2.18995500	-0.95655800
C	-0.02680200	2.60703600	-1.35868300
C	2.34681400	3.23855200	-0.04291600
H	3.22780300	1.62620300	-1.17235600
C	0.00748500	3.64054300	-0.43492400
H	-0.93827900	2.37809100	-1.89440900
C	1.19192100	3.97348700	0.23531200
H	3.27102800	3.48187800	0.46778700
H	-0.89730100	4.20220800	-0.23309500
C	1.20695400	5.10083300	1.23102900
H	2.17947200	5.19017800	1.71626300
H	0.97905500	6.05306500	0.74344500
H	0.45119500	4.93941400	2.00361400

CONFORMER 8

	0	1	
C	-1.71301300	2.93373600	-0.69484500
C	-0.79857500	1.87189300	-0.68282800
C	-0.15934700	1.51278500	0.50533700
C	-0.42482800	2.24808600	1.66822200
C	-1.35631800	3.28290500	1.66221500
C	-2.01269800	3.61619900	0.46802900
H	-2.18175200	3.20828400	-1.62904000
H	0.09371700	1.97849600	2.57742300
H	-2.72473100	4.43179400	0.47194400
C	0.83867800	0.37682200	0.57269700
C	1.41476300	-0.06962700	-0.81841000
H	1.28886000	-1.12607200	-1.03150800
N	-0.41526400	1.25056800	-1.91802100
C	0.99829600	0.83484400	-1.98304600
H	1.13980300	0.31386200	-2.92689000
C	2.28732000	0.86202500	0.96492100
H	2.70724300	0.35156200	1.83019900
H	2.36640600	1.93890900	1.11370900
C	2.84132900	0.37584100	-0.40654300
C	1.93781900	2.05652900	-1.92290600
H	2.03558600	2.53752100	-2.89631800
H	1.54055800	2.79673300	-1.22547200
C	3.25987500	1.48574100	-1.39919900
H	3.89763600	2.23407800	-0.92676200
H	3.82413600	1.03772000	-2.22263000
C	3.89612800	-0.69250600	-0.31828300
O	3.80143600	-1.82040700	-0.75080000
C	0.34052300	-0.79846500	1.41285900
C	-0.90610200	-0.80449400	2.04195400
C	1.15500800	-1.93069900	1.56985500
C	-1.31206400	-1.88182600	2.82805600
H	-1.57894800	0.03048600	1.91578200
C	0.74929100	-3.00977700	2.34695100
H	2.11316500	-1.99000400	1.07147600
C	-0.48610700	-2.98675400	2.99227300
H	-2.28771000	-1.85641300	3.29926500
H	1.40122600	-3.86998300	2.44787800
H	-0.80354000	-3.82503300	3.60092200
O	-1.68870800	4.02563200	2.75144900
C	-1.05612700	3.71746500	3.99393000
H	-1.47037300	4.41515700	4.71818200
H	-1.27700200	2.69226300	4.30551700
H	0.02724700	3.85619300	3.93141300

O	4.99148600	-0.22806900	0.30292500
C	6.09103200	-1.15362400	0.44022000
H	6.42732800	-1.48851900	-0.54093300
H	6.87606900	-0.59780600	0.94540000
H	5.78621400	-2.01415700	1.03601200
S	-1.55953800	0.28038000	-2.69607800
O	-2.74789100	1.11220200	-2.88765800
O	-0.87988000	-0.29150600	-3.86170100
C	-2.00577300	-1.04087600	-1.58756500
C	-1.23929800	-2.20404900	-1.56240100
C	-3.11289400	-0.88774900	-0.75595100
C	-1.59759500	-3.22720100	-0.69562500
H	-0.39126000	-2.31498200	-2.22444600
C	-3.46207000	-1.92870700	0.09434400
H	-3.69539300	0.02254400	-0.78947900
C	-2.71626200	-3.11115400	0.13622500
H	-1.00147000	-4.13136900	-0.66707100
H	-4.32360000	-1.81762700	0.74246400
C	-3.12408700	-4.24745400	1.03340800
H	-2.25601100	-4.82174400	1.35907900
H	-3.65029100	-3.88474700	1.91753900
H	-3.79661500	-4.92948300	0.50266500

CONFORMER 10

	0	1	
C	-2.28551100	-2.40956100	0.68578600
C	-1.14452800	-1.60905500	0.65175500
C	-0.47939100	-1.38451400	-0.56327300
C	-0.96574500	-2.00347200	-1.71160500
C	-2.12426400	-2.78202900	-1.68580600
C	-2.79935400	-2.97453200	-0.47519000
H	-2.77033600	-2.58610800	1.63540900
H	-0.46039400	-1.86812400	-2.66012100
H	-3.69230900	-3.58019000	-0.41925300
C	0.76126400	-0.52178200	-0.65404200
C	1.48114000	-0.26755600	0.71857800
H	1.62369900	0.78159400	0.95614000
N	-0.57157200	-1.12951200	1.87658800
C	0.90208500	-1.07530800	1.88447400
H	1.20466000	-0.63137200	2.82973700
C	2.03317700	-1.33031600	-1.11843400
H	2.53117400	-0.90930000	-1.99036000
H	1.84352000	-2.38918200	-1.29364900
C	2.73968900	-1.03408000	0.23705100
C	1.50978300	-2.48726500	1.75979900
H	1.52376800	-3.00574900	2.71869200
H	0.91670200	-3.08756200	1.06689300
C	2.91048900	-2.24132100	1.18907700
H	3.32662500	-3.10858500	0.67470900
H	3.59828100	-1.96950900	1.99542300
C	4.01971400	-0.25260400	0.12427500
O	4.22031300	0.85064900	0.58342900
C	0.53281800	0.76352300	-1.44872200
C	1.58995700	1.67294600	-1.60889600
C	-0.69368600	1.08602000	-2.03282700
C	1.43234300	2.84079000	-2.34642600
H	2.54860000	1.48644300	-1.14388900
C	-0.85242000	2.25291900	-2.77885300
H	-1.54296900	0.43209500	-1.90222300
C	0.20898900	3.13328400	-2.94730700

H	2.26832600	3.52293600	-2.45126900
H	-1.81888900	2.47550700	-3.21580300
H	0.08397200	4.04126300	-3.52513800
O	-2.51162700	-3.31065200	-2.87760600
C	-3.68942500	-4.11748300	-2.90613300
H	-3.81171700	-4.42542300	-3.94210600
H	-3.57842100	-5.00263700	-2.27302100
H	-4.56737700	-3.54714700	-2.58880900
O	4.94394000	-0.95084200	-0.55378900
C	6.23102300	-0.31806900	-0.71977900
H	6.83696700	-1.03393300	-1.26821800
H	6.12506700	0.60766700	-1.28565700
H	6.67465200	-0.10390700	0.25247900
S	-1.41083200	0.07153500	2.71811300
O	-2.75435000	-0.45379800	2.96276400
O	-0.55977000	0.44071700	3.85271200
C	-1.57815100	1.48246500	1.64346600
C	-0.56001200	2.43216200	1.59278000
C	-2.72596700	1.61222900	0.86466300
C	-0.70530300	3.53013500	0.75613300
H	0.31937500	2.32519600	2.21334400
C	-2.85671900	2.72412000	0.04303600
H	-3.50516500	0.86448800	0.91753600
C	-1.85598300	3.69908400	-0.02117100
H	0.08570000	4.26885300	0.70802300
H	-3.74795500	2.83316200	-0.56395800
C	-2.02487300	4.91965500	-0.88379900
H	-2.66369700	4.71168100	-1.74337700
H	-2.49053400	5.72904400	-0.31179100
H	-1.06188700	5.27991700	-1.24740200

CONFORMER 11

	0	1	
C	-2.91187900	-1.46693200	0.98045800
C	-1.57010800	-1.15030900	0.76354000
C	-1.03634900	-1.22582100	-0.53228800
C	-1.86704800	-1.62304800	-1.57624700
C	-3.21675400	-1.90746200	-1.36629100
C	-3.74573100	-1.81866500	-0.07344200
H	-3.30099000	-1.42981400	1.98751800
H	-1.47583000	-1.69598200	-2.58387700
H	-4.78302600	-2.04552600	0.12624300
C	0.41421900	-0.91576000	-0.83248500
C	1.33993700	-0.83743600	0.43268000
H	1.84855600	0.11459900	0.55055700
N	-0.71123000	-0.87057100	1.87826500
C	0.68087800	-1.32948900	1.72680700
H	1.23915900	-0.96443000	2.58521900
C	1.23266500	-2.17504400	-1.30151300
H	1.71010700	-2.07908200	-2.27390500
H	0.64694400	-3.09365000	-1.28263900
C	2.19510700	-2.03330400	-0.09841500
C	0.76320700	-2.86702000	1.68510700
H	0.71588800	-3.29880000	2.68500400
H	-0.07334700	-3.26952300	1.10977500
C	2.09159700	-3.14237500	0.97357400
H	2.14053900	-4.13757100	0.52740400
H	2.92091700	-3.04259300	1.67659700
C	3.62383300	-1.71941700	-0.45661300
O	4.13436100	-1.88799800	-1.54256800

C	0.56643100	0.31134300	-1.72672600
C	1.78572200	0.58258000	-2.36450200
C	-0.47446400	1.22919200	-1.88967300
C	1.95147400	1.72594300	-3.14094300
H	2.61969700	-0.09989300	-2.27055800
C	-0.31389700	2.36864500	-2.67427000
H	-1.42141900	1.05986900	-1.39834500
C	0.89866400	2.62436300	-3.30573700
H	2.90443900	1.90891200	-3.62423100
H	-1.13998000	3.06137800	-2.78127000
H	1.02391700	3.51093900	-3.91616700
O	-3.92950500	-2.26542700	-2.46803100
C	-5.31462500	-2.57135800	-2.30412300
H	-5.45484000	-3.42698600	-1.63708400
H	-5.86688400	-1.71010900	-1.91680700
H	-5.68170000	-2.82130500	-3.29701000
O	4.28410700	-1.21096600	0.59644400
C	5.66760800	-0.86375200	0.37838200
H	6.23458000	-1.74337900	0.07396100
H	5.74534400	-0.09436400	-0.39006200
H	6.02583200	-0.48822200	1.33290600
S	-0.98239800	0.53112200	2.78060300
O	-2.39858100	0.53027300	3.14580900
O	0.03824600	0.53164700	3.83200600
C	-0.70369500	1.94053900	1.72538200
C	-1.78660800	2.54861600	1.09813100
C	0.59527600	2.41774300	1.54847100
C	-1.55945200	3.65744200	0.28971200
H	-2.78727700	2.16993000	1.25466800
C	0.80163000	3.51719600	0.72926600
H	1.42471200	1.95125000	2.06283500
C	-0.26945400	4.15460000	0.08949200
H	-2.39897800	4.13714900	-0.19947500
H	1.80898900	3.89068900	0.58598100
C	-0.02239100	5.34874200	-0.79121300
H	-0.93944400	5.67956500	-1.27989800
H	0.37545300	6.18498500	-0.20900300
H	0.71183200	5.10927600	-1.56423200

CONFORMER 12

	0	1	
C	-1.71364800	2.93342000	-0.69494100
C	-0.79901200	1.87172100	-0.68290600
C	-0.15960000	1.51288100	0.50523300
C	-0.42509000	2.24825900	1.66807900
C	-1.35676500	3.28290500	1.66205700
C	-2.01332200	3.61595400	0.46787700
H	-2.18253100	3.20776200	-1.62912800
H	0.09362100	1.97884900	2.57724300
H	-2.72548900	4.43143700	0.47180400
C	0.83869200	0.37715600	0.57259900
C	1.41463700	-0.06943200	-0.81851400
H	1.28884700	-1.12592200	-1.03145200
N	-0.41575400	1.25029000	-1.91803600
C	0.99786400	0.83480000	-1.98323500
H	1.13930900	0.31368400	-2.92701700
C	2.28729100	0.86274300	0.96449900
H	2.70744600	0.35261200	1.82986000
H	2.36616000	1.93968700	1.11298600
C	2.84118600	0.37631200	-0.40689600

C	1.93723300	2.05661200	-1.92344000
H	2.03478400	2.53748300	-2.89693800
H	1.54000600	2.79687300	-1.22604200
C	3.25944500	1.48605100	-1.39987800
H	3.89724500	2.23454200	-0.92772900
H	3.82356200	1.03789200	-2.22333700
C	3.89616300	-0.69186900	-0.31871900
O	3.80187500	-1.81951100	-0.75200200
C	0.34093200	-0.79812900	1.41299500
C	1.15571000	-1.93014100	1.57008600
C	-0.90566000	-0.80439400	2.04215500
C	0.75031300	-3.00923200	2.34733400
H	2.11386000	-1.98927400	1.07166300
C	-1.31130100	-1.88173100	2.82842300
H	-1.57871700	0.03041300	1.91591800
C	-0.48505600	-2.98643400	2.99272500
H	1.40247200	-3.86926400	2.44832800
H	-2.28691400	-1.85649200	3.29971300
H	-0.80224000	-3.82471300	3.60151200
O	-1.68918800	4.02570400	2.75121600
C	-1.05638700	3.71785600	3.99367600
H	-1.27702500	2.69265600	4.30544300
H	0.02695300	3.85678600	3.93098800
H	-1.47068200	4.41558500	4.71786700
O	4.99114500	-0.22759900	0.30325400
C	6.09088000	-1.15298000	0.44033500
H	6.87570500	-0.59720100	0.94589300
H	5.78613600	-2.01383000	1.03571300
H	6.42740500	-1.48738000	-0.54091000
S	-1.55996300	0.27990500	-2.69590600
O	-2.74850600	1.11151800	-2.88726900
O	-0.88036600	-0.29181600	-3.86164900
C	-2.00573900	-1.04144700	-1.58731600
C	-1.23897600	-2.20443200	-1.56220800
C	-3.11278100	-0.88855800	-0.75554100
C	-1.59690700	-3.22764800	-0.69534400
H	-0.39100800	-2.31519300	-2.22437700
C	-3.46159900	-1.92957900	0.09482200
H	-3.69549900	0.02159900	-0.78902000
C	-2.71550700	-3.11185900	0.13663000
H	-1.00055800	-4.13167600	-0.66685400
H	-4.32307200	-1.81869500	0.74305700
C	-3.12302800	-4.24824800	1.03384000
H	-3.64863500	-3.88560200	1.91835700
H	-3.79603900	-4.93001100	0.50336200
H	-2.25489900	-4.82281700	1.35888100

CONFORMER 13

	0	1	
C	-2.17394700	1.68721400	-2.01383100
C	-1.04219500	1.03280100	-1.50254800
C	-0.40634000	1.54082200	-0.36339700
C	-0.94276200	2.67116000	0.26630500
C	-2.09529400	3.28471000	-0.21440600
C	-2.71063400	2.78464100	-1.37037400
H	-2.63368300	1.30762100	-2.91386000
H	-0.44609600	3.05459300	1.14486000
H	-3.59119600	3.28306100	-1.75552900
C	0.89300100	0.96183900	0.17031900
C	1.49432200	-0.19881600	-0.68005100

H	1.54100400	-1.16466300	-0.18462100
N	-0.51513600	-0.10817800	-2.19535800
C	0.93946400	-0.31158800	-2.10899400
H	1.14982500	-1.30661800	-2.49189500
C	2.16158700	1.82341100	-0.16717200
H	2.70478800	2.22046100	0.68560000
H	1.95706000	2.62996800	-0.87018400
C	2.83381300	0.59676700	-0.82285900
C	1.70624100	0.71772300	-2.95874300
H	1.70726300	0.44431500	-4.01413700
H	1.23338300	1.69893400	-2.87095300
C	3.10533800	0.72747800	-2.33423800
H	3.67302700	1.63101000	-2.56592800
H	3.67956800	-0.13538700	-2.67810000
C	3.99456300	0.04098800	-0.03966700
O	4.58549400	0.61067300	0.85007500
C	0.76709600	0.61943700	1.65024700
C	1.13014000	1.53120600	2.64656300
C	0.23074800	-0.60940900	2.04221900
C	0.96384500	1.22271100	3.99542000
H	1.55049300	2.49210600	2.37781400
C	0.07227000	-0.92626500	3.38818100
H	-0.06675200	-1.32816300	1.29274800
C	0.43813900	-0.01060200	4.37263600
H	1.25309200	1.94555200	4.74945600
H	-0.33494300	-1.89011100	3.66638600
H	0.31710100	-0.25659400	5.42101900
O	-2.68252800	4.37122200	0.35430600
C	-2.09119500	4.91264100	1.53585700
H	-2.07509700	4.17480600	2.34344700
H	-1.07373300	5.26549800	1.34270200
H	-2.71892800	5.75313600	1.82298200
O	4.30057900	-1.20187400	-0.45073600
C	5.39306500	-1.84966300	0.23269100
H	5.16624100	-1.95090900	1.29425100
H	5.48798600	-2.82689800	-0.23279600
H	6.31102600	-1.27486500	0.10890000
S	-1.48912700	-1.48594600	-2.32797700
O	-2.76645900	-1.05061900	-2.89198400
O	-0.68985900	-2.48456400	-3.04097900
C	-1.81462500	-2.08781800	-0.68276900
C	-1.13226300	-3.20688000	-0.21427400
C	-2.75222300	-1.42501300	0.11090800
C	-1.40890200	-3.67586600	1.06645900
H	-0.40900500	-3.70486100	-0.84580000
C	-3.00472600	-1.90309500	1.38882700
H	-3.27869500	-0.55946900	-0.26729300
C	-2.34741200	-3.03715200	1.88292600
H	-0.88524700	-4.54998500	1.43516400
H	-3.72616200	-1.38948600	2.01346900
C	-2.66328700	-3.56173600	3.25786400
H	-2.79037400	-2.74480700	3.97127900
H	-3.59826000	-4.13063700	3.24414100
H	-1.87647900	-4.22382800	3.62197000

CONFORMER 13b

	0	1	
C	2.56279300	-1.73767000	-1.25601500
C	1.28996800	-1.22122400	-1.00475600
C	0.69602900	-1.41905300	0.25553300

C	1.42283400	-2.08997300	1.23470600
C	2.71518400	-2.55940900	0.99824900
C	3.28980800	-2.38392500	-0.26449900
H	2.99218900	-1.61020400	-2.23841600
H	0.99535500	-2.25437900	2.21512000
H	4.27799200	-2.75689100	-0.49162700
C	-0.73559100	-1.00425700	0.55213400
C	-1.50745600	-0.38938500	-0.65588600
H	-1.80065700	0.65039100	-0.54182000
N	0.58204100	-0.54341300	-2.05303500
C	-0.88417300	-0.66198600	-2.03430600
H	-1.27562000	0.05887200	-2.74716700
C	-1.75626300	-2.19758600	0.55398400
H	-2.26156400	-2.38589600	1.49692600
H	-1.32729200	-3.12815500	0.18432700
C	-2.62781100	-1.46880800	-0.49271700
C	-1.34376800	-2.07063500	-2.45143300
H	-1.32434000	-2.19406900	-3.53447700
H	-0.67792100	-2.82219100	-2.02028000
C	-2.75050200	-2.18054200	-1.85415500
H	-3.09010400	-3.21217700	-1.74147200
H	-3.47040100	-1.64941600	-2.48042200
C	-3.93707700	-0.95517500	0.04741700
O	-4.45973500	-1.30015400	1.08333100
C	-0.80678600	-0.14452100	1.80861500
C	-1.03289600	-0.70782300	3.06852400
C	-0.59762700	1.23435000	1.72891200
C	-1.05237900	0.08451600	4.21472400
H	-1.20011000	-1.77303800	3.16563100
C	-0.62600200	2.03142300	2.86961400
H	-0.41155500	1.69447600	0.76944800
C	-0.85367800	1.45977900	4.11970700
H	-1.23027200	-0.37493500	5.18013800
H	-0.47311900	3.09956500	2.77965400
H	-0.87838100	2.07922100	5.00851000
O	3.32315900	-3.18119800	2.04407400
C	4.64546500	-3.68443200	1.85096500
H	4.66704900	-4.45197700	1.07178900
H	5.34072300	-2.88022900	1.59282700
H	4.93632400	-4.12473300	2.80205400
O	-4.46865400	-0.03544200	-0.77660900
C	-5.72339600	0.54326400	-0.36324500
H	-5.60536500	1.05508400	0.59209900
H	-5.98880100	1.24964100	-1.14508300
H	-6.48522100	-0.23099900	-0.27085700
S	1.24364500	0.88770900	-2.66801400
O	2.62084000	0.58639200	-3.05791100
O	0.30007400	1.37425500	-3.67683800
C	1.31709700	2.07265500	-1.33882300
C	0.39329900	3.11283600	-1.29500300
C	2.30559800	1.93894300	-0.36214800
C	0.47435900	4.04123900	-0.26122200
H	-0.36499500	3.19741200	-2.06162800
C	2.36043700	2.86861800	0.66622400
H	3.02039400	1.12902500	-0.41046400
C	1.45555800	3.93619800	0.72925900
H	-0.23817100	4.85683500	-0.22462800
H	3.11990700	2.76612800	1.43251300
C	1.55473600	4.95321900	1.83427800
H	1.76192400	4.47275500	2.79287000
H	2.37251600	5.65349500	1.63743600
H	0.63488800	5.53230100	1.92628300

CONFORMER 14

	0	1	
C	-0.48002300	-3.08549600	-0.65631300
C	-0.46987500	-1.70727900	-0.44971100
C	-1.67022300	-0.98537300	-0.47232300
C	-2.85915000	-1.66966600	-0.70783000
C	-2.87488100	-3.05303000	-0.89266200
C	-1.67154600	-3.76945500	-0.86059200
H	0.45838100	-3.62285800	-0.64843600
H	-3.80029100	-1.13352800	-0.73549400
H	-1.65061800	-4.83948300	-1.00877100
C	-1.70926100	0.51536700	-0.28232300
C	-0.31124300	1.22720700	-0.35630800
H	-0.03997300	1.76635200	0.54567500
N	0.78828900	-1.02857000	-0.29730500
C	0.82389500	0.33215400	-0.86653800
H	1.78168600	0.77888300	-0.59687100
C	-2.12734300	1.28414300	-1.58511500
H	-3.01605700	1.90490800	-1.50575400
H	-2.23884600	0.62160300	-2.44283500
C	-0.79107700	2.06361200	-1.58683400
C	0.69885800	0.31568000	-2.39972200
H	1.65010500	0.08471900	-2.87974400
H	-0.02086100	-0.44665800	-2.70550000
C	0.18020000	1.71907200	-2.73833900
H	-0.31373300	1.76811400	-3.71075200
H	1.00594100	2.43320300	-2.73910100
C	-0.92632100	3.54579400	-1.35540800
O	-1.95039400	4.18640500	-1.45198300
C	-2.45049600	0.90078200	0.99190900
C	-2.42403700	0.04676200	2.10183200
C	-3.08834300	2.13880000	1.12787700
C	-3.02437000	0.41095900	3.30335000
H	-1.93244200	-0.91404400	2.02502600
C	-3.69159500	2.50456500	2.33064200
H	-3.11277700	2.83778200	0.30266600
C	-3.66541800	1.64266600	3.42360100
H	-2.99171100	-0.27031600	4.14595300
H	-4.18308400	3.46766600	2.40896600
H	-4.13677000	1.92658900	4.35723900
O	-4.09728500	-3.61158700	-1.10161300
C	-4.16953800	-5.02422100	-1.29661500
H	-3.79458100	-5.56399300	-0.42214400
H	-5.22427400	-5.24953000	-1.43744300
H	-3.60930500	-5.33048700	-2.18489300
O	0.25150100	4.08989900	-1.00797500
C	0.24779000	5.50770500	-0.74110000
H	1.27393700	5.75714200	-0.48542800
H	-0.07251300	6.05826100	-1.62563000
H	-0.42016900	5.73190500	0.09078000
S	1.53500700	-1.14815300	1.22843800
O	1.11090900	-0.07417300	2.13776600
O	1.35950700	-2.53308400	1.67272200
C	3.23492300	-0.85466100	0.77951600
C	3.93391800	0.17607400	1.39548700
C	3.84198700	-1.68655200	-0.16158600
C	5.27038900	0.37565900	1.05902200
H	3.43726600	0.81122200	2.11645700
C	5.17217800	-1.46908500	-0.48616400

H	3.27829200	-2.47700400	-0.63930800
C	5.90705500	-0.43771600	0.11845500
H	5.82203800	1.17886800	1.53301100
H	5.65112900	-2.10634100	-1.22072900
C	7.35136900	-0.22161800	-0.24681900
H	7.46065800	-0.06191300	-1.32289900
H	7.76862700	0.64160000	0.27251000
H	7.95096600	-1.09900400	0.01190500

CONFORMER 14b

	0	1	
C	-0.37193800	-3.05173500	-0.60078400
C	-0.40089800	-1.67193900	-0.40292200
C	-1.62042000	-0.98080600	-0.46197600
C	-2.78400000	-1.70216500	-0.71377300
C	-2.75965400	-3.08667500	-0.88630100
C	-1.53930400	-3.77014500	-0.82458100
H	0.57934100	-3.56456000	-0.56891200
H	-3.74006100	-1.19646500	-0.76756500
H	-1.48545400	-4.84017200	-0.96422100
C	-1.70093700	0.52833900	-0.30450800
C	-0.32214800	1.26238100	-0.29458300
H	-0.09567300	1.79861100	0.62159000
N	0.83647200	-0.96416700	-0.22613100
C	0.85815400	0.40516100	-0.76921300
H	1.78831100	0.87493300	-0.44793800
C	-2.06505000	1.28954400	-1.62610000
H	-2.96112000	1.90252200	-1.58283000
H	-2.11666700	0.64068200	-2.50001600
C	-0.75666700	2.10708300	-1.53603900
C	0.80871800	0.41672400	-2.30610500
H	1.78593300	0.20847100	-2.74236300
H	0.11592000	-0.34958000	-2.66120000
C	0.28535300	1.81960000	-2.63771300
H	-0.15248300	1.88814600	-3.63549800
H	1.09547200	2.54841400	-2.56954200
C	-0.96346800	3.57576800	-1.27100200
O	-2.00607600	4.17815000	-1.39625600
C	-2.56962700	0.86653100	0.90018800
C	-2.02603100	0.77345000	2.18714700
C	-3.91819000	1.20353700	0.76734800
C	-2.81095000	1.02200900	3.30921300
H	-0.98388500	0.50492600	2.31142100
C	-4.70679000	1.44985300	1.89121600
H	-4.36688800	1.27614400	-0.21531600
C	-4.15600000	1.36262600	3.16661700
H	-2.37127900	0.94880500	4.29754400
H	-5.75098500	1.71229800	1.76561300
H	-4.76659100	1.55813900	4.04037800
O	-3.96342800	-3.67830700	-1.11459200
C	-3.99484600	-5.09378800	-1.29814000
H	-3.62269800	-5.61605600	-0.41187700
H	-5.04036500	-5.34831000	-1.45698800
H	-3.40975500	-5.39292300	-2.17276800
O	0.17677400	4.15442800	-0.85518400
C	0.10517200	5.56272800	-0.55296600
H	1.10497700	5.84193800	-0.23176000
H	-0.18380800	6.12601400	-1.44048100
H	-0.61743000	5.74098600	0.24363200
S	1.62400500	-1.12128200	1.27050400

O	1.22635000	-0.06916400	2.21929700
O	1.46331200	-2.51483700	1.69182600
C	3.30906100	-0.80819900	0.78096500
C	4.04147600	0.16657300	1.44731000
C	3.87397200	-1.57558400	-0.23800300
C	5.36883600	0.37532000	1.08189200
H	3.57711600	0.75320200	2.22836100
C	5.19578800	-1.34958100	-0.58995700
H	3.28344500	-2.32079500	-0.75455000
C	5.96364900	-0.37361700	0.06354600
H	5.94646600	1.13502600	1.59499500
H	5.64181200	-1.93642400	-1.38474600
C	7.39546300	-0.14113000	-0.33893400
H	7.45517900	0.19678500	-1.37748500
H	7.86944000	0.61121400	0.29214200
H	7.97455600	-1.06562900	-0.26653900

CONFORMER 15

	0	1	
C	-2.63029600	1.94507800	-0.65472600
C	-1.36664500	1.35221400	-0.70011100
C	-0.52027100	1.43143100	0.42084500
C	-0.99000000	2.07343300	1.56309300
C	-2.27062000	2.62319100	1.62345400
C	-3.10016300	2.55823000	0.49959400
H	-3.25575200	1.90701100	-1.53393000
H	-0.36519100	2.14892300	2.44320400
H	-4.08914800	2.99326700	0.50210400
C	0.90824800	0.90723100	0.40297400
C	1.39352000	0.37480000	-0.98007000
H	1.63830700	-0.68371700	-1.00729100
N	-0.91567900	0.73202800	-1.91233700
C	0.52966000	0.79964300	-2.17789500
H	0.73577000	0.13926000	-3.01603500
C	1.99898900	2.02993700	0.31215900
H	2.68078000	2.08400800	1.15533000
H	1.58088800	3.01854000	0.12429600
C	2.59734900	1.38852100	-0.97260400
C	0.96747800	2.22787500	-2.54907900
H	0.73540400	2.45949200	-3.58880000
H	0.43819500	2.95110200	-1.92352700
C	2.46786200	2.23385100	-2.24319500
H	2.87294700	3.23898300	-2.10664200
H	3.02682800	1.75408200	-3.04895600
C	3.94667800	0.73397300	-0.81964100
O	4.78944000	0.65888700	-1.68681100
C	1.12718400	-0.07195300	1.55018700
C	0.81915500	-1.42391600	1.39180300
C	1.59428600	0.35922200	2.79537800
C	0.98826200	-2.32557100	2.43934400
H	0.44680200	-1.78312100	0.44350100
C	1.75576500	-0.53648400	3.84984900
H	1.84768500	1.40052500	2.94998900
C	1.45853000	-1.88648800	3.67477600
H	0.75552800	-3.37195700	2.28686500
H	2.12204400	-0.17871400	4.80525100
H	1.59335900	-2.58734900	4.49023000
O	-2.61254000	3.20647400	2.80393500
C	-3.91165100	3.78843200	2.91491500
H	-3.97425600	4.18191400	3.92699700

H	-4.04265900	4.60389100	2.19758000
H	-4.69463200	3.03921300	2.76523500
O	4.09653900	0.18825500	0.39776400
C	5.31436600	-0.54407600	0.63313300
H	5.39940200	-1.37212200	-0.07102200
H	6.17815800	0.11293700	0.52987800
H	5.23527000	-0.91501900	1.65145500
S	-1.76852600	-0.59878200	-2.50998500
O	-3.17333500	-0.20018000	-2.59538000
O	-1.06519700	-1.02353900	-3.72223800
C	-1.66367400	-1.90753700	-1.30513200
C	-2.44530800	-1.83422100	-0.15102000
C	-0.80764900	-2.98147800	-1.53170800
C	-2.36160600	-2.85944600	0.78014100
H	-3.10959000	-0.99646800	0.01085100
C	-0.74784800	-4.00441700	-0.59002300
H	-0.21011200	-3.01774800	-2.43259000
C	-1.52203800	-3.96153600	0.57353300
H	-2.95943300	-2.80553400	1.68247300
H	-0.08734600	-4.84584500	-0.76337700
C	-1.47316900	-5.08005800	1.57944400
H	-2.33838500	-5.73971900	1.45998600
H	-0.57396400	-5.68568300	1.45845700
H	-1.49834900	-4.69227800	2.59994000

CONFORMER 15b

	0	1	
C	-2.04293800	2.62017400	-0.74305800
C	-1.02390600	1.65623000	-0.79934500
C	-0.07478300	1.59247500	0.22743900
C	-0.18766700	2.47366600	1.31065400
C	-1.22861700	3.39356300	1.38617100
C	-2.16229700	3.46406100	0.34312200
H	-2.74703400	2.68329300	-1.55893700
H	0.54742100	2.41695100	2.09912800
H	-2.95495900	4.19969600	0.39508300
C	1.11804900	0.64915600	0.18154500
C	1.26289200	-0.15859400	-1.14404500
H	1.17270800	-1.23657600	-1.03946300
N	-0.91976000	0.80303300	-1.94764600
C	0.43864000	0.38142200	-2.32350700
H	0.33997000	-0.39854800	-3.07377200
C	2.47996000	1.35528500	-0.14201500
H	3.23629300	1.28379800	0.63376800
H	2.36309600	2.39846500	-0.43438600
C	2.70874400	0.42100300	-1.36578500
C	1.24292100	1.54974000	-2.92174900
H	0.97669200	1.72520300	-3.96427300
H	1.02933100	2.46722800	-2.36757100
C	2.69955000	1.11952900	-2.72851400
H	3.40126600	1.95583800	-2.76259600
H	2.99487500	0.40364900	-3.49813800
C	3.81137200	-0.59616400	-1.21887300
O	4.52254400	-0.99225600	-2.11604000
C	1.15373500	-0.21435000	1.43714600
C	1.86941800	0.17886900	2.57197600
C	0.42378000	-1.40246500	1.49515200
C	1.86013300	-0.59586100	3.72970800
H	2.45188400	1.09164800	2.55883600
C	0.41968200	-2.18636300	2.64589600

H	-0.14602400	-1.72570800	0.63616600
C	1.13852600	-1.78701800	3.77026100
H	2.42474700	-0.27102700	4.59609700
H	-0.14361800	-3.11083600	2.66099900
H	1.13805300	-2.39700800	4.66592900
O	-1.41219000	4.26496200	2.41390400
C	-0.48715400	4.22556800	3.50075800
H	-0.49017200	3.24553800	3.98702200
H	0.52670800	4.46445300	3.16586000
H	-0.82484500	4.98248900	4.20500800
O	3.89250300	-1.05735900	0.03944300
C	4.86206200	-2.09332500	0.28758100
H	5.86704100	-1.73289400	0.06715000
H	4.76408400	-2.33277900	1.34299500
H	4.64562000	-2.96834300	-0.32577900
S	-2.19760000	-0.24373700	-2.30354700
O	-3.41584900	0.56530000	-2.33228200
O	-1.79635700	-0.98484700	-3.50107100
C	-2.35880500	-1.39316400	-0.95207500
C	-1.88120500	-2.69268900	-1.09617900
C	-2.96004900	-0.96873900	0.23372700
C	-2.02496800	-3.58333300	-0.03674400
H	-1.41733200	-3.00035200	-2.02361200
C	-3.08370700	-1.87025900	1.28140700
H	-3.33020300	0.04269900	0.33071500
C	-2.62860700	-3.18951900	1.16165200
H	-1.66015800	-4.59803100	-0.14432500
H	-3.54278100	-1.54572300	2.20789400
C	-2.80537500	-4.16292700	2.29599300
H	-2.64143900	-3.67804800	3.26048400
H	-3.82430100	-4.56282600	2.30081200
H	-2.11852000	-5.00591600	2.20775700

M06-2x Optimization

b3lyp/6-311g(d,p) opt freq scrf(solvent=acetonitrile) EmpiricalDispersion=GD3BJ

CONFORMER 4

	0	1	
C	2.39718600	-2.22040800	-1.16294600
C	1.20396300	-1.53445600	-0.89838800
C	0.70677000	-1.47854900	0.40086200
C	1.40766700	-2.11991100	1.43005700
C	2.60874600	-2.76856200	1.17218300
C	3.10649800	-2.80819800	-0.13789100
H	2.75287700	-2.27973700	-2.18262600
H	0.99783500	-2.07775300	2.43199300
H	4.03454500	-3.33348300	-0.32572000
C	-0.58617000	-0.77307300	0.74787900
C	-1.49152100	-0.42471100	-0.48001900
H	-1.72488100	0.63401900	-0.57677000
N	0.42823300	-1.00986200	-1.98686900
C	-1.03018700	-1.07002600	-1.79230900
H	-1.49702700	-0.56572100	-2.63714900
C	-1.70859900	-1.75120400	1.24661900
H	-2.11341100	-1.51815500	2.23064000
H	-1.40756600	-2.79966900	1.21892300
C	-2.62250200	-1.34355500	0.07198400
C	-1.52064600	-2.52652200	-1.73540300
H	-1.61072100	-2.95848100	-2.73165600
H	-0.81534600	-3.13734400	-1.16575400
C	-2.85807600	-2.42593000	-1.00098800
H	-3.17492400	-3.37053700	-0.55560800
H	-3.63680200	-2.08765700	-1.68799700
C	-3.90524300	-0.65962800	0.46495500
O	-4.41660800	-0.69925800	1.55661000
C	-0.35981900	0.43379700	1.65464000
C	0.90943800	0.96355000	1.88976600
C	-1.45795000	1.07641500	2.24300400
C	1.07964400	2.08714600	2.69575600
H	1.78101100	0.50735000	1.43802100
C	-1.29047800	2.20212300	3.03975300
H	-2.46171900	0.69449900	2.09493700
C	-0.01591300	2.71179500	3.27599400
H	2.07824400	2.47801700	2.85795900
H	-2.15791000	2.67631800	3.48377800
H	0.11816900	3.58531400	3.90314600
O	3.35961500	-3.39448400	2.10899000
C	2.89539800	-3.36859200	3.45023100
H	1.92652700	-3.86719700	3.53956400
H	3.63673300	-3.90704000	4.03456600
H	2.81527300	-2.34151300	3.81662800
O	-4.42750800	0.01581100	-0.56237300
C	-5.65740800	0.70382400	-0.29975900
H	-5.93299200	1.18207000	-1.23463300
H	-6.42494000	-0.00438700	0.01039700
H	-5.51018400	1.44776100	0.48276700
S	1.05922600	0.28624500	-2.83200500
O	2.38911600	-0.10523000	-3.26413700
O	0.05774500	0.64665000	-3.82312900
C	1.24888500	1.64498600	-1.70656900
C	2.48218800	1.85702100	-1.10148700
C	0.16801600	2.49121600	-1.47012000
C	2.63031500	2.94247100	-0.24710100
H	3.31214100	1.19379200	-1.31194100

C	0.33291900	3.56032200	-0.60333400
H	-0.77491600	2.32982600	-1.97914400
C	1.56316900	3.80209400	0.01657900
H	3.58898100	3.11858600	0.22794700
H	-0.50230500	4.22428600	-0.40944800
C	1.72544300	4.97970900	0.93781800
H	2.63163500	4.89024400	1.53737500
H	1.78834400	5.90707000	0.36240900
H	0.86880900	5.06185300	1.60927700

CONFORMER 8

0 1

C	-1.76690800	2.91323400	-0.69792200
C	-0.84205000	1.86166400	-0.68274300
C	-0.20317500	1.50883100	0.50287800
C	-0.47881800	2.23659400	1.66754500
C	-1.42001400	3.25899200	1.65879500
C	-2.07525800	3.58781700	0.46396800
H	-2.23229200	3.18717700	-1.63534600
H	0.04472000	1.96758600	2.57692200
H	-2.79371900	4.39788000	0.47079400
C	0.81579700	0.39126700	0.57044200
C	1.40155100	-0.04723600	-0.81411000
H	1.29435800	-1.10812100	-1.02886600
N	-0.44205000	1.25035000	-1.91853900
C	0.97815800	0.86137500	-1.97390300
H	1.14302600	0.35603800	-2.92446100
C	2.24968100	0.89961200	0.96667600
H	2.67453100	0.39624500	1.83548700
H	2.31072400	1.97992700	1.10988800
C	2.81491100	0.42081900	-0.39694400
C	1.89190400	2.09778200	-1.88609800
H	1.97633000	2.60471900	-2.84687100
H	1.48801900	2.81127500	-1.16322200
C	3.22215000	1.53315100	-1.38497700
H	3.86129300	2.28039000	-0.91285800
H	3.77561800	1.08919000	-2.21814400
C	3.89252500	-0.62298200	-0.30692600
O	3.82902500	-1.74354100	-0.74879900
C	0.33682600	-0.79343800	1.40811800
C	-0.90675200	-0.83015400	2.03844300
C	1.17546600	-1.90813400	1.55274400
C	-1.28816800	-1.92639400	2.81048000
H	-1.60057900	-0.00764800	1.92530400
C	0.79370900	-3.00461200	2.31374100
H	2.13809100	-1.93605800	1.05443200
C	-0.44181000	-3.01555400	2.95727700
H	-2.26293100	-1.92605500	3.28584300
H	1.46403900	-3.85124000	2.40577300
H	-0.74187100	-3.86814900	3.55513700
O	-1.76229700	3.99472600	2.74273700
C	-1.12863500	3.68651100	3.97496800
H	-1.54545700	4.37347100	4.70659500
H	-1.34017200	2.65698400	4.27682900
H	-0.04752000	3.83505200	3.90821200
O	4.96922100	-0.14061100	0.31797800
C	6.07905400	-1.04052600	0.43968600
H	6.42291700	-1.34741400	-0.54750200
H	6.85353300	-0.48471800	0.95918200
H	5.78728900	-1.91951100	1.01371000

S	-1.55999100	0.26674700	-2.67816600
O	-2.76240800	1.06341300	-2.84888000
O	-0.88788600	-0.28158700	-3.84572400
C	-1.95999900	-1.06627000	-1.57830800
C	-1.17226500	-2.21260100	-1.58298300
C	-3.06329800	-0.94616300	-0.73834000
C	-1.49635800	-3.25193800	-0.72197100
H	-0.33643700	-2.29920800	-2.26704500
C	-3.38147000	-2.00459400	0.10001000
H	-3.66750100	-0.04763000	-0.75990500
C	-2.60540300	-3.16651600	0.12254200
H	-0.88551500	-4.14761500	-0.71413300
H	-4.24171500	-1.92508400	0.75562900
C	-2.97729200	-4.31744500	1.01644700
H	-2.10206900	-4.91974000	1.26169000
H	-3.42720800	-3.96274300	1.94486200
H	-3.70488700	-4.96315200	0.51677200

CONFORMER 10

	0	1	
C	-2.45341700	-2.26325500	0.68850200
C	-1.27072000	-1.53014000	0.65343300
C	-0.59332500	-1.34502200	-0.55845800
C	-1.11265000	-1.93355900	-1.70580400
C	-2.31243200	-2.64323700	-1.67990700
C	-2.99750600	-2.79732300	-0.47182600
H	-2.94512700	-2.41564800	1.64011900
H	-0.59697800	-1.82931200	-2.65484300
H	-3.92315500	-3.35273900	-0.41516400
C	0.70263000	-0.56736100	-0.64864800
C	1.43505100	-0.35396200	0.71931400
H	1.64597200	0.68650600	0.95639600
N	-0.66659800	-1.09032700	1.87921200
C	0.80637000	-1.13256800	1.88052300
H	1.14503700	-0.72319400	2.83115500
C	1.91481500	-1.45650600	-1.10860300
H	2.43810200	-1.07202000	-1.98430100
H	1.65678000	-2.50405600	-1.27347000
C	2.63843700	-1.19826400	0.23941800
C	1.31766100	-2.57749000	1.73435000
H	1.28160000	-3.11509500	2.68139800
H	0.70134100	-3.12207400	1.01433000
C	2.73792400	-2.40731700	1.19241600
H	3.11817700	-3.29408400	0.68370900
H	3.42204300	-2.16484500	2.01145000
C	3.96857400	-0.50790300	0.12549100
O	4.24958900	0.56565800	0.59818500
C	0.56319200	0.72719800	-1.44849900
C	1.68290200	1.55920200	-1.59385400
C	-0.62940500	1.13386700	-2.04582900
C	1.61672400	2.73815600	-2.32357400
H	2.62289100	1.29798600	-1.12071700
C	-0.69581100	2.31305600	-2.78655200
H	-1.52716100	0.54103900	-1.93142600
C	0.42372500	3.11843400	-2.93425800
H	2.49969700	3.35961500	-2.41701700
H	-1.63865900	2.60323600	-3.23705400
H	0.36854900	4.03626700	-3.50777300
O	-2.72853000	-3.14976700	-2.86528600
C	-3.94093500	-3.88857400	-2.87780800

H	-4.09140000	-4.19906700	-3.90830100
H	-3.86949400	-4.77131800	-2.23691100
H	-4.78174900	-3.26811800	-2.55656200
O	4.83496500	-1.25697600	-0.56056300
C	6.15273600	-0.71182600	-0.71143300
H	6.71415900	-1.45011300	-1.27563600
H	6.10748200	0.23212600	-1.25381700
H	6.60551800	-0.54926900	0.26606000
S	-1.42060400	0.15737700	2.69704600
O	-2.79717300	-0.25677800	2.90455500
O	-0.57757500	0.45493400	3.84443200
C	-1.44881000	1.57568300	1.63240100
C	-0.36587300	2.44844500	1.63134500
C	-2.56011800	1.79483900	0.82339100
C	-0.39985200	3.55685200	0.79641200
H	0.47629500	2.27592200	2.29100100
C	-2.58158900	2.91853300	0.01020700
H	-3.39539600	1.10593800	0.84921100
C	-1.50655900	3.81085300	-0.01681900
H	0.44097700	4.24115100	0.78446900
H	-3.44348000	3.10247900	-0.62188900
C	-1.55422600	5.04045900	-0.88149100
H	-2.11646500	4.85334600	-1.79742200
H	-2.04572900	5.85838600	-0.34722000
H	-0.54926100	5.36700500	-1.15061400

CONFORMER 11

	0	1	
C	-2.83760500	-1.61517600	0.94118000
C	-1.51385500	-1.23420200	0.73373600
C	-0.98449300	-1.22258600	-0.56314100
C	-1.80112700	-1.60413000	-1.62105600
C	-3.13529200	-1.95323400	-1.42000000
C	-3.66131500	-1.94840100	-0.12526200
H	-3.21999300	-1.64899000	1.95233700
H	-1.41146500	-1.61494600	-2.63374000
H	-4.68752300	-2.22845000	0.06723300
C	0.45015700	-0.83661300	-0.85180400
C	1.38273900	-0.80097800	0.40453900
H	1.86590600	0.15949500	0.57376500
N	-0.65537800	-0.98471800	1.85736500
C	0.74613000	-1.39439900	1.66699800
H	1.30462900	-1.07828700	2.54683200
C	1.31099600	-2.02597800	-1.40681900
H	1.78480300	-1.83623600	-2.36898600
H	0.76146600	-2.96733400	-1.45482700
C	2.26703100	-1.93308700	-0.19914800
C	0.86210200	-2.92017100	1.51323700
H	0.81692000	-3.42523100	2.47767300
H	0.04267800	-3.29836100	0.89627100
C	2.20133500	-3.10682600	0.79906100
H	2.28662800	-4.06977800	0.29264500
H	3.02159800	-3.01707700	1.51458100
C	3.68806100	-1.56281700	-0.53264600
O	4.20100900	-1.65387200	-1.62048900
C	0.54924000	0.44633000	-1.67273900
C	1.78361200	0.83186100	-2.21357300
C	-0.54184900	1.29396200	-1.86680500
C	1.91778900	2.01678700	-2.92645500
H	2.65689100	0.20066900	-2.09413400

C	-0.41039100	2.47878300	-2.58795200
H	-1.50806800	1.04037700	-1.44977400
C	0.81662600	2.84659500	-3.12288900
H	2.88392100	2.28728700	-3.33618500
H	-1.27577200	3.11909800	-2.71989500
H	0.91716200	3.76779900	-3.68469000
O	-3.83691800	-2.28738600	-2.52936600
C	-5.19760900	-2.65698100	-2.36267900
H	-5.28858300	-3.54505300	-1.73177400
H	-5.77649100	-1.83716900	-1.92918700
H	-5.57153200	-2.87887200	-3.35863900
O	4.33491400	-1.10845300	0.54417800
C	5.70265700	-0.73072900	0.34044600
H	6.27870400	-1.58414800	-0.01549400
H	5.76286600	0.07851100	-0.38685100
H	6.06493400	-0.40141200	1.30945200
S	-0.96367300	0.36828700	2.78793100
O	-2.35909500	0.29504800	3.18302900
O	0.07240500	0.39778900	3.80823600
C	-0.78023700	1.80526400	1.76302800
C	-1.90616200	2.36354100	1.16946000
C	0.48405200	2.36543100	1.59448400
C	-1.75643700	3.50815900	0.39600200
H	-2.88093100	1.91891100	1.32783400
C	0.61364600	3.49922500	0.80785400
H	1.34373000	1.93595700	2.09531500
C	-0.50173800	4.08639100	0.20109400
H	-2.62864500	3.95385300	-0.06903600
H	1.59315700	3.94302700	0.66759300
C	-0.33996700	5.32698400	-0.63344800
H	-1.24013000	5.53415700	-1.21253200
H	-0.13814700	6.19146200	0.00435500
H	0.50058800	5.21811700	-1.32150400

CONFORMER 13

	0	1	
C	-2.50160800	1.55923300	-1.78186800
C	-1.28676500	0.99198700	-1.36669600
C	-0.61538600	1.53017300	-0.26707600
C	-1.19325200	2.60151100	0.42650600
C	-2.42115500	3.12348000	0.04293300
C	-3.07554300	2.59398000	-1.07650500
H	-2.98860400	1.16673600	-2.66298500
H	-0.66049300	3.01268500	1.27353000
H	-4.01769500	3.02889100	-1.38566000
C	0.76541000	1.06026900	0.15955100
C	1.40151000	-0.01935300	-0.76241900
H	1.57014500	-0.99284700	-0.30354500
N	-0.70764600	-0.07126000	-2.13932400
C	0.76130300	-0.13616500	-2.15545200
H	1.04458500	-1.09142400	-2.59485400
C	1.92038800	2.03841700	-0.23675300
H	2.48919600	2.45971700	0.58833700
H	1.59654800	2.83953100	-0.90181100
C	2.64792000	0.89705000	-0.97265800
C	1.36547200	0.99042400	-3.00734200
H	1.30478700	0.76199000	-4.07106600
H	0.82062100	1.92236900	-2.83195600
C	2.80153500	1.08939000	-2.48899400
H	3.28031700	2.04051200	-2.72884200
H	3.40810800	0.27995700	-2.90103300

C	3.89398900	0.41733600	-0.27493400
O	4.43730100	0.96572300	0.65041700
C	0.77313900	0.67452300	1.63439900
C	1.13598700	1.58232300	2.63186000
C	0.35260400	-0.59894800	2.02080300
C	1.08336500	1.22474100	3.97648700
H	1.46385100	2.58142900	2.36979300
C	0.30461900	-0.96222300	3.36196700
H	0.05904700	-1.31751900	1.26574200
C	0.67180900	-0.05060700	4.34723600
H	1.37071100	1.94540700	4.73289600
H	-0.01616800	-1.96084900	3.63578500
H	0.63885800	-0.33209500	5.39281900
O	-3.04942700	4.14519200	0.67137100
C	-2.41289600	4.71110200	1.80697100
H	-2.27213600	3.96232600	2.59134100
H	-1.44677300	5.14704200	1.53837500
H	-3.07750200	5.49289400	2.16480000
O	4.33010000	-0.73172000	-0.80140300
C	5.50029800	-1.29237600	-0.19363700
H	5.30919600	-1.51055500	0.85673900
H	5.70893100	-2.20597400	-0.74195000
H	6.33544300	-0.59729300	-0.27455900
S	-1.54529100	-1.51385600	-2.26042900
O	-2.91688900	-1.18238100	-2.59965600
O	-0.76866000	-2.35888800	-3.15185000
C	-1.56923900	-2.27185300	-0.65705900
C	-0.65729700	-3.27999200	-0.36274600
C	-2.51238100	-1.84589400	0.27523000
C	-0.70428400	-3.87815500	0.89082200
H	0.06087300	-3.59960700	-1.10804200
C	-2.53909800	-2.45414900	1.52229700
H	-3.21938800	-1.06488500	0.02154000
C	-1.64581800	-3.48057900	1.84406200
H	-0.00324500	-4.66990800	1.12945100
H	-3.26812000	-2.13092600	2.25669600
C	-1.71805800	-4.16584700	3.18185700
H	-2.09604900	-3.49038500	3.95036600
H	-2.39647100	-5.02150300	3.12854100
H	-0.73920500	-4.53740000	3.48761100

CONFORMER 13b

	0	1	
C	2.87388300	-1.21217600	-1.29274000
C	1.53589400	-0.91305900	-1.03645900
C	0.95274300	-1.32325500	0.17403900
C	1.74893300	-1.97999900	1.10563000
C	3.09833500	-2.23172500	0.86891300
C	3.66652800	-1.84574900	-0.34658400
H	3.29842600	-0.93260700	-2.24641300
H	1.32967800	-2.31069500	2.04886800
H	4.70279100	-2.04956800	-0.57707900
C	-0.53054600	-1.15814800	0.46289000
C	-1.36094700	-0.55279300	-0.70574300
H	-1.81248100	0.41903800	-0.51106800
N	0.75115300	-0.26338400	-2.04870400
C	-0.67752400	-0.60892200	-2.08210300
H	-1.17115200	0.09548200	-2.74989200
C	-1.35629000	-2.48028400	0.32559400
H	-1.85018500	-2.82485200	1.23083300

H	-0.78665100	-3.30051900	-0.11220900
C	-2.30389600	-1.79645300	-0.67825100
C	-0.90048400	-2.03038500	-2.61988600
H	-0.82622500	-2.06189000	-3.70657500
H	-0.14293600	-2.70533900	-2.21155000
C	-2.29242900	-2.38837900	-2.09614000
H	-2.48463000	-3.46277500	-2.08636000
H	-3.06014900	-1.90211200	-2.70200100
C	-3.68064500	-1.52213700	-0.13175700
O	-4.13421800	-1.97033900	0.89071200
C	-0.74833100	-0.44416100	1.79174700
C	-0.90844800	-1.14983100	2.98656700
C	-0.73444600	0.95019000	1.84410000
C	-1.05525300	-0.47909800	4.19754400
H	-0.91961300	-2.23349800	2.98382700
C	-0.88696100	1.62416900	3.05079800
H	-0.60393100	1.51944300	0.93225400
C	-1.05000400	0.91107700	4.23440900
H	-1.17903100	-1.04725300	5.11185900
H	-0.88300400	2.70815400	3.06316800
H	-1.17289200	1.43341400	5.17550300
O	3.76842600	-2.86499600	1.86137800
C	5.14315500	-3.14987000	1.64986700
H	5.27886600	-3.81594200	0.79371100
H	5.71472400	-2.23097300	1.49459400
H	5.48890900	-3.64474700	2.55349400
O	-4.35681500	-0.68538300	-0.92587700
C	-5.67646200	-0.33891900	-0.48823900
H	-5.63245700	0.15118700	0.48401800
H	-6.06871600	0.33862500	-1.24049700
H	-6.29552100	-1.23274500	-0.41713400
S	1.18392700	1.28289100	-2.51694800
O	2.61381000	1.26761400	-2.76488300
O	0.27304000	1.65101100	-3.58787800
C	0.90053100	2.37337700	-1.14683900
C	-0.24990900	3.15436200	-1.12048800
C	1.84823400	2.43528500	-0.12768300
C	-0.44371500	4.02274500	-0.05262300
H	-0.96756400	3.09373600	-1.92948500
C	1.63217400	3.30529700	0.93147200
H	2.74256200	1.82502700	-0.17316300
C	0.49309300	4.11497400	0.98006700
H	-1.33305100	4.64207000	-0.02495500
H	2.36158300	3.36152500	1.73152000
C	0.29654200	5.08990700	2.10944000
H	0.75829500	4.72574900	3.02812900
H	0.76007600	6.04865000	1.86207800
H	-0.76307700	5.27136100	2.29374800

conformer 14

	0	1	
C	-0.37453900	-3.08509900	-0.67120400
C	-0.40834400	-1.70982300	-0.46285000
C	-1.62868200	-1.02873100	-0.46641600
C	-2.79649800	-1.75049000	-0.68532400
C	-2.76836200	-3.13114700	-0.87218100
C	-1.54390600	-3.80739200	-0.85890100
H	0.58363500	-3.58923500	-0.67754400
H	-3.75649600	-1.24500200	-0.70057700
H	-1.48891000	-4.87647500	-1.00903200

C	-1.71631500	0.46950300	-0.27582000
C	-0.34933400	1.22786300	-0.35766700
H	-0.08518800	1.77372300	0.54497700
N	0.83116200	-0.99007200	-0.32910600
C	0.80643200	0.37253800	-0.89227000
H	1.75476200	0.85531100	-0.64234300
C	-2.17045800	1.21929500	-1.57217500
H	-3.08569700	1.80227100	-1.48997000
H	-2.25290100	0.55243200	-2.43155100
C	-0.86907800	2.04792000	-1.57677000
C	0.64796900	0.35539800	-2.41944700
H	1.59138000	0.14033400	-2.92097300
H	-0.07163100	-0.41435200	-2.71097300
C	0.10270400	1.75096600	-2.73584300
H	-0.39621000	1.80512900	-3.70497600
H	0.91477500	2.48132000	-2.72193900
C	-1.05822300	3.52297400	-1.34071600
O	-2.10030900	4.12243400	-1.44066700
C	-2.46486300	0.83200700	1.00100600
C	-2.42897400	-0.02576200	2.10575400
C	-3.11780900	2.06006600	1.14045300
C	-3.03851000	0.32477100	3.30516500
H	-1.92184300	-0.98058600	2.02830900
C	-3.72951900	2.41100100	2.34141800
H	-3.15165200	2.76391800	0.31745000
C	-3.69635200	1.54482700	3.42800100
H	-2.99998800	-0.35951500	4.14463000
H	-4.23429800	3.36653100	2.42298500
H	-4.17573000	1.81725300	4.36057800
O	-3.96816500	-3.72987600	-1.06435300
C	-3.98091000	-5.13573300	-1.26179200
H	-3.56910700	-5.65770700	-0.39402300
H	-5.02462200	-5.41039900	-1.38922300
H	-3.41858700	-5.41149400	-2.15781000
O	0.09069300	4.10999000	-0.99469000
C	0.02204500	5.51888200	-0.74037000
H	1.03140200	5.82075000	-0.47811100
H	-0.31685600	6.04540600	-1.63197800
H	-0.66386400	5.71748800	0.08269600
S	1.56667900	-1.08455500	1.18242000
O	1.11056700	-0.01674400	2.06452800
O	1.41743000	-2.45876000	1.63352900
C	3.25993500	-0.76808200	0.76137900
C	3.91929300	0.30232900	1.34641600
C	3.90192000	-1.62885300	-0.12634400
C	5.25858800	0.51338900	1.03238500
H	3.39273700	0.95641100	2.03004500
C	5.23330000	-1.39936200	-0.42824900
H	3.36330700	-2.45473600	-0.57606600
C	5.93004100	-0.32794500	0.14660400
H	5.78493100	1.34701300	1.48246200
H	5.74573100	-2.05830000	-1.12029300
C	7.37752900	-0.10254300	-0.19614800
H	7.50057500	0.02769400	-1.27344100
H	7.77055200	0.78047100	0.30657200
H	7.97858800	-0.96523500	0.09979600

conformer 14b

	0	1	
C	-0.24529900	-3.04647400	-0.59224000

C	-0.32910500	-1.67031700	-0.40121500
C	-1.57282800	-1.02954400	-0.45355500
C	-2.70690700	-1.79746300	-0.69352400
C	-2.62750200	-3.17847000	-0.85944500
C	-1.38258900	-3.81194500	-0.80331400
H	0.72834000	-3.51891400	-0.56554600
H	-3.68443600	-1.33050600	-0.74630000
H	-1.28578700	-4.88003200	-0.93823300
C	-1.71408200	0.47620700	-0.30908800
C	-0.36892500	1.26156600	-0.29632200
H	-0.15709400	1.80532700	0.62204900
N	0.88368000	-0.91401800	-0.24102600
C	0.84085000	0.45329900	-0.78449400
H	1.75486900	0.96649700	-0.47503000
C	-2.10028200	1.20855100	-1.63490400
H	-3.02577800	1.77870800	-1.60514400
H	-2.10544100	0.55282800	-2.50660200
C	-0.83701700	2.08578600	-1.53572400
C	0.77257900	0.46307900	-2.31737000
H	1.74884200	0.27718300	-2.76507000
H	0.08814100	-0.31578000	-2.66490700
C	0.21651800	1.85484900	-2.63223200
H	-0.21746600	1.92601100	-3.63109400
H	1.00646100	2.60347800	-2.54207800
C	-1.11839700	3.53646700	-1.24288600
O	-2.20197700	4.06309100	-1.27191700
C	-2.60594600	0.79391100	0.88414300
C	-2.06513100	0.75609500	2.17318100
C	-3.96827800	1.05536900	0.73817200
C	-2.86645800	0.98648200	3.28534300
H	-1.00891700	0.54356300	2.30531100
C	-4.77252300	1.28365900	1.85275700
H	-4.41816300	1.07944200	-0.24742600
C	-4.22444300	1.25372900	3.12946000
H	-2.42948000	0.95728300	4.27669600
H	-5.82832300	1.48718800	1.71819900
H	-4.84847900	1.43632300	3.99606800
O	-3.80152400	-3.81932300	-1.07640200
C	-3.76169800	-5.22744600	-1.25213900
H	-3.35658800	-5.72228000	-0.36547300
H	-4.79162700	-5.53948600	-1.40353000
H	-3.16580400	-5.49726300	-2.12808400
O	0.00127900	4.18856200	-0.91203000
C	-0.15737300	5.57352900	-0.58124700
H	0.83713600	5.93484700	-0.33775800
H	-0.56567000	6.11880600	-1.43167200
H	-0.82445600	5.68086400	0.27364200
S	1.66313200	-1.03042500	1.24240300
O	1.23883000	0.02927300	2.15233000
O	1.52675200	-2.40777100	1.68665400
C	3.34198500	-0.70498600	0.77244300
C	4.03687800	0.32022000	1.39607900
C	3.93976200	-1.51899000	-0.18730500
C	5.36701600	0.53334200	1.04674700
H	3.54388400	0.93921000	2.13506500
C	5.26293200	-1.28832600	-0.52271500
H	3.37300000	-2.30804300	-0.66772700
C	5.99470400	-0.26167500	0.08902900
H	5.92073100	1.33212000	1.52616900
H	5.74114700	-1.91093100	-1.27060800
C	7.43026100	-0.02953600	-0.29662500
H	7.50405500	0.22928500	-1.35527900

H	7.87146500	0.77748900	0.28727100
H	8.02046900	-0.93475400	-0.13932000

CONFORMER 15

	0	1	
C	3.04189000	-1.25744700	-0.73875600
C	1.68806500	-0.92157000	-0.76194500
C	0.84608900	-1.36396500	0.27136900
C	1.40231900	-2.09786300	1.31325300
C	2.76290600	-2.39132000	1.35889800
C	3.59250400	-1.96493900	0.32001900
H	3.67051700	-0.95290300	-1.56318100
H	0.77922500	-2.45633000	2.12452100
H	4.64857800	-2.19542500	0.30789200
C	-0.65853700	-1.13631800	0.25899200
C	-1.20872600	-0.48823300	-1.04412900
H	-1.66821500	0.49103000	-0.91709000
N	1.14831500	-0.22333800	-1.89383500
C	-0.24484000	-0.53964100	-2.24131200
H	-0.57027600	0.18107900	-2.99004400
C	-1.49419000	-2.41538100	-0.06524100
H	-2.18141800	-2.73089800	0.71611800
H	-0.88525800	-3.26531000	-0.37591700
C	-2.17080200	-1.70210000	-1.26940500
C	-0.36434600	-1.95192500	-2.83531200
H	-0.04641200	-1.97361800	-3.87729100
H	0.27309500	-2.64312400	-2.27611300
C	-1.84200100	-2.29160400	-2.63939400
H	-2.04727300	-3.36288500	-2.68235600
H	-2.45305800	-1.79907000	-3.39934300
C	-3.63433100	-1.41041300	-1.07526500
O	-4.50076700	-1.61792700	-1.88722700
C	-1.08775300	-0.42435200	1.53635900
C	-1.51034400	-1.13233400	2.66287800
C	-1.00903700	0.96534100	1.61922300
C	-1.85510600	-0.46743100	3.83613800
H	-1.57909300	-2.21364800	2.63604400
C	-1.35748800	1.63448100	2.78778700
H	-0.67565800	1.53544200	0.76099700
C	-1.78568600	0.92019100	3.90234100
H	-2.18320400	-1.03743200	4.69738700
H	-1.29767000	2.71626700	2.82411400
H	-2.06186700	1.43899100	4.81239800
O	3.18286400	-3.10137300	2.43370800
C	4.56182100	-3.43084900	2.50710300
H	4.86174600	-4.05637400	1.66213100
H	5.17964000	-2.52934400	2.53433000
H	4.68819800	-3.98604000	3.43276300
O	-3.87150300	-0.87276900	0.12497600
C	-5.23485700	-0.54360900	0.41190600
H	-5.85460600	-1.43905800	0.37236700
H	-5.23141700	-0.12528800	1.41426900
H	-5.60512600	0.18674500	-0.30710200
S	1.71417500	1.30532200	-2.25509500
O	3.16223900	1.25516500	-2.17317500
O	1.07660000	1.68496700	-3.50470900
C	1.15503900	2.41578900	-0.99067600
C	0.00967500	3.17590600	-1.20529600
C	1.87960900	2.50709800	0.19474000
C	-0.40714800	4.05122700	-0.21025900

H	-0.53144800	3.09435700	-2.14018000
C	1.44379300	3.38590800	1.17690400
H	2.77465900	1.91308200	0.33605200
C	0.30438300	4.17301200	0.98686700
H	-1.29442600	4.65374900	-0.36857200
H	1.99923600	3.46558400	2.10443400
C	-0.13171500	5.15705300	2.03864400
H	0.20051400	4.84713000	3.03013900
H	0.30033100	6.14035900	1.83454800
H	-1.21690300	5.26836500	2.04787100

CONFORMER 15b

	0	1	
C	-2.08546100	2.66601700	-0.72284800
C	-1.12536700	1.64392200	-0.78846800
C	-0.02841900	1.67305900	0.07447900
C	0.07020900	2.70590000	1.01620800
C	-0.90890300	3.68521600	1.11017700
C	-1.99536800	3.65988500	0.22660500
H	-2.90429200	2.66167900	-1.42776200
H	0.92715500	2.72011300	1.67614700
H	-2.73849600	4.44490600	0.28899800
C	1.11047700	0.66782600	-0.00763100
C	1.02374700	-0.31646400	-1.20860000
H	0.91433700	-1.36650700	-0.94096100
N	-1.22069500	0.65171600	-1.82102800
C	0.05452100	0.11657900	-2.32141600
H	-0.17150900	-0.74397700	-2.94978500
C	2.42776400	1.24409500	-0.61768400
H	3.29306600	1.22469600	0.04051800
H	2.31185300	2.24624500	-1.03266500
C	2.42969800	0.14568100	-1.71803100
C	0.80288000	1.15704700	-3.16954700
H	0.38322800	1.22835600	-4.17258700
H	0.72149700	2.14228300	-2.70129500
C	2.24769500	0.65755700	-3.14522300
H	2.97543000	1.43106300	-3.39753100
H	2.37872700	-0.17172600	-3.84432800
C	3.53100300	-0.87014200	-1.57701000
O	4.23966300	-1.26023600	-2.47063300
C	1.29849700	-0.01433900	1.34254900
C	2.20471400	0.46680400	2.28928000
C	0.50930700	-1.11292300	1.68117000
C	2.32308300	-0.13903200	3.53699300
H	2.83420600	1.31948900	2.06194900
C	0.62707500	-1.72436000	2.92479100
H	-0.20549400	-1.49970200	0.96560800
C	1.53760800	-1.24078700	3.85913100
H	3.03526500	0.25015500	4.25508400
H	0.00716400	-2.58156000	3.16167200
H	1.63419400	-1.71731700	4.82720900
O	-0.89197400	4.70314200	2.00330500
C	0.19383100	4.76058800	2.91562400
H	0.23363000	3.86015900	3.53490200
H	1.14337300	4.88499100	2.38791500
H	0.01140200	5.62761700	3.54488200
O	3.63185800	-1.31037900	-0.31922800
C	4.64352500	-2.29265100	-0.07212000
H	5.62669400	-1.88925800	-0.31327200
H	4.57489300	-2.52491900	0.98668400

H	4.45841100	-3.18284100	-0.67275700
S	-2.55242000	-0.35482800	-1.87069800
O	-3.72238800	0.47162000	-1.63892400
O	-2.43626800	-1.11067800	-3.10654600
C	-2.43538400	-1.49507600	-0.51766000
C	-1.85343100	-2.74251300	-0.72461000
C	-2.92778600	-1.11814400	0.72807500
C	-1.77533900	-3.62818900	0.34197900
H	-1.48745000	-3.01739400	-1.70652900
C	-2.83960400	-2.01913200	1.78128900
H	-3.38474400	-0.14529100	0.86356000
C	-2.27122900	-3.28320000	1.60330000
H	-1.32960200	-4.60501000	0.19184100
H	-3.22036200	-1.73698200	2.75626600
C	-2.21770700	-4.27012900	2.73813400
H	-2.27310300	-3.76561500	3.70325300
H	-3.06101700	-4.96273600	2.67352800
H	-1.30181200	-4.86199700	2.70041600

10.2 DFT-Calculation Coordinates for Chapter 7.2

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Coordinates from ORCA-job Int2ent E -5376.952775163048

P	3.72445815984455	0.55637000455039	1.15781692484196
C	2.71805997723366	1.10285841685893	-0.27944972711736
C	5.10683687492747	-0.43545119025191	0.47290461700273
C	4.52678798271919	2.06552704272140	1.76678968188585
C	1.80189840307908	2.17950235110102	-0.12087008136846
C	2.85583545826258	0.48171529741534	-1.51492052466130
C	4.83322168406799	-1.67625629870087	-0.10564358231707
C	6.42805615491447	-0.06003682627289	0.65506217265067
C	5.20489400760136	2.86809825887778	0.85991375718767
C	4.53583987510998	2.39228239923672	3.11912614164955
C	1.55335973947929	2.86787818468369	1.16502174226885
C	1.15332782559588	2.59928486181033	-1.26218823944045
C	2.12341791657937	0.87905754071297	-2.63830165987212
H	3.56363821573019	-0.32107473366992	-1.63563615288131
C	5.83501691423440	-2.50904382175772	-0.59286224069990
H	3.80598346895152	-1.99642168447183	-0.16533894033363
C	7.47205602268733	-0.87548718681915	0.23069160126472
H	6.67158620551123	0.86200219881830	1.16059070014450
C	5.97379311843857	3.93597844324643	1.29429642260753
H	5.14869314418843	2.65999394284719	-0.20092596074798
C	5.25994571293895	3.48200740779866	3.60547703857111
H	3.95530337652738	1.78331512044527	3.79406197873691
C	0.72245816604468	2.33707956391259	2.18922829842972
C	2.07033631406242	4.12051799527712	1.40009201557426
C	1.28466346782713	1.95250841738717	-2.48492979897729
H	2.23759520086777	0.37476078088904	-3.58621058907926
C	7.16806232305605	-2.07286193849840	-0.42931349735999
C	6.04244240823054	4.19358547114498	2.67234147703512
C	0.54484483030535	3.02258522876118	3.38573456148810
C	1.87389402862466	4.80450013293232	2.59397414888228
C	-1.44315921178101	0.65873535795956	3.21301297046212
C	-1.49101880175890	1.67638263501954	0.51392510574829
C	1.13807957288917	4.26624819337490	3.61909136865094
H	-0.09870131775119	2.61379694470278	4.14768085182370
C	-0.90977631803175	0.25847676094763	4.42890426466697
C	-2.81897136082770	0.79954011179185	3.08414330313017
C	-2.04514005169553	2.93419534440381	0.73614210112503
C	-1.81559590758250	0.97156365654295	-0.63663782378937
H	0.99112150088122	4.79076263562147	4.55088741606115
C	-1.70921496731490	0.11667968932490	5.56737334376247
H	0.15307745537082	0.08081383563762	4.49720025674467
C	-3.66955644232187	0.68574455868713	4.17346591672803
H	-3.22628923461944	1.02895683780297	2.11702887389898
C	-2.95019331220974	3.48083513194748	-0.16099102695261
H	-1.77720388375280	3.49718823337266	1.62050557258382
C	-2.70845410771834	1.49161513434921	-1.56838368671849
H	-1.35371409671933	0.01077593812093	-0.82752024890197
C	-3.07452136918176	0.45062035893857	5.43426854640189
C	-3.28144577025833	2.73913813464912	-1.30248957749560
C	-0.05480079583670	3.72070387731675	-2.77765920565752
H	-1.13362430923251	3.74552812618470	-2.89179716837852
H	0.42431610680352	4.60044359258204	-3.20772884943097
O	0.27749983177179	3.63532476284520	-1.38059039931841
O	0.46806851126677	2.53611329866701	-3.40791890099006
H	2.83895777528047	6.94169468244976	0.72010265432301
C	3.17360535828278	6.06903812890950	1.27443180317558
H	4.24752682988616	6.07883315095570	1.44774275339788
O	2.49089627101929	6.01446654727007	2.54226103255315

O	2.81603021443815	4.87863008242397	0.55026369226273
O	8.18802679038968	-2.89674617241768	-0.84679034093510
O	6.84638459729092	5.21783799382061	3.11879627615518
O	-4.13617450961188	3.30818201382181	-2.22104465829765
O	-3.88690417521609	0.53642962775052	6.54217782988671
C	8.25841598954622	4.99796784646422	2.98836508678632
C	5.20135691098156	3.87353946879917	5.08634980794924
C	6.66862378652617	4.79805548472819	0.28656989134780
C	8.87985978265240	-0.46850494916222	0.53880621120517
C	9.02095282170213	-2.40110865955828	-1.90496278685105
H	9.52188861184096	-3.26728283075444	-2.32702227919525
H	8.41903741040881	-1.92122034044817	-2.67527441262564
H	9.76855221133133	-1.70045935795469	-1.54246785673468
C	5.48164771146092	-3.85214051440632	-1.23831326119164
C	-3.53407795100447	4.83819084718292	0.06550110442896
C	-3.01827544856299	0.74085166758496	-2.82400568776834
C	-5.50366487095546	2.89074501380044	-2.09682686241599
H	-5.89362164422094	3.13207038666310	-1.10772784165189
H	-6.06167323172508	3.43741121454137	-2.85029432320104
H	-5.60989702039519	1.82085601503845	-2.27221513355144
C	-1.01560525642510	-0.37270939113911	6.85397135133988
C	-5.18638407766911	0.80099077235915	3.96044623048184
C	-3.75154034784841	1.76781668577649	7.26380264402043
H	-4.53275495382984	1.76914833801464	8.01755647699907
H	-2.78212647178319	1.84465399097580	7.74975737529850
H	-3.88014916166110	2.62260553565765	6.60223216040100
Au	2.86862878391310	-1.02617309795133	2.63315057188294
Au	0.46306258002971	-0.98210197276002	1.05324263123406
P	-0.38808815563345	0.96036507349848	1.76252475531643
H	8.73946899084468	5.76297353781903	3.59002095112763
H	8.52879866764074	4.01349346825545	3.36837052699839
H	8.59374132849323	5.08927138163997	1.95823886052980
C	-5.77756122247806	2.03433576878393	4.65445665222729
C	-5.53919003438278	0.91564416381069	2.47402069178817
C	-5.87190975282230	-0.46561948484834	4.48876684441092
C	-0.12595346850846	0.75093379078749	7.40626136503971
C	-1.94934122641983	-0.87897938949806	7.95684933967639
C	-0.11319831688806	-1.56783098933238	6.51037025023906
H	-3.28658643677945	5.51215598314655	-0.75392796220420
H	-4.62080605908859	4.80364183020143	0.12548201853536
H	-3.15746633987557	5.26936586480181	0.98906226559873
H	-3.96593756829817	0.20703223407522	-2.74697127562118
H	-3.09899299891489	1.41265512545091	-3.67533433933397
H	-2.24557734927839	0.00499252251864	-3.03050986183751
C	6.05041208813727	-3.94983054655405	-2.66056363281302
C	6.02620813685891	-4.99452759148125	-0.36939018432379
C	3.97069706244919	-4.04550565832166	-1.35625055145677
C	4.78674108207546	5.34374993411036	5.24029312681096
C	4.17234926134864	3.04399003294098	5.85085363614948
C	6.56330631027364	3.64084453803126	5.75394251827757
H	6.77859327496145	5.81981685826505	0.64004896178874
H	7.66472290645912	4.42333200000545	0.04967504748711
H	6.10306238833013	4.81410959149748	-0.64224982680352
C	2.61410989371336	-2.81497487490164	3.61732913742649
C	2.84042794611420	-3.18130142711351	4.90020193563833
C	2.32478573465423	-3.96423352605951	2.69211330042041
H	2.65915165860370	-4.91401060866739	3.11494212914856
H	2.87336574194417	-3.83328716035799	1.76401756807539
N	3.15424501724699	-2.46885104197036	6.05311491069376
H	2.77769516523441	-4.23903551882561	5.14090847735071
S	3.76248409241646	-0.86317865099014	6.03513407184736
C	3.46138893279858	-3.24626062429789	7.25912097959641

O	4.06877804528783	-0.52807647324784	7.43903627844020
O	2.80306230091800	-0.01371764653247	5.30695343319057
C	5.30746912198247	-0.97559117730086	5.12568539382828
H	5.70252318481780	0.03221530425815	5.05625976981738
H	5.09636562244484	-1.37193499942862	4.13778024157889
H	5.96760635744695	-1.62401746370458	5.69133863023772
H	3.26833556351026	-2.64944548524593	8.13987717278346
H	4.49639134833865	-3.58725636307706	7.26950517089142
H	2.79987688017145	-4.10550222161858	7.27608222911391
O	0.65065225294893	-3.00446814613785	0.24602510884866
C	0.60636294157924	-4.05736954660992	0.90079891100246
O	0.46716958027541	-5.21823000451805	0.30531420844089
C	0.80078529350461	-4.14020475408732	2.37925954068643
C	-0.89804029021043	-4.41114720407209	3.61792712561328
C	0.11618127411817	-5.34782914404183	3.08439063444339
C	-0.15599551388363	-3.23129269641030	3.19907202755936
H	0.74892597557664	-5.75188930942881	3.88016572143086
H	-0.24002921368502	-6.18207708349793	2.48454682741660
H	-0.69030969471401	-2.39341040439822	2.74888840491888
H	0.44732160003212	-2.80332121060428	4.02454737634456
C	-2.11968472013378	-4.59626671756347	4.26388832533626
C	0.32355380786735	-5.22568206877047	-1.14152257667549
H	0.22162965308105	-6.26951942003383	-1.40626548151881
H	1.20469406793962	-4.79317801362945	-1.60095447881873
H	-0.56227048761553	-4.66538394895675	-1.42177372326656
H	4.73842541494461	5.59585151197202	6.29967601260868
H	5.48767571422322	6.01847419963044	4.76322741785350
H	3.80154609642724	5.51214730937602	4.81156960071231
H	6.48183575899338	3.82730679689390	6.82482118193890
H	6.88914793625512	2.61026525393975	5.61566420805091
H	7.32900968504450	4.29959916309371	5.35999305238552
H	4.11795605831338	3.40659964548543	6.87578424485131
H	3.17746454199611	3.11999895723956	5.41666449934955
H	4.44238296075600	1.99433069725418	5.89432673047158
C	-2.89289075197598	-3.48251555206754	4.67443633702887
C	-4.04502190655674	-3.67930412361623	5.39782748808340
C	-4.46537586883176	-4.97478995065358	5.69972439237129
C	-3.73045174411021	-6.08431082437395	5.28222829410178
C	-2.56644382882221	-5.90431560024167	4.57212609270491
H	-2.56698046968095	-2.48188638338287	4.43011645865442
H	-4.62580752148673	-2.83379721995024	5.73145564490595
H	-5.37592217472353	-5.12063877886361	6.26438560254586
H	-4.07279321854829	-7.08040370731603	5.52221424874043
H	-1.98224177502498	-6.75601618473989	4.25466034767384
H	9.50886799326942	-1.33111632230033	0.74459758133129
H	9.33636081503624	0.07968358927991	-0.28556461888793
H	8.89810791534861	0.18556881514247	1.40715695633660
H	5.76879486255291	-5.95549081339129	-0.81524859497546
H	7.10583878188141	-4.94361883995441	-0.27103189315009
H	5.58667131565729	-4.95784370852497	0.62726601831587
H	5.68230772414101	-4.85876666021102	-3.13553104191261
H	5.72849186803746	-3.10226733380778	-3.26497943043798
H	7.13206463686357	-3.98683724705478	-2.66947943753022
H	3.77347260737295	-5.00400537612005	-1.83223945981972
H	3.48129246709330	-4.06186221320954	-0.38605530030117
H	3.50374686901030	-3.27082327209161	-1.96309261039227
H	0.39988634975964	0.40343734003065	8.29542220101785
H	0.61907671033756	1.05534570398543	6.67529661094375
H	-0.70663058748199	1.62891666538125	7.68130405667383
H	0.41026163136582	-1.89342663007391	7.40709741941679
H	-0.70190576121915	-2.40702920352261	6.14753879364272
H	0.64429686744601	-1.33070172158454	5.77458712450486

H	-1.33748938217708	-1.35441558773719	8.72288705970640
H	-2.51803525198958	-0.09618061312923	8.44201791160132
H	-2.64694508957608	-1.62304726729794	7.57877534002810
H	-6.94771398671532	-0.39550533674968	4.32952843629968
H	-5.51145777699353	-1.34563647560053	3.95797056142586
H	-5.69481049491451	-0.60373138764924	5.55030186394766
H	-6.81604874425415	2.15737780945893	4.34804759821138
H	-5.76353155092952	1.94169661672136	5.73335388689065
H	-5.23786929208335	2.93831263770356	4.37455040645168
H	-6.62279268570149	0.92597419844420	2.37429712571998
H	-5.16290310553697	1.83493524223874	2.02682419314211
H	-5.16504832972583	0.07265203396949	1.89514399708561

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Coordinates from ORCA-job Int2ent E -5376.952107488716

P	3.76620409745973	0.58813997160506	1.14857254075221
C	2.73128556871966	1.15050102339229	-0.26151568181163
C	5.11682613211884	-0.41508941724009	0.42077475943641
C	4.59350745816550	2.08623304376531	1.74930732601169
C	1.82233018717971	2.22790665268116	-0.07323832460095
C	2.85577387162753	0.55396607926737	-1.51055347840243
C	4.80951093816147	-1.64999454517191	-0.15346345103539
C	6.44715266914140	-0.05658879936280	0.56405442544042
C	5.25805178160531	2.89652985696114	0.83949120576959
C	4.62383756696291	2.40069244709486	3.10423640722679
C	1.57981886232701	2.88962915711953	1.22783074738982
C	1.17413451456909	2.68004783969264	-1.20231522783374
C	2.12071931715005	0.98181207830972	-2.62102381160172
H	3.55668337669997	-0.25145631941199	-1.65265517008698
C	5.78457898394422	-2.49444507827907	-0.67272320745653
H	3.77621876828842	-1.95420358653052	-0.18577761430167
C	7.46708241416182	-0.88629172709293	0.10920857904343
H	6.71762722075028	0.86129580911214	1.06388794581991
C	6.03077228965480	3.96270236712000	1.27195276434393
H	5.18576603694467	2.69767036052545	-0.22217940251177
C	5.35489569027408	3.48550181157138	3.59005634227579
H	4.05197858234057	1.78582105379242	3.78125671546451
C	0.74243979720363	2.34714312406324	2.24113849029444
C	2.10031369798939	4.13696897983928	1.48300369454512
C	1.29564877097371	2.06158900911706	-2.44056240042854
H	2.22525390662313	0.49721233511101	-3.58025027807676
C	7.12783430075361	-2.07765571442327	-0.54469945097792
C	6.11935794776383	4.20896290653080	2.65118819455004
C	0.55985996821555	3.01893333424172	3.44487078677780
C	1.89976318305000	4.80642194299006	2.68432389128294
C	-1.44171435340132	0.65947044752738	3.22591201011022
C	-1.44078930914753	1.66993256541212	0.52524298793513
C	1.15537010455346	4.25783628218644	3.69767134123467
H	-0.08901378574177	2.60332649177493	4.19830485009397
C	-0.93377917871433	0.28050635273562	4.45952642912999
C	-2.81702602926017	0.76382501925728	3.05827329868940
C	-2.03697531648040	2.90806138399016	0.74842762463304
C	-1.71068113376341	0.97391606776482	-0.64478062050866
H	1.00269897693880	4.77161039669883	4.63456436479142
C	-1.76082965440958	0.13345412015042	5.57756934836831
H	0.13008895356664	0.12424599510516	4.55876881227244
C	-3.69419501916259	0.63933286658540	4.12490068627301
H	-3.20406774289693	0.97155796666273	2.07804937360496
C	-2.93211202215680	3.44165523997819	-0.16671024485889
H	-1.81197996683679	3.46485996902417	1.64859897240752
C	-2.58893926812319	1.48297268358030	-1.59588539357259
H	-1.21536897729114	0.02982254367576	-0.83523707032921
C	-3.12853054996337	0.43530020830225	5.40442968808923

C	-3.20751709074570	2.70813977578903	-1.32810794274743
C	-0.02463043499228	3.85078225419966	-2.68714575330677
H	-1.10307964161329	3.89197981286482	-2.79950938971424
H	0.46526257425752	4.73477232865278	-3.09578613714313
O	0.30765597221491	3.72660654229302	-1.29310720117775
O	0.48309200795939	2.67576133085239	-3.34690471506085
H	2.89255408796165	6.96581424909904	0.84412447170315
C	3.21232496522220	6.08168490413286	1.38870841187808
H	4.28486552910355	6.07633737964583	1.57127405961672
O	2.51726808384025	6.01681263932870	2.64942659879837
O	2.84774772895923	4.90598044806669	0.64473471822263
O	8.12335219903629	-2.91512742021657	-0.99303331543238
O	6.91927950318540	5.23703632737850	3.09520427643761
O	-4.05200168981513	3.26274454311163	-2.26494055181550
O	-3.96879365041307	0.52582494533433	6.49103237302594
C	8.33182587550779	5.03794676252996	2.93987303509886
C	5.32003205187865	3.86005719875298	5.07590823661014
C	6.70405615199861	4.83910059387473	0.26209077381772
C	8.88849895309278	-0.50124886107643	0.38053071304618
C	8.93926646868661	-2.42671090562503	-2.06777088416149
H	9.40876897230231	-3.29931915223499	-2.51215727740616
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C	-3.56179376890755	4.77808770454157	0.06234379423155
C	-2.83693109464636	0.74641685989738	-2.87338913642077
C	-5.41351608214732	2.81844349802744	-2.17332998673100
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H	-5.49337823479447	1.74555208448230	-2.34485181282944
C	-1.09174701647479	-0.32897654874002	6.88636062358966
C	-5.20714594239230	0.70167984115019	3.86880326929586
C	-3.86766927976029	1.77111924564788	7.19422083800548
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H	-4.02131135556879	2.61230234772506	6.52046932777140
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P	-0.35679465655300	0.96569049882338	1.79737814125951
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H	8.61907523791364	4.04631302650265	3.28745484376314
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C	-5.86081260339029	1.91343678537703	4.54405494882451
C	-5.52067977407204	0.80269037272917	2.37302205753958
C	-5.86024461568853	-0.58904094905571	4.38014317850818
C	-0.22169089053489	0.81039879647502	7.43788345824773
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C	-0.17546607349758	-1.52296979529366	6.57988205980462
H	-3.33218657154037	5.46343986953304	-0.75259085120057
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C	5.94700891552550	-4.98529582024999	-0.47328998252849
C	3.87659746853598	-3.99983652649401	-1.39148287004072
C	4.90748939192877	5.32807170814145	5.25329384765107
C	4.30359394867813	3.02091996574801	5.84647706730450
C	6.69263424316816	3.61973890264828	5.71828666819798
H	6.80088833080851	5.86089324074590	0.61960418202429
H	7.70397999474460	4.48135646905236	0.01552327586536

H	6.13077046374172	4.85062341277773	-0.66198884349468
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C	2.77434994353710	-3.14558646596663	4.92543220080385
C	2.36335283374360	-3.89904625202654	2.67855711991821
H	2.75653585884901	-4.85091067425776	3.04407842318586
H	2.84641422877068	-3.71522419515952	1.72506995265239
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H	2.66361309665384	-4.20115072336106	5.15919435487590
S	3.64744667676237	-0.84379611668497	6.13135742031632
C	3.24623860739884	-3.23558325429210	7.31711312444722
O	3.86547003985650	-0.52145793924302	7.55448394966547
O	2.74271275843802	0.01692491187862	5.34877856922643
C	5.24785145380430	-0.96342985435016	5.32516950359187
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H	5.09597538695426	-1.29495485959776	4.30315682982119
H	5.84389964007144	-1.66736658117812	5.89591619011962
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C	0.57623882710186	-4.06699234170162	0.97851306979586
O	0.39049427661190	-5.23033086127644	0.40187272984992
C	0.83115767472970	-4.12962964642870	2.45012959951188
C	-0.83861998421479	-4.42514635999465	3.71759187115503
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C	-0.12900155022257	-3.23173850984506	3.28041078119649
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C	-2.05840582510550	-4.63265020461722	4.35986026329255
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H	0.07358712268974	-6.29461338618817	-1.28999469588887
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H	6.63014636959580	3.79960102098091	6.79156294610507
H	7.01325791294671	2.58917884453627	5.56782063367516
H	7.45302631419886	4.27900126708575	5.31505137391424
H	4.27088362648151	3.36470503289010	6.87863274749128
H	3.30041412703952	3.10588408533174	5.43371768664087
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H	5.66305819869955	-5.93848853833638	-0.91973948725422
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Coordinates from ORCA-job Int2ent E -5376.949853618285

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C	2.12778230037500	4.15576366699531	1.54826841664639
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C	0.57709670130627	3.01897335875376	3.49047060914414
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C	-2.89845943618942	3.42289720071312	-0.17117954565727
H	-1.82058270668408	3.44408812192525	1.66967657047905
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C	-3.16708923359448	0.40989186589930	5.37021972617357
C	-3.13374336231426	2.69869520979571	-1.34702890989133
C	0.01871683503641	3.95735380907764	-2.62070799234131
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O	0.51876444601299	2.79158028802499	-3.30203599566395
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H	4.31270694548678	6.09119687264266	1.66721024824313
O	2.53832662648363	6.02466235257412	2.73428927991643
O	2.87856065354255	4.93314593115402	0.72078105798593
O	8.05878887146791	-2.91262048900937	-1.14747032429413
O	6.99621215545286	5.23871721479236	3.10096649919135
O	-3.96709434238529	3.24952046134931	-2.29606819795037
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H	9.24610978369829	-3.31273466700869	-2.74138099266179
H	8.21868237242059	-1.88161782913330	-2.95401420463731
H	9.66264490284547	-1.80041912832854	-1.92345085608348
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C	-3.55569913926092	4.74611767581677	0.05717178743348
C	-2.68999048294644	0.76399695421192	-2.90726829144101
C	-5.32057525256133	2.77536909115981	-2.24473753856484
H	-5.76829156161554	2.98470110962485	-1.27317233926828
H	-5.86339192383132	3.31070618027992	-3.01722086097885
H	-5.37375853042292	1.70492737244892	-2.44016153927359
C	-1.14914914876198	-0.28938246526258	6.90692121262781
C	-5.21380557940993	0.60340658878696	3.78479988929170
C	-3.98985079303535	1.73664155090566	7.12695577464024
H	-4.77364571811742	1.70272914416862	7.87722854570657
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P	-0.32318090534013	0.97180464092464	1.82323320396672
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C	-0.30701706366163	0.87194632557278	7.45620587353212
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C	-0.21027510525001	-1.47382158596439	6.63589822779529
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C	5.89213758977816	-4.97293118990518	-0.53289596818163
C	3.79486238318808	-3.97391905798829	-1.37262510628037
C	4.97800208211828	5.32861089851045	5.26681388444260
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C	6.77291262759112	3.62592402619222	5.71572136573624
H	6.85545494528875	5.88248265608026	0.62770179680652
H	7.75925714853085	4.50559278959733	0.01870545997046
H	6.18494945026620	4.87511822332300	-0.65622967058881
C	2.70900637851204	-2.73784884952637	3.63758778280797
C	2.68889697077572	-3.10261955890175	4.94036845438695
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H	2.81232080294320	-4.78422512105917	2.97119404741971
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C	3.05093077286739	-3.20897961079236	7.34978056229963
O	3.77353266985199	-0.51937064071120	7.61195358112076
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Coordinates from ORCA-job Int2ent E -5376.946442528371

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H	-7.05715595430688	1.52574457024366	3.75292293676852
H	-6.14751674711364	1.47970093507470	5.25087440322174
H	-5.60395827406717	2.50596371976825	3.92179830393429
H	-6.48868040849905	0.30684612414319	1.85276093024863
H	-5.11150729754881	1.37325060292175	1.64056799690567
H	-4.89834245649639	-0.37962762201539	1.56760469020150

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Coordinates from ORCA-job Int2ent E -5376.941478588336

P	3.90754565598928	0.68571988806148	1.17592570404402
C	2.81264966099777	1.31606740070649	-0.15862872227818
C	5.13787213874555	-0.36044316335009	0.31668117784327
C	4.82203958116732	2.14757182542444	1.73781354403010
C	1.91674404672932	2.38015047992240	0.12842391918099
C	2.92993961419053	0.83399664784611	-1.45728796864453
C	4.70546494787061	-1.56545859594557	-0.23899243181257
C	6.48797663006216	-0.05493711247277	0.28991851611159
C	5.46141252151505	2.95220156480810	0.80515367843813
C	4.90628981947703	2.46188339629960	3.09059862531282
C	1.68402919312367	2.93617315215972	1.47987389429360
C	1.27855594780992	2.94478319454838	-0.95455720980725
C	2.20356173028525	1.37323841727819	-2.52425353091664
H	3.62221021205743	0.03711235041171	-1.67264111344543
C	5.56725325196900	-2.43596042470080	-0.89554918068113
H	3.65934955208884	-1.81471391481709	-0.16069932296971
C	7.40321657713951	-0.91027458296701	-0.31653982314590
H	6.85775381859210	0.84054056123951	0.76697927944822

C	6.26417732134067	4.00728313055474	1.20927511693972
H	5.33886591701379	2.76185876195640	-0.25342896033728
C	5.67255457159891	3.53298974872531	3.55079454851628
H	4.34888324749786	1.85568364920876	3.78762463263834
C	0.82019378549114	2.34656072060428	2.44476162424233
C	2.22589684502180	4.15377210580701	1.82223942411488
C	1.39804383632318	2.44660812402069	-2.24575400073004
H	2.30319956736341	0.97812523569372	-3.52419492790937
C	6.93177196528434	-2.07259930174060	-0.94106836041055
C	6.40989920954688	4.24923808092287	2.58487773801358
C	0.61882423429937	2.95689828302316	3.67815882017292
C	2.00775836108267	4.75948086739466	3.05346504508415
C	-1.43035854504125	0.61650775052263	3.25930261077981
C	-1.25411961673906	1.65611625150062	0.58893917437372
C	1.22478154787699	4.17081872553871	4.01346771294939
H	-0.05568630103941	2.51687389129977	4.39292021516466
C	-1.03318536177017	0.31855660681475	4.55394780408951
C	-2.78241742998635	0.56866900755711	2.93643008844926
C	-1.93170448504393	2.85256147508128	0.80881952024216
C	-1.39840062107486	0.99183593678310	-0.62012810260874
H	1.05024811763992	4.63596638076953	4.97176237499442
C	-1.96582652555958	0.13881163896518	5.58106123105287
H	0.02145314727008	0.24944261665465	4.77442312855933
C	-3.75871234179371	0.38419148594887	3.90244362930388
H	-3.07400869956384	0.69970401577137	1.91064649399300
C	-2.78222259913044	3.37354732004026	-0.15437294465811
H	-1.80919094810696	3.38185894986742	1.74480366822842
C	-2.22405873987597	1.49368079011553	-1.62124048970542
H	-0.84400579641471	0.07962256581230	-0.80213402686341
C	-3.32591429921324	0.29473911299182	5.24541801051014
C	-2.92471992759416	2.67544006764055	-1.36110597325340
C	0.11299007492649	4.27487579851226	-2.32620485281340
H	-0.96268116816667	4.35187085180272	-2.44580198270256
H	0.62749495601227	5.18335605190004	-2.64011974851453
O	0.42524408806104	4.00619135312641	-0.94812601419249
O	0.60311675807529	3.15951619539597	-3.09328942086057
H	3.03755441339867	7.00363213357549	1.34997532440370
C	3.35309273648587	6.09274458501549	1.85176106612376
H	4.42326263335532	6.08088222341362	2.04754043734875
O	2.63994833478389	5.96178044809303	3.09778407725732
O	3.00122104305839	4.95648892590388	1.04353265325980
O	7.81840554649028	-2.93455617002896	-1.54104459301607
O	7.23187505412699	5.26743307372544	3.00643719946303
O	-3.72210467077625	3.23285747014383	-2.33638976633572
O	-4.28806648028395	0.34917517643036	6.22852626920734
C	8.63469162859706	5.10834092674005	2.74954556124901
C	5.71577182384967	3.88886551387192	5.04117422664370
C	6.90088772642349	4.88400194906446	0.17695005494425
C	8.86264517838266	-0.58502485482690	-0.23895889190768
C	8.55022861206230	-2.44183631214375	-2.67329486690238
H	8.78267549297489	-3.30699066301205	-3.28791611904169
H	7.94619405981403	-1.74287819992429	-3.24954485337557
H	9.47757923872085	-1.95944274203400	-2.37538474933796
C	5.03709984820090	-3.73042450152775	-1.51862092487162
C	-3.50112683000864	4.66497125933286	0.06843829509755
C	-2.32794957945887	0.78853179474049	-2.93581943989020
C	-5.03391377019950	2.65917742993968	-2.43187034791514
H	-5.56722451198832	2.75978522454642	-1.48618011884919
H	-5.55654034057106	3.21352536474732	-3.20484134545692
H	-4.98859619331469	1.60656878533611	-2.70822064222597
C	-1.41087411556042	-0.20142879693737	6.97641520745423
C	-5.22844229086120	0.24985335430477	3.48011478753235

C	-4.39349807909670	1.63742127376997	6.84893685653446
H	-5.23192877206356	1.58022187701106	7.53614838240913
H	-3.49139365602496	1.89189067593504	7.40041921504313
H	-4.58036686305782	2.41179570616787	6.10681795208322
Au	3.15072012829773	-0.84189902306388	2.75090007023928
Au	0.61649017768355	-1.01242202672670	1.29439505832620
P	-0.24095781944807	0.96053582057044	1.92302126645266
H	9.14679918977078	5.75058590718683	3.45999126335819
H	8.94074350236991	4.07554431769588	2.91044342238945
H	8.90118064839725	5.41059615515879	1.73996829861708
C	-6.09842457984315	1.39602496463640	4.01074348677458
C	-5.37494570488034	0.24959103462719	1.95551446783866
C	-5.77074382583535	-1.09238414210715	3.98900362714892
C	-0.68942884628692	1.02767597173445	7.54723083714272
C	-2.43362979812863	-0.71004948687508	7.99669087198904
C	-0.38778379276864	-1.33534823006668	6.83175453792324
H	-3.17715929314070	5.42001529374629	-0.64767915145518
H	-4.57665447349553	4.55387148756365	-0.05835620634272
H	-3.31188079125672	5.04182839678956	1.06976842295682
H	-3.15804710188019	0.08106047173279	-2.94366773231268
H	-2.49463762216104	1.49013732161008	-3.74892939243775
H	-1.41986497231819	0.22630908137711	-3.13884296227835
C	5.32344844419000	-3.75802587826144	-3.02588582613696
C	5.68244495413681	-4.94160993110140	-0.83074996905891
C	3.52386276586452	-3.86620094715758	-1.35170776522735
C	5.36376759090131	5.36645470971613	5.26548757942198
C	4.70395376940748	3.07459904368513	5.84419110814234
C	7.10976508843475	3.58814403229590	5.60686976948683
H	6.94823711567409	5.91900369326522	0.50709305896276
H	7.91798665942736	4.56868399119251	-0.05619234460756
H	6.33154956584720	4.84413086200338	-0.74845800783887
C	2.76808465666250	-2.60590670609372	3.74844269788395
C	2.52709368402449	-2.89560577749821	5.04724874118690
C	2.37178664445528	-3.65462778840134	2.73634901004032
H	2.92834311264267	-4.57932800495675	2.92751941051225
H	2.67524068879163	-3.34028174434571	1.74842658345786
N	2.72878449565797	-2.19657100927441	6.23433923370892
H	2.22326364358530	-3.90633755839384	5.30014055435583
S	3.47903413475290	-0.65713886013770	6.31343232134276
C	2.74390152680899	-2.98315694334785	7.47287391804446
O	3.56533037632628	-0.31646374745446	7.74660666990341
O	2.74235439377484	0.25816549317365	5.42316803230638
C	5.14272473878126	-0.94756418844647	5.70239950099137
H	5.67169998047480	-0.00251068855879	5.75241524151238
H	5.07601705526008	-1.29960637729463	4.67865178936646
H	5.59616444338630	-1.68548333536272	6.35551184148061
H	2.53120683539153	-2.34391374449843	8.31787152541019
H	3.70237281521237	-3.48000629373735	7.62118884166233
H	1.95926788868899	-3.72902421324280	7.40139504535538
O	0.51778576879643	-3.09641080654502	0.54262519873629
C	0.47565950486277	-4.10941828072502	1.25750989122288
O	0.12857457696713	-5.27605012115965	0.77257505705969
C	0.87746874840534	-4.09362324041475	2.70382883635785
C	-0.70884000181958	-4.48627880734218	4.04595121754363
C	0.41469129236934	-5.31453536682133	3.54176808512731
C	-0.14165683620247	-3.24831655779524	3.52902299693999
H	1.12727533359208	-5.56748123754153	4.32993967223558
H	0.16048492978109	-6.23562532719305	3.02349668488484
H	-0.78352666974554	-2.49870397051463	3.07005442098451
H	0.44976576602115	-2.72473198937655	4.30584677715131
C	-1.89951359727911	-4.78239114851775	4.70430475284166
C	-0.24045028481888	-5.33989608074431	-0.63351234967970

H	-0.50955151097222	-6.37349955974164	-0.80461365991962
H	0.60738026592005	-5.05232065935603	-1.24551087453560
H	-1.08245801161417	-4.68176965293272	-0.81941870824909
H	5.37950318684286	5.58258340969896	6.33374046851248
H	6.06257999706487	6.03282845684437	4.77456179305759
H	4.36432445210158	5.58195804350794	4.89545682013726
H	7.12255767853929	3.78352134414626	6.67933879339733
H	7.37062938447017	2.54131880850751	5.45249363482043
H	7.87550153510908	4.20285577551594	5.14638734277999
H	4.73079156426956	3.39909788250032	6.88273158193541
H	3.68777096762313	3.20789298014296	5.47841826436847
H	4.92964305042512	2.01380497064565	5.83153440088631
C	-2.81766243939012	-3.74953502799318	5.01966681130027
C	-3.96131386796081	-4.04211219621428	5.72306470271935
C	-4.22269982659803	-5.35733503933768	6.10912917015469
C	-3.33805016970534	-6.38957176052327	5.79474806788808
C	-2.18523444527600	-6.11269065916663	5.09820435028135
H	-2.60959082174789	-2.73480655160245	4.71375886317963
H	-4.65847999353765	-3.25772652174739	5.97563911261224
H	-5.12661443677304	-5.58038263392124	6.65899119950112
H	-3.55957677304918	-7.40176688507262	6.10017314702346
H	-1.48917956027910	-6.90185366759422	4.85298667851341
H	9.46290690829725	-1.48001303782834	-0.09049105237370
H	9.22329127221117	-0.09959544187823	-1.14571583172380
H	9.05096935331437	0.09551125206887	0.58756954487647
H	5.28686577078433	-5.86332639532445	-1.25758478215048
H	6.76050116768975	-4.94576650416834	-0.95110171047034
H	5.45477994929580	-4.94096285701268	0.23515529212065
H	4.86407878530399	-4.64166803344785	-3.46851364210612
H	4.90029515981229	-2.88015137592434	-3.51348508960554
H	6.38397905166468	-3.79192157207406	-3.24145374616964
H	3.19947722801707	-4.79389324292246	-1.81941995905475
H	3.22885448116262	-3.91031611454334	-0.30660310698943
H	2.97981863925345	-3.05081353222522	-1.82633987851774
H	-0.27637605888930	0.79289699983034	8.52811826562505
H	0.13246670997424	1.34107045053326	6.90578044587070
H	-1.36454226261962	1.87370682643740	7.66073118470173
H	0.05595568847396	-1.54618636688301	7.80238090043864
H	-0.86544051610729	-2.24711356945271	6.47912608536272
H	0.42279628616087	-1.09208680534652	6.15791313046226
H	-1.88728049976367	-1.08002171632467	8.86393619400104
H	-3.11491583208717	0.05334495062675	8.34952647474659
H	-3.01894197487510	-1.53343752424681	7.59549939521207
H	-6.80634955588644	-1.21672244792415	3.67287580906226
H	-5.19295635446746	-1.92002256448994	3.57925906690923
H	-5.73750943113654	-1.15268348234375	5.07186852799823
H	-7.08726203435683	1.33938050294370	3.55654199407171
H	-6.22797143863188	1.34704135981415	5.08484918186000
H	-5.66912618693278	2.36417356187017	3.75511642397553
H	-6.42174566817663	0.08963240790887	1.70459097561873
H	-5.07529055186362	1.19809532004528	1.51165044831459
H	-4.79986319853268	-0.54693363510045	1.48590975938340

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Coordinates from ORCA-job Int2ent E -5376.934731473295

P	3.95738898364023	0.71701199572738	1.19673149358869
C	2.84754488316220	1.36263621026958	-0.11798859627339
C	5.15223233851392	-0.34568831210912	0.30947609213646
C	4.90357597466970	2.16927889471322	1.73054615241663
C	1.95431052292408	2.42149579910047	0.19430695214185
C	2.96216967345441	0.90967039815942	-1.42720883240018
C	4.69355368895789	-1.54749474906137	-0.23134711956504
C	6.50203629969226	-0.04672682734590	0.23646590932221

C	5.50907388138561	2.97780936586138	0.77904030269875
C	5.04475703881517	2.47195039146387	3.08114678830841
C	1.72538707999222	2.94460047722526	1.55917239710200
C	1.31740696790712	3.01361920915373	-0.87443118438901
C	2.23617667818381	1.47550861083682	-2.48076115614620
H	3.65230338767115	0.11599653762716	-1.66071438815497
C	5.52829487642903	-2.42280193257428	-0.91646804930711
H	3.64804612899240	-1.78803941379734	-0.12134087104706
C	7.39105331448340	-0.90588961911974	-0.40270841186684
H	6.89152727547607	0.84780396526322	0.69974627866860
C	6.32351406346595	4.03320283765146	1.15775984992721
H	5.34592197939345	2.79338814196214	-0.27511254415637
C	5.83107499385655	3.53832310365104	3.51822139143934
H	4.52057281041070	1.85667433873971	3.79599507628437
C	0.85401000922515	2.33859078338384	2.50771807228546
C	2.27791254254159	4.14812367063571	1.93268260816869
C	1.43507581865146	2.54533124474747	-2.17698360467450
H	2.33278540830233	1.10275184019664	-3.48954583355213
C	6.89157826765736	-2.06505101718215	-1.01101347220047
C	6.52034452257046	4.26920502765268	2.52808801331448
C	0.65561137333945	2.92125505529608	3.75468511385204
C	2.06854876893217	4.72198387400736	3.18066098523504
C	-1.43032619050279	0.59971270548942	3.25358091209351
C	-1.20540528582800	1.68792451906147	0.61604654992338
C	1.27676562408125	4.11757718323511	4.12332856654494
H	-0.02712243765746	2.47474928791398	4.45665197732985
C	-1.08482416633951	0.33729429718015	4.57003747514934
C	-2.76199841499322	0.47982143870580	2.86767736554807
C	-1.90257110246905	2.86855581999030	0.85771979615080
C	-1.32927757055651	1.04902280437124	-0.60864932526619
H	1.10582698257681	4.55892691799368	5.09347158869694
C	-2.05822299725047	0.13692303042972	5.55533544881179
H	-0.04082055889622	0.30924367279851	4.84275657447997
C	-3.77430262803939	0.26127226826670	3.78757934663973
H	-3.00999686654852	0.58044444917110	1.82712039010814
C	-2.75426146979327	3.39754036893219	-0.10008082159404
H	-1.79448825965463	3.37908934987354	1.80588629399169
C	-2.15715839700610	1.55895102461865	-1.60379858854609
H	-0.75763733181322	0.15077952094142	-0.80640507907566
C	-3.40550728436825	0.22257154904743	5.15206683238153
C	-2.87952127226595	2.72246226996200	-1.32178844232126
C	0.15231387412939	4.37696773099025	-2.21355034531583
H	-0.92355782232597	4.45634294779713	-2.33014764769381
H	0.66608370586719	5.29277630813010	-2.50657436807285
O	0.46612720851107	4.07603952479341	-0.84244530657595
O	0.64191034886424	3.28009462863704	-3.00719484882731
H	3.06979251582326	7.00348915032182	1.53103462422654
C	3.40766705434477	6.08513610485919	2.00468375592441
H	4.48078075179496	6.08514090878725	2.18176588783265
O	2.71768031199489	5.91303859083197	3.25897442181530
O	3.05894146202513	4.96412570348467	1.17428096454830
O	7.75237978089330	-2.92852278133394	-1.64611912469715
O	7.34388564234485	5.29613748669576	2.92367385230055
O	-3.68319579052276	3.28518407100680	-2.28897339862679
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C	6.91543383196086	4.91868421601720	0.10654070679473
C	8.85366251445604	-0.58675271570340	-0.37967832995376
C	8.42854241918520	-2.43698911782616	-2.81284316747207
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C	4.97293859700890	-3.71592665720232	-1.52019035975238
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P	-0.20943320076447	0.96860981900565	1.95062042282782
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H	9.06085778804666	4.13259860501103	2.70910307973076
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C	-6.16913120323449	1.13810852980159	3.75973504764222
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Coordinates from ORCA-job Int2ent E -5376.920083536236

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H	-6.04038725641816	1.76636137748800	3.14252985651194
H	-6.18445002274200	-0.54885736944809	1.02252901776564
H	-4.98189613167884	0.72946933569305	1.00413169717559
H	-4.47851261409004	-0.96476080349783	1.01979175884938

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Coordinates from ORCA-job Int2ent E -5376.913946794001

P	4.19125972630747	0.75994914172488	1.30862674122474
C	2.99317696758187	1.34461925953965	0.04227439970287
C	5.30834089640875	-0.35807570027544	0.39226016684614
C	5.19505002829016	2.22016136677917	1.68276058226948
C	2.04057087420942	2.34509505005131	0.37861695391911
C	3.13353975224909	0.93344886044553	-1.27845024876005
C	4.81400060875452	-1.58990818300886	-0.03541021924211
C	6.64073506093489	-0.05226923903345	0.17445908396916
C	5.60986148485943	3.06588056044379	0.66500036762522
C	5.58268374708970	2.47704290035217	2.99255920405599
C	1.75586732742711	2.81545909433519	1.75485692397786
C	1.40049243157299	2.95100495153511	-0.68117147286917
C	2.39080932621394	1.49515872234725	-2.32257414835245
H	3.85925477504735	0.17618406520553	-1.52599051622073
C	5.59508240494170	-2.50099178984331	-0.73693010509015
H	3.78251964099252	-1.82403206270248	0.17483925790671
C	7.47997015781749	-0.94453026412086	-0.48618581645824
H	7.05667785224800	0.87553106386889	0.53994830698945
C	6.43151997955580	4.14991318332347	0.93225648326929
H	5.27046443747464	2.90338664116292	-0.34984234055114
C	6.41195150998820	3.54880124133864	3.31954494030631
H	5.22186125463068	1.81616766997187	3.76501073410878
C	0.75958089090992	2.24435494443240	2.59966304018724
C	2.35461463442418	3.96172080356851	2.22655811932822
C	1.55228136405792	2.52895829445150	-1.99723176832903
H	2.51101184655875	1.15549767059215	-3.34046985232380
C	6.94211678942815	-2.14470404863853	-0.97013218084201
C	6.85258260947236	4.36324634222615	2.25550400016744
C	0.49584282068343	2.79661930579807	3.84886904479632
C	2.09747998706396	4.48879005328068	3.48820669849014
C	-1.62939963195744	0.53343207691993	3.16201415657920
C	-1.35750841938961	1.87350627520188	0.66759660057697
C	1.18101217099583	3.91473668295960	4.33024290853107
H	-0.28472925887506	2.38875075864154	4.46603470369845
C	-1.36660563389432	0.26810386444100	4.49615170039171
C	-2.91906374042319	0.33143756029895	2.67631384143394
C	-2.01938611656644	3.04151810009620	1.03531962085699
C	-1.52688905926819	1.35256903202971	-0.60643582969893
H	0.96136559909533	4.32660461083320	5.30358987594864
C	-2.39795246923567	-0.00231185839784	5.40619551568814

H	-0.34751007226053	0.29564843419289	4.84794256619086
C	-3.97741440416186	0.01780970778271	3.51174367954902
H	-3.09578030030214	0.43848114492717	1.62131020657681
C	-2.87843513097713	3.67715093024342	0.15221914583824
H	-1.87778889383979	3.45908074333587	2.02366366306829
C	-2.37106652913320	1.96692605371815	-1.52646701982319
H	-0.98531378776694	0.46270223948743	-0.90116910858497
C	-3.71172416560972	-0.01319126684456	4.90095517003050
C	-3.05628171434371	3.11566200199866	-1.12002491458482
C	0.25174874958960	4.34574878567909	-1.99990552278837
H	-0.81978158552746	4.43654884865637	-2.13974277697496
H	0.77957048279115	5.26645634092441	-2.25068341372056
O	0.53097483276064	3.99828988999289	-0.63220098914017
O	0.75393016989042	3.27108220629523	-2.81573932560308
H	3.11925179064350	6.78091314130218	1.99763580549625
C	3.51751939092429	5.86774993398547	2.43736950754078
H	4.58728476004399	5.92967044935683	2.61056638184331
O	2.84367150725584	5.60687717761516	3.68538884848861
O	3.23550704442594	4.75948305342434	1.56705461707588
O	7.75309430215634	-3.04575013692619	-1.61805732640194
O	7.64429528127712	5.44618137821505	2.55015029922263
O	-3.87756496133261	3.77542370312736	-2.00713712739082
O	-4.79067010405444	-0.07540455000548	5.75326502550491
C	8.95019587635059	5.49255668694267	1.95501224283060
C	6.81192297972562	3.81281707650917	4.77429627670266
C	6.77924679813812	5.09629696321697	-0.17369198295683
C	8.93434316907394	-0.61435974962188	-0.61745334308607
C	8.33729222784602	-2.62938685180164	-2.86127966579456
H	8.48493446723845	-3.53165577870476	-3.44826537050132
H	7.66854719392396	-1.95743713535271	-3.39659418408613
H	9.29778808255669	-2.14303711564601	-2.71201309374835
C	4.99963907833558	-3.82838493154720	-1.21376393310029
C	-3.58041840641720	4.94130700186970	0.53114918801970
C	-2.51210375632101	1.41644908175080	-2.90943662162128
C	-5.20148679412395	3.22970774176917	-2.10491223708531
H	-5.70001100324604	3.25113136932469	-1.13541214663489
H	-5.74218174920670	3.85813465705283	-2.80534171326041
H	-5.18330760014973	2.20570534451433	-2.47550097893543
C	-1.99118022562803	-0.23212632588497	6.87366483307223
C	-5.34442855820533	-0.33066989199082	2.90837761826540
C	-5.14786036194888	1.19768777137186	6.30855441424237
H	-6.02969453642187	1.03057727640575	6.91910714067346
H	-4.35013107519274	1.60182819375469	6.92751924874063
H	-5.37768327904749	1.91480873615770	5.52246763915106
Au	3.42508391612637	-0.58634801010750	3.00670456358854
Au	0.30768669996473	-0.96289199861136	1.08169159980440
P	-0.37407136962510	0.99535858701234	1.91251884702081
H	9.58928293342778	6.02171672986858	2.65653150611733
H	9.33977847147397	4.48795139954553	1.80055485319447
H	8.94132411330385	6.02871880032350	1.00962917143807
C	-6.44849200147878	0.65159266654245	3.31915853078836
C	-5.29760238413856	-0.32685726334354	1.37738382831521
C	-5.72263851290308	-1.75145790202317	3.35213763372931
C	-1.48537419596609	1.09403790479785	7.46196859196596
C	-3.07046230681579	-0.81143449126917	7.79239252552257
C	-0.84032126033306	-1.24355580555488	6.91201903574084
H	-3.30026765511369	5.75752101526259	-0.13393220209049
H	-4.66195232269885	4.83687569094981	0.46002268169406
H	-3.33253366019632	5.23005159543700	1.54899025641810
H	-3.38761189754724	0.77220447375346	-2.99631452470597
H	-2.62584840366662	2.21303906862591	-3.64046058023922
H	-1.64201026715370	0.82084510402868	-3.17310964605396

C	5.10523435855257	-3.95014177143183	-2.74027676316202
C	5.72489949906491	-4.99940436289943	-0.53595086792899
C	3.51848558071628	-3.94591406812609	-0.85761922381553
C	6.30128020505951	5.18827275968814	5.22414276460865
C	6.21505377185567	2.77401379844891	5.72179945007309
C	8.33673286410070	3.73614237267712	4.93255853743028
H	6.74304607289380	6.13025236573632	0.16325894169743
H	7.77927340255541	4.91906899470691	-0.56836352033248
H	6.07992771716529	4.97989522335548	-0.99742802971492
C	2.54543675210536	-2.22624890050658	3.95833621825448
C	2.02448223494273	-2.34867540033438	5.18227927605185
C	2.00642885737282	-2.98123411654921	2.76541300806359
H	2.79974702170286	-3.66831419605298	2.44678713834599
H	1.94954234910571	-2.28940358695188	1.93110441057130
N	2.35903842436628	-1.75088227044944	6.42444157487088
H	1.29129594449542	-3.11522097707854	5.40059908025549
S	3.30915167620317	-0.36049716258137	6.60052881422534
C	2.36909120272324	-2.67865429639155	7.56209666515749
O	3.29034645077164	-0.02835135759403	8.04186269602721
O	2.81264163163961	0.65779383572241	5.65390216407870
C	4.98589196523261	-0.84604453438604	6.18132499134271
H	5.62160718102513	0.01232330399056	6.36360900607340
H	5.00237574921453	-1.13465894575531	5.13555825545619
H	5.25654363654705	-1.67418257747827	6.82798214817961
H	2.37219646993016	-2.12617167496102	8.49135918898065
H	3.22698791990189	-3.35186760044807	7.52845063312795
H	1.45904431025760	-3.26973659167383	7.51815138872672
O	0.30387779449344	-3.10306158744623	0.46097743132958
C	0.39277422537928	-4.02890976975351	1.28327515369551
O	0.20064332682595	-5.27459220536931	0.93417903286351
C	0.71444325611379	-3.80166585881896	2.74138122787991
C	-0.75948317618961	-4.41549052808410	4.14806003563276
C	0.50976393269449	-5.02288681731685	3.67394530666554
C	-0.54447726205281	-3.15556710349936	3.42274548574736
H	1.26268120373921	-5.12824375806510	4.45429484665370
H	0.40524628870265	-5.99981682224570	3.20514059246427
H	-1.36669185163343	-2.78384967231547	2.81262514584719
H	-0.26009796201950	-2.33582597932005	4.09010963526869
C	-1.81572398560825	-4.86671198073453	4.92340686162375
C	-0.16581571002601	-5.54503204836554	-0.44872856075414
H	-0.29051582338709	-6.61821086944754	-0.49835451015665
H	0.62840122983225	-5.21447701085376	-1.10814191122081
H	-1.09270378928691	-5.03308687558410	-0.68417059579168
H	6.57779236244162	5.35909787163893	6.26453737557052
H	6.71955159975878	5.99039066013917	4.62565346650305
H	5.21558782900812	5.23575825704840	5.15440704584413
H	8.60138957669952	3.84456931133310	5.98427328478515
H	8.71073326371500	2.77125657654231	4.59103306253558
H	8.84546372807471	4.51567618734829	4.37921852602696
H	6.51634884669792	3.00826679680360	6.74102265065573
H	5.12713547236616	2.76044274713343	5.69605847198942
H	6.57875682749126	1.77409739904405	5.49394493910847
C	-2.93449592530581	-4.02073921162967	5.14663338376557
C	-3.97050198634474	-4.45397550142125	5.93548453043172
C	-3.91596307062787	-5.72531909524807	6.51036321372309
C	-2.82506311702983	-6.57276067291286	6.30138184730733
C	-1.78033427726438	-6.15659954646287	5.51361926093582
H	-2.96079079841676	-3.03876498172523	4.69808104844912
H	-4.82434432372665	-3.81672632196315	6.11068861789910
H	-4.73582520669329	-6.06202142254046	7.12971179021647
H	-2.80891705187082	-7.55148784308683	6.75754965915077
H	-0.92996403405692	-6.79967987462277	5.33871512911309

H	9.55686259227022	-1.49587626025125	-0.47975106261848
H	9.17377214141885	-0.19900386224119	-1.59625087022870
H	9.21872629020929	0.12615196659664	0.12572453716149
H	5.29151899522208	-5.94326546706430	-0.86699850838827
H	6.78330941972897	-5.00935438939632	-0.77273788733026
H	5.61428231984623	-4.94100895275337	0.54674845177298
H	4.58977595355371	-4.85184123052741	-3.07031537748933
H	4.63415232135940	-3.09756764596639	-3.22877474758498
H	6.13269714894989	-4.01284542486913	-3.07640449983724
H	3.14480439601867	-4.90443221525179	-1.21238282151978
H	3.35430667434418	-3.91148915546415	0.21631183956900
H	2.91716455585293	-3.16563125099496	-1.32161108612203
H	-1.17945405247450	0.94860195715830	8.49776822585281
H	-0.62696636687590	1.46930690170558	6.90820700801180
H	-2.25693003566561	1.86160005609364	7.44259910411433
H	-0.51045585471363	-1.37657483566256	7.94064212193225
H	-1.15955708469914	-2.21398937786139	6.53805645958282
H	0.02442883586867	-0.92733756763769	6.34363709293232
H	-2.59665982364946	-1.07957644541528	8.73629636136392
H	-3.86736609542378	-0.11617778545391	8.02166390794330
H	-3.51195532388756	-1.71232152512649	7.37495041047125
H	-6.68501564712110	-2.02830238496484	2.92228673858847
H	-4.98051510915483	-2.47131225213130	3.00854222444035
H	-5.79804624574425	-1.82807823208292	4.43235526823171
H	-7.34787253502924	0.44369649497982	2.74030509381272
H	-6.70597865398005	0.56393165967661	4.36725411173850
H	-6.15300431732492	1.68040106673504	3.11657734995811
H	-6.26903479457171	-0.63664405386097	0.99708710368701
H	-5.09116082421546	0.66438891757942	0.97427489304086
H	-4.55537525617361	-1.01993931441054	0.98437625984918

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Coordinates from ORCA-job Int2ent E -5376.910350971163

P	4.26639623654187	0.69456344234726	1.33937429357727
C	3.07985557296626	1.23585980651448	0.03763909309392
C	5.40664910150485	-0.44430785434226	0.47534838912550
C	5.27153416118201	2.15291861988294	1.70567706288866
C	2.07510488743113	2.20432751139411	0.32049187243375
C	3.26610338409381	0.79672129322717	-1.26947133426834
C	4.92358008377517	-1.67444369946774	0.02864823010339
C	6.75145394086932	-0.15233717115526	0.32202729622189
C	5.72868822814810	2.96937908701409	0.68216836191697
C	5.62975098878342	2.42774570997254	3.01961874822567
C	1.73097144597487	2.72518346331079	1.66568338488060
C	1.43745714250981	2.75039466153157	-0.77315798652703
C	2.52177101748020	1.28956190992738	-2.34609462329397
H	4.02739283544854	0.06438788247920	-1.48122724539022
C	5.72900186632438	-2.59241918292660	-0.63597199937465
H	3.88117769213880	-1.89972368840613	0.18723731759091
C	7.61236300604800	-1.05101105075971	-0.30049904642914
H	7.15923604938827	0.77093659785177	0.70698513589014
C	6.55911028257312	4.04610637328150	0.94994085864565
H	5.41523476501862	2.78958833404985	-0.33814598920852
C	6.47093389055562	3.48980862499138	3.34743243382385
H	5.23973726019601	1.78547349976548	3.79387074279876
C	0.63955737929107	2.25180199785627	2.45300056170456
C	2.36696399233149	3.85010630360973	2.14260051854579
C	1.63015145802422	2.29288425974785	-2.07145859385509
H	2.68127522323366	0.92438244184110	-3.34961976240527
C	7.08678384095034	-2.24463352416862	-0.81232982066287
C	6.94840141887486	4.27922313821505	2.28040484848531
C	0.33308625051961	2.86414274095699	3.66585086237030
C	2.06610475836683	4.43229940745182	3.37009193031252

C	-1.76487028551658	0.57859477119114	3.03056579173947
C	-1.60345915742124	2.08109976986959	0.61597581828642
C	1.06219896827906	3.94499903059902	4.16531548928828
H	-0.51749525280000	2.53553502399595	4.23661494056297
C	-1.45145622964064	0.34309028257726	4.35882595576627
C	-3.05363664133967	0.29781146681324	2.58059268053353
C	-2.16996279558234	3.26496172424894	1.07820486668340
C	-1.88468416340761	1.63101028104496	-0.66577276198586
H	0.80612881282564	4.40106673803351	5.10960018617368
C	-2.44427837545392	0.04026871477555	5.30222545234994
H	-0.42690808869730	0.42990342047873	4.68320837775014
C	-4.06643956329081	-0.06964325283082	3.44944490250531
H	-3.26300289892410	0.37842457890368	1.52782313828775
C	-3.03328933823449	3.99712847409775	0.27702229652563
H	-1.94130423130225	3.62594110254445	2.07252135393587
C	-2.74542659930965	2.33665303436993	-1.50105965876717
H	-1.41539670676494	0.72679588779368	-1.03287994261045
C	-3.76574262956701	-0.04880010064071	4.83266044976648
C	-3.32214335932743	3.51034349015956	-1.00587780714120
C	0.28269144537893	4.07142546316526	-2.16028968981892
H	-0.78668953925422	4.13767168971623	-2.32506379315630
H	0.80020928294488	4.99239305160530	-2.43110747684333
O	0.53934480169100	3.77547702506442	-0.77603297866444
O	0.82114895316226	2.97857049809907	-2.92827812280524
H	3.22407642615003	6.61745751089392	1.86564832973492
C	3.59215687069147	5.71550545603482	2.35330435061673
H	4.65446468836407	5.76922831876899	2.56552362774215
O	2.86659390910746	5.50930386445966	3.58211210033514
O	3.32544751565164	4.58013685982835	1.51364523309259
O	7.91779655480740	-3.14639934697735	-1.43357457096158
O	7.74133644722749	5.35865848947715	2.57828513408050
O	-4.14201623169920	4.26649633215493	-1.81311306610939
O	-4.81979152940243	-0.13462610637804	5.71412704606997
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C	9.07393437723750	-0.73294540819943	-0.36456078072458
C	8.54089897893214	-2.72615366182628	-2.65647208363105
H	8.73008715896135	-3.62958676915244	-3.22927197829189
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P	-0.57576729738264	1.09486383160472	1.73941581881100
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C	-5.39964535641041	-0.61880504126136	1.36853624148580

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H	2.50113963533023	-3.18642143493840	1.96603349531078
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H	4.79100711051098	-0.75533057509528	5.31097169374562
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Coordinates from ORCA-job Int2ent E -5376.907319410184

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O	3.34949872435879	4.56892022453437	1.52724908154966
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H	-6.10649686133105	4.68297690319138	-2.46755687705651
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C	-5.22841109272557	1.08682466020875	6.18216931487347
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C	3.64696960590557	-4.08168803407242	-0.64825280705291
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H	7.99645075159465	4.77374112516348	-0.51987079721351
H	6.31427107707140	4.82953755022743	-1.01314075024400
C	2.25197181261155	-2.15884887391171	3.81418511231015
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H	2.27825231799412	-2.78134059764213	1.81429607228832
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H	2.57219114750798	-2.62826266875899	8.29913819448407
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C	-0.69605114032928	-4.39114385855451	4.03057501951102
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H	-1.80975794004450	-3.36655673072924	2.50517953496802
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H	8.64566407936181	3.78582907377373	6.04431934114915
H	8.75150363561397	2.68600308855750	4.67154835673841
H	8.93141915235379	4.42263183174861	4.43191878532455
H	6.52814186254005	3.00360231736809	6.77666967811989
H	5.15013106263766	2.78062536817219	5.71121530532463
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Coordinates from ORCA-job Int2ent E -5376.915595416253

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C	4.56302458290142	2.56336935767538	3.28303717192012

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C	2.70107843926474	1.12906086922988	-0.21517803285246
C	4.63221647922868	-0.64284096672971	1.08091665796693
C	4.30738514993342	2.06840065482913	2.06634305262233
C	1.82259181619314	2.24303094239856	-0.28634174522600
C	3.00486790881378	0.40905234768652	-1.36531845323813
C	4.20099436304091	-1.84933573301705	0.52807809672259
C	5.94475178270326	-0.53103834074804	1.50740569107059
C	5.27978323828484	2.71237048942227	1.31642247333751
C	4.05875101326988	2.47902835549276	3.37117542914870
C	1.48880390998737	3.07319278941489	0.88869843435183
C	1.35147785446551	2.57660635588541	-1.53631994186871
C	2.46455143490492	0.73416704865879	-2.61377949002197
H	3.69200380231015	-0.41859630652758	-1.31454227217827
C	5.06417238989482	-2.91141345299614	0.28912443123126
H	3.15955995034988	-1.94933469489798	0.27164953982261
C	6.83638633514943	-1.58923627589067	1.35885205722055
H	6.28676608164800	0.36913114231671	1.99730971089315
C	6.04592690372285	3.72520374802273	1.87614954826082
H	5.44556325343038	2.43488382516355	0.28306905823204
C	4.79413785432262	3.48821747544051	3.98394231010873
H	3.26603940855259	1.98467981760673	3.91020388133259
C	0.48368566289454	2.73546762275435	1.83052884678920
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C	1.63815116880000	1.82728361024296	-2.67034205858186
H	2.70825195524060	0.15803348218643	-3.49388093036765
C	6.40282535923029	-2.75395596467117	0.70985739750190
C	5.82464732799778	4.07484501156208	3.21969335288571
C	0.25974588454376	3.54393898371533	2.94104035093592
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C	-1.83962041194452	1.35752881263614	2.82840165953680
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H	-0.51477492791308	3.29037408524484	3.64509670757625
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C	-3.18627435972286	1.66312427426497	2.68517336591342
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C	-1.90317764231220	1.34047434901593	-1.10843230965469
H	0.80316427441153	5.32971961275251	4.03141436685162
C	-2.12378736668737	1.11742546561793	5.22852366713607
H	-0.31216461300312	0.69934848539446	4.15382741231830
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C	-2.63415029557838	1.84915740875781	-2.17686142420519
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O	0.99339486385628	2.35393358500104	-3.74932500829261
H	3.23503303746804	6.88421345838623	0.31396073922858
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H	4.55317746826400	6.02859647517540	1.20044326830398
O	2.73556740178641	6.14448176786656	2.18649413776911
O	3.11805290612990	4.81602166516126	0.32592264720613
O	7.26313070298539	-3.81232894351147	0.54797921377146
O	6.58009979146951	5.06871604233912	3.79309343915917
O	-3.80053520022128	3.71788379262941	-3.13214716072829

O	-4.18868921284029	1.96053783698736	6.16208807413651
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C	4.48725833099166	3.90555085301563	5.42529422537074
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C	8.20913354664910	-1.46810697431842	1.94364679282366
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H	8.68241058207516	-4.55830993466154	-0.69716009079858
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C	4.55685454669919	-4.17342304379823	-0.41529227141233
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C	-5.20055645973128	3.40402926394374	-3.16966191640016
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C	-3.85135821935218	3.25213501753184	6.68563108053828
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P	-0.71411454328686	1.42808455128583	1.40716633837816
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C	-5.90326770660605	1.95612498470568	2.10197808864199
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C	-2.40528569221853	0.51519673419553	7.74506605575460
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H	-2.93484196721033	5.95877721691483	-1.72574757256639
H	-4.43068430347584	5.43226096882424	-0.99047210419734
H	-3.05465320602021	5.84547248960307	0.03055008186362
H	-3.84878249175098	0.57487306008491	-3.41146354881400
H	-2.77561261113893	1.63165295013853	-4.30480947469413
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C	5.33373570967942	-4.39732125917685	-1.71995343607950
C	4.70044482441612	-5.39829322493937	0.49731605881643
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C	3.29207657281877	3.13795173838157	5.99361053289385
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H	7.11272354828503	5.49587052975828	1.28340363831084
H	8.04528547139719	4.01817240202654	1.12170974856802
H	6.76530301250112	4.36552840757912	-0.02435156645663
C	1.43726133200606	-2.24681594514997	3.91648700691535
C	2.40003473886786	-3.05531645052196	4.38566910409168
C	0.07966416053666	-2.73716337516523	3.49777777007317
H	-0.43110761740633	-1.95598433662561	2.94529762502260
H	-0.53655600276714	-2.84942381454783	4.39417346689465
N	3.74665249462381	-2.62795275978949	4.56510606741257
H	2.21598875352211	-4.06713241613173	4.74248483826260
S	4.13622870469428	-1.70404636540444	5.97437760247341
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H	6.12212660513317	-1.03103768248094	4.84842721737952
H	5.74510030965003	-3.26402311843403	4.36259025065949
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H	4.64113141855258	-4.53633337945495	4.91307629690993
O	-0.29112023775253	-2.87615051856144	0.62304342972360
C	-0.64842223390016	-3.80503743883625	1.35813125852232
O	-1.48501316484651	-4.72662320749712	0.93892652613965
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C	0.65338294935640	-5.90724660052352	3.51382668671716
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H	-1.42958670682373	-5.81393725527882	3.03854953724003
H	-1.05117314389758	-4.99321206382732	4.54933482852113
C	1.23281117822816	-6.94496238648976	4.23052861204017
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H	4.95102650936900	6.02104181544603	5.13511417305562
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H	2.85787879425574	-9.82746023212109	6.20299641610814
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H	8.95521187666951	-1.20081947192873	1.19577480056719
H	8.22224440710245	-0.69305784668065	2.70556366538525
H	4.32697406747621	-6.28563751741064	-0.01375654478548
H	5.73309079111355	-5.57525785246369	0.77785986038783
H	4.11552327698904	-5.26881834153525	1.40512530204055
H	4.90639303769019	-5.24466490017867	-2.25573358786516
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H	2.75969420333955	-4.97660120703439	-1.27168865250692
H	2.44473186943518	-3.90206412534625	0.07844259215749
H	2.89779105849305	-3.23761259469674	-1.48925442850307
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H	-0.74240325479751	2.67155618871155	7.09011264995152
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H	-5.99466390037651	-0.12070645839800	3.85295407437018
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H	-7.04392199760135	3.49613938957854	3.84460831572216
H	-5.96819150228649	3.36469471015368	5.22424170982997
H	-5.41345546105273	4.15440197575744	3.74634383863363
H	-6.98425158470056	2.04439818421441	2.01227397958979
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Coordinates from ORCA-job Int2ent E -5376.934447783265

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C	5.25754400905688	2.71989580598557	1.28989170364133
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H	3.67584502910343	-0.42167647787752	-1.34414405585981
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C	1.91210904250718	5.07357872908751	2.16725294223927
C	-1.86401410846819	1.40210866868546	2.84945019716534
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H	-1.92869394287659	4.05466813915984	0.94884393950632
C	-2.65186457809861	1.85902318829570	-2.17050046044115
H	-1.53354471604595	0.34496763341123	-1.15073422334175
C	-3.44812927490437	1.64504022646618	5.09373824557020
C	-3.13108409917934	3.16966386198949	-2.07721099228530
C	0.36678557991115	3.57760228869191	-3.30441512204949
H	-0.68763448169922	3.59470288407928	-3.56175449694887
H	0.90859549376581	4.41735616612189	-3.73921718243643

O	0.51139908379630	3.60906269886990	-1.87351000390045
O	0.95300074509992	2.34304292682959	-3.76169882185150
H	3.19871237442137	6.87105273648654	0.22322971761733
C	3.47068303172444	6.04982563571205	0.88357332915720
H	4.53351062164904	6.03951868065975	1.10755234490756
O	2.72742603611222	6.15924691614200	2.11379566728798
O	3.09659046340329	4.80265201886132	0.27124977223573
O	7.29715657650409	-3.80257437066881	0.57074675205453
O	6.55198028118823	5.07201242413716	3.77380063139228
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H	8.26729736691017	-2.89914734180515	-1.04130012847925
H	9.30639498313496	-3.24107809317667	0.35900407491405
C	4.59769551167842	-4.19242864031201	-0.39891346654839
C	-3.35494429957237	5.39327938433935	-0.91796050659939
C	-2.86909013365097	1.03229683628874	-3.39740573563913
C	-5.20376653422114	3.41517274724048	-3.19035870886789
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H	-5.36691385550962	2.34446312708355	-3.30510470147180
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C	-5.54247662233738	2.06604569894116	3.62704849409769
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Au	2.12336631556703	-0.60251443278017	2.88773607454912
Au	-0.09650182608634	-0.65920487865825	1.04826948051480
P	-0.74520083079420	1.44897745013435	1.42210566002652
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H	8.12582342862670	3.77200904901565	4.20258044356600
H	8.51993419737972	5.05696099541682	3.04140801605706
C	-6.00664248195217	3.40742258741757	4.20763077272819
C	-5.91994339328888	2.06683388906684	2.14316840797349
C	-6.31539928978429	0.91752302044637	4.29225983562028
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H	-2.93193710412343	5.97244430240626	-1.73813267073171
H	-4.43754141085635	5.45686327974012	-1.01555013555839
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H	-3.85522570178268	0.56701594880027	-3.39761952159381
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C	4.73144428096353	-5.39349890277123	0.54689704542877
C	3.12485401642029	-4.08279540342695	-0.79673682535508
C	4.10726714610947	5.37180401627344	5.48709968602859
C	3.30038568268223	3.09544151651961	5.98544095185931
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H	6.72898177850572	4.38929947927329	-0.04720265397476
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C	2.39225759611491	-3.02652883807791	4.47090119886539
C	0.08307664015472	-2.78884084721504	3.58058314341997

H	-0.51774231473354	-2.01735062325555	3.10980258469331
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N	3.74688661065779	-2.61027491079846	4.61555714035411
H	2.18303552677424	-4.00361419439710	4.90628058318543
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O	4.82267213614812	-2.41512404550207	7.02514255017164
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H	4.85626352969839	0.06919835176921	4.47759650973805
H	6.17105637388055	-1.08835624724746	4.83441836086662
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H	4.59657846018362	-4.51781472522730	5.06410924290234
O	-0.19708794673413	-2.83676307177019	0.66474623786286
C	-0.55255760655765	-3.79701168043116	1.35881929931413
O	-1.34112619614498	-4.73002932564358	0.87616762796568
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C	1.24670943511214	-4.98432040793740	2.56718183895223
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H	-1.39995637618332	-5.85072423976018	2.94333367174844
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H	3.21885510687499	5.57927757677907	4.89538528927151
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H	4.36444052499214	-6.29411973028691	0.05452019240747
H	5.76145407253769	-5.56213473355636	0.84206810338573
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H	2.47831557666284	-3.91608275456914	0.06065383218487
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Coordinates from ORCA-job Int2ent E -5376.940673204655

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C	1.77767347118959	2.21661940401425	-0.35440298620789
C	2.97808152417449	0.40714591776082	-1.45946525948749
C	4.44078748601229	-1.78456739806703	0.42254759809200
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O	3.05908428959139	4.80824666640336	0.19173816300972
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O	-4.05480583809909	3.63768036283742	-3.02428424950136
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C	8.76991751531425	-3.26825777035827	-0.42354486759173
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H	8.51777279734629	-2.55771176842385	-1.20863952881311
H	9.61727423469669	-2.89537102933627	0.14588222532498
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C	-3.47309618559755	5.34757572109105	-0.86883292274826
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C	-5.42570049938900	2.18260038151918	3.84027851426567
C	-3.54624883262293	3.12101910753994	6.95129323293386
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H	-3.16138057010762	1.51328340937756	-4.18588052496725
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C	5.17452324617905	-5.26973320034044	0.61629873678271

C	3.44008091387012	-4.14324183403767	-0.72221665037135
C	3.97915385017730	5.39538486802035	5.44088693257228
C	3.19248710841380	3.10391222234945	5.90102372430385
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H	7.93781054573543	4.22108565896749	1.06353221604336
H	6.64510550155791	4.57625771759616	-0.06483183826496
C	1.56650345627248	-2.35557526253406	3.73746415857015
C	2.45264103968604	-3.07187376055317	4.43973576214468
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H	-0.45046113192912	-2.18629394840970	2.99182615536324
H	-0.26460242860897	-3.23741879749614	4.34414652143994
N	3.81195626244014	-2.67213607746522	4.62060086263415
H	2.18435245348744	-3.98413456586025	4.97276216090908
S	4.16348845442764	-1.57588382365595	5.90921117417496
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