Supporting Material

$n \rightarrow \pi^*$ Interaction and $n)(\pi$ Pauli Repulsion are Antagonistic for Protein Stability

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1. Materials and General Procedures

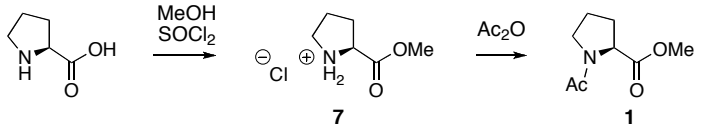
Column chromatography was performed with 60 Å 40–63 μm silia–P flash silica gel. **Solvents** for reactions (acetonitrile, DMF, DCM, ether, THF, and toluene) were dried using a Glass Contour purification system. Other solvents were used as received. **Bases** (triethylamine, Hünig's base) were dried by distillation from calcium hydride. **Chemicals** were purchased and used as received unless noted otherwise. The **High Vacuum** pump was measured to pull 0.25 mmHg. **NMR Spectra** were measured in $CDCl_3$ at ambient temperature unless otherwise noted.

^{1}H NMR spectra were recorded on either a Bruker 500 MHz or a Bruker 400 MHz spectrometer. Chemical shifts are reported in ppm (δ) relative to tetramethylsilane using the solvent or TMS as a reference ($CDCl_3$ = 7.26 ppm, DMSO-d_6 = 2.49 ppm, D_2O = 4.80 ppm, CD_2Cl_2 = 5.32). The following is an example data point: chemical shift (multiplicity [s = singlet, d = doublet, t = triplet, q = quartet, pent = pentet, sext = sextet, sept = spetet, oct = octet, m = multiplet, br = broad, and combinations thereof], coupling constants [Hz], integration, assignment [if any]). **^{13}C NMR** spectra were recorded on a Bruker 500 MHz (125 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm (δ) relative to tetramethylsilane using the solvent or TMS as a reference ($CDCl_3$ = 77.0 ppm, DMSO-d_6 = 39.5 ppm, CD_3OD = 49.0 ppm). **^{19}F NMR** spectra were recorded on a Bruker 400 MHz (376 MHz) spectrometer without proton decoupling. Chemical shifts are reported in ppm (δ) relative to trichlorofluoromethane. **^{1}H–^{1}H NOESY** spectra were recorded at approximately 0.05 M. Solvents were degassed by the freeze-pump-thaw protocol that follows. Under a nitrogen atmosphere, the solvent (approximately 3 mL) was frozen in a liquid nitrogen bath (–196 °C) and maintained under high vacuum (3 min). Under static vacuum, the flask was transferred to an ambient temperature water bath, allowed to warm (melting the solid and evolving gas), evacuated briefly under dynamic vacuum, and backfilled with nitrogen. The process was repeated three times, and the degassed solvent was used immediately. NMR tubes were filled under an argon atmosphere and sealed with parafilm. **IR** spectra were recorded on a Nicolet 6700 FT–IR spectrometer, using a thin film from solution evaporation on a salt plate. Spectra are partially reported (υ_{max}, cm^{-1}). **$[\alpha]_D$** Optical rotations were measured on a Perkin Elmer 341 polarimeter at 20 °C with 589 nm radiation. Sample concentrations (c) are reported in cg·mL^{-1}. **HRMS** was performed at either the University of Illinois at Urbana–Champaign or at The Keck Center at Yale Medical School. Unless otherwise noted, data were obtained by positive mode electrospray ionization. **TLC** was performed on 60 Å F_{254} precoated silica gel plates. Samples were visualized by either ultraviolet irradiation (UV), potassium permanganate staining ($KMNO_4$), or cerium ammonium molybdenate staining (CAM). **Yield** refers to isolated material. **Conversion** refers to the amount of product divided by the sum of the amounts of product, starting material, and byproducts.

2. Standard Experimental Procedures

Boc Deprotection The Boc-protected amine (0.1–5 mmol, 1.0 equiv) was placed in a flask. The flask was capped with a septum and flushed with nitrogen. Hydrogen chloride (4.0 M in dioxane, 3–5 mL) was added, the nitrogen line and vent needle were removed, and the mixture was stirred (30 min, occasionally venting pressure). Volatiles were removed under a stream of nitrogen (3 h) and under high vacuum (1 h). Crude deprotected amine hydrochloride was used directly for the next step.

3. Experimental Procedures

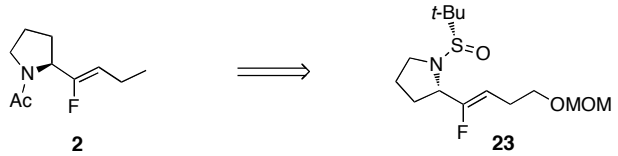


Synthesis of Ester 1 Into a flask were added L-proline (2.30 g, 20.0 mmol, 1.0 equiv) and methanol (40 mL, 0.5 M, giving a homogeneous solution). The flask was fit with a condenser, capped with a rubber septum, and maintained under a nitrogen atmosphere. Thionyl chloride (2.0 mL, 26 mmol, 1.3 equiv) was added dropwise by syringe (producing a vigorous reaction). The mixture was heated to reflux (2 h), and most of the solvent was removed by distillation. Remaining volatiles were removed under reduced pressure to yield hydrochloride **7** (quantitative, contaminated with methanol), a fraction of which was used directly in the next step.

Into a flask were added hydrochloride **7** (245 mg, 1.48 mmol, 1.0 equiv), DCM (15 mL, 0.1 M), and DMAP (45 mg, 0.37 mmol, 0.25 equiv). The flask was capped with a rubber septum and maintained under a nitrogen atmosphere. To the flask were added triethylamine (820 μL, 5.93 mmol, 4.0 equiv) and acetic anhydride (280 μL, 2.96 mmol, 2.0 equiv). The mixture was stirred (2.5 h), diluted with DCM (40 mL), washed with sodium carbonate (10% aqueous, 40 mL) and citric acid (10% aqueous, 40 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by column chromatography (20 mL silica gel, EtOAc) to yield acetamide **1** (156 mg, 0.912 mmol, 62% yield overall). NMR spectra show two rotational isomers (3.7:1 in $CDCl_3$). Published data assigns the major rotational isomer (*trans*) as the one with the acetamide's carbonyl pointing toward the ester.[1]

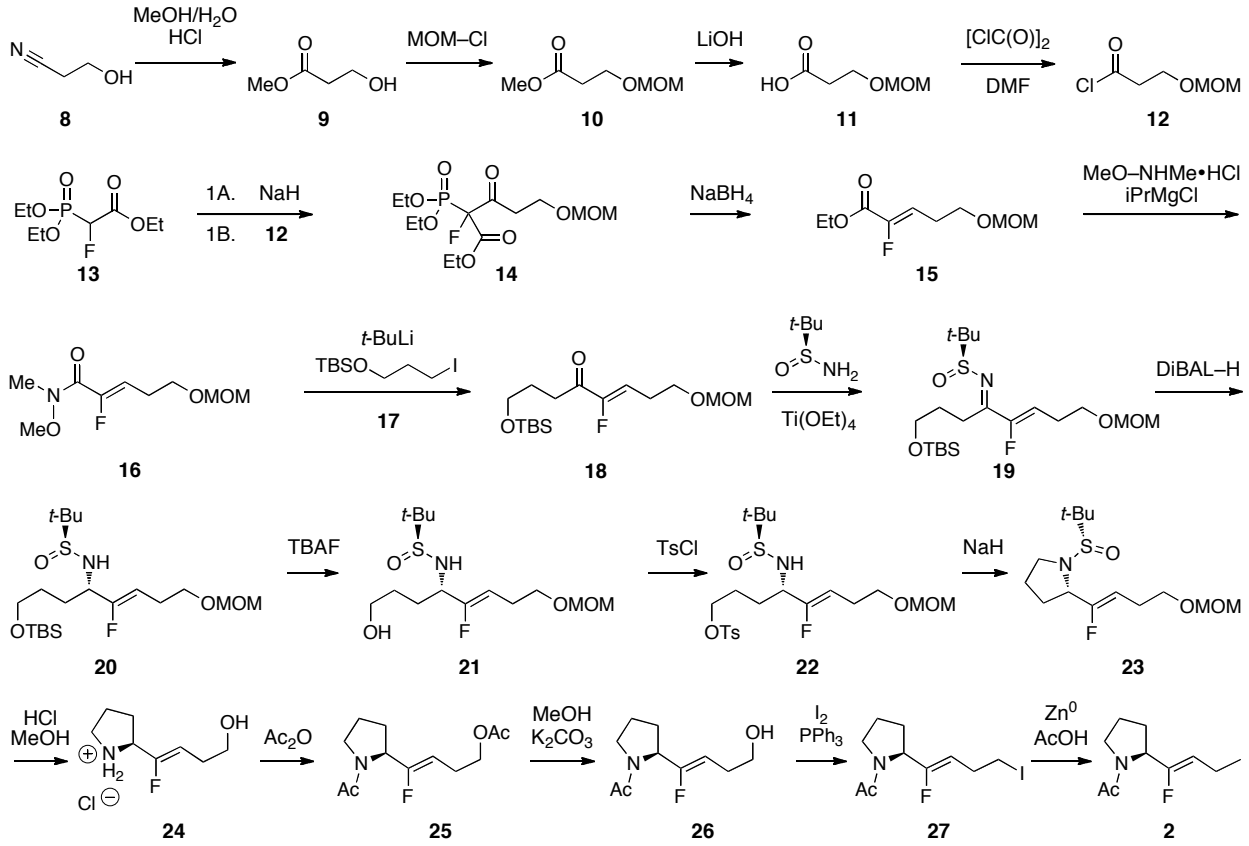
^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.45 (dd, J_1 = 8.7 Hz, J_2 = 3.7 Hz, 0.8H), 4.35 (dd, J_1 = 8.6 Hz, J_2 = 2.8 Hz, 0.2H), 3.73 (s, 0.6H), 3.69 (s, 2.4H), 3.65–3.43 (m, 2H), 2.30–1.84 (m, 4H), 2.05 (s, 2.4H), 1.94 (s, 0.6H); **TLC** EtOAc, $KMNO_4$, R_f = 0.25. Compound analysis is consistent with published data.[1]

[1] Hinderaker, M. P.; Raines, R. T. *Protein Sci.* **2003**, *12*, 1188–1194.

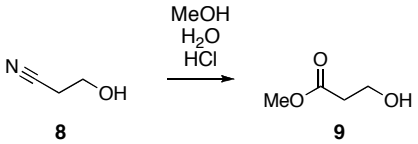


Acetamide **2** was made from intermediate **23**, which had been made for other reasons.

Scheme S1



Scheme S1 summarizes the synthetic approach used to access acetamide **2** via intermediate **23**.

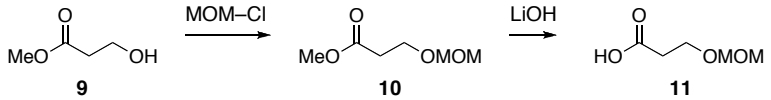


Synthesis of Ester 9[2] Methanol (200 mL, 3.7 M) was placed in a flask, which was cooled in an ice bath (0 °C). Hydrochloric acid (concentrated aqueous, 12.1 M, 16.0 mL, 194 mmol HCl, 0.26 equiv, 888 mmol H_2O, 1.2 equiv) was added. A condenser and an addition funnel were attached. Thionyl chloride (26.5 mL, 366 mmol, 0.5 equiv) was added dropwise (over 10 min), and the mixture was allowed to return to ambient temperature. 3-Hydroxypropionitrile (**8**, 50.0 mL, 732 mmol, 1.0 equiv) was added dropwise (over 20 min). The mixture was heated to reflux (5 h, producing precipitate), cooled in an ice bath, and neutralized with sodium bicarbonate. Solids

[2] Esterification procedure and partial compound data from: Ogawa, T.; Nakazato, A.; Sato, M.; Hatayama, K. *Synthesis* **1990**, 459–460.

were removed by vacuum filtration, and the filtrate was concentrated under reduced pressure (producing additional precipitate). Toluene (200 mL) was added, and solids were again removed by vacuum filtration. The biphasic filtrate was concentrated under reduced pressure, and the crude material was purified by distillation (0.25 mmHg, 41–44 °C, collecting fractions in an ice bath) to yield ester **9** (33.2 g, 319 mmol, 44% yield).

^{1}**H NMR** ($CDCl_3$, 500 MHz) δ 3.86 (q, J = 5.6 Hz, 2H), 3.71 (s, 3H), 2.58 (t, J = 5.6 Hz, 2H), 2.42–2.35 (brs, 1H); **BP** 41–44 °C, 0.25 mmHg. Product analysis is consistent with published data.[2]



Synthesis of Carboxylic Acid 11[3,4] Into a dried flask were added alcohol **9** (31.5 g, 303 mmol, 1 equiv), DCM (300 mL, 1.0 M), and Hünig's base (158 mL, 909 mmol, 3.0 equiv). The flask was fit with an addition funnel, capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in an ice bath (0 °C). Chloromethyl methy ether (42 mL, 553 mmol, 1.8 equiv) was added dropwise (over 20 min). The mixture was allowed to warm to slightly above ambient temperature, stirred (4 h), quenched with ammonium chloride (50% saturated aqueous, 300 mL), and stirred vigorously (10 min). The organic phase was isolated, and the aqueous phase was further extracted with DCM (2 × 50 mL). The combined organic phases were dried with sodium sulfate. Volatiles were removed gently under reduced pressure (400 mBar, 29 °C) to yield ether **10** (contaminated with DCM and Hünig's base), which was used directly in the next step.

^{1}**H NMR** ($CDCl_3$, 400 MHz) δ 4.61 (s, 2H), 3.80 (t, J = 6.2 Hz, 2H), 3.70 (s, 3H), 3.35 (s, 3H), 2.60 (t, J = 6.2 Hz, 2H).

Into a flask were added crude ester **10** (303 mmol, 1.0 equiv) and THF (200 mL, 1.5 M). The solution was cooled in an ice bath (0 °C). Into an Erlenmeyer flask were added lithium hydroxide monohydrate (37.3 g, 909 mmol, 3.0 equiv) and water (200 mL, 1.5 M, producing a suspension). The suspension was mixed vigorously and added to the THF solution. Remaining lithium hydroxide was chased into the reaction with additional water (100 mL). The mixture was stirred (30 min), allowed to return to ambient temperature (additional 7 h), cooled in an ice bath, acidified with hydrochloric acid (concentrated aqueous, 12.1 M, 93 mL, ***dropwise***, to pH 1), and extracted with ether (200 mL). The aqueous phase was further acidified with potassium hydrogen sulfate (1.0 M, 50 mL, to pH 0) and further extracted with DCM (2 × 100 mL). The combined organic phases were dried with sodium sulfate, and volatiles were gently removed under reduced pressure (120 mBar, 29 °C) to yield acid **11** (34.1 g, 254 mmol, 84% yield, contaminated with solvent).

^{1}**H NMR** ($CDCl_3$, 400 MHz) δ 4.63 (s, 2H), 3.81 (t, J = 6.1 Hz, 2H), 3.37 (s, 3H), 2.65 (t, J = 6.1 Hz, 2H). Product analysis is consistent with published data.[4]

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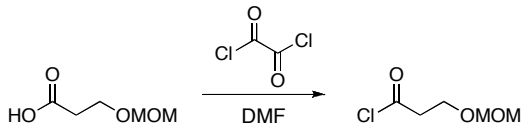
[3] Etherification procedure from: Durham, T. B.; Blanchard, N.; Savall, B. M.; Powell, N. A.; Roush, W. R. *J. Am. Chem. Soc.* **2004**, *126*, 9307–9317.

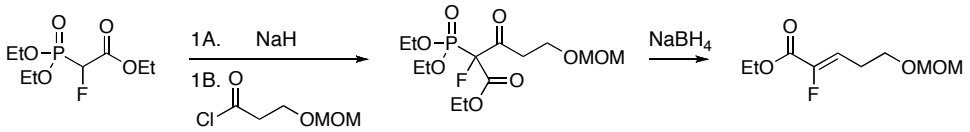
[4] Compound data from: Hirata, Y.; Nakamura, S.; Watanabe, N.; Kataoka, O.; Kurosaki, T.; Anada, M.; Kitagaki, S.; Shiro, M.; Hashimoto, S. *Chem. Eur. J.* **2006**, *12*, 8898–8925.



11 **12**

Synthesis of Acid Chloride 12[5] Into a dried flask were added acid **11** (3.35 g, 25.0 mmol, 1.0 equiv), ether (50 mL, 0.5 M), and DMF (5.69 mL, 72.5 mmol, 2.9 equiv). The flask was capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in an ice bath (0 °C). Oxalyl chloride (5.69 mL, 65.0 mmol, 2.6 equiv) was added ***dropwise*** (over 10 min, evolving gas and producing gooey precipitate). The mixture was returned to ambient temperature with a water bath (10 min), diluted with hexane (100 mL, 0.25 M), mixed vigorously, and allowed to sit without stirring (5 min). The supernatant was isolated by decantation and chased with additional hexanes (25 mL). Volatiles were gently removed under reduced pressure (180 mBar, 29 °C) to yield crude acid chloride **12** (quantitative, contaminated with solvent), which was used directly in the next step. Acid chloride **12** was not fully characterized due to its reactivity.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.31 (s, 2H), 3.84 (t, J = 5.8 Hz, 2H), 3.37 (s, 3H), 3.15 (t, J = 5.8 Hz, 2H).



13 **12** **14** **15**

Synthesis of Ketone 15[6] Phosphonate ester **13** was prepared as previously described.[7] Sodium hydride (95%, 900 mg, 37.5 mmol, 1.5 equiv) was weighed directly into a flame-dried flask. The flask was capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in an ice bath (0 °C). THF (40 mL, 0.6 M) was added by syringe (producing a colorless suspension). Phosphonate ester **13** (10.7 g, 44.2 mmol, 1.8 equiv) was added ***dropwise*** (over 30 min, evolving gas). The mixture was allowed to return to ambient temperature and stirred (30 min, giving a clear orange solution). Into a second flask were added crude acid chloride **12** (25.0 mmol, 1.0 equiv) and THF (30 mL, 0.8 M). This flask was capped with a rubber septum and maintained under a nitrogen atmosphere. Both flasks were cooled in an acetonitrile/dry ice bath (–40 °C). The phosphonate solution was transferred by cannula into the acid chloride solution. The mixture was stirred (1 h), quenched with ammonium chloride (saturated, 100 mL), allowed to warm to ambient temperature, diluted with water (100 mL), extracted with ether (200 + 100 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure to yield crude phosphonate ester **14** (full conversion by NMR), which was used directly in the next step.

^{1}H NMR ($CDCl_3$, 400 MHz, partially reported) δ 3.81 (d, J = 7.2 Hz, 2H), 3.08–3.03 (m, 2H); **TLC** (3:2) EtOAc/hexane, R_f = 0.34, indistinguishable from starting phosphonate ester **13**.

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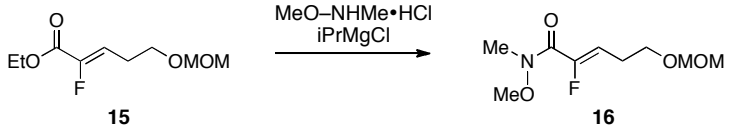
[5] Acid chloride formation procedure modified from: Ward, D. E.; Rhee, C. K. *Tetrahedron Lett.* **1991**, *32*, 7165–7166.

[6] Example coupling constants from and acylation and reduction procedures modified from: a) Sano, S.; Kuroda, Y.; Saito, K.; Ose, Y.; Nagao, Y. *Tetrahedron* **2006**, 11881–11890. b) Sano, S.; Saito, K.; Nago, Y. *Tetrahedron Lett.* **2003**, 3987–3990.

[7] Jakobsche, C. E.; Peris, G.; Miller, S. J. *Angew. Chem., Int. Ed.* **2008**, *47*, 6707–6711.

Into a flask were added crude phosphonate ester **14** (25.0 mmol, 1.0 equiv) and ethanol (HPLC grade, 50 mL, 0.5 M). The flask was capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in an acteone/dry ice bath (–78 °C). Into another flask were added sodium borohydride (***powdered***, 3.80 g, 100 mmol, 4.0 equiv) and ethanol (100 mL, 0.3 M). The suspension was mixed in an ultrasonic water bath (2 min, dissolving most of the solid and evolving some gas), capped with a rubber septum, maintained under a nitrogen atmosphere, cooled in the bath (accidentally it was not cooled for long enough to reach equilibrium), quickly poured into the phosphonate solution, and chased with additional ethanol (25 mL). The mixture was stirred (2 h), transferred to an ice bath (0 °C, 10 min), quenched with ammonium chloride (saturated aqueous, 150 mL), diluted with water (100 mL), extracted with ether (200 + 100 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by column chromatography (350 mL silica gel, [3:1] hexanes/ether) to yield enoate **15** (2.7 g, 13 mmol, 52% yield from carboxylic acid **11**) as a single diastereomer. Olefin geometry (*Z*) was assigned by $^3J_{H,F}$ coupling.[6]

^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.18 (dt, J_d = 33.2 Hz, J_t = 7.6 Hz, 1H), 4.61 (s, 2H), 4.26 (q, J = 7.1 Hz, 2H), 3.60 (t, J = 6.4 Hz, 2H), 3.34 (s, 3H), 2.55–2.50 (m, 2H), 1.30 (t, J = 7.4 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 160.6 (d, J = 35.5 Hz), 148.8 (d, J = 257.1 Hz), 117.1 (d, J = 11.4 Hz), 96.4, 65.7 (d, J = 2.0 Hz), 61.6, 55.3, 25.1 (d, J = 2.7 Hz), 14.1; **IR** (film, cm^{-1}) 2981, 2937, 2888, 1740, 1682, 1312, 1113, 1076, 1035; **HRMS** calculated for $[C_9H_{15}FO_4Na]^+$, requires m/z = 229.0852, found m/z = 229.0840 (ESI); **TLC** (3:1) hexane/ether, R_f = 0.29.



Synthesis of Weinreb Amide 16[8] *N*,*O*-Dimethylhydroxyamine hydrochloride was finely ground and dried in a desiccator over phosphorous pentaoxide (overnight). Isopropylmagnesium chloride was analyzed by titration as follows.[9] Into a flame-dried flask were added 1,10-phenylanthroline (9 mg), *sec*-butyl alcohol (100 μL, 1.09 mmol), and ether (4 mL, 0.3 M). The Grignard reagent was added dropwise by syringe until the light pink mixture suddenly became a deep violet color.

Into a flame-dried flask were added ester **15** (5.00 g, 24.3 mmol, 1.0 equiv), *N*,*O*-dimethylhydroxyamine hydrochloride (4.73 g, 48.5 mmol, 2.0 equiv), and THF (80 mL, 0.3 M, giving a suspension). The flask was capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in an ice bath (0 °C). Isopropylmagnesium chloride (2.0 M in THF, 46.0 mL, 92.3 mmol, 3.8 equiv) was added dropwise (over 30 min). The mixture was stirred (additional 1 h), quenched with ammonium chloride (saturated, 100 mL), diluted with water (100 mL), extracted with ether (2 × 100 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by short column chromatography (100 mL silica gel, 7 cm wide × 2 cm high, [2:1] ether/hexane) to yield slightly contaminated amide **16** (4.94 g, 22.3 mmol, 92% yield), which was used in the next step. ^{1}H NMR signals were assigned by comparison to previous spectra.

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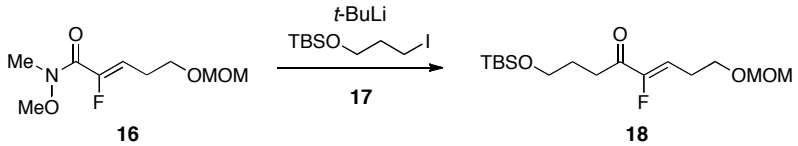
[8] Amination procedure from: He, W.; Huang, J.; Sun, X.; Frontier, A. J. *J. Am. Chem. Soc.* **2007**, *129*, 498–499.

[9] Titration procedure from: Watson, S. C.; Eastman, J. F. *J. Organomet. Chem.* **1967**, *9*, 165–168.

^{1}H NMR ($CDCl_3$, 500 MHz) δ 5.91 (dt, J_d = 35.1 Hz, J_t = 7.5 Hz, 1H, vinyl), 4.60 (s, 2H, MOM), 3.71 (s, 3H, CH_3–O–N), 3.59 (t, J = 6.5 Hz, 2H, CH_2–OMOM), 3.34 (s, 3H, MOM), 3.21 (s, 3H, CH_3–N), 2.53–2.47 (m, 2H, CH_2–C=C); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 162.4 (d, J = 28.9 Hz), 151.7 (d, J = 256.6 Hz), 114.8 (d, J = 11.8 Hz), 96.4, 65.9, 61.7, 55.2, 33.8, 24.9; **IR** (film, cm^{-1}) 2938, 2886, 1649, 1379, 1144, 1108, 1045; **HRMS** calculated for $[C_9H_{16}FNO_4H]^+$, requires m/z = 222.1142, found m/z = 222.1132 (ESI); **TLC** (3:2) ether/hexane, R_f = 0.29.



Synthesis of Enone 18[10] *tert*-Butyllithium (1.7 M in pentane) was transferred by cannula from its original sure-seal bottle into an oven-dried storage flask with a Teflon screw-seal top. The flask was flushed with argon and stored at –20 °C. The reagent slowly decomposes at ambient temperature, and even at –20 °C it completely decomposed over six months. For use, the reagent was warmed to ambient temperature, maintained under an argon atmosphere, and transferred into a syringe with positive pressure. Pulling the solution into syringes can cause significant solvent evaporation. Excess material was quenched with a 5:1 mixture of hexane and *sec*-butyl alcohol. *tert*-Butyllithium was analyzed by titration as follows.[11] Into a flame-dried flask were added 1,10-phenylanthroline (18 mg), *sec*-butanol (50 μL, 0.55 mmol), and hexane (2 mL, 0.3 M). The flask was capped with a rubber septum and maintained under an argon atmosphere. The organolithium reagent was added dropwise by syringe until the yellow mixture suddenly became deep maroon. Iodide **17** was prepared as previously described.[12]

Iodide **17** (17.0 g, 56.7 mmol, 3.5 equiv) was added into a flame-dried flask. The flask was dried under high vacuum, capped with a rubber septum, flushed with argon (10 min), and maintained under an argon atmosphere. Ether (180 mL, 0.09 M) was added, and the mixture was cooled in a dry ice/acetone bath (–78 °C, 20 min). *tert*-Butyllithium (1.43 M in pentane, 80 ± 5 mL, 114 mmol, 7.2 equiv) was cooled in the bath and added by cannula to the iodide solution. The mixture was stirred (20 min, producing precipitate), transferred to an ice bath (0 °C, 40 min, producing a clear yellow solution), and returned to the dry ice bath (20 min, producing precipitate). Into a separate flame-dried flask were added amide **16** (3.54 g, 16.0 mmol, 1.0 equiv) and ether (40 mL, 0.4 M). This flask was capped with a rubber septum, flushed with argon (10 min), maintained under an argon atmosphere, and cooled in the dry ice bath (20 min). The amide solution was transferred by cannula into the lithium solution. The mixture was stirred (2 h), quenched with ammonium chloride (saturated aqueous, 100 mL), allowed to warm to ambient temperature, and diluted with water (200 mL). The organic phase was isolated, the

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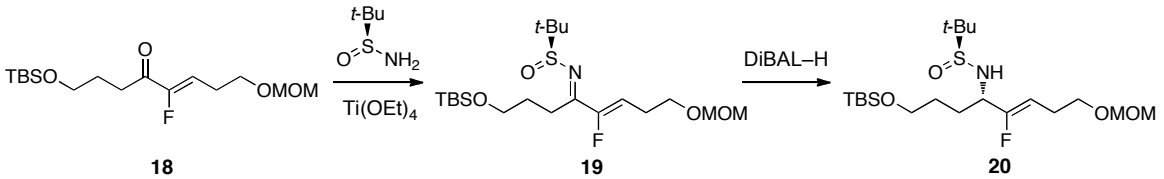
[10] Lithium–halogen exchange procedure from: a) Bailey, W. F.; Punzalan, E. R. *J. Org. Chem.* **1990**, *55*, 5404–5406. b) Negishi, E.–I.; Swanson, D. R.; Rousset, C. J. *J. Org. Chem.* **1990**, *55*, 5406–5409. Addition to Weinreb amide procedure from: c) Jung, W.–H.; Harrison, C.; Shin, Y.; Fournier, J.–H.; Balachandran, R.; Raccor, B. S.; Sikorsku, R. P.; Vogt, A.; Curran, D. P.; Day, B. W. *J. Med. Chem.* **2007**, *50*, 2951–2966. d) Fearnley, S. P.; Funk, R. L.; Gregg, R. J. *Tetrahedron* **2000**, *56*, 10275–10281.

[11] Titration procedure from: Watson, S. C.; Eastman, J. F. *J. Organomet. Chem.* **1967**, *9*, 165–168.

[12] Jakobsche, C. E.; Peris, G.; Miller, S. J. *Angew. Chem., Int. Ed.* **2008**, *47*, 6707–6711.

aqueous phase was further extracted with ether (100 mL), and the combined organic phases were dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by column chromatography (200 mL silica gel, [4:1 to 5:2] hexanes/ether) to yield ketone **18** (5.34 g, 16.0 mmol, quantitative), which was used directly in the next step. ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY and by comparison to previous spectra.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.11 (dt, J_d = 34.4 Hz, J_t = 7.6 Hz, 1H, vinyl), 4.62 (s, 2H, MOM), 3.65–3.60 (m, 4H, CH_2–OTBS, CH_2–OMOM), 3.35 (s, 3H, MOM), 2.69 (td, J_t = 7.2 Hz, J_d = 1.6 Hz, 2H, CH_2–C=O), 2.57–2.50 (m, 2H, allyl), 1.83 (pent, J = 6.6 Hz, 2H, CH_2–C–OTBS), 0.87 (s, 9H, TBS), 0.03 (s, 6H, TBS); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 193.7 (d, J = 30.9 Hz), 155.8 (d, J = 262.8 Hz), 115.3 (d, J = 12.4 Hz), 96.4, 67.7, 61.9, 55.3, 34.2, 26.6, 25.9, 25.0, 18.3, –5.4; **IR** (film, cm^{-1}) 2957, 2929, 2881, 2853, 1699, 1659, 1101, 837; **HRMS** calculated for $[C_{16}H_{31}FO_4SiH]^+$, requires m/z = 335.2054, found m/z = 335.2035 (ESI); **TLC** (2:1) hexane/ether, R_f = 0.54.



Synthesis of Sulfinamide 20[13] Into a flask were added ketone **18** (6.49 g, 19.4 mmol, 1.0 equiv), (*S*)-2-methyl-2-propanesulfinamide (5.26 g, 43.5 mmol, 2.2 equiv), and THF (100 mL, 0.2 M). Titanium (IV) ethoxide (16.5 g, 79.4 mmol, 4.1 equiv) was added by syringe. The flask was fit with a reflux condenser, capped with a rubber septum, and maintained under a nitrogen atmosphere. The mixture was heated to reflux (3 h, giving a yellow solution), allowed to cool to ambient temperature, diluted with EtOAc (150 mL), quenched with citric acid (10% aqueous, 75 mL), diluted with brine (75 mL), and mixed vigorously (giving a clear organic phase over a chunky, gooey aqueous phase). The organic phase was decanted through filter paper and chased with EtOAc (4 × 50 mL). Allowing too much of the aqueous goo onto the filter paper caused it to become clogged. The filtrate was washed with sodium chloride (50% saturated aqueous, 100 mL) and dried with sodium sulfate. Volatiles were removed under reduced pressure to yield crude sulfinimide **19** (full conversion, a brown oil), which was used directly in the next step.

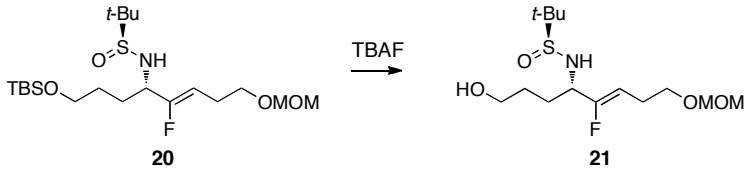
^{1}H NMR ($CDCl_3$, 500 MHz) δ 5.91 (dt, J_d = 34.1 Hz, J_t = 7.5 Hz, 1H), 4.58 (s, 2H), 3.65–3.55 (m, 4H), 3.31 (s, 3H), 3.00–2.92 (m, 1H), 2.85–2.77 (m, 1H), 2.58–2.49 (m, 2H), 1.83–1.76 (m, 2H), 1.21 (s, 9H), 0.85 (s, 9H), 0.00 (s, 6H); **TLC** (2:1) hexane/ether, UV/$KMNO_4$, R_f = 0.36.

Crude sulfinimide **19** (19.4 mmol, 1.0 equiv) was placed in a flask and dried under high vacuum. THF (100 mL, 0.2 M) was added. The flask was capped with a rubber septum, flushed with nitrogen, and cooled in a dry ice/acetone bath (–78 °C, 20 min). Diisobutylaluminum hydride (1.0 M in THF, 100 mL, 100 mmol, 5.0 equiv) was maintained under a nitrogen atmosphere, cooled in the bath (20 min), and added by cannula to the sulfinimide solution (over 20 min). The mixture was stirred (additional 2.5 h), quenched with ammonium chloride (saturated aqueous, 150 mL), allowed to warm to ambient temperature, diluted with water (150 mL) and EtOAc (200 mL), mixed with potassium sodium tartrate (75 g), and stirred vigorously

[13] Reductive amination procedure from: Dutheuil, G.; Couve–Bonnaire, S.; Pannecoucke, X. *Angew. Chem., Int. Ed.* **2007**, *46*, 1290–1292.

(2 h, giving clear organic and aqueous phases). The organic phase was isolated, the aqueous phase was further extracted with EtOAc (2 × 50 mL), and the combined organic phases were dried with sodium sulfate. Volatiles were removed under reduced pressure, and an aliquot of the crude material was purified by column chromatography (silica gel, [1:1] hexanes/EtOAc) for characterization. Crude sulfinamide **20** (full consumption of sulfinimide **19**, contaminated by an unidentified minor byproduct [approximately 10%]) was used directly in the next step. ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY and by comparison to previous spectra.

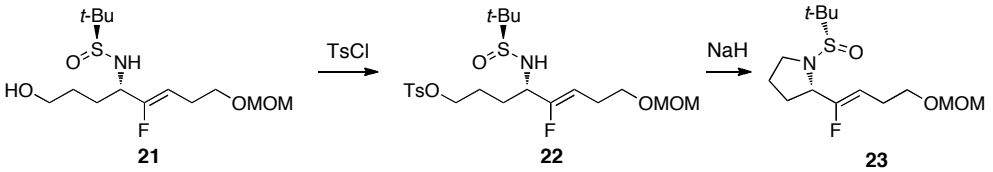
^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.92 (dt, J_d = 37.3 Hz, J_t = 7.3 Hz, 1H, vinyl), 4.61 (s, 2H, MOM), 3.79–3.70 (m, 1H, CH–N), 3.61 (t, J = 6.2 Hz, 2H, CH_2–OTBS), 3.55 (t, J = 6.7 Hz, 2H, CH_2–OMOM), 3.38 (d, J = 8.4 Hz, 1H, NH), 3.35 (s, 3H, MOM), 2.45–2.35 (m, 2H, CH_2–C=C), 1.76–1.70 (m, 2H, CH_2–C–N), 1.60–1.50 (m, 2H, CH_2–C–C–N), 1.21 (s, 9H, *t*-Bu–S), 0.88 (s, 9H, TBS), 0.04 (s, 6H, TBS); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 158.9 (d, J = 258.5 Hz), 104.1 (d, J = 14.1 Hz), 96.2, 66.5, 62.3, 57.3 (d, J = 34.7 Hz), 56.0, 55.0, 29.5, 28.7, 25.8, 24.2, 22.4, 18.2, –5.5; **IR** (film, cm^{-1}) 3203, 2956, 2928, 2855, 1112, 1063, 833; $[\alpha]_D$ = +41.4° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{20}H_{42}FNO_4SSiH]^+$, requires m/z = 440.2666, found m/z = 440.2657 (ESI); **TLC** (1:1) hexane/EtOAc, $KMNO_4$, R_f = 0.27.



Synthesis of Alcohol 21[14] Into a flask were added crude TBS ether **20** (19.4 mmol, 1.0 equiv) and THF (100 mL, 0.2 M). The flask was capped with a rubber septum and maintained under a nitrogen atmosphere. Tetrabutylammonium fluoride (1.0 M in THF, a bright pink solution, 40.0 mL, 40.0 mmol, 2.1 equiv) was added by syringe. The mixture was stirred (1 h), quenched with ammonium chloride (saturated aqueous, 100 mL), diluted with water (100 mL) and brine (100 mL), extracted with EtOAc (200 + 2 × 50 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by column chromatography (300 mL silica gel, [5:1] toluene/acetone to remove byproducts, then [1:1] toluene/acetone) to yield pure alcohol **21** (3.50 g, 10.8 mmol, 56% yield from ketone **18**) as a single diastereomer. ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY.

^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.88 (dt, J_d = 37.3 Hz, J_t = 7.3 Hz, 1H, vinyl), 4.56 (s, 2H, MOM), 3.70 (dq, J_d = 20.4 Hz, J_q = 7.5 Hz, 1H, CH–N), 3.60–3.54 (m, 3H, CH_2–OH, NH), 3.49 (t, J = 6.7 Hz, 2H, CH_2–OMOM), 3.30 (s, 3H, MOM), 2.55–2.60 (m, 1H, OH), 2.40–2.30 (m, 2H, CH_2–C=C), 1.80–1.50 (m, 4H, CH_2–CH_2–C–N), 1.15 (s, 9H, *t*-Bu); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 158.8 (d, J = 258.5 Hz), 104.3 (d, J = 14.1 Hz), 96.2, 66.6, 61.9, 57.2 (d, J = 27.9 Hz), 56.1, 55.1, 29.4, 28.7, 24.2, 22.4; **IR** (film, cm^{-1}) 3403, 3237, 2952, 2924, 2871, 1045; $[\alpha]_D$ = +54.8° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{14}H_{28}FNO_4SH]^+$, requires m/z = 326.1801, found m/z = 326.1790 (ESI); **TLC** (3:2) toluene/acetone, $KMnO_4$, R_f = 0.27.

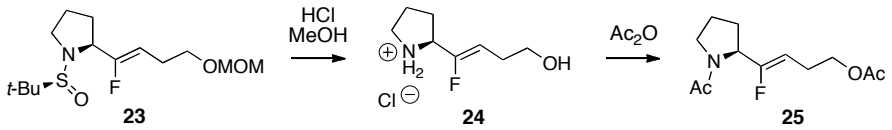
[14] TBS deprotection procedure from: Kim, Y.–J.; Wang, P.; Navarro–Villalobos, M.; Rohde, B. D.; Derryberry, J.; Gin, D. Y. *J. Am. Chem. Soc.* **2006**, *128*, 11906–11915.



Synthesis of Pyrrolidine 23[15] Into a flask were added alcohol **21** (2.3 g, 7.1, mmol, 1.0 equiv), DCM (24 mL, 0.3 M), DMAP (268 mg, 2.20 mmol, 0.3 equiv), triethylamine (3.0 mL, 22 mmol, 3.1 equiv), and *para*-toluenesulfonyl chloride (2.78 g, 14.6 mmol, 2.1 equiv). The flask was capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in an ambient temperature water bath (to prevent significant warming). The mixture was stirred (1 h), diluted with DCM (100 mL), quenched with sodium carbonate (10% aqueous, 60 mL), and stirred (5 min). The organic phase was isolated, washed with citric acid (10% aqueous, 60 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure and by azeotropic distillation (THF) to yield crude tosylate **22** (full conversion by NMR, a brown oil), which was used directly in the next step.

Sodium hydride (95%, 900 mg, 37.5 mmol, 5.3 equiv) was weighed directly into a flame-dried flask. The flask was capped with a rubber septum and maintained under an argon atmosphere. THF (10 mL, 1.4 M) was added (producing a suspension). Crude tosylate **22** (7.1 mmol, 1.0 equiv) was dissolved in THF (40 mL, 0.2 M) and added to the hydride suspension by cannula (evolving gas). The mixture was stirred (1 h), cooled in an ice bath (0 °C), quenched with ammonium chloride (saturated aqueous, dropwise until bubbling ceased, then in one portion, 60 mL total), diluted with water (60 mL), extracted with EtOAc (100 + 50 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by column chromatography (150 mL silica gel, [3:1] hexane/EtOAc to remove byproducts, then [1:1] hexane/EtOAc) to yield pure pyrrolidine **23** (1.33 g, 4.33 mmol, 61% yield from alcohol **21**). ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY.

^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.82 (dt, J_d = 37.0 Hz, J_t = 7.4 Hz, 1H, vinyl), 4.60 (s, 2H, MOM), 4.43–4.36 (m, 1H, Pro-α), 3.51 (t, J = 6.7 Hz, 2H, CH_2–OMOM), 3.45–3.35 (m, 2H, Pro-δ), 3.34 (s, 3H, MOM), 2.40–2.34 (m, 2H, CH_2–C=C), 1.91–1.79 (m, 4H, Pro-β, Pro-γ), 1.16 (s, 9H, *t*-Bu); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 160.3 (d, J = 264.4 Hz), 102.9 (d, J = 14.2 Hz), 96.4, 66.9, 57.6, 55.1, 54.4 (d, J = 32.0 Hz), 53.8, 30.9, 24.5, 24.2, 22.9; **IR** (film, cm^{-1}) 2952, 2919, 2874, 1111, 1070, 1034; $[\alpha]_D$ = –45.6° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{14}H_{26}FNO_3SNa]^+$, requires m/z = 330.1515, found m/z = 330.1499 (ESI); **TLC** (3:1) chloroform/ether, $KMNO_4$, R_f = 0.48.



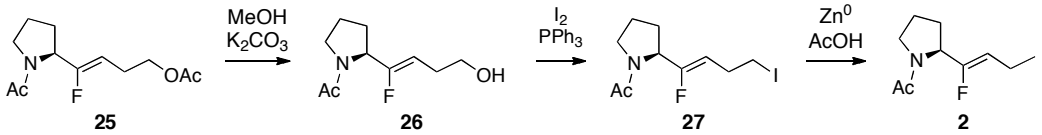
Synthesis of Acetamide 25 Into a flask were added sulfinamide **23** (27 mg, 0.088 mmol, 1.0 equiv) and methanol (1 mL, 0.09 M). The flask was capped with a septum and flushed with nitrogen. Hydrogen chloride (4.0 M in dioxane, 1 mL, 4.0 mmol, 45 equiv) was added, the nitrogen line and vent needle were removed, and the mixture was stirred (2.5 h, occasionally

[15] a) Tosylation procedure from: Yadav, J. S.; Bhaskar–Reddy, K.; Prasad, A. R.; Ur–Rehman, H. *Tetrahedron* **2008**, *64*, 2063–2070. b) Cyclization procedure modified from: Voituriez, A.; Ferreira, F.; Pérez–Luna, A.; Chemla, F. *Org. Lett.* **2007**, *9*, 4705–4708.

venting pressure). Volatiles were removed under a stream of nitrogen (1 h), under high vacuum (1 h), and by azeotropic distillation (2× toluene). Crude amine hydrochloride **24** was used directly in the next step.

Into a flask were added crude amine hydrochloride **24**, DCM (3 mL, 0.03 M), triethylamine (277 μL, 2.0 mmol, 22 equiv), DMAP (61 mg, 0.50 mmol, 6 equiv), and acetic anhydride (142 μL, 1.5 mmol, 17 equiv). The mixture was stirred (18 h), diluted with DCM (40 mL), washed with citric acid (10% aqueous, 40 mL) and sodium carbonate (10% aqueous, 40 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by column chromatography (20 mL silica gel, [4:1 to 1:0] EtOAc/hexanes) to yield acetamide **25** (12 mg, 0.049 mmol, 56% yield from sulfinamide **23**). NMR spectra show two rotational isomers (1:1 in $CDCl_3$). ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY.

^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.75–4.70 (m, 0.5H, vinyl), 4.67–4.60 (m, 1H, vinyl, Pro-α), 4.33–4.28 (m, 0.5H, Pro-α), 4.08–4.02 (m, 2H, CH_2–O), 3.57–3.40 (m, 2H, Pro-δ), 2.45–2.36 (m, 2H, CH_2–C=C), 2.10–1.86 (m, 4H, Pro-β, Pro-γ), 2.06 (s, 1.5H, Ac), 2.06 (s, 1.5H, Ac), 2.03 (s, 3H, Ac); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 171.0, 170.9, 169.8, 169.3, 159.0 (d, J = 260.3 Hz), 158.8 (d, J = 259.2 Hz), 101.9 (d, J = 13.6 Hz), 101.1 (d, J = 14.0 Hz), 63.3, 63.1, 58.4 (d, J = 38.4 Hz), 56.7 (d, J = 32.8 Hz), 47.7, 46.0, 30.7, 29.1, 24.1, 23.3 (d, J = 5.0 Hz), 23.2 (d, J = 5.0 Hz), 22.7, 22.1, 21.9, 20.9, 20.8; **IR** (film, cm^{-1}) 1738, 1653, 1409, 1242, 1026; $[\alpha]_D$ = –41.7° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{12}H_{18}FNO_3H]^+$, requires m/z = 244.1349, found m/z = 244.1341 (ESI); **TLC** EtOAc, $KMNO_4$, R_f = 0.19.



Synthesis of Vinylfluoride 2[16,17,18] Into a flask were added acetamide **25** (43 mg, 0.177 mmol, 1.0 equiv), methanol (6 mL, 0.03 M), and powdered potassium carbonate (140 mg, 1.01 mmol, 5.7 equiv). The heterogeneous mixture was stirred (16 h, becoming homogeneous), concentrated under reduced pressure, diluted with THF (5 mL), mixed in an ultrasonic water bath (producing precipitate), and filtered through Celite. Volatiles were removed under reduced pressure to yield crude alcohol **26** (full conversion by NMR), which was used directly in the next step.

Into a flask were added crude alcohol **26** (0.177 mmol, 1.0 equiv), DCM (4 mL, 0.04 M), polymer supported triphenylphosphine (3.08 mmol·g^{-1}, 584 mg, 1.80 mmol, 10 equiv) and imidazole (100 mg, 1.47 mmol, 8.3 equiv). The flask was capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in an ice bath (0 °C). Iodine (228 mg, 0.898 mmol, 5.1 equiv) was added. The mixture was covered with aluminum foil, stirred (2 h), and diluted with hexane (20 mL). Solids were removed by vacuum filtration, and washed with a mixture of hexane and EtOAc (2:1, 2 × 5 mL). The filtrate was concentrated under reduced pressure to yield crude iodide **27** (full conversion), which was used directly in the next step.

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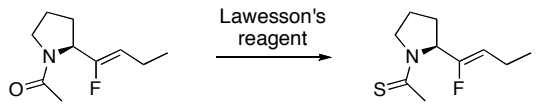
[16] Methanolysis procedure from: Matsuo, G.; Kawamura, K.; Hori, N.; Matsukura, H. Nakata, T. *J. Am. Chem. Soc.* **2004**, 14374–6.

[17] Iodination procedure modified from: Smith, A. B., III; Fox, R. J.; Vanecko, J. A. *Org. Lett.* **2005**, *7*, 3099–3102.

[18] Reduction procedure from: Shi, M.; Liu, L.–P.; Tang, J. *J. Org. Chem.* **2005**, 10420–10425.

Into a flask were added crude iodide **27** (0.177 mmol, 1.0 equiv), THF (4 mL, 0.04 M), zinc dust (350 mg, 5.38 mmol, 30 equiv), and acetic acid (350 μL, 6.12 mmol, 35 equiv). The flask was capped with a rubber septum and maintained under a nitrogen atmosphere. The mixture was stirred (1 h), and filtered through cotton. Volatiles were removed under reduced pressure and by azeotropic distillation (toluene), and the crude mixture was purified by column chromatography (20 mL silica gel, [2:1] EtOAc/hexanes) to yield acetamide **2** (6 mg, 0.03 mmol, 18% yield from acetamide **25**). NMR spectra show two rotational isomers (1.7:1 in $CDCl_3$), whose signals coalesce at 100 °C in DMSO-d_6. ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY. Isomers were assigned by ^{1}H–^{1}H NOESY at –70 °C. The major rotational isomer (*cis*) has the acetamide's methyl group pointing towards the fluorobutenyl group.

^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.70–4.66 (m, 0.4H, vinyl), 4.66–4.63 (m, 0.4H, Pro-α), 4.63–4.58 (m, 0.6H, vinyl), 4.33–4.25 (m, 0.6H, Pro-α), 3.57–3.40 (m, 2H, Pro-δ), 2.14–2.03 (m, 2H, CH_2–Me), 2.08 (s, 1.1H, Ac), 2.07 (s, 1.9H, Ac), 2.03–1.83 (m, 4H, Pro-β, Pro-γ), 0.98–0.93 (m, 3H, CH_3); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 170.1, 169.5, 156.5 (d, J = 256.5 Hz), 156.3 (d, J = 255.5 Hz), 108.2 (d, J = 14.1 Hz), 107.7 (d, J = 14.4 Hz), 58.4 (d, J = 35.9 Hz), 56.8 (d, J = 33.1 Hz), 47.7, 46.0, 30.7, 29.0, 24.0, 22.8, 22.2, 21.9, 16.9 (d, J = 5.1 Hz), 16.8 (d, J = 5.1 Hz), 14.0; **^{19}F NMR** ($CDCl_3$, 376 MHz) δ –121.5 (dd, J_1 = 36.9 Hz, J_2 = 8.3 Hz, 0.6H), –125.0 (dd, J_1 = 38.5 Hz, J_2 = 15.6 Hz, 0.4H); **IR** (film, cm^{-1}) 2967, 2874, 1651, 1409; $[\alpha]_D$ = –78.2° (c = 0.5, $CHCl_3$); **HRMS** calculated for $[C_{10}H_{16}FNOH]^+$, requires m/z = 186.1294, found m/z = 186.1285 (ESI); **TLC** EtOAc, $KMNO_4$, R_f = 0.42.



2 **3**

Synthesis of Thioacetamide 3[19] Lawesson's reagent was purified by recrystallization (toluene, reflux to ambient temperature) and stored under a nitrogen atmosphere. For use, it was transferred and weighed under regular atmosphere.

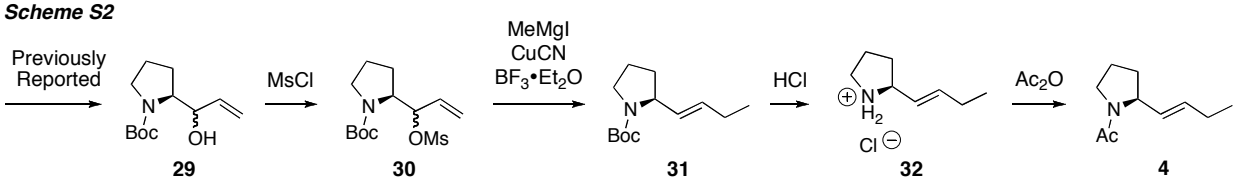
Into a Woodward condenser were added acetamide **2** (approximately 2 mg, 0.01 mmol, 1.0 equiv), sodium bicarbonate (84 mg, 1.0 mmol, 100 equiv), Lawesson's reagent (40 mg, 0.10 mmol, 10 equiv), and toluene (1 mL, 0.01 M, forming a suspension). The mixture was heated to reflux with a sand bath (3 h, bath temperature = 130 °C), allowed to cool to ambient temperature, diluted with toluene (5 mL), washed with sodium bicarbonate (saturated aqueous, 3 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by preparatory TLC (DCM) to yield pure thioacetamide **3** (approximately 1 mg, 0.005 mmol, 50% yield). NMR spectra show two rotational isomers (2.2:1 in $CDCl_3$). The sample was allowed to equilibrate for 5 h in $CDCl_3$ before it was analyzed. Further equilibration (4 d) did not alter the conformational ratio. ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY. Conformational isomers were assigned by ^{19}F NMR analogy to acetamide **2**. The major rotational isomer (*cis*) has the acetamide's methyl group pointing towards the fluorobutenyl group.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.31–5.24 (m, 0.3H, Pro-α), 4.69 (dt, J_d = 38.0 Hz, J_t = 7.4 Hz, 0.3H, vinyl), 4.66–4.51 (m, 1.4H, Pro-α, vinyl), 3.98–3.58 (m, 2H, Pro-δ), 2.65 (s, 2.1H,

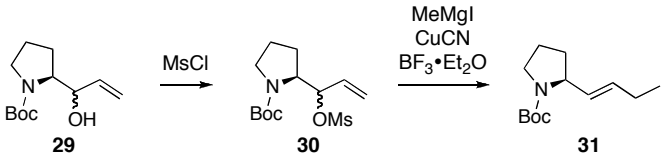
[19] Sulfurization procedure from: Liu, Z.; Qu, H.; Gu, X.; Min, B. J.; Nyberg, J.; Hruby, V. J. *Org. Lett.* **2008**, *10*, 4105–4108.

Ac), 2.60 (s, 0.9H, Ac), 2.25–1.95 (m, 6H, Pro-β, Pro-γ, CH_2–Me), 0.97 (t, J = 7.5 Hz, 2.1H, CH_3), 0.96 (t, J = 7.5 Hz, 0.9H, CH_3); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 198.7, 198.2, 154.3 (d, J = 256.9 Hz), 153.8 (d, J = 255.4 Hz), 109.8 (d, J = 13.9 Hz), 109.1 (d, J = 13.8 Hz), 63.1 (d, J = 33.0 Hz), 61.8 (d, J = 36.4 Hz), 53.8, 51.3, 33.7, 32.5, 30.9 (d, J = 2.0 Hz), 29.2 (d, J = 1.0 Hz), 24.3 (d, J = 1.0 Hz), 22.0, 17.0 (d, J = 5.1 Hz), 16.9 (d, J = 5.0 Hz), 14.0 (d, J = 1.6 Hz), 13.9 (d, J = 1.6 Hz); **^{19}F NMR** ($CDCl_3$, 376 MHz) δ –121.2 (dd, J_1 = 36.9 Hz, J_2 = 7.9 Hz, 0.7H), –125.4 (dd, J_1 = 38.0 Hz, J_2 = 16.9 Hz, 0.3H); **IR** (film, cm^{-1}) 2968, 2931, 2875, 1704, 1469, 1452, 1426, 1018; **$[\alpha]_D$** = –27° (c = 0.1, $CHCl_3$); **HRMS** calculated for $[C_{10}H_{16}FNSH]^+$, requires m/z = 202.1066, found m/z = 202.1074 (ESI); **TLC** DCM, UV/CAM, R_f = 0.30.

Scheme S2



Scheme S2 summarizes the synthetic approach used to access acetamide **4**.



Synthesis of Alkene 31[20] Alcohol **29** was made as previously described.[21] Into a flask were added a diastereomeric mixture of alcohol **29** (1.40 g, 6.17 mmol, 1.0 equiv), chloroform (6 mL, 0.6 M), and pyridine (12.3 mL, 123 mmol, 20 equiv). The flask was capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in an ice bath (0 °C). Methanesulfonyl chloride (4.81 mL, 61.7 mmol, 10 equiv) was added by syringe. The mixture was stirred (1 h), quenched with water (60 mL), allowed to warm to ambient temperature, extracted with ether (60 mL), washed with citric acid (10% aqueous, 30 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude mixture was passed through a short silica gel plug (100 mL silica gel, [2:1] hexane/EtOAc) to yield mostly pure mesylate **30** (1.31 g, 4.30 mmol, 70% yield), a fraction of which was used directly in the next step.

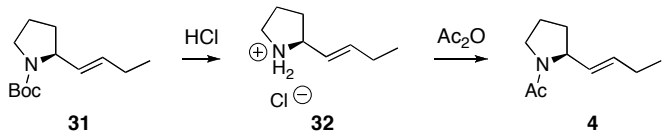
TLC (2:1) hexane/EtOAc, $KMNO_4$, R_f = 0.38.

Into a flame-dried flask were added dry copper (I) cyanide (290 mg, 3.24 mmol, 3.0 equiv) and THF (15 mL, 0.07 M, giving a suspension). The flask was capped with a rubber septum, maintained under a nitrogen atmosphere, and cooled in a dry ice/acetone bath (–78 °C). Methylmagnesium iodide (3.0 M in ether, 1.08 mL, 3.24 mmol, 3.0 equiv) was added. The mixture was transferred to an ice bath (0 °C), stirred (15 min), and returned to the dry ice/acetone bath. Borontrifluoride etherate (407 μL, 3.24 mmol, 3.0 equiv) was added, and the mixture was stirred (5 min). One quarter of mesylate **30** (329 mg, 1.08 mmol, 1.0 equiv) was placed in a flask,

[20] Mesylation and allylic alkylation procedures from: Ibuka, T.; Taga, T.; Habashita, H.; Nakai, K.; Tamamura, H.; Fujii, N. *J. Org. Chem.* **1993**, *58*, 1207–1214.
[21] Jakobsche, C. E.; Peris, G.; Miller, S. J. *Angew. Chem., Int. Ed.* **2008**, *47*, 6707–6711.

flushed with nitrogen, dissolved in THF (8 mL, 0.1 M), and added to the reaction mixture. The mixture was stirred (additional 30 min), transferred to the ice bath, stirred (additional 15 min), quenched with a mixture of ammonium hydroxide and saturated ammonium chloride (1:1, 40 mL), allowed to return to ambient temperature, extracted with ether (40 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude mixture was purified by column chromatography (40 mL silica gel, [4:1] hexane/ether) to yield alkene **31** (223 mg, 1.00 mmol, 93% yield, 65% yield from alcohol **29**). Diastereoselectivity was assayed after further transformations, at which time only a single diastereomer was observed.

^{1}H NMR ($CDCl_3$, 500 MHz) δ 5.55–5.42 (m, 1H), 5.35–5.25 (m, 1H), 4.37–4.10 (m, 1H), 3.40–3.28 (m, 2H), 2.04–1.90 (m, 3H), 1.88–1.71 (m, 2H), 1.68–1.60 (m, 1H), 1.41 (s, 9H), 0.95 (t, J = 7.4 Hz, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 154.6, 131.8, 129.6, 78.8, 58.6, 46.1, 32.5, 28.5, 25.1, 22.9, 13.7; **IR** (film, cm^{-1}) 2970, 2929, 2873, 1693, 1389, 1166; $[\alpha]_D$ = –12.2° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{13}H_{23}NO_2Na]^+$, requires m/z = 248.1626, found m/z = 248.1616 (ESI); **TLC** (4:1) hexane/ether, $KMNO_4$, R_f = 0.27.

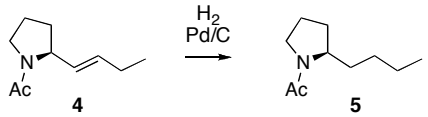


Synthesis of Alkene 4 The standard Boc deprotection was followed using carbamate **31** (113 mg, 0.500 mmol, 1.0 equiv) and hydrogen chloride (4.0 M in dioxane, 3 mL). Crude amine hydrochloride **32** was used directly in the next step.

^{1}H NMR (DMSO-d_6, 400 MHz) δ 9.30–9.15 (brs, 1H), 8.82–8.65 (brs, 1H), 5.89 (dt, J_d = 15.5 Hz, J_t = 6.3 Hz, 1H), 5.52 (dd, J_1 = 15.4 Hz, J_2 = 8.1 Hz, 1H), 3.92 (q, J = 8.4 Hz, 1H), 3.20–3.07 (m, 2H), 2.09–2.00 (m, 3H), 2.00–1.80 (m, 2H), 1.70–1.58 (m, 1H), 0.96 (t, J = 7.4 Hz, 3H).

Into a flask were added crude amine hydrochloride **32**, DCM (3 mL, 0.2 M), triethylamine (277 μL, 2.0 mmol, 4.0 equiv), DMAP (61 mg, 0.50 mmol, 0.5 equiv), and acetic anhydride (142 μL, 1.5 mmol, 3.0 equiv). The mixture was stirred (1.5 h), diluted with DCM (40 mL), washed with sodium carbonate (10% aqueous, 40 mL) and citric acid (10% aqueous, 40 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by column chromatography (20 mL silica gel, [2:1 to 3:1] EtOAc/hexanes) to yield acetamide **4** (40 mg, 0.24 mmol, 48% yield from carbamate **31**). Only a single olefin diastereomer was observed by NMR (*trans*, assigned by coupling constants). NMR spectra show two rotational isomers (2.9:1 in $CDCl_3$), whose signals coalesce at 100 °C in DMSO-d_6. ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY. Isomers were assigned by ^{1}H–^{1}H NOESY at –70 °C. The major rotational isomer (*cis*) has the acetamide's methyl group pointing towards the butenyl group.

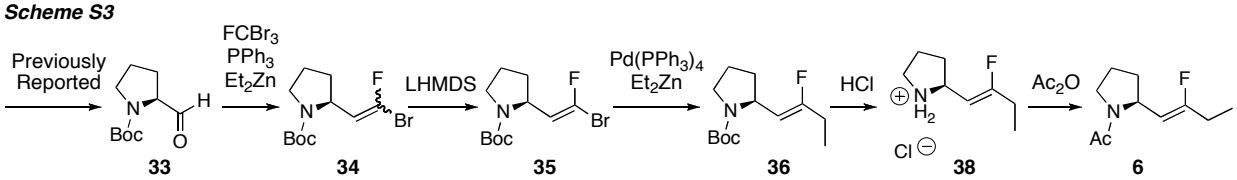
^{1}H NMR ($CDCl_3$, 500 MHz) δ 5.56 (dt, J_d = 15.4 Hz, J_t = 6.3 Hz, 1H, CH–Et), 5.34 (dd, J_1 = 15.3 Hz, J_2 = 6.1 Hz, 1H, Pro-vinyl), 4.61 (t, J = 5.5 Hz, 0.3H, Pro-α), 4.23 (t, J = 6.8 Hz, 0.7H, Pro-α), 3.52–3.34 (m, 2H, Pro-δ), 2.04 (s, 0.7H, Ac), 2.00 (s, 2.3H, Ac), 2.10–1.65 (m, 6H, Pro-β, Pro-γ, Et), 0.96 (t, J = 7.5 Hz, 3H, Et); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 169.9, 168.9, 133.1, 132.0, 128.8, 128.0, 60.0, 57.6, 47.6, 45.9, 33.1, 31.0, 25.0, 23.7, 22.8, 22.4, 22.0, 13.5, 13.4; **IR** (film, cm^{-1}) 2966, 2929, 2868, 1646, 1414; $[\alpha]_D$ = –16.0° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{10}H_{17}NOH]^+$, requires m/z = 168.1388, found m/z = 168.1382 (ESI); **TLC** (2:1) EtOAc/hexane, $KMNO_4$, R_f = 0.21.



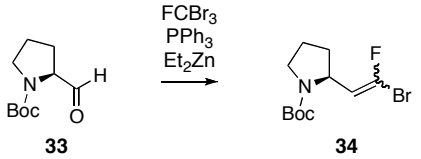
Synthesis of Acetamide 5 Into a flask were added alkene **4** (18 mg, 0.11 mmol, 1.0 equiv) and methanol (1 mL, 0.1 M). The flask was flushed with argon. Into another flask was added palladium on carbon (10%, 20 mg). This flask was capped with a rubber septum and flushed with argon. Methanol (1 mL, 0.1 M) was added by syringe to the palladium-containing flask. The flask was uncapped, and the suspension was transferred into the alkene-containing flask, which was flushed with argon and capped with a rubber septum. A hydrogen balloon was attached, and the system was flushed briefly with hydrogen. The mixture was stirred (3 h), the balloon was removed, and the system was flushed with argon. The crude mixture was filtered through Celite with methanol. Volatiles were removed to yield pure alkane **5** (15 mg, 0.89 mmol, 81% yield). NMR spectra show two rotational isomers (1.4:1 in $CDCl_3$), whose signals coalesce at 100 °C in DMSO-d_6. ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY. Isomers were assigned by ^{1}H–^{1}H NOESY at –70 °C. The major rotational isomer (*trans*) has the acetamide's carbonyl pointing towards the butyl group.

^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.60–4.40 (m, 0.6H), 3.69–3.75 (m, 0.4H), 5.55–3.48 (m, 0.4H), 3.45–3.33 (m, 1.6H), 2.06 (s, 1.3H), 2.01 (s, 1.7H), 1.98–1.15 (m, 12H), 0.92–0.85 (m, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 168.9, 58.7, 57.1, 47.6, 45.3, 34.6, 32.9, 30.3, 29.2, 28.6, 28.5, 24.0, 23.0, 22.7, 22.6, 22.2, 22.1, 14.1, 14.0; **IR** (film, cm^{-1}) 2960, 2928, 2863, 1646, 1411; **$[\alpha]_D$** = –39.2° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{10}H_{19}NOH]^+$, requires m/z = 170.1545, found m/z = 170.1537 (ESI); **TLC** EtOAc, $KMNO_4$, R_f = 0.37. Compound analysis is consistent with published data.[22]

Scheme S3



Scheme S3 summarizes the synthetic approach used to access acetamide **6**.

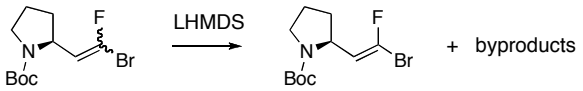


Synthesis of Bromofluoroalkene 34[23] Aldehyde **33** was prepared as previously described.[24] Into a flask were added crude aldehyde **33** (3.38 g, 17.0 mmol, 1.0 equiv), triphenylphosphine (5.34 g, 20.4 mmol, 1.2 equiv), THF (170 mL, 0.1 M), and tribromofluoromethane (2.00 mL, 20.4 mmol, 1.2 equiv). The flask was capped with a rubber septum, maintained under a nitrogen

[22] Compound data from: Lucwig, C.; Wistrand, L.–G. *Acta. Chem. Scand.* **1990**, *44*, 707–710.
[23] Olefination and kinetic resolution procedures and example coupling constants from: Lei, X.; Dutheuil, G.; Pannecoucke, X. Quirion, J.–C. *Org. Lett.* **2004**, *6*, 2101–2104.
[24] Jakobsche, C. E.; Peris, G.; Miller, S. J. *Angew. Chem., Int. Ed.* **2008**, *47*, 6707–6711.

atmosphere, and placed in an ambient temperature water bath. Diethylzinc (1.0 M in hexanes, 20.4 mL, 20.4 mL, 1.2 equiv) was added dropwise (over 30 min). The mixture was stirred (additional 30 min), quenched with ammonium chloride (saturated aqueous, 40 mL), stirred (20 min), concentrated under reduced pressure (to remove the THF), diluted with ammonium chloride (saturated aqueous, additional 40 mL) and brine (40 mL), extracted with DCM (2 × 40 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure to give an orange oil. Hexane (50 mL) was added (producing gooey precipitate), and the supernatant was isolated by vacuum filtration. Volatiles were removed under reduced pressure, and the crude mixture was purified by column chromatography (200 mL silica gel, [10:1] hexanes/EtOAc) to yield bromoalkene **34** (2.74 g, 9.32 mmol, 55% yield from Boc–Pro–OH). The product was isolated as a mixture of olefin geometric isomers (1.3:1 *Z*/*E*, assigned after the next step). By ^{19}F NMR, each isomer shows two rotational isomers (each approximately 2.5:1).

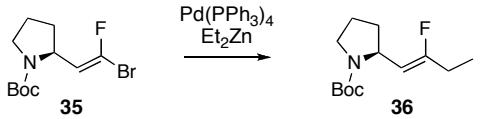
^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.48 (dd, J_1 = 12.0 Hz, J_2 = 9.1 Hz, 0.6H), 5.00 (dd, J_1 = 30.0 Hz, J_2 = 11.4 Hz, 0.4H), 4.65–4.50 (m, 0.4H), 4.40–4.20 (m, 0.6H), 3.50–3.30 (m, 2H), 2.20–2.04 (m, 1H), 1.90–1.80 (m, 2H), 1.76–1.65 (m, 1H), 1.45 (s, 9H); **^{19}F NMR** ($CDCl_3$, 376 MHz) δ –72.3 to –72.5 (brs, 0.3H), –73.4 to –73.8 (m, 1H), –74.6 (d, J = 29.7 Hz, 0.7H); **TLC** (10:1) hexane/EtOAc, $KMNO_4$, R_f = 0.25.



34 **35**

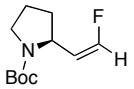
Kinetic Resolution of Bromofluoroalkene 35[23] Into a flask were added a diastereomeric mixture of bromofluoroalkene **34** (1.3:1 *Z*/*E*, 2.74 g, 9.32 mmol, 1.0 equiv) and THF (95 mL, 0.1 M). The flask was capped with a rubber septum and maintained under a nitrogen atmosphere. Lithium bis(trimethylsilyl)amide (1.0 M in hexane, 5.6 mL, 5.6 mmol, 0.6 equiv) was added portionwise (over 5 min, slightly exothermic, causing the solution to become deep green and then deep brown). After 15 min (at which time NMR analysis indicated approximately 70% consumption of one diastereomer), additional lithium bis(trimethylsilyl)amide (3.5 mL, 3.5 mmol, 0.4 equiv) was added. The mixture was stirred (20 min), quenched with ammonium chloride (saturated aqueous, 30 mL), diluted with water (30 mL) and brine (60 mL), extracted with EtOAc (2 × 60 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude mixture was purified by column chromatography (80 mL silica gel, [10:1] hexanes/EtOAc) to yield nearly pure *E*-alkene **35** (581 mg, 1.98 mmol, 48% yield based on *E*-isomer, 21% yield based on mixture **34**) and impure material (349 mg, containing a more polar contaminant). The product was recovered as a single olefin isomer (*E*, assigned by $^{3}J_{H,F}$ coupling).[23] By ^{19}F NMR alkene **35** shows two rotational isomers (3.0:1).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.00 (dd, J_1 = 30.0 Hz, J_2 = 11.4 Hz, 1H), 4.65–4.50 (m, 1H), 3.50–3.30 (m, 2H), 2.20–2.04 (m, 1H), 1.90–1.80 (m, 2H), 1.76–1.65 (m, 1H), 1.45 (s, 9H); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 154.2, 132.4 (d, J = 329.5 Hz), 114.8 (d, J = 10.2 Hz), 79.6, 53.0, 46.0, 32.5, 28.4, 23.3; **^{19}F NMR** ($CDCl_3$, 376 MHz) δ –73.7 (d, J = 26.9 Hz, 0.3H), –74.5 (d, J = 29.2 Hz, 0.7H); **IR** (film, cm^{-1}) 2973, 2932, 2876, 1695, 1666, 1394, 1362, 1167; $[\alpha]_D$ = –31.2° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{11}H_{17}BrFNO_2Na]^+$, requires m/z = 316.0324, found m/z = 316.0313 (ESI); **TLC** (10:1) hexane/EtOAc, $KMNO_4$, R_f = 0.25.



Synthesis of Fluoroalkene 36[25] Into a flame-dried flask were added bromofluoroalkene **35** (168 mg, 0.571 mmol, 1.0 equiv), THF (1.7 mL, 0.3 M), and tetrakis(triphenylphosphine)palladium (33 mg, 0.029 mmol, 0.05 equiv). The flask was fit with an oven-dried reflux condenser, capped with a rubber septum, and flushed with argon. Diethylzinc (1.0 M in hexane, 1.7 mL, 1.7 mmol, 3.0 equiv) was added by syringe. The mixture was heated to reflux (4 h, becoming yellow then dark brown), allowed to cool to ambient temperature, *carefully* quenched with ammonium chloride (saturated aqueous, 20 mL, briefly and vigorously evolving gas), diluted with brine (20 mL), extracted with ether (40 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure. Crude ^{1}H NMR showed full consumption of bromoalkene **35** and approximately 60% conversion to fluoroalkene **36**. The crude mixture was purified by column chromatography (40 mL silica gel, [15:1] hexanes/EtOAc) to yield fluoroalkene **36** (56 mg, 0.23 mmol, 40% yield). By ^{19}F NMR fluoroalkene **36** shows two rotational isomers (approximately 3.2:1). ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY.

^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.65–4.55 (brs, 1H, Pro-α), 4.55–4.40 (brd, J = 37.2 Hz, 1H, vinyl), 3.40–3.30 (brs, 1H, Pro-δ), 2.17–2.09 (m, 2H, CH_2–Me), 2.10–2.00 (m, 1H, Pro-β), 1.87–1.73 (m, 2H, Pro-γ), 1.66–1.59 (m, 1H, Pro-β), 1.40 (s, 9H, Boc), 1.03 (t, J = 7.5 Hz, 3H, CH_3); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 160.7 (d, J = 260.3 Hz), 154.6, 106.7 (d, J = 13.0 Hz), 78.9, 51.7, 46.0, 33.1, 28.4, 25.0 (d, J = 28.0 Hz), 23.4, 10.7; **^{19}F NMR** ($CDCl_3$, 376 MHz) δ –106.7 to –107.2 (brs, 0.2H), –108.7 to –109.2 (m, 0.8H); **IR** (film, cm^{-1}) 2971, 2935, 2877, 1694, 1396, 1171; $[\alpha]_D$ = +11.3° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{13}H_{22}FNO_2Na]^+$, requires m/z = 266.1532, found m/z = 266.1538 (ESI); **TLC** (5:1) hexane/EtOAc, $KMNO_4$, R_f = 0.37, (8:1) toluene/EtOAc, R_f = 0.38.



37

Fluoroalkene **37**[26] was also recovered from the reaction (approximately 25% conversion by crude ^{1}H NMR).

^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.39 (dd, J_1 = 84.7 Hz, J_2 = 3.8 Hz, 1H), 4.85–4.60 (m, 2H), 3.45–3.30 (m, 2H), 2.18–2.04 (m, 1H), 1.90–1.75 (m, 2H), 1.72–1.65 (m, 1H), 1.42 (s, 9H); **TLC** (5:1) hexane/EtOAc, $KMNO_4$, R_f = 0.31.

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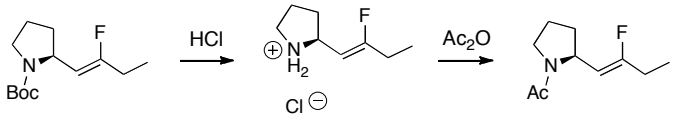
[25] Cross coupling procedure modified from: a) Schachtschabel, D.; Boland, W. *J. Org. Chem.* **2007**, *72*, 1366–1372; b) Andrei, D.; Wnuk, S. *J. Org. Chem.* **2006**, *71*, 405–408.

[26] Formation of this type of byproduct has been reported. An example from: Fürstner, A.; Leitner, A. *Angew. Chem., Int. Ed.* **2002**, *41*, 609–612.



36 **38** **6**

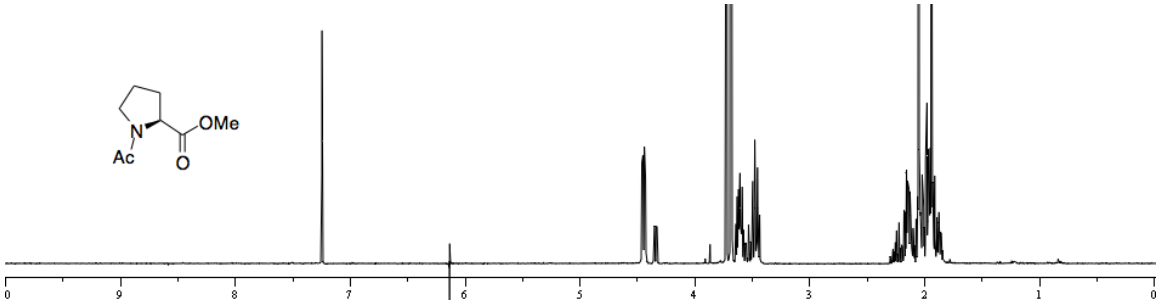
Synthesis of Acetamide 6 The standard Boc deprotection was followed using carbamate **36** (56 mg, 0.23 mmol, 1.0 equiv) and hydrogen chloride (4.0 M in dioxane, 2 mL). Crude amine hydrochloride **38** was used directly in the next step.

Into a flask were added crude amine hydrochloride **38** (0.23 mmol, 1.0 equiv), DCM (1 mL, 0.2 M), triethylamine (127 μL, 0.92 mmol, 4.0 equiv), DMAP (28 mg, 0.23 mmol, 1.0 equiv), and acetic anhydride (65 μL, 0.69 mmol, 3.0 equiv). The mixture was stirred (15 h), diluted with sodium carbonate (10% aqueous, 15 mL) and brine (15 mL), extracted with DCM (40 mL), washed with citric acid (10% aqueous, 30 mL), and dried with sodium sulfate. Volatiles were removed under reduced pressure, and the crude material was purified by column chromatography (15 mL silica gel, [4:0] EtOAc/hexanes) to yield acetamide **6** (14 mg, 0.076 mmol, 33% yield from carbamate **36**). NMR spectra show two rotational isomers (4.0:1 in $CDCl_3$), whose signals coalesce at 100 °C in DMSO-d_6. ^{1}H NMR signals were assigned by ^{1}H–^{1}H COSY. Isomers were assigned by ^{1}H–^{1}H NOESY at –70 °C. The major rotational isomer (*cis*) has the acetamide's methyl group pointing towards the fluorobutenyl group.

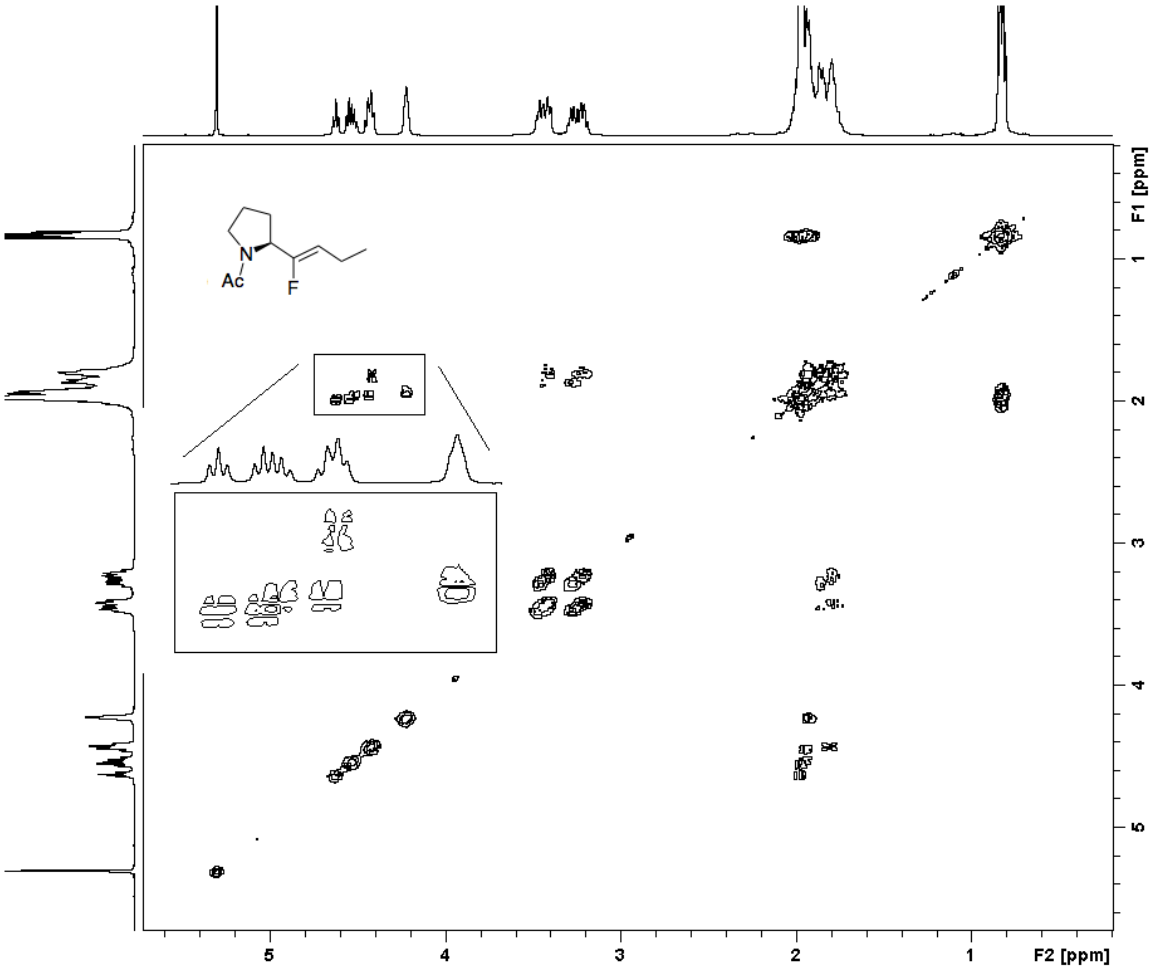
^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.83 (td, J_t = 7.7 Hz, J_d = 3.0 Hz, 0.2H, Pro-α), 4.68 (td, J_t = 9.4 Hz, J_d = 2.8 Hz, 0.8H, Pro-α), 4.55 (dd, J_1 = 36.0 Hz, J_2 = 9.3 Hz, 0.8H, vinyl), 4.52 (dd, J_1 = 37.1 Hz, J_2 = 7.3 Hz, 0.2H, vinyl), 3.54–3.35 (m, 2H, Pro-δ), 2.23–2.12 (m, 3H, Pro-β, CH_2–Me), 2.02 (s, 3H, Ac), 2.00–1.84 (m, 2H, Pro-γ),1.79–1.73 (m, 1H, Pro-β), 1.08–1.00 (m, 3H, CH_3); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ 169.8, 168.8, 161.5 (d, J = 261.5 Hz), 161.2 (d, J = 261.7 Hz), 105.8 (d, J = 12.7 Hz), 105.7 (d, J = 12.9 Hz), 52.8 (d, J = 6.1 Hz), 52.1 (d, J = 5.1 Hz), 47.6, 45.7, 33.8, 32.3, 25.1 (d, J = 27.8 Hz), 24.9 (d, J = 27.6 Hz), 228, 22.0, 10.5, 10.5; **^{19}F NMR** ($CDCl_3$, 376 MHz) δ –105.7 (dt, J_d = 37.8 Hz, J_t = 14.0 Hz, 0.2H), –107.1 (dt, J_d = 35.8 Hz, J_t = 14.8 Hz, 0.8H); **IR** (film, cm^{-1}) 2972, 2939, 2879, 1700, 1648, 1411; $[\alpha]_D$ = +47.3° (c = 1.0, $CHCl_3$); **HRMS** calculated for $[C_{10}H_{16}FNOH]^+$, requires m/z = 186.1294, found m/z = 186.1301 (ESI); **TLC** EtOAc, $KMNO_4$, R_f = 0.23.

4. Spectra

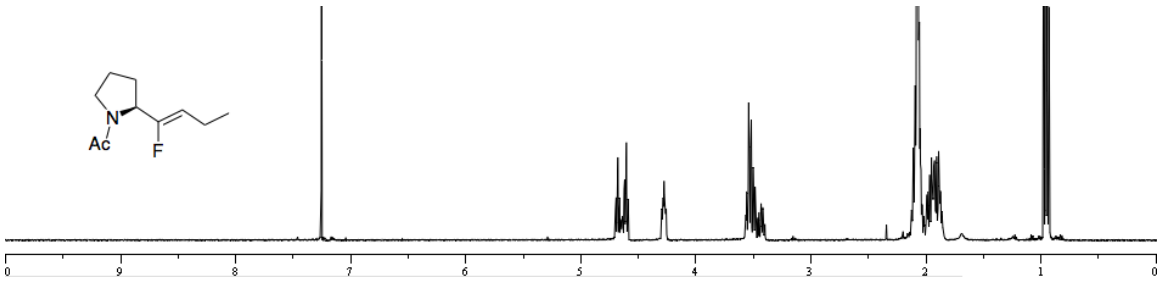
^{1}H NMR Spectrum of 1



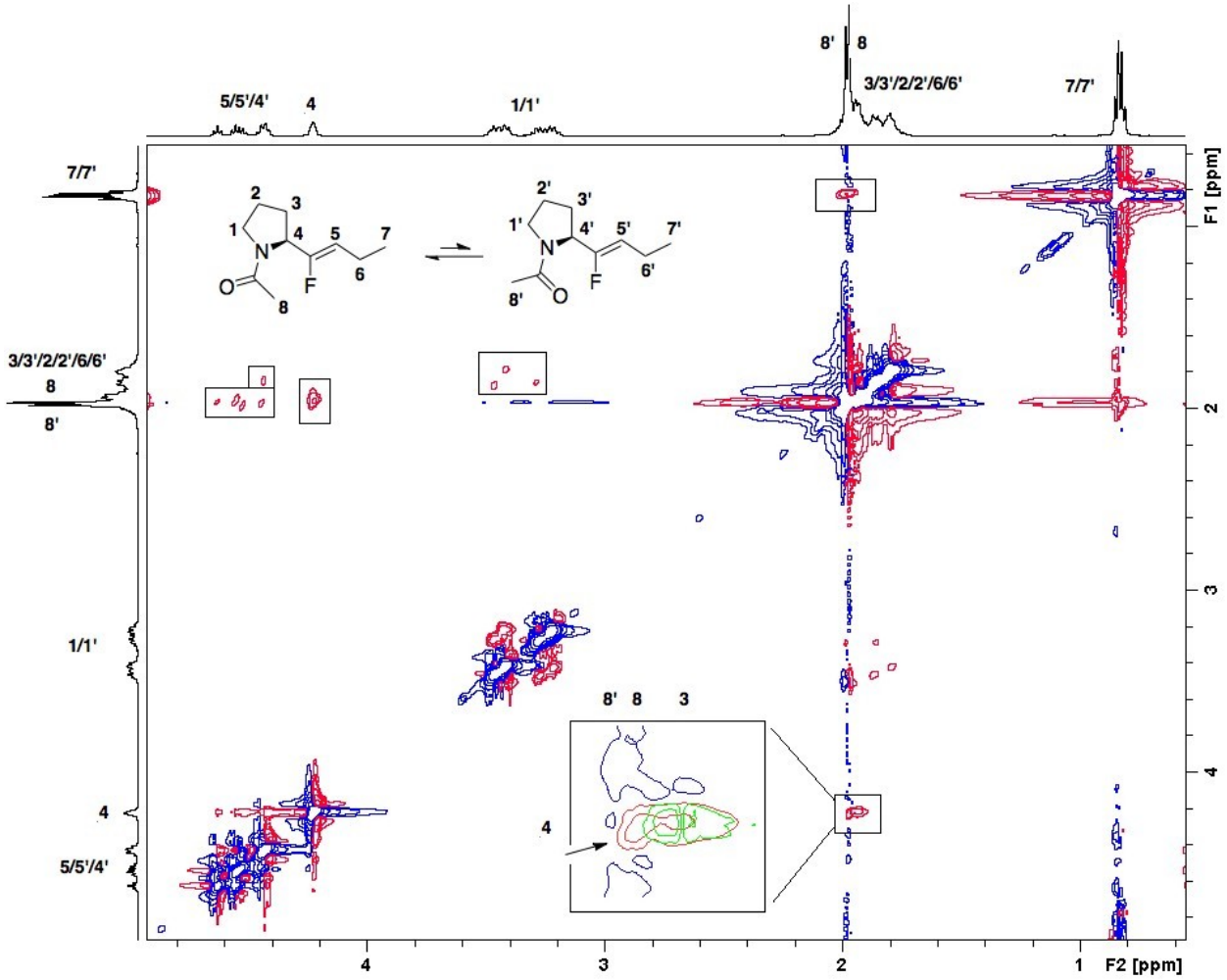
^{1}H–^{1}H COSY Spectrum of 2 (DCM-d_2, –70 °C)



^{1}H NMR Spectrum of 2

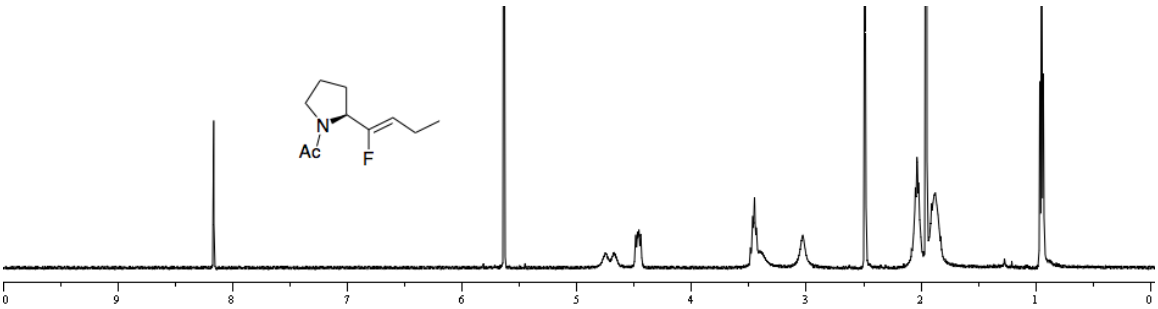


^{1}H–^{1}H NOESY Spectrum of 2 (DCM-d_2, –70 °C)

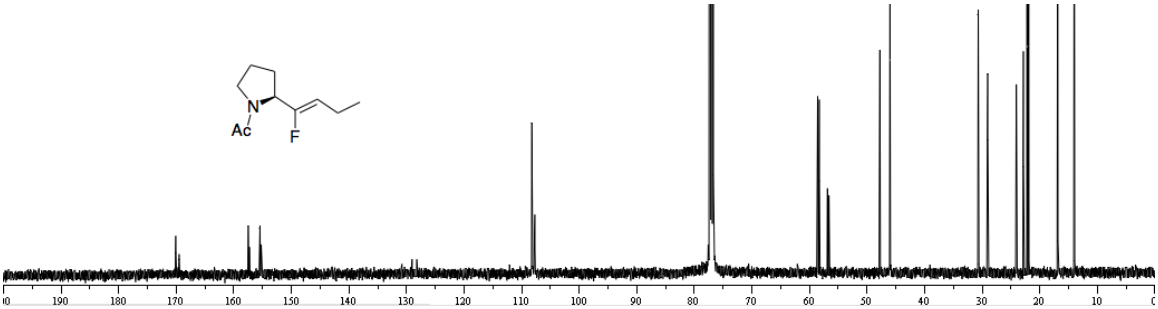


This spectrum is not symmetrized. Legitimate signals are enclosed in rectangles. The zoom in the lower region has a ^{1}H–^{1}H COSY signal overlaid in green. This overlay shows that the red NOE signal is actually two partially overlapping signals: one between **H4** and **H3** (which overlaps the COSY signal) and one between **H4** and **H8** (which is not in the COSY spectrum and proves that the major conformation is *cis*).

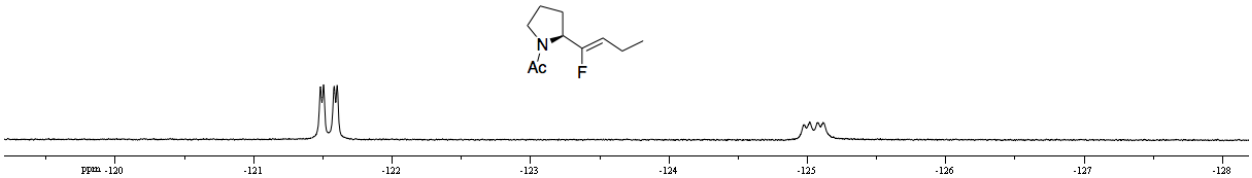
^{1}H NMR Spectrum of 2 (DMSO-d_6, 100 °C)



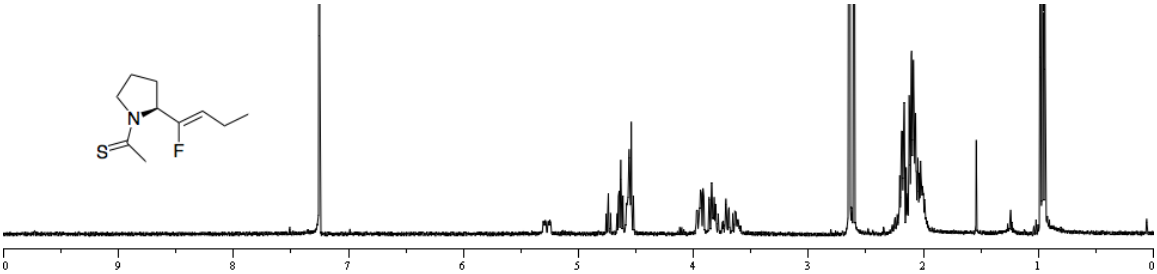
^{13}C NMR Spectrum of 2



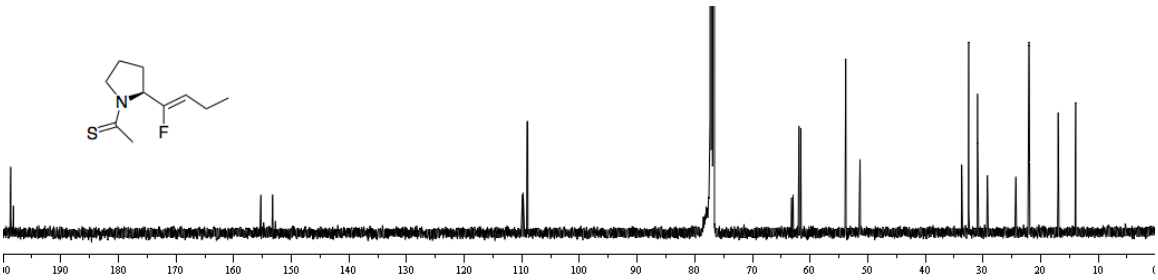
^{19}F NMR Spectrum of 2



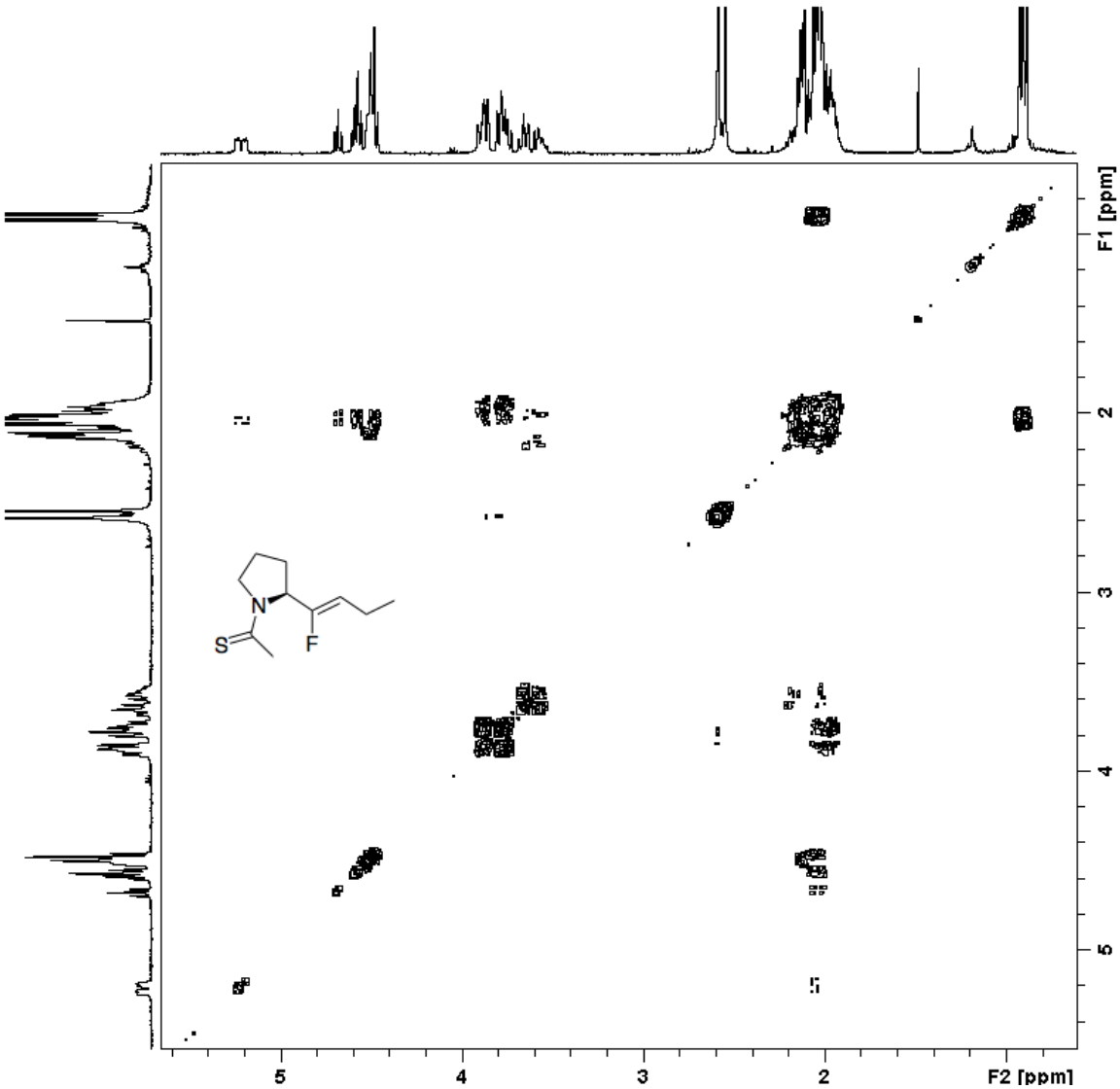
^{1}H NMR Spectrum of 3



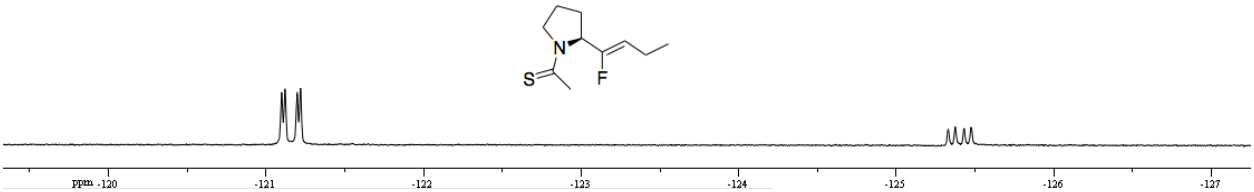
^{13}C NMR Spectrum of 3



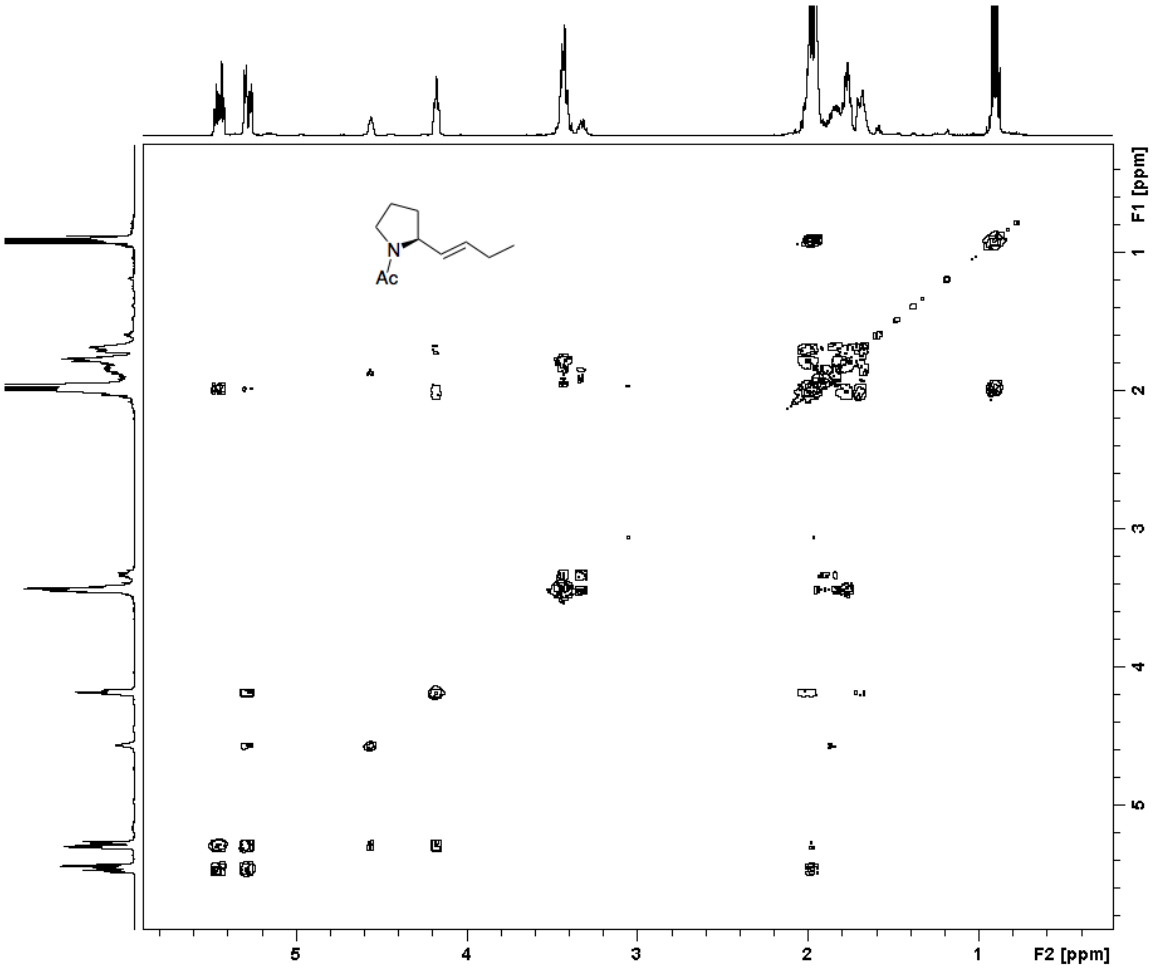
^{1}H–^{1}H COSY Spectrum of 3



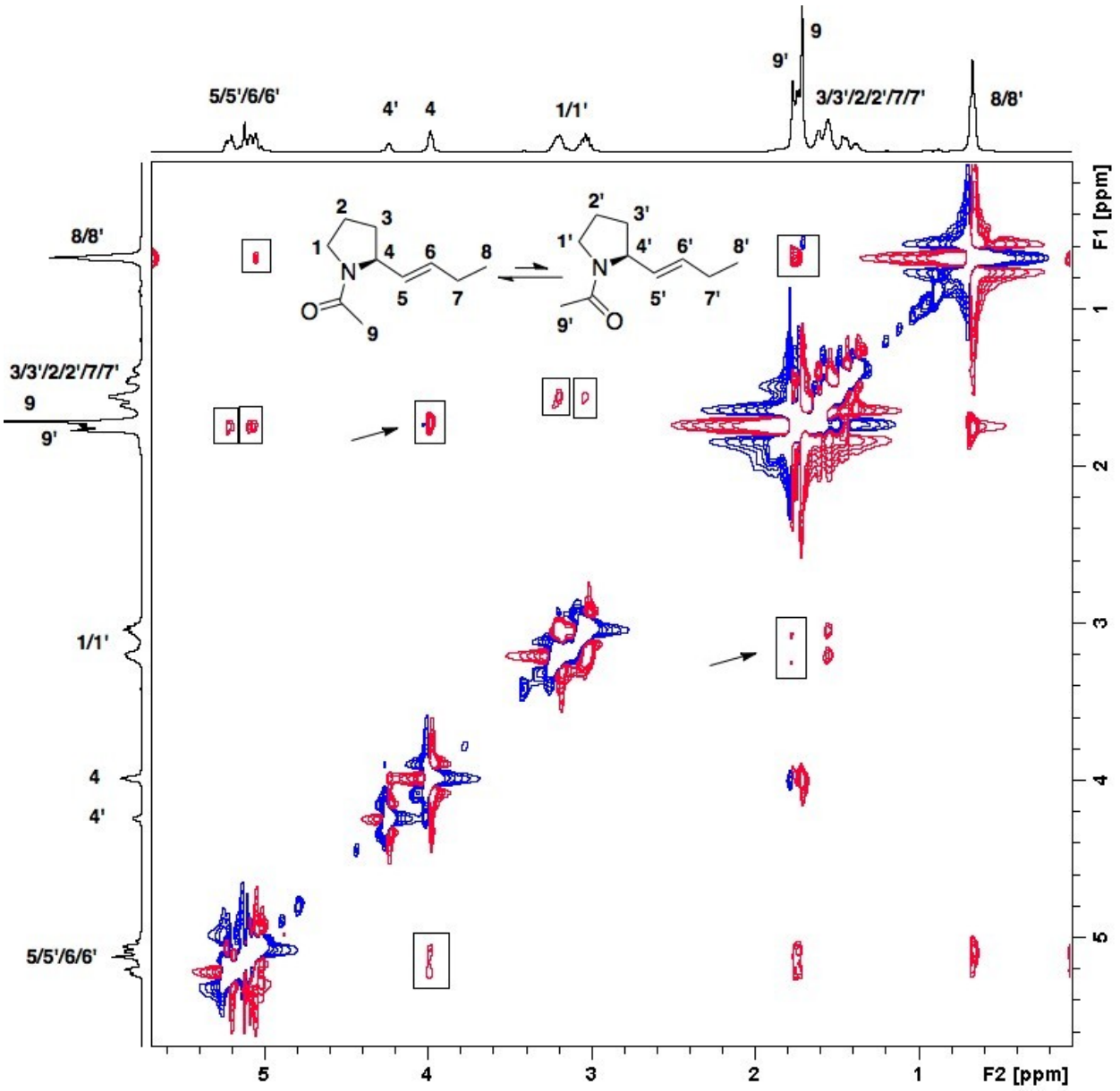
^{19}F NMR Spectrum of 3



^{1}H–^{1}H COSY Spectrum of 4

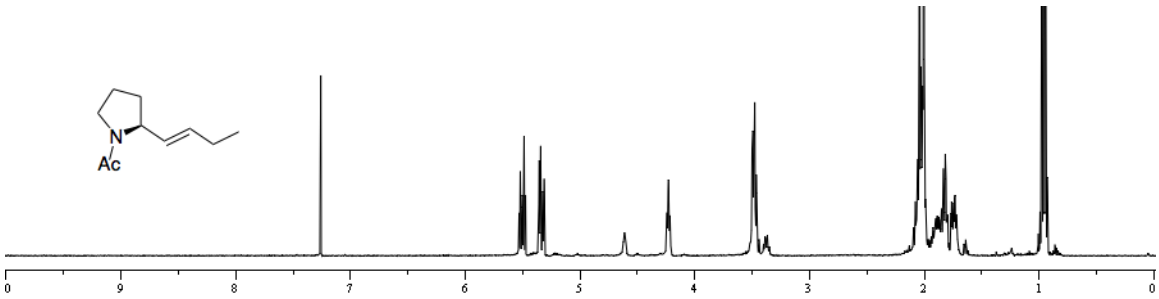


^{1}H–^{1}H NOESY Spectrum of 4 (DCM-d_2, –70 °C)

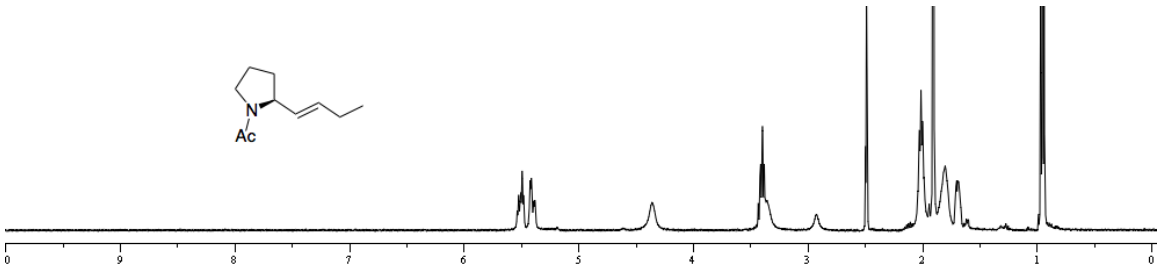


This spectrum is not symmetrized. Legitimate signals are enclosed in rectangles. The signals between **H4** and **H9** and between **H1'** and **H9'** prove that the major conformation is *cis*.

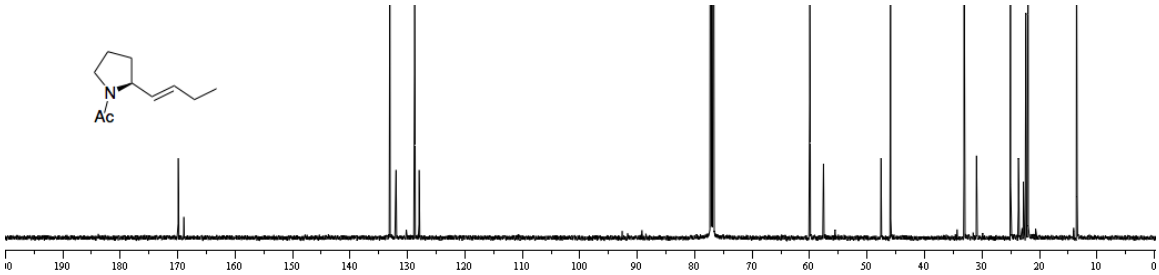
^{1}H NMR Spectrum of 4



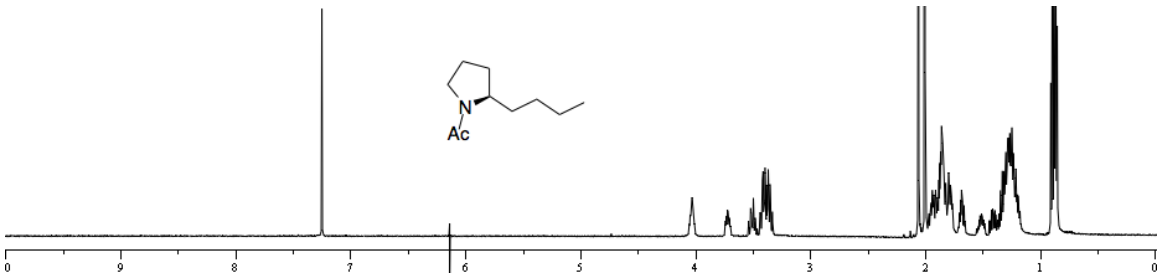
^{1}H NMR Spectrum of 4 (DMSO-d_6, 100 °C)



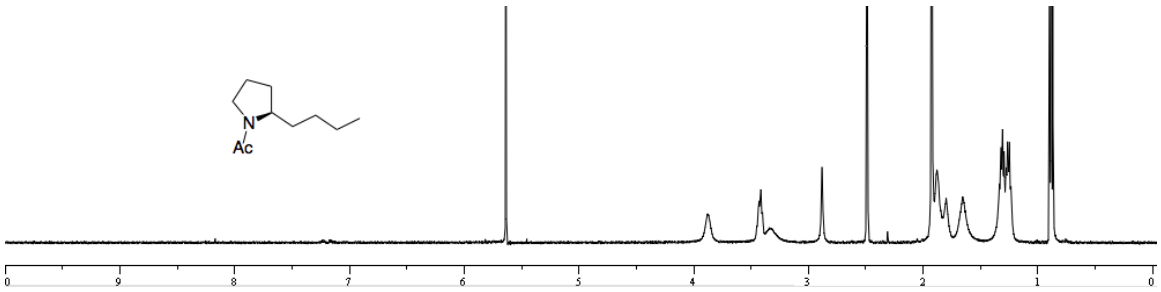
^{13}C NMR Spectrum of 4



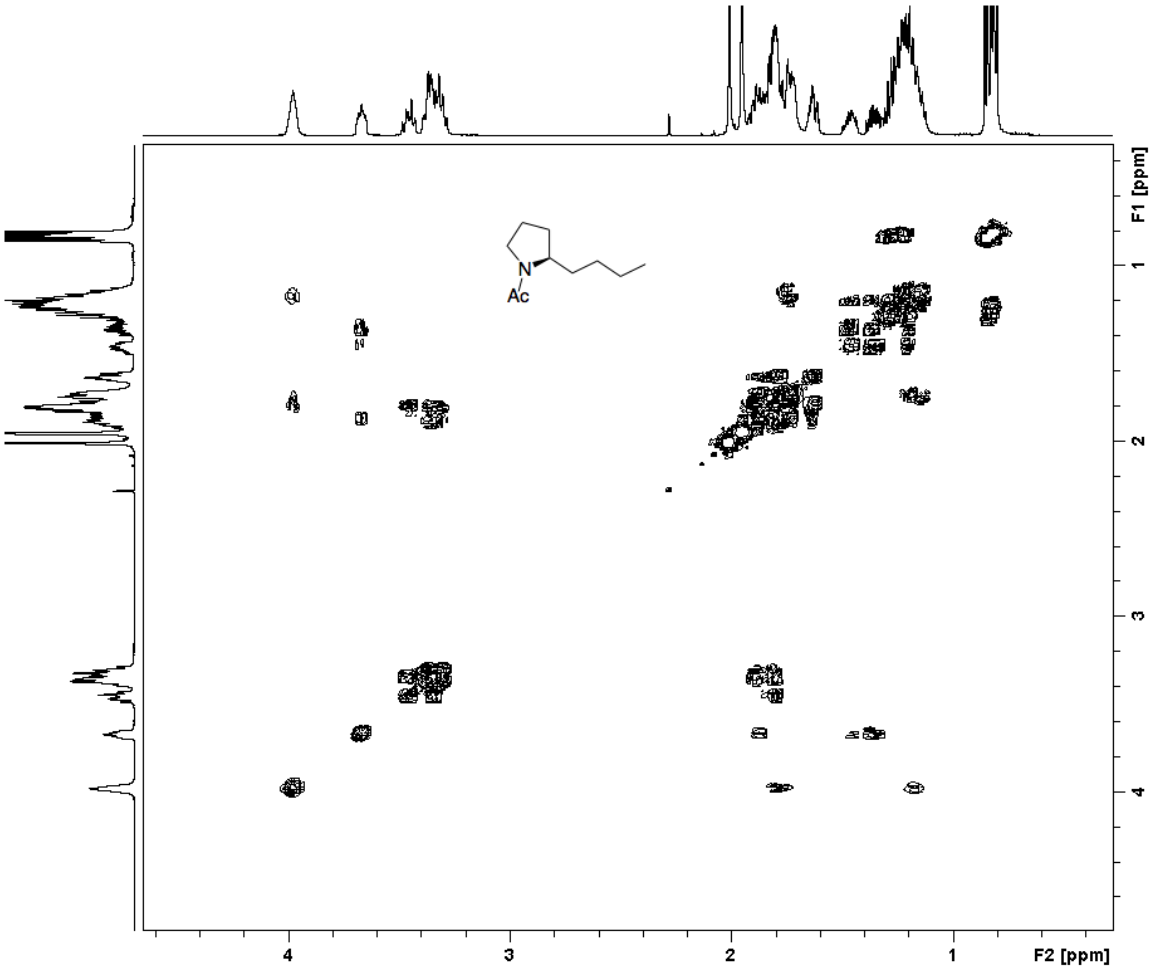
^{1}H NMR Spectrum of 5



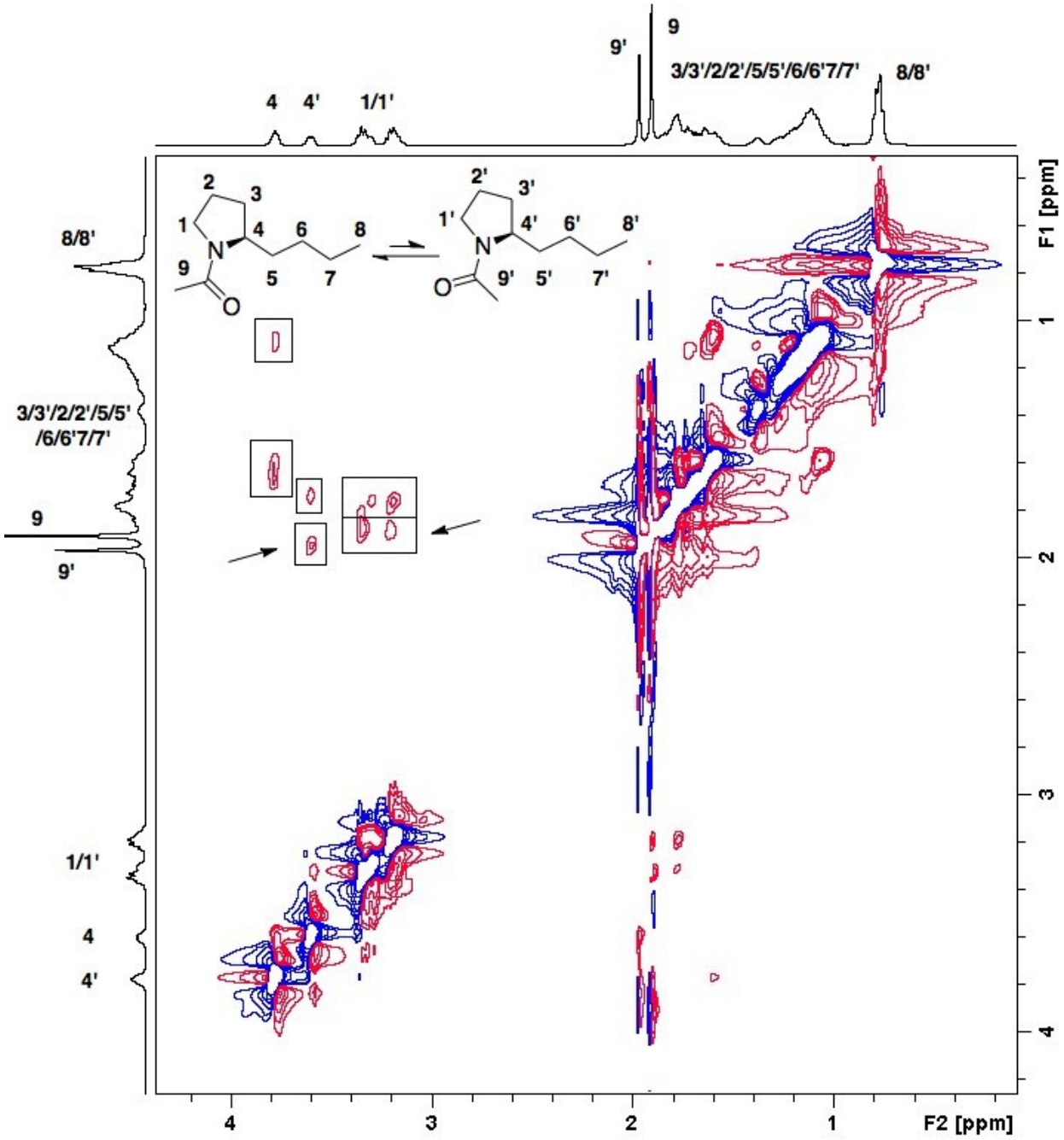
^{1}H NMR Spectrum of 5 (DMSO-d_6, 100 °C)



^{1}H–^{1}H COSY Spectrum of 5

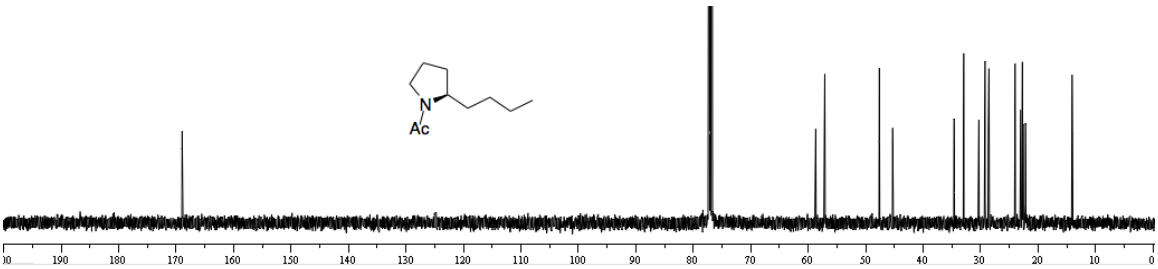


^{1}H–^{1}H NOESY Spectrum of 5 (DCM-d_2, –70 °C)

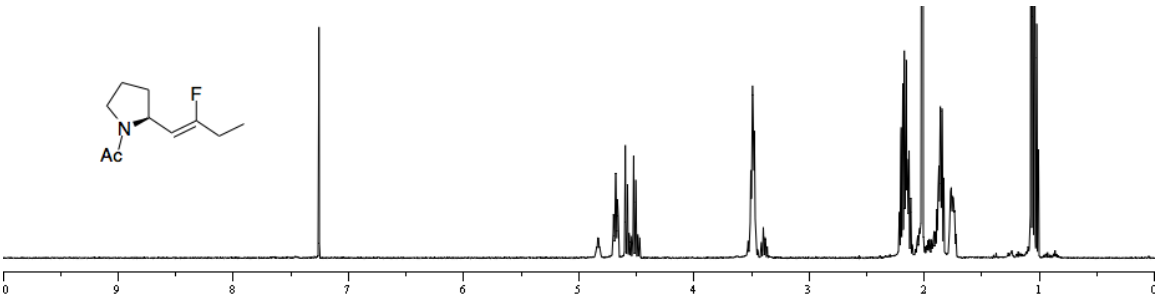


This spectrum is not symmetrized. Legitimate signals are enclosed in rectangles. The signals between **H4'** and **H9'** and between **H1** and **H9** prove that the major conformation is *trans*.

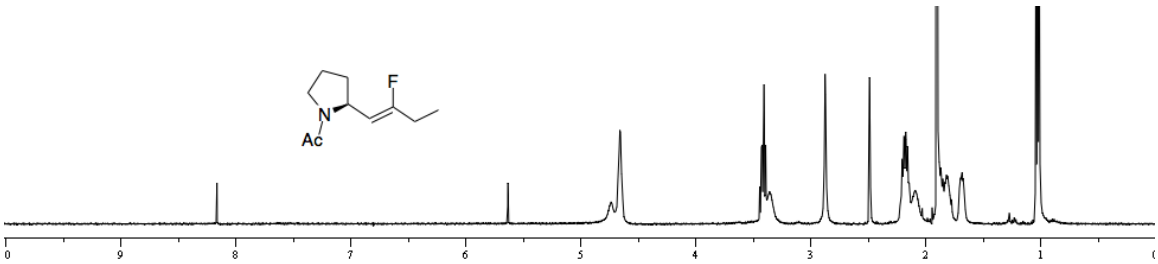
^{13}C NMR Spectrum of 5



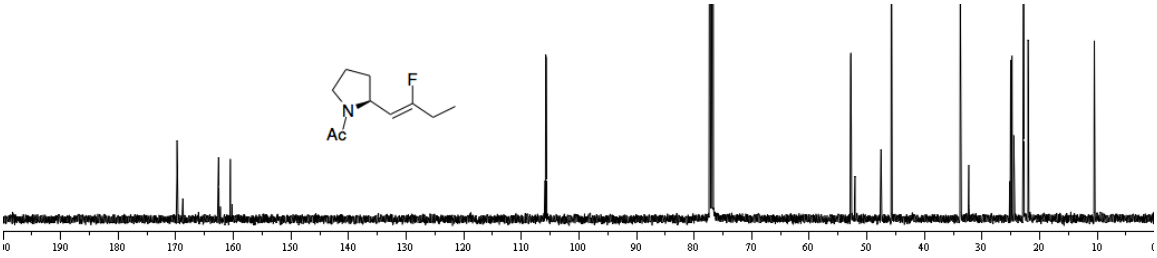
^{1}H NMR Spectrum of 6



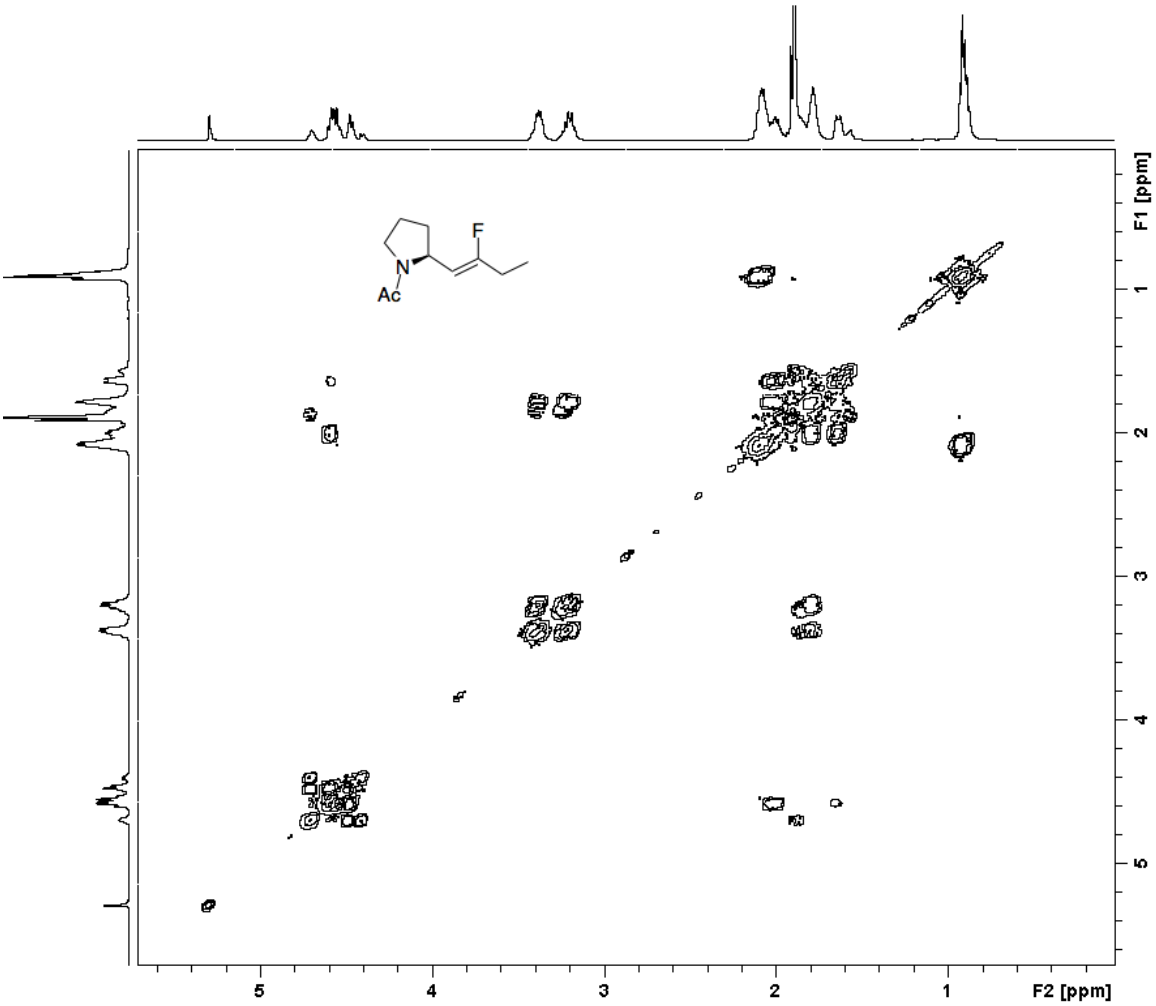
^{1}H NMR Spectrum of 6 (DMSO-d_6, 100 °C)



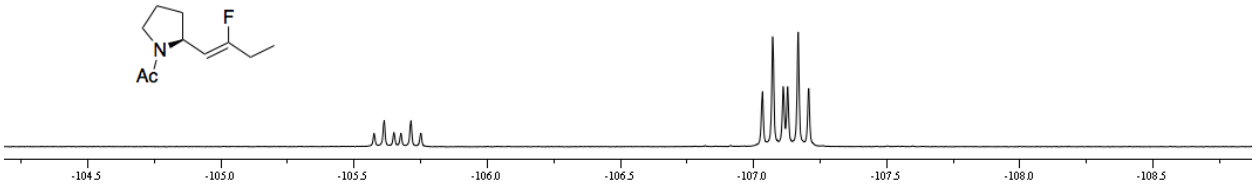
^{13}C NMR Spectrum of 6



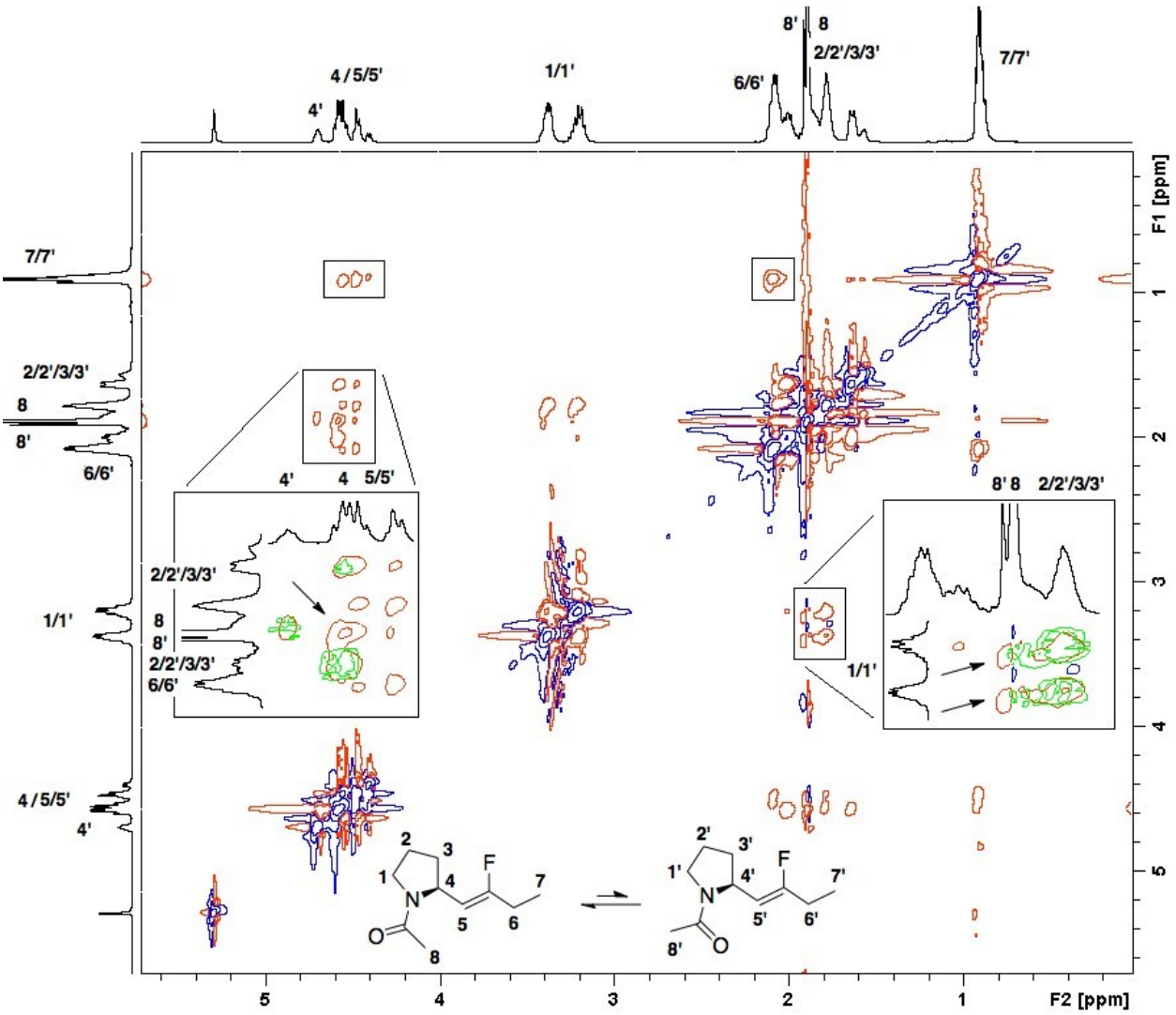
^{1}H–^{1}H COSY Spectrum of 6 (DCM-d_2, –70 °C)



^{19}F NMR Spectrum of 6

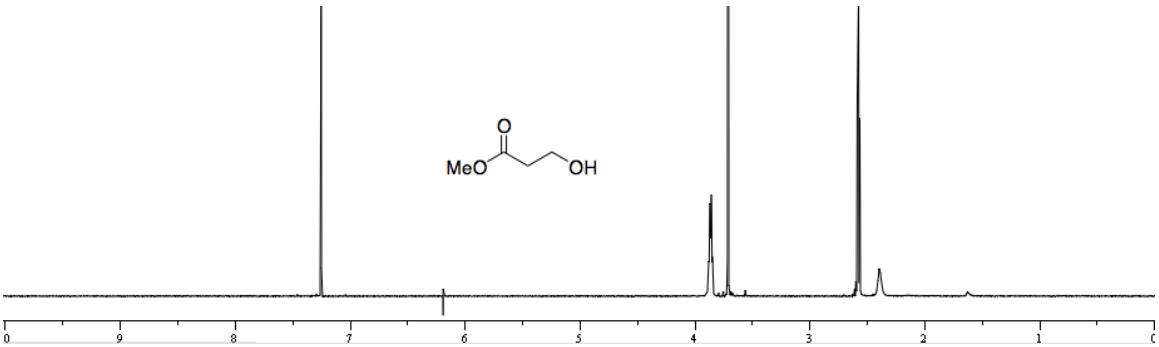


^{1}H–^{1}H NOESY Spectrum of 6 (DCM-d_2, –70 °C)

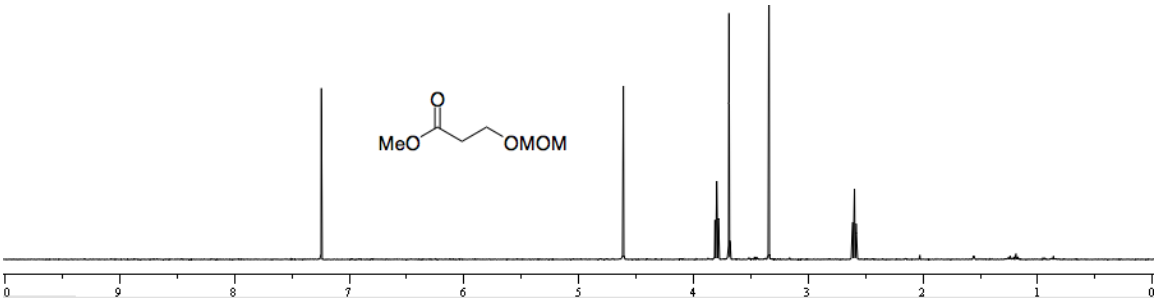


This spectrum is not symmetrized. Legitimate signals are enclosed in rectangles. The two zooms have a ^{1}H–^{1}H COSY signal overlaid in green. These overlays show that in addition to the signals between **H4** and **H3** and between **H1/H1'** and **H2/H2'** (which overlap the COSY signals) there are signals between **H4** and **H8** and between **H1'** and **H8'** (which are not in the COSY spectra and prove that the major conformation is *cis*).

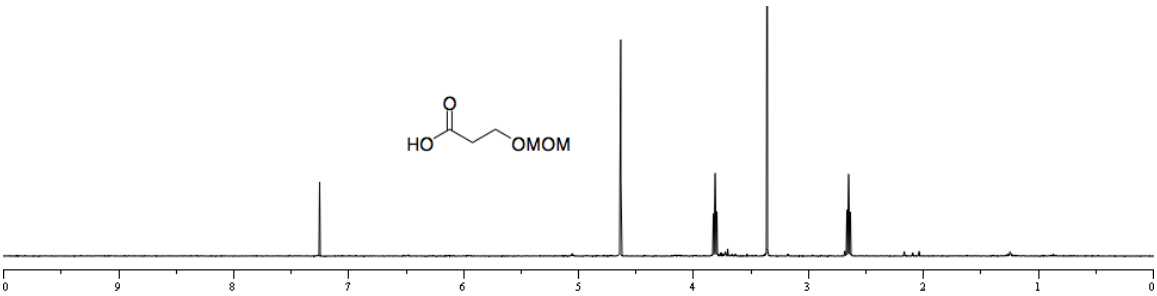
^{1}H NMR Spectrum of 9



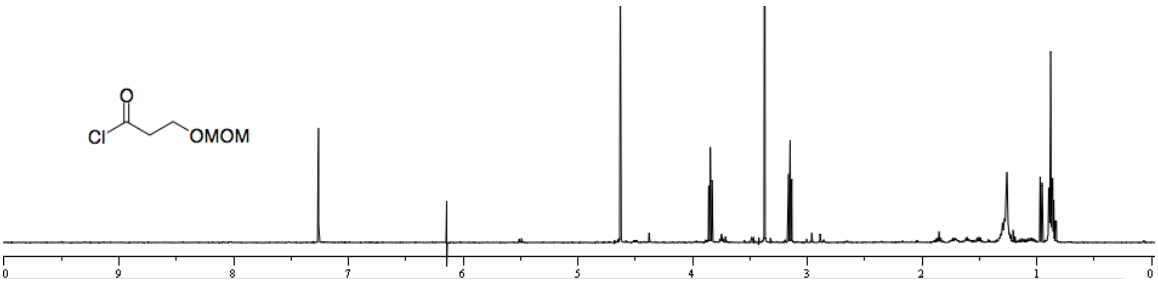
^{1}H NMR Spectrum of 10



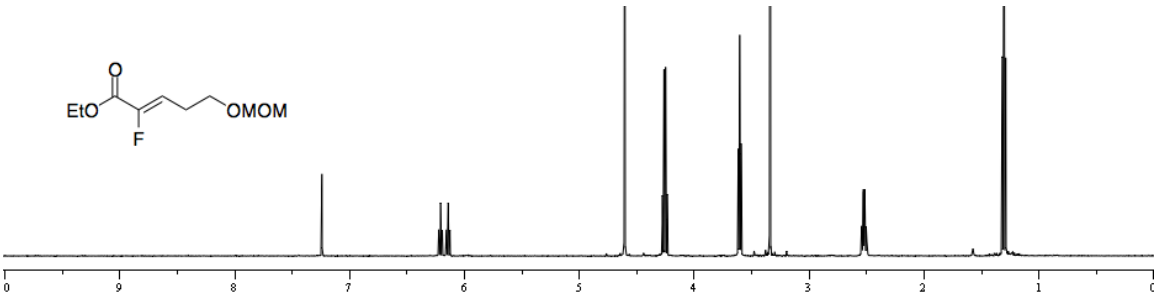
^{1}H NMR Spectrum of 11



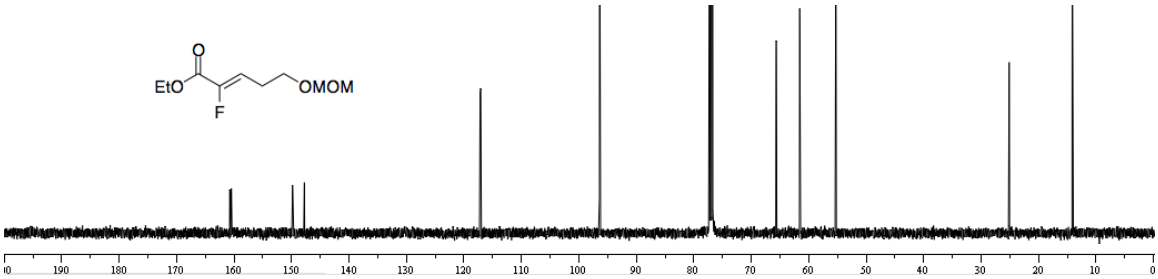
Semi-Pure ^{1}H NMR Spectrum of 12



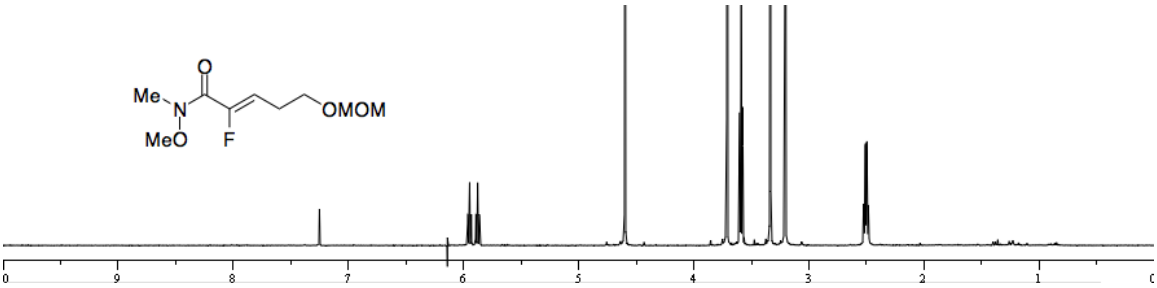
^{1}H NMR Spectrum of 15



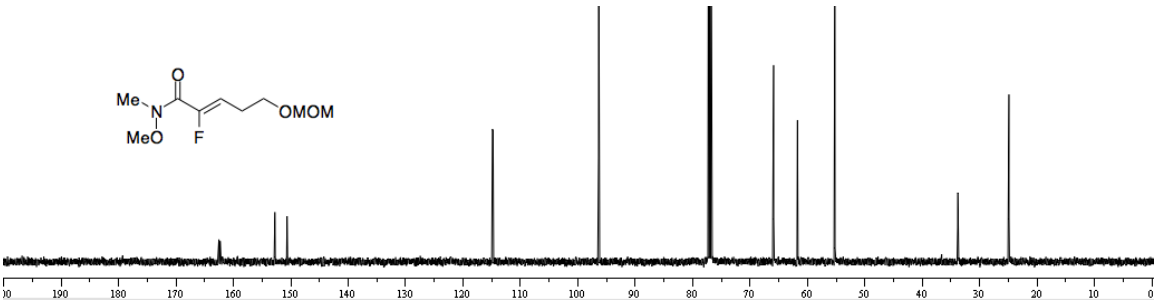
^{13}C NMR Spectrum of 15



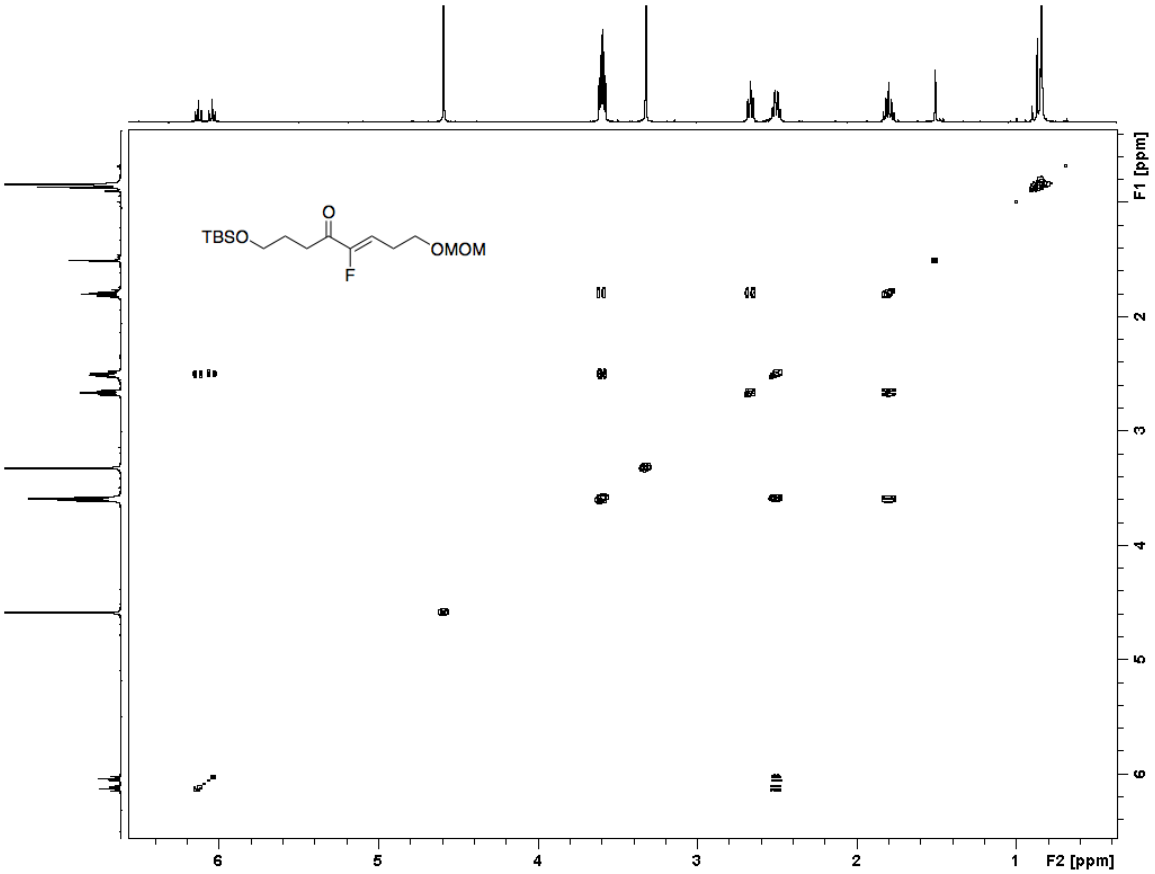
^{1}H NMR Spectrum of 16



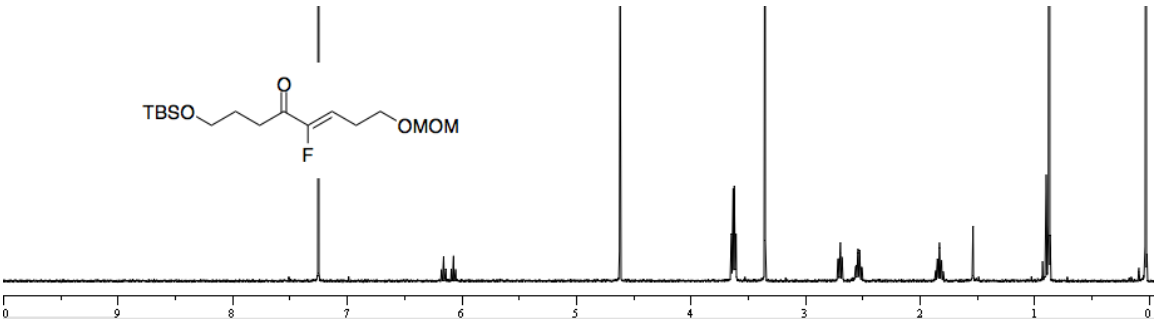
^{13}C NMR Spectrum of 16



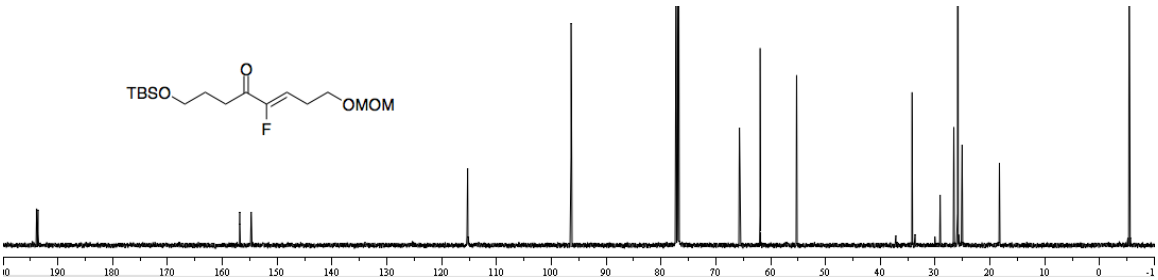
^{1}H–^{1}H COSY Spectrum of 18



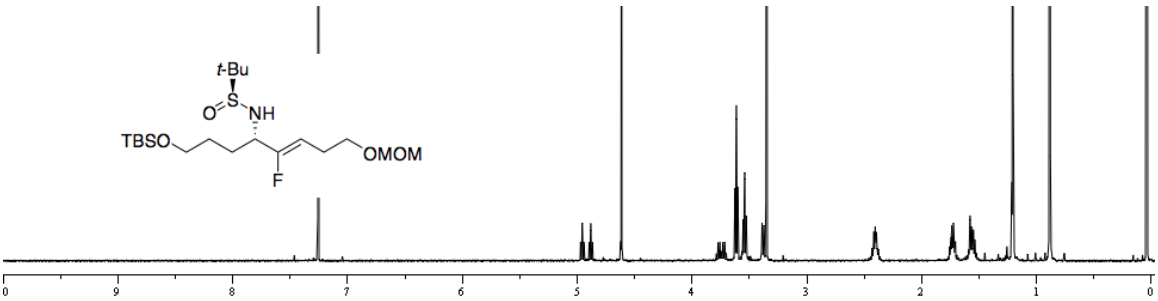
^{1}H NMR Spectrum of 18



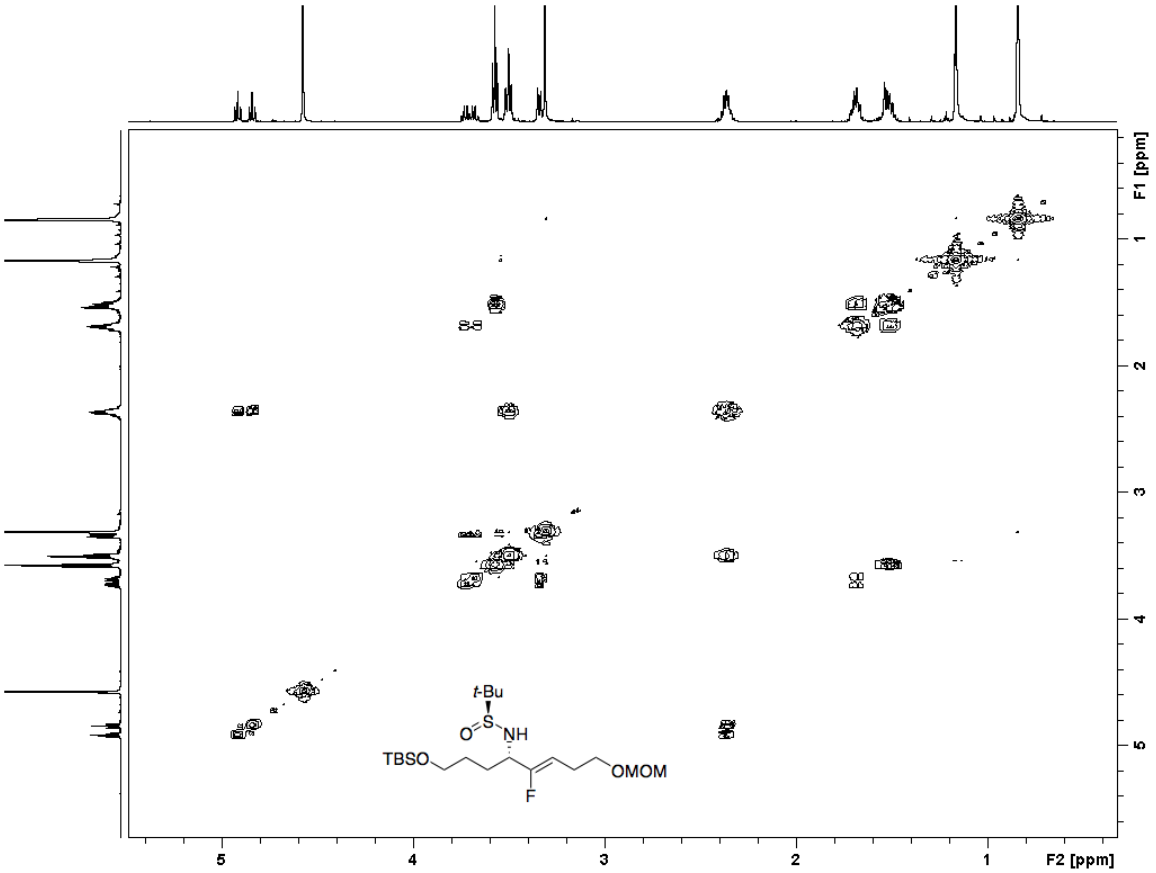
^{13}C NMR Spectrum of 18



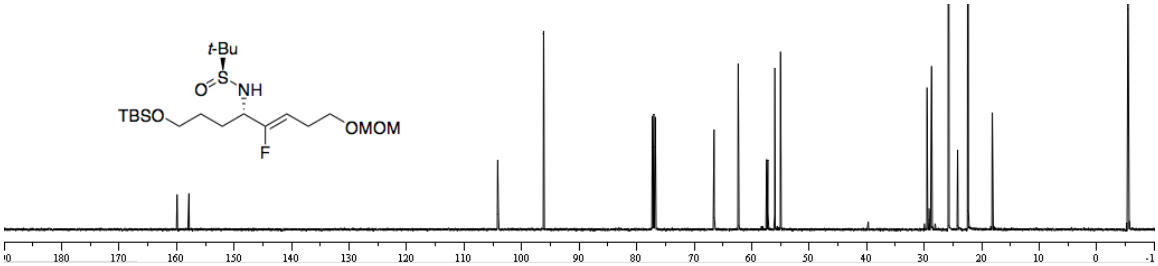
^{1}H NMR Spectrum of 20



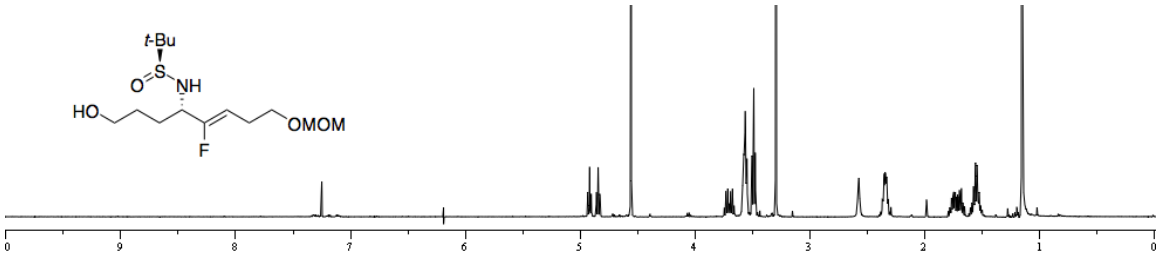
^{1}H–^{1}H COSY Spectrum of 20



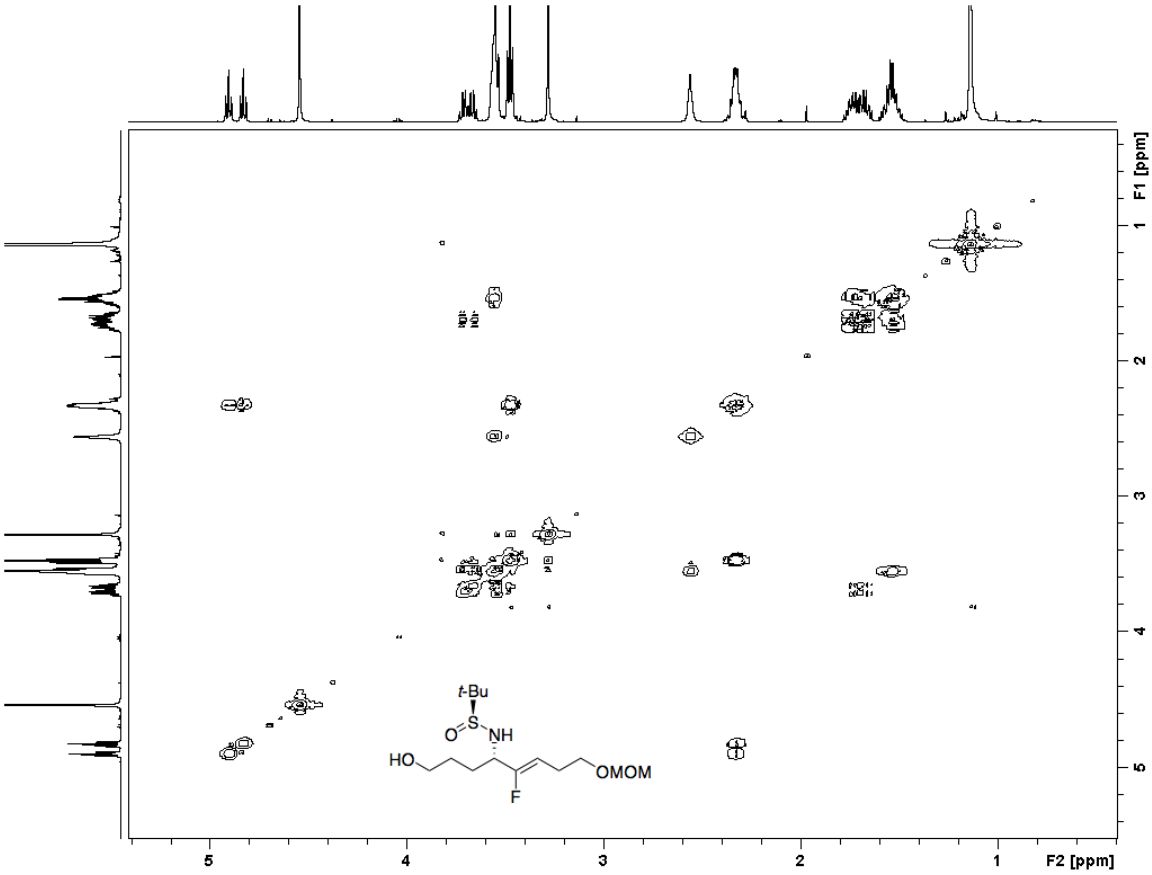
^{13}C NMR Spectrum of 20



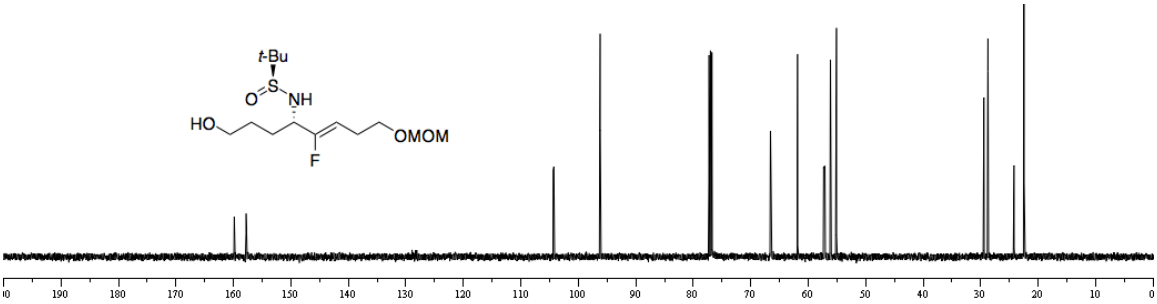
^{1}H NMR Spectrum of 21



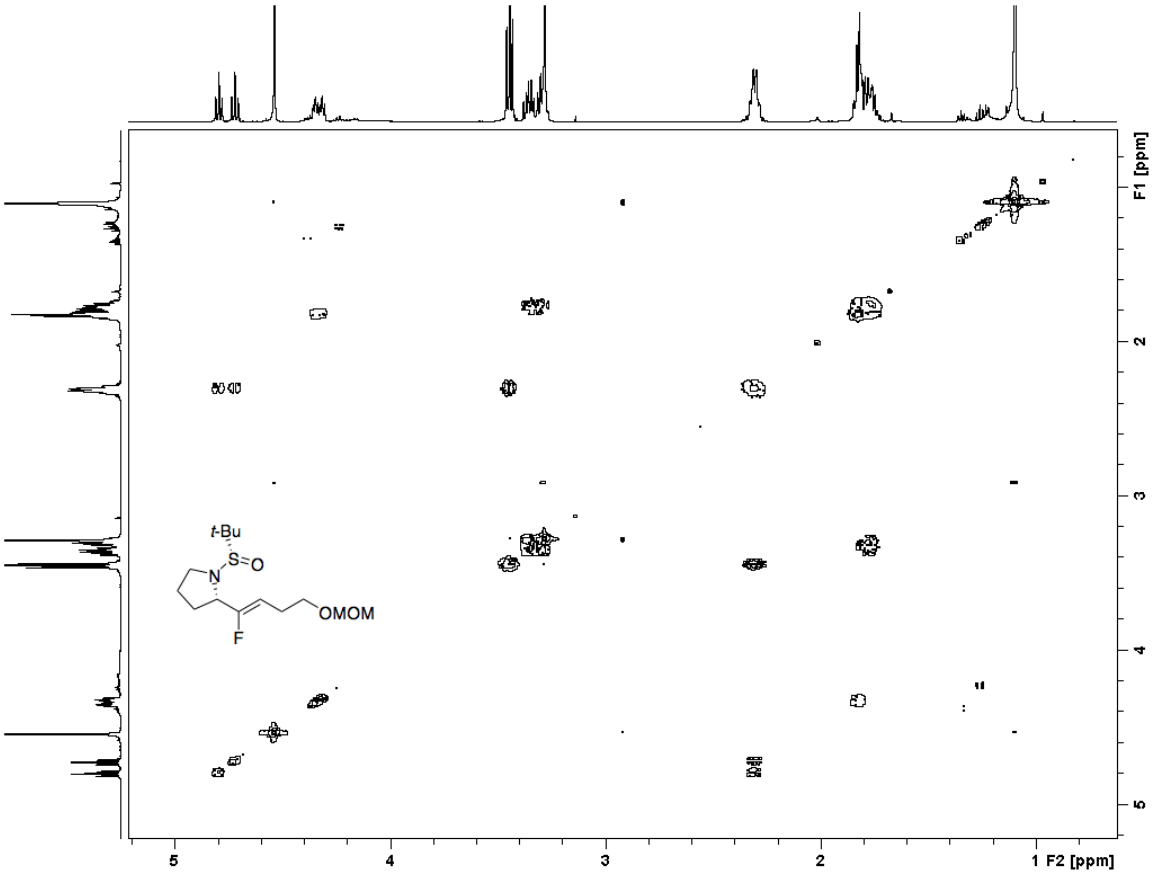
^{1}H–^{1}H COSY Spectrum of 21



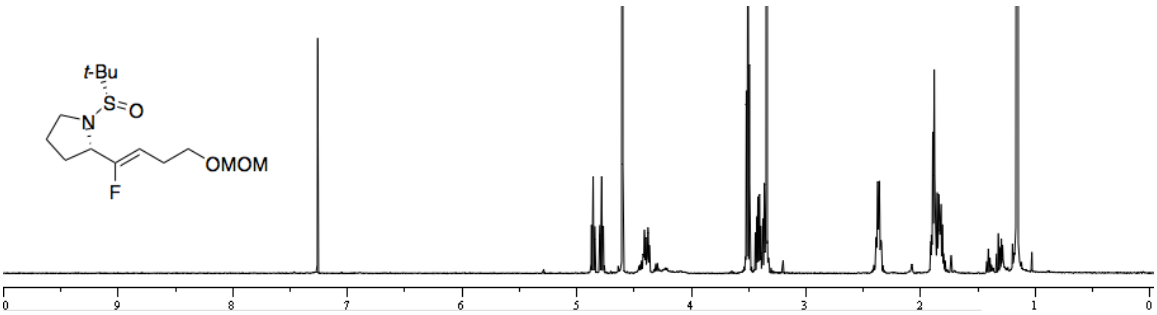
^{13}C NMR Spectrum of 21



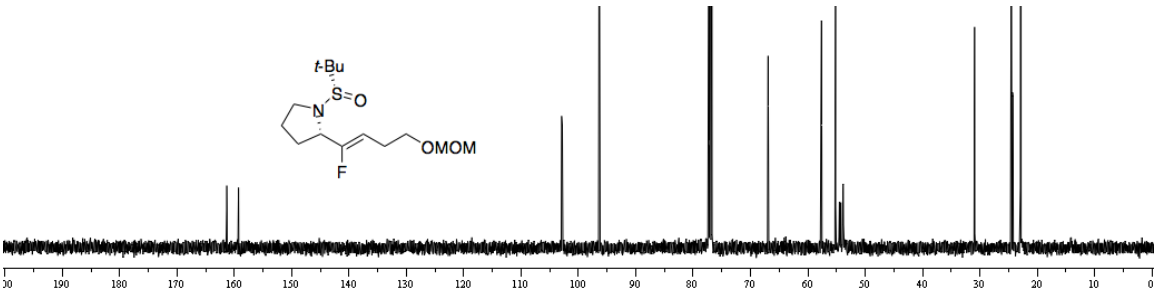
^{1}H–^{1}H COSY Spectrum of 23



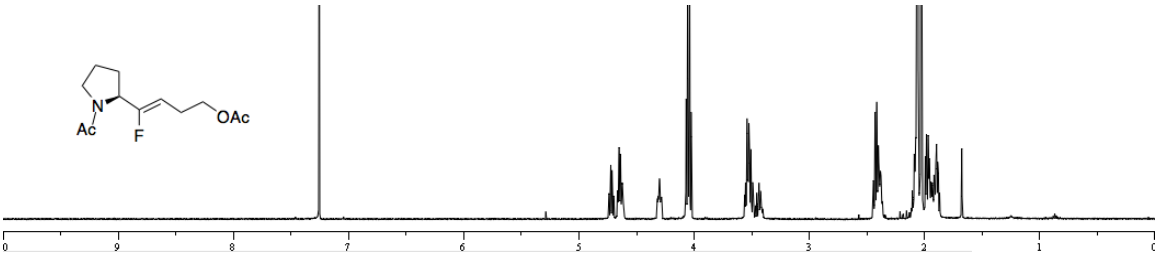
^{1}H NMR Spectrum of 23



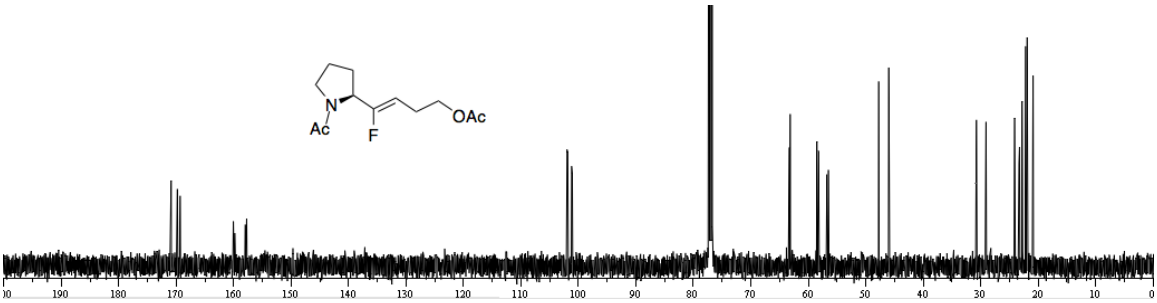
^{13}C NMR Spectrum of 23



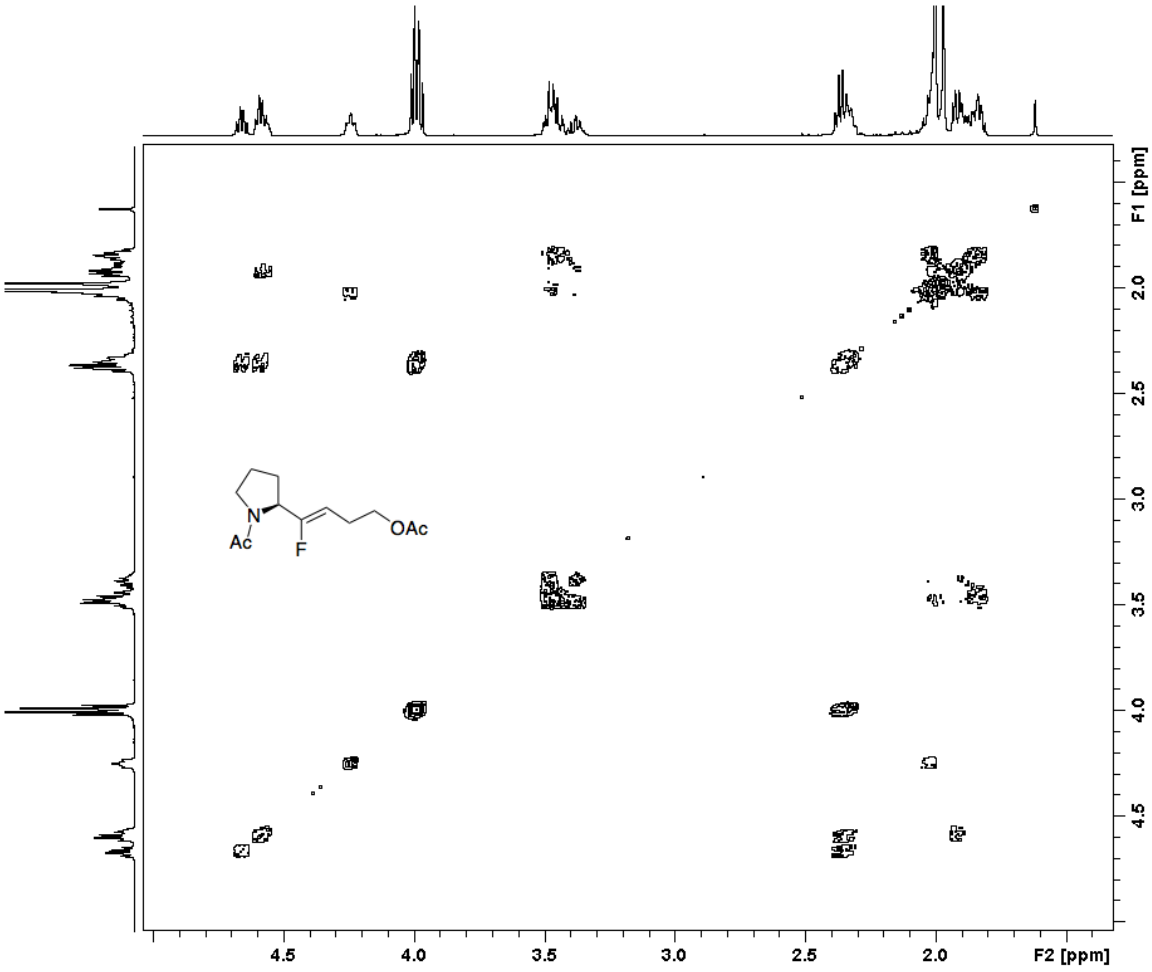
^{1}H NMR Spectrum of 25



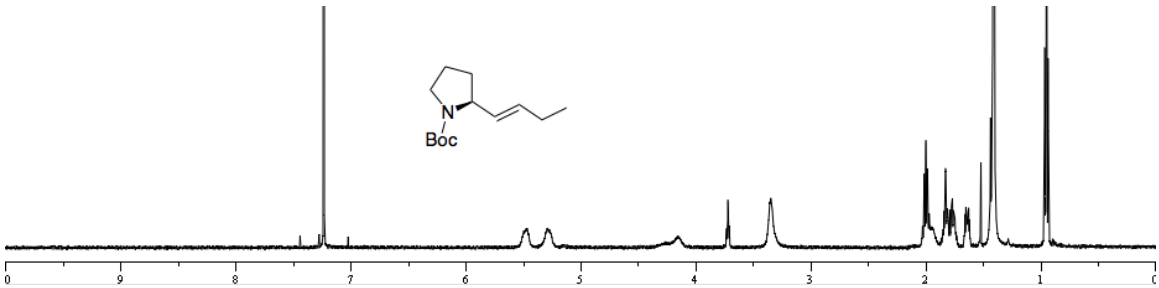
^{13}C NMR Spectrum of 25



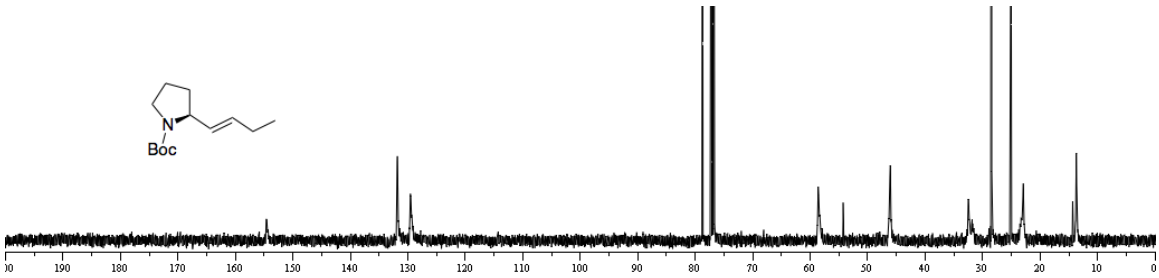
^{1}H–^{1}H COSY Spectrum of 25



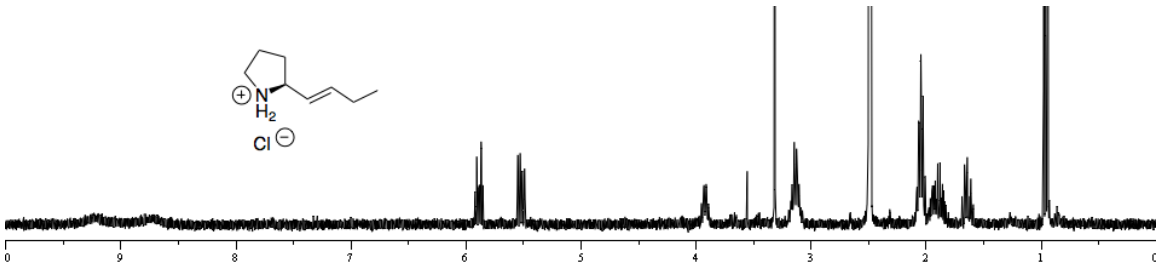
^{1}H NMR Spectrum of 31



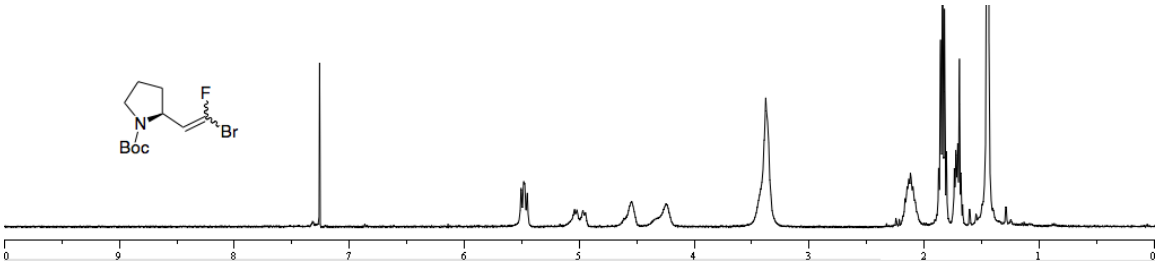
^{13}C NMR Spectrum of 31



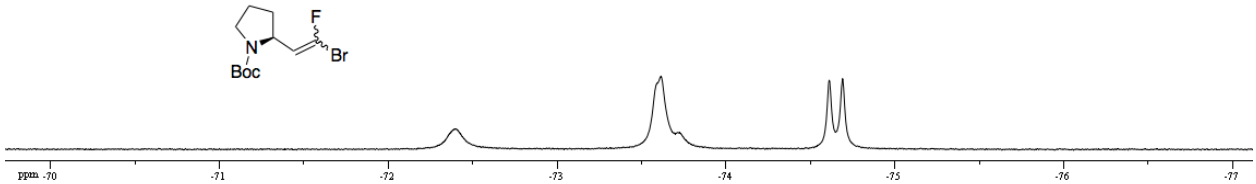
^{1}H NMR Spectrum of 32 (DMSO-d_6)



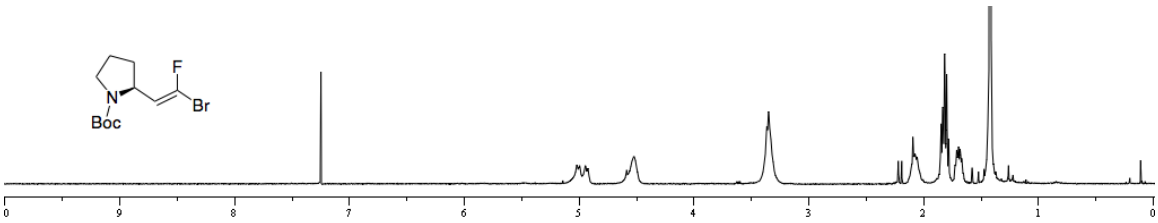
^{1}H NMR Spectrum of 34



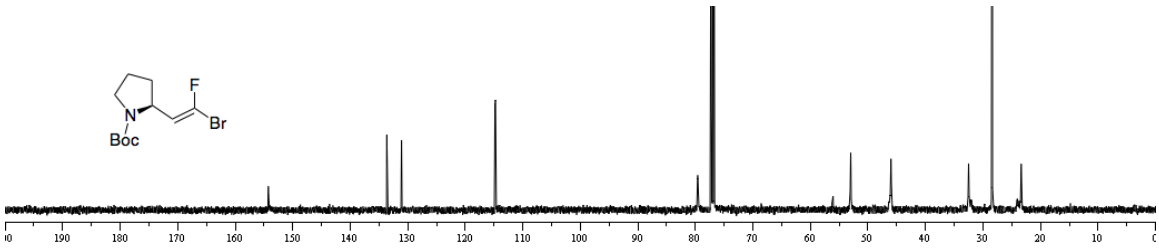
^{19}F NMR Spectrum of 34



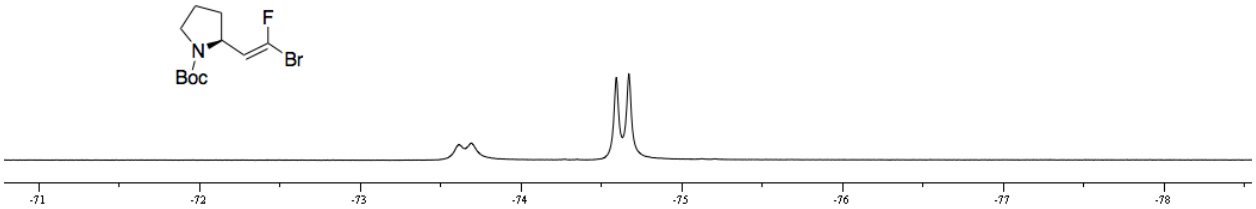
^{1}H NMR Spectrum of 35



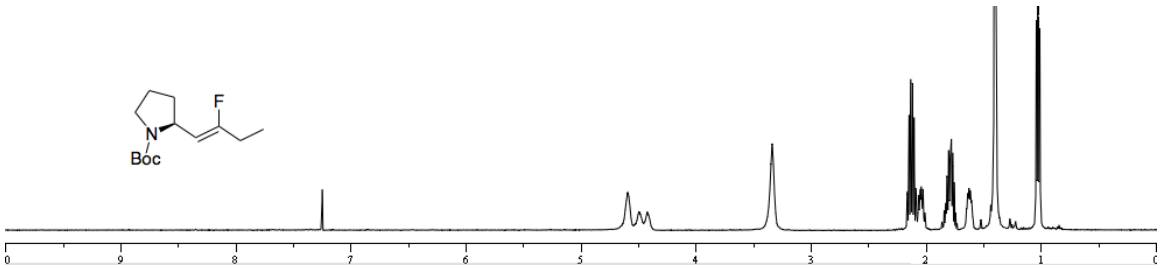
^{13}C NMR Spectrum of 35



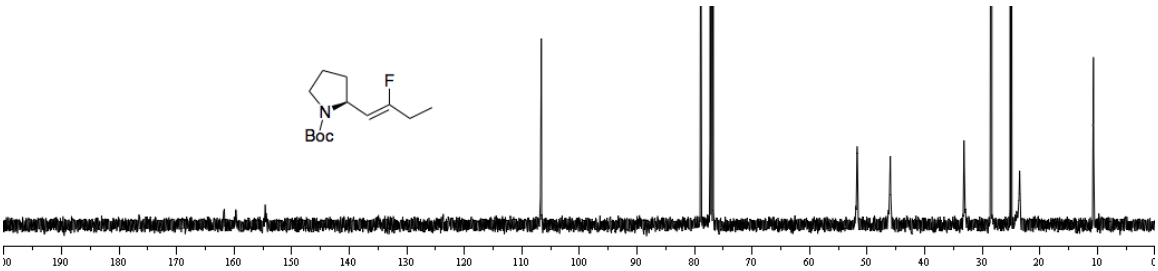
^{19}F NMR Spectrum of 35



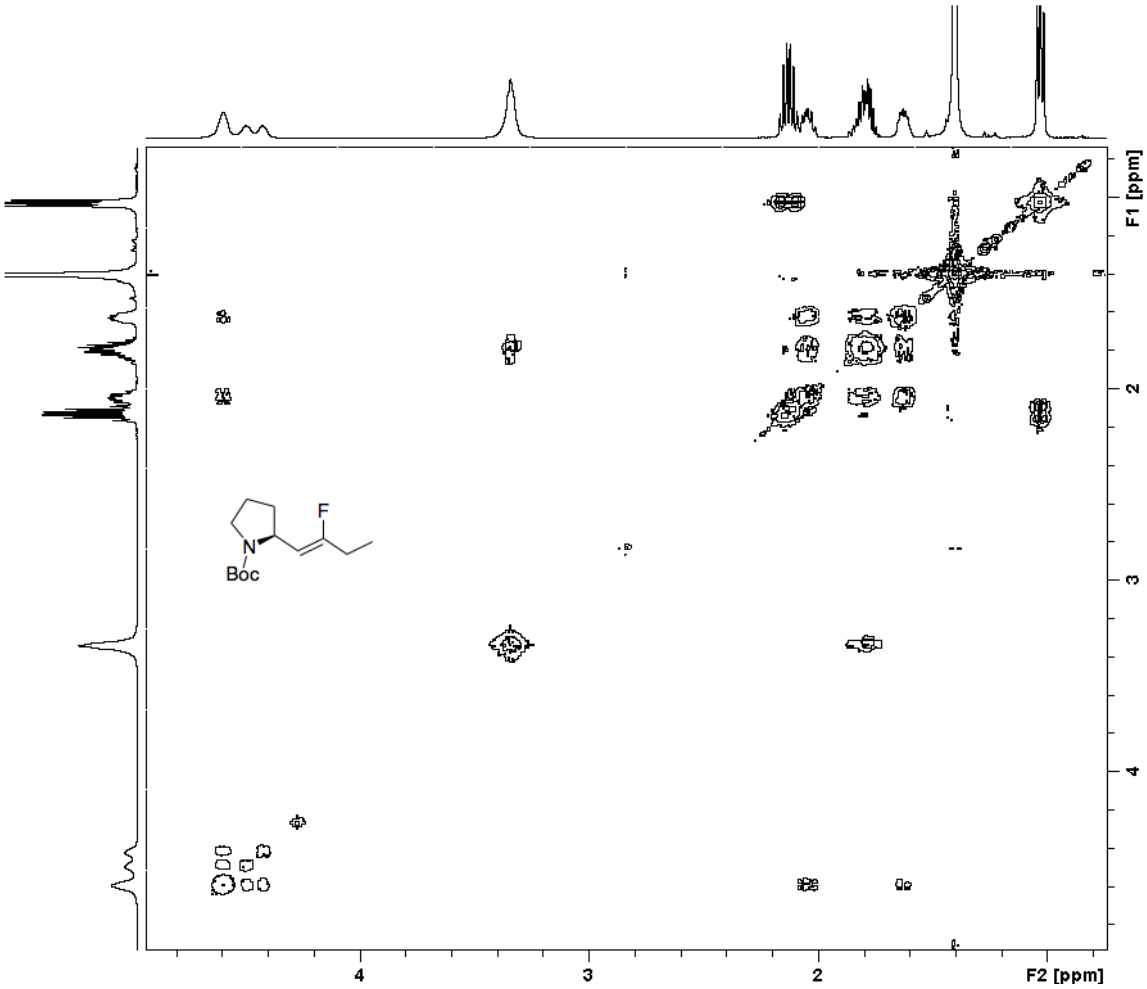
^{1}H NMR Spectrum of 36



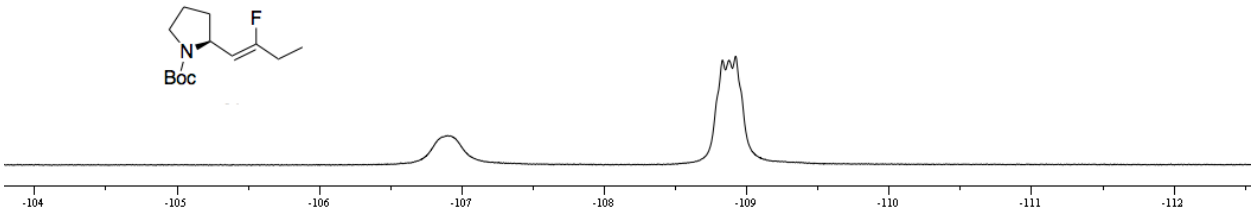
^{13}C NMR Spectrum of 36



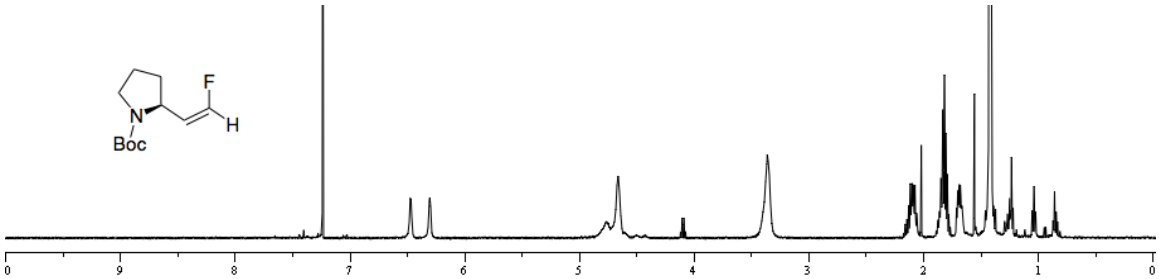
^{1}H–^{1}H COSY Spectrum of 36



^{19}F NMR Spectrum of 36



^{1}H NMR Spectrum of Semi-Pure 37



5. Computational Data

Computational methodology. Hybrid density functional theory as implemented in Gaussian '03[27] was employed to determine the conformational preferences of compounds **1–6**. Gas phase full geometry optimizations and frequency calculations were performed at the B3LYP/6-311+G (2d,p) level of theory[28,29] employing Berny algorithm and a tight SCF convergence criteria. The geometry optimization and frequency calculations were performed on *endo* and *exo* conformers in both *trans* and *cis* geometries of compounds **1–6**. The ester moiety in each of these conformations was either over the pyrrolidine ring (proximal conformations) or not over the pyrrolidine ring (distal conformation). Additionally, the conformations differing in the orientation of the terminal methyl group were designated with different numbers. Frequency calculations of the optimized structures yielded no imaginary frequencies, indicating a true stationary point on the potential energy surface has been attained. The resulting self-consistent field (SCF) energies were corrected by the zero-point vibrational energy (ZPVE) determined in the frequency calculations, and are listed in Table S2. Optimized geometries were analyzed by NBO 5.0 at B3LYP/6-311+G(2d,p). The energy landscapes in Figure 3 were generated by computing the energies of the conformations generated by systematically varying the torsion angles ϕ and ψ (Tables S3 and S4). The energies were computed at the B3LYP/6-311+G(2d,p) level of theory using Gaussian '03.

Table S1. Conformational parameters of compounds **1–6**.

Compound	Conformation	d (Å)	θ (°)	$n\rightarrow\pi^*$ (kcal/mol)	$S(i,j)$ Lp2[a]	$S(i,j)$ Lp1[b]
1c	trans, endo, distal	3.08021	99.514	0.40	0.0589	0.0197
1d	trans, endo, proximal	3.13508	121.526	0.32	0.0462	0.0151
1g	trans, exo, distal	2.88076	99.248	1.33	0.0774	0.0290
1h	trans, exo, proximal	2.92006	115.407	1.12	0.0680	0.0270
2e	trans, endo, distal 1	3.27978	124.885	0.01	0.0641	0.0171

[27] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.
[28] Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648–5652.
[29] Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785–789.

2f	trans, endo, distal 2	3.27592	125.954	0.01	0.0672	0.0186
2g	trans, endo, proximal 1	3.36266	125.494	0.00	0.0509	0.0194
2h	trans, endo, proximal 2	3.36288	125.957	0.00	0.0530	0.0200
2m	trans, exo, distal 1	3.17736	119.550	0.00	0.0726	0.0247
2n	trans, exo, distal 2	3.18378	119.554	0.00	0.0744	0.0256
2o	trans, exo, proximal 1	3.25832	127.585	0.00	0.0205	0.0064
2p	trans, exo, proximal 2	3.25917	126.909	0.00	0.0269	0.0569
3e	trans, endo, distal 1	3.58781	126.305	0.05	0.0838	0.0224
3f	trans, endo, distal 2	3.57744	126.147	0.06	0.0899	0.0248
3g	trans, endo, proximal 1	3.60398	120.400	0.03	0.0730	0.0224
3h	trans, endo, proximal 2	3.60550	121.513	0.02	0.0822	0.0235
3m	trans, exo, distal 1	3.49841	123.071	0.03	0.0912	0.0280
3n	trans, exo, distal 2	3.49708	123.096	0.04	0.0964	0.0300
3o	trans, exo, proximal 1	3.52618	123.422	0.03	0.0860	0.0296
3p	trans, exo, proximal 2	3.52230	122.013	0.05	0.0779	0.0287
4e	trans, endo, distal 1	3.31974	126.353	0.02	0.0638	0.0168
4f	trans, endo, distal 2	3.32087	127.962	0.02	0.0674	0.0181
4g	trans, endo, proximal 1	3.40992	130.270	0.00	0.0476	0.0223
4h	trans, endo, proximal 2	3.40339	129.906	0.00	0.0521	0.0232
4m	trans, exo, distal 1	3.16376	118.859	0.00	0.0767	0.0281
4n	trans, exo, distal 2	3.17008	120.089	0.00	0.0803	0.0299
4o	trans, exo, proximal 1	3.26551	131.451	0.00	0.0117	0.0029
4p	trans, exo, proximal 2	3.26856	131.175	0.00	0.0117	0.0029
6e	trans, endo, distal 1	3.24587	104.143	0.03	0.0694	0.0191
6e′	trans, endo, distal 2	3.24653	108.463	0.01	0.0720	0.0204
6f	trans, endo, distal 3	3.23822	106.557	0.02	0.0687	0.0195
6f′	trans, endo, distal 4	3.24444	103.925	0.03	0.0695	0.0192
6g	trans, endo, proximal 1	3.14369	52.764	0.00	0.0159	0.0000
6g′	trans, endo, proximal 2	3.15168	52.878	0.00	0.0159	0.0000
6h	trans, endo, proximal 3	3.15522	52.858	0.00	0.0197	0.0000
6h′	trans, endo, proximal 4	3.14314	52.766	0.00	0.0202	0.0000
6m	trans, exo, distal 1	3.03204	100.699	0.19	0.0924	0.0362
6m′	trans, exo, distal 2	3.02337	96.617	0.27	0.0891	0.0337
6n	trans, exo, distal 3	3.02403	96.815	0.27	0.0891	0.0337
6n′	trans, exo, distal 4	3.03062	100.014	0.21	0.0877	0.0339
6o	trans, exo, proximal 1	3.00383	86.673	0.53	0.0791	0.0230
6o′	trans, exo, proximal 2	3.00535	85.698	0.53	0.0808	0.0223
6p	trans, exo, proximal 3	3.00534	85.715	0.53	0.0808	0.0223
6p′	trans, exo, proximal 4	3.00771	85.597	0.52	0.0817	0.0238

[a]$S(i, j)$ Lp2 is a measure of the magnitude of the Pauli repulsion between the *p*-type oxygen lone pair and the π-orbital.
[b]$S(i, j)$ Lp1 is a measure of the magnitude of the Pauli repulsion between the *s*-type oxygen lone pair and the π-orbital.

Table S2. Energies of various conformations of compounds **1**–**6**.

Compound	Conformation	Energy	ZPE Correction	Energy (Corrected)
1a	cis, endo, distal	-593.3135009	0.209105	-593.1043959
1b	cis, endo, proximal	-593.3129724	0.209100	-593.1038724
1c	trans, endo, distal	-593.3155741	0.209177	-593.1063971
1d	trans, endo, proximal	-593.3139762	0.209085	-593.1048912
1e	cis, exo, distal	-593.3126368	0.209127	-593.1035098
1f	cis, exo, proximal	-593.3122207	0.209065	-593.1031557
1g	trans, exo, distal	-593.3149713	0.209233	-593.1057383
1h	trans, exo, proximal	-593.3136820	0.209242	-593.1044400
2a	cis, endo, distal 1	-620.7114748	0.248307	-620.4631678
2b	cis, endo, distal 2	-620.7114191	0.248174	-620.4632451
2c	cis, endo, proximal 1	-620.7128325	0.248243	-620.4645895
2d	cis, endo, proximal 2	-620.7128635	0.248277	-620.4645865
2e	trans, endo, distal 1	-620.7125579	0.248098	-620.4644599
2f	trans, endo, distal 2	-620.7125547	0.248153	-620.4644017
2g	trans, endo, proximal 1	-620.7118019	0.247995	-620.4638069
2h	trans, endo, proximal 2	-620.7117274	0.247914	-620.4638134
2i	cis, exo, distal 1	-620.7109373	0.248207	-620.4627303
2j	cis, exo, distal 2	-620.7110105	0.248212	-620.4627985
2k	cis, exo, proximal 1	-620.7105230	0.248226	-620.4622970
2l	cis, exo, proximal 2	-620.7104616	0.248154	-620.4623076
2m	trans, exo, distal 1	-620.7119522	0.248258	-620.4636942
2n	trans, exo, distal 2	-620.7119027	0.248182	-620.4637207
2o	trans, exo, proximal 1	-620.7096387	0.248054	-620.4615847
2p	trans, exo, proximal 2	-620.7096541	0.248049	-620.4616051
3a	cis, endo, distal 1	-943.6666647	0.246352	-943.4203127
3b	cis, endo, distal 2	-943.6666373	0.246244	-943.4203933
3c	cis, endo, proximal 1	-943.6681217	0.246319	-943.4218027
3d	cis, endo, proximal 2	-943.6682042	0.246370	-943.4218342
3e	trans, endo, distal 1	-943.6670368	0.246283	-943.4207538
3f	trans, endo, distal 2	-943.6670677	0.246196	-943.4208717
3g	trans, endo, proximal 1	-943.6661316	0.246027	-943.4201046
3h	trans, endo, proximal 2	-943.6661103	0.246023	-943.4200873

3i	cis, exo, distal 1	-943.6653321	0.246165	-943.4191671
3j	cis, exo, distal 2	-943.6654116	0.246157	-943.4192546
3k	cis, exo, proximal 1	-943.6647672	0.246229	-943.4185382
3l	cis, exo, proximal 2	-943.6648203	0.246190	-943.4186303
3m	trans, exo, distal 1	-943.6658896	0.246293	-943.4195966
3n	trans, exo, distal 2	-943.6659553	0.246305	-943.4196503
3o	trans, exo, proximal 1	-943.6632968	0.246184	-943.4171128
3p	trans, exo, proximal 2	-943.6632695	0.246081	-943.4171885
4a	cis, endo, distal 1	-521.4387752	0.255663	-521.1831122
4b	cis, endo, distal 2	-521.4388032	0.255800	-521.1830032
4c	cis, endo, proximal 1	-521.4388680	0.255839	-521.1830290
4d	cis, endo, proximal 2	-521.4388571	0.255770	-521.1830871
4e	trans, endo, distal 1	-521.4381156	0.255435	-521.1826806
4f	trans, endo, distal 2	-521.4381445	0.255580	-521.1825645
4g	trans, endo, proximal 1	-521.4376834	0.255523	-521.1821604
4h	trans, endo, proximal 2	-521.4376802	0.255709	-521.1819712
4i	cis, exo, distal 1	-521.4383452	0.255505	-521.1828402
4j	cis, exo, distal 2	-521.4384560	0.255539	-521.1829170
4k	cis, exo, proximal 1	-521.4365479	0.255891	-521.1806569
4l	cis, exo, proximal 2	-521.4365240	0.255924	-521.1806000
4m	trans, exo, distal 1	-521.4374863	0.255578	-521.1819083
4n	trans, exo, distal 2	-521.4374432	0.255512	-521.1819312
4o	trans, exo, proximal 1	-521.4355874	0.255960	-521.1796274
4p	trans, exo, proximal 2	-521.4355716	0.255780	-521.1797916
5a	cis, endo	-522.6686972	0.279356	-522.3893412
5b	trans, endo	-522.6703561	0.279652	-522.3907041
5c	cis , exo	-522.6676816	0.279563	-522.3881186
5d	trans, exo	-522.6697910	0.279485	-522.3903060
6a	cis, endo, distal 1	-620.7135089	0.247914	-620.4655949
6a′	cis, endo, distal 2	-620.7138192	0.248045	-620.4657742
6b	cis, endo, distal 3	-620.7137853	0.248061	-620.4657243
6b′	cis, endo, distal 4	-620.7135089	0.247913	-620.4655959
6c	cis, endo, proximal 1	-620.7092542	0.248391	-620.4608632
6c′	cis, endo, proximal 2	-620.7096440	0.248271	-620.4613730
6d	cis, endo, proximal 3	-620.7096530	0.248273	-620.4613800
6d′	cis, endo, proximal 4	-620.7092543	0.248390	-620.4608643
6e	trans, endo, distal 1	-620.7118220	0.247927	-620.4638950
6e′	trans, endo, distal 2	-620.7121156	0.247935	-620.4641806
6f	trans, endo, distal 3	-620.7122082	0.247917	-620.4642912
6f′	trans, endo, distal 4	-620.7118202	0.247922	-620.4638982

6g	trans, endo, proximal 1	-620.7107247	0.248446	-620.4622787
6g′	trans, endo, proximal 2	-620.7110677	0.248424	-620.4626437
6h	trans, endo, proximal 3	-620.7111175	0.248400	-620.4627175
6h′	trans, endo, proximal 4	-620.7107245	0.248448	-620.4622765
6i	cis, exo, distal 1	-620.7134544	0.248052	-620.4654024
6i'	cis, exo, distal 2	-620.7130929	0.248137	-620.4649559
6j	cis, exo, distal 3	-620.7130929	0.248137	-620.4649559
6j′	cis, exo, distal 4	-620.7133176	0.248126	-620.4651916
6k	cis, exo, proximal 1	-620.7088655	0.248280	-620.4605855
6k′	cis, exo, proximal 2	-620.7084729	0.248276	-620.4601969
6l	cis, exo, proximal 3	-620.7084735	0.248271	-620.4602025
6l′	cis, exo, proximal 4	-620.7088252	0.248056	-620.4607692
6m	trans, exo, distal 1	-620.7119914	0.247962	-620.4640294
6m′	trans, exo, distal 2	-620.7116902	0.247962	-620.4637282
6n	trans, exo, distal 3	-620.7116907	0.247959	-620.4637317
6n′	trans, exo, distal 4	-620.7120858	0.247970	-620.4641158
6o	trans, exo, proximal 1	-620.7110013	0.248411	-620.4625903
6o′	trans, exo, proximal 2	-620.7106295	0.248267	-620.4623625
6p	trans, exo, proximal 3	-620.7106296	0.248267	-620.4623626
6p′	trans, exo, proximal 4	-620.7108939	0.248387	-620.4625069

Table S3. Data used to generate Figure 3A.

ϕ (°)	ψ (°)	d (Å)	θ (°)	Energy (au)	Relative Energy (au)	Relative Energy (kcal/mol)
-67	110	3.00931	130.373	-593.3101736	0.0054005	3.389
-67	115	3.00931	126.313	-593.3112981	0.0042760	2.683
-67	120	3.00931	122.276	-593.3123011	0.0032730	2.054
-67	125	3.00931	118.269	-593.3131798	0.0023943	1.502
-67	130	3.00931	114.299	-593.3139222	0.0016519	1.037
-67	135	3.00931	110.374	-593.3145144	0.0010597	0.665
-67	140	3.00931	106.500	-593.3149527	0.0006214	0.390
-67	145	3.00931	102.686	-593.3152420	0.0003321	0.208
-67	150	3.00931	98.941	-593.3153686	0.0002055	0.129
-67	155	3.00931	95.274	-593.3153062	0.0002679	0.168
-67	160	3.00931	91.696	-593.3150557	0.0005184	0.325
-67	165	3.00931	88.220	-593.3146278	0.0009463	0.594
-67	170	3.00931	84.859	-593.3140247	0.0015494	0.972
-67	175	3.00931	81.628	-593.3132280	0.0023461	1.472
-67	180	3.00931	78.546	-593.3122443	0.0033298	2.089
-72	110	3.09538	133.154	-593.3106235	0.0049506	3.107
-72	115	3.09538	129.115	-593.3115785	0.0039956	2.507
-72	120	3.09538	125.104	-593.3124639	0.0031102	1.952

-72	125	3.09538	121.128	-593.3132716	0.0023025	1.445
-72	130	3.09538	117.192	-593.3139867	0.0015874	0.996
-72	135	3.09538	113.303	-593.3145788	0.0009953	0.625
-72	140	3.09538	109.467	-593.3150308	0.0005433	0.341
-72	145	3.09538	105.693	-593.3153468	0.0002273	0.143
-72	150	3.09538	101.988	-593.3155280	0.0000461	0.029
-72	155	3.09538	98.362	-593.3155457	0.0000284	0.018
-72	160	3.09538	94.825	-593.3153900	0.0001841	0.116
-72	165	3.09538	91.389	-593.3150660	0.0005081	0.319
-72	170	3.09538	88.065	-593.3145868	0.0009873	0.620
-72	175	3.09538	84.869	-593.3139336	0.0016405	1.029
-72	180	3.09538	81.816	-593.3130980	0.0024761	1.554
-72	-175	3.09538	78.924	-593.3120948	0.0034793	2.183
-77	110	3.18142	135.659	-593.3103683	0.0052058	3.267
-77	115	3.18142	131.654	-593.3111775	0.0043966	2.759
-77	120	3.18142	127.681	-593.3119592	0.0036149	2.268
-77	125	3.18142	123.746	-593.3127027	0.0028714	1.802
-77	130	3.18142	119.855	-593.3133922	0.0021819	1.369
-77	135	3.18142	116.011	-593.3139882	0.0015859	0.995
-77	140	3.18142	112.224	-593.3144616	0.0011125	0.698
-77	145	3.18142	108.498	-593.3148114	0.0007627	0.479
-77	150	3.18142	104.843	-593.3150431	0.0005310	0.333
-77	155	3.18142	101.267	-593.3151323	0.0004418	0.277
-77	160	3.18142	97.780	-593.3150548	0.0005193	0.326
-77	165	3.18142	94.392	-593.3148080	0.0007661	0.481
-77	170	3.18142	91.115	-593.3143985	0.0011756	0.738
-77	175	3.18142	87.964	-593.3138313	0.0017428	1.094
-77	180	3.18142	84.951	-593.3130877	0.0024864	1.560
-77	-175	3.18142	82.094	-593.3121758	0.0033983	2.132
-77	-170	3.18142	79.410	-593.3110976	0.0044765	2.809
-82	110	3.26681	137.870	-593.3092799	0.0062942	3.950
-82	115	3.26681	133.916	-593.3099887	0.0055854	3.505
-82	120	3.26681	129.996	-593.3107132	0.0048609	3.050
-82	125	3.26681	126.116	-593.3114375	0.0041366	2.596
-82	130	3.26681	122.280	-593.3121367	0.0034374	2.157
-82	135	3.26682	118.494	-593.3127708	0.0028033	1.759
-82	140	3.26681	114.765	-593.3133012	0.0022729	1.426
-82	145	3.26681	111.099	-593.3137081	0.0018660	1.171
-82	150	3.26681	107.504	-593.3139897	0.0015844	0.994
-82	155	3.26681	103.987	-593.3141312	0.0014429	0.905
-82	160	3.26681	100.559	-593.3141070	0.0014671	0.921
-82	165	3.26682	97.229	-593.3139132	0.0016609	1.042
-82	170	3.26681	94.009	-593.3135508	0.0020233	1.270

-82	175	3.26682	90.911	-593.3130216	0.0025525	1.602
-82	180	3.26681	87.948	-593.3123140	0.0032601	2.046
-82	-175	3.26682	85.137	-593.3114208	0.0041533	2.606
-82	-170	3.26681	82.491	-593.3103429	0.0052312	3.283
-82	-165	3.26681	80.030	-593.3090775	0.0064966	4.077
-87	110	3.35098	139.770	-593.3073212	0.0082529	5.179
-87	115	3.35098	135.885	-593.3079900	0.0075841	4.759
-87	120	3.35098	132.036	-593.3087072	0.0068669	4.309
-87	125	3.35098	128.226	-593.3094572	0.0061169	3.838
-87	130	3.35098	124.461	-593.3102049	0.0053692	3.369
-87	135	3.35098	120.746	-593.3109062	0.0046679	2.929
-87	140	3.35098	117.088	-593.3115171	0.0040570	2.546
-87	145	3.35098	113.492	-593.3120004	0.0035738	2.243
-87	150	3.35098	109.968	-593.3123367	0.0032374	2.031
-87	155	3.35098	106.521	-593.3125203	0.0030538	1.916
-87	160	3.35098	103.162	-593.3125369	0.0030372	1.906
-87	165	3.35098	99.900	-593.3123784	0.0031957	2.005
-87	170	3.35098	96.745	-593.3120431	0.0035310	2.216
-87	175	3.35098	93.710	-593.3115201	0.0040540	2.544
-87	180	3.35098	90.808	-593.3107963	0.0047778	2.998
-87	-175	3.35098	88.051	-593.3098580	0.0057161	3.587
-87	-170	3.35098	85.456	-593.3087096	0.0068645	4.308
-87	-165	3.35098	83.037	-593.3073469	0.0082272	5.163
-87	-160	3.35098	80.811	-593.3057766	0.0097975	6.148
-87	-155	3.35098	78.795	-593.3040203	0.0115538	7.250

Table S4. Data used to generate Figure 3B.

ϕ (°)	ψ (°)	d (Å)	θ (°)	Energy (au)	Relative Energy (au)	Relative Energy (kcal/mol)
-67	101	3.01806	132.419	-620.7076410	0.0049169	3.085
-67	104	3.01806	129.721	-620.7079422	0.0046157	2.896
-67	107	3.01806	127.029	-620.7081818	0.0043761	2.746
-67	110	3.01806	124.345	-620.7083620	0.0041959	2.633
-67	113	3.01806	121.670	-620.7084961	0.0040618	2.549
-67	116	3.01806	119.003	-620.7085961	0.0039618	2.486
-67	119	3.01806	116.346	-620.7086569	0.0039010	2.448
-67	122	3.01806	113.700	-620.7086694	0.0038885	2.440
-67	125	3.01806	111.065	-620.7086297	0.0039282	2.465
-67	128	3.01806	108.443	-620.7085357	0.0040222	2.524
-67	131	3.01806	105.834	-620.7083869	0.0041710	2.617
-67	134	3.01806	103.239	-620.7081879	0.0043700	2.742
-67	137	3.01806	100.661	-620.7079426	0.0046153	2.896

-67	140	3.01806	98.100	-620.7076500	0.0049079	3.080
-67	143	3.01806	95.557	-620.7073146	0.0052433	3.290
-67	146	3.01806	93.035	-620.7069460	0.0056119	3.522
-67	149	3.01806	90.536	-620.7065532	0.0060047	3.768
-67	152	3.01806	88.060	-620.7061372	0.0064207	4.029
-67	155	3.01806	85.611	-620.7056909	0.0068670	4.309
-67	158	3.01806	83.191	-620.7052162	0.0073417	4.607
-67	161	3.01806	80.803	-620.7047234	0.0078345	4.916
-67	164	3.01806	78.449	-620.7042165	0.0083414	5.234
-67	167	3.01806	76.133	-620.7036954	0.0088625	5.561
-70	101	3.06754	133.815	-620.7091187	0.0034392	2.158
-70	104	3.06754	131.140	-620.7093882	0.0031697	1.989
-70	107	3.06754	128.471	-620.7096055	0.0029524	1.853
-70	110	3.06754	125.810	-620.7097312	0.0028267	1.774
-70	113	3.06754	123.156	-620.7098684	0.0026895	1.688
-70	116	3.06754	120.511	-620.7099344	0.0026235	1.646
-70	119	3.06754	117.876	-620.7099294	0.0026285	1.649
-70	122	3.06754	115.252	-620.7099064	0.0026515	1.664
-70	125	3.06754	112.638	-620.7098599	0.0026980	1.693
-70	128	3.06754	110.038	-620.7097299	0.0028280	1.775
-70	131	3.06754	107.451	-620.7095492	0.0030087	1.888
-70	134	3.06754	104.878	-620.7093224	0.0032355	2.030
-70	137	3.06754	102.321	-620.7090534	0.0035045	2.199
-70	140	3.06754	99.782	-620.7087406	0.0038173	2.395
-70	143	3.06754	97.262	-620.7083865	0.0041714	2.618
-70	146	3.06754	94.762	-620.7080013	0.0045566	2.859
-70	149	3.06754	92.284	-620.7075949	0.0049630	3.114
-70	152	3.06754	89.831	-620.7071733	0.0053846	3.379
-70	155	3.06754	87.404	-620.7067328	0.0058251	3.655
-70	158	3.06754	85.006	-620.7062723	0.0062856	3.944
-70	161	3.06754	82.640	-620.7058021	0.0067558	4.239
-70	164	3.06754	80.307	-620.7053305	0.0072274	4.535
-73	107	3.11725	129.794	-620.7107231	0.0018348	1.151
-73	110	3.11725	127.159	-620.7108706	0.0016873	1.059
-73	113	3.11725	124.532	-620.7109610	0.0015969	1.002
-73	116	3.11725	121.913	-620.7110069	0.0015510	0.973
-73	119	3.11725	119.303	-620.7110094	0.0015485	0.972
-73	122	3.11725	116.703	-620.7109592	0.0015987	1.003
-73	125	3.11725	114.115	-620.7108504	0.0017075	1.071
-73	128	3.11725	111.538	-620.7106874	0.0018705	1.174
-73	131	3.11725	108.976	-620.7104792	0.0020787	1.304
-73	134	3.11725	106.428	-620.7102315	0.0023264	1.460
-73	137	3.11725	103.895	-620.7099451	0.0026128	1.640

-73	140	3.11725	101.381	-620.7096153	0.0029426	1.847
-73	143	3.11725	98.885	-620.7092423	0.0033156	2.081
-73	146	3.11725	96.409	-620.7088383	0.0037196	2.334
-73	149	3.11725	93.956	-620.7084167	0.0041412	2.599
-73	152	3.11725	91.527	-620.7079857	0.0045722	2.869
-73	155	3.11725	89.124	-620.7075458	0.0050121	3.145
-73	158	3.11725	86.750	-620.7070936	0.0054643	3.429
-73	161	3.11725	84.408	-620.7066373	0.0059206	3.715
-73	164	3.11725	82.099	-620.7061879	0.0063700	3.997
-73	167	3.11725	79.828	-620.7057513	0.0068066	4.271
-73	170	3.11725	77.597	-620.7053296	0.0072283	4.536
-76	107	3.16706	130.996	-620.7115322	0.0010257	0.644
-76	110	3.16706	128.392	-620.7116786	0.0008793	0.552
-76	113	3.16706	125.795	-620.7117659	0.0007920	0.497
-76	116	3.16706	123.205	-620.7118042	0.0007537	0.473
-76	119	3.16706	120.624	-620.7117948	0.0007631	0.479
-76	122	3.16706	118.053	-620.7116981	0.0008598	0.540
-76	125	3.16706	115.492	-620.7115959	0.0009620	0.604
-76	128	3.16706	112.944	-620.7114076	0.0011503	0.722
-76	131	3.16706	110.408	-620.7111768	0.0013811	0.867
-76	134	3.16706	107.887	-620.7109112	0.0016467	1.033
-76	137	3.16706	105.382	-620.7106106	0.0019473	1.222
-76	140	3.16706	102.894	-620.7102674	0.0022905	1.437
-76	143	3.16706	100.425	-620.7098782	0.0026797	1.682
-76	146	3.16706	97.976	-620.7094566	0.0031013	1.946
-76	149	3.16706	95.550	-620.7090204	0.0035375	2.220
-76	152	3.16706	93.147	-620.7085800	0.0039779	2.496
-76	155	3.16706	90.771	-620.7081381	0.0044198	2.773
-76	158	3.16706	88.423	-620.7076915	0.0048664	3.054
-76	161	3.16706	86.107	-620.7072447	0.0053132	3.334
-76	164	3.16706	83.824	-620.7068088	0.0057491	3.608
-76	167	3.16706	81.579	-620.7063919	0.0061660	3.869
-76	170	3.16706	79.373	-620.7059999	0.0065580	4.115
-76	173	3.16706	77.211	-620.7056329	0.0069250	4.345
-79	107	3.21682	132.074	-620.7120396	0.0005183	0.325
-79	110	3.21682	129.506	-620.7121897	0.0003682	0.231
-79	113	3.21682	126.944	-620.7122807	0.0002772	0.174
-79	116	3.21682	124.388	-620.7123189	0.0002390	0.150
-79	119	3.21682	121.839	-620.7123050	0.0002529	0.159
-79	122	3.21682	119.300	-620.7122298	0.0003281	0.206
-79	125	3.21682	116.771	-620.7120872	0.0004707	0.295
-79	128	3.21682	114.253	-620.7118849	0.0006730	0.422
-79	131	3.21682	111.748	-620.7116377	0.0009202	0.577

-79	134	3.21682	109.257	-620.7113562	0.0012017	0.754
-79	137	3.21682	106.782	-620.7110430	0.0015149	0.951
-79	140	3.21682	104.324	-620.7106904	0.0018675	1.172
-79	143	3.21682	101.884	-620.7102911	0.0022668	1.422
-79	146	3.21682	99.464	-620.7098569	0.0027010	1.695
-79	149	3.21682	97.066	-620.7094090	0.0031489	1.976
-79	152	3.21682	94.693	-620.7089609	0.0035970	2.257
-79	155	3.21682	92.345	-620.7085164	0.0040415	2.536
-79	158	3.21682	90.026	-620.7080727	0.0044852	2.815
-79	161	3.21682	87.738	-620.7076320	0.0049259	3.091
-79	164	3.21682	85.483	-620.7072049	0.0053530	3.359
-79	167	3.21682	83.265	-620.7067990	0.0057589	3.614
-79	170	3.21682	81.087	-620.7064220	0.0061359	3.850
-79	173	3.21682	78.952	-620.7060780	0.0064799	4.066
-79	176	3.21682	76.864	-620.7057632	0.0067947	4.264
-82	110	3.26641	130.500	-620.7124068	0.0001511	0.095
-82	113	3.26641	127.977	-620.7125043	0.0000536	0.034
-82	116	3.26641	125.459	-620.7125456	0.0000123	0.008
-82	119	3.26641	122.947	-620.7125319	0.0000260	0.016
-82	122	3.26641	120.444	-620.7124569	0.0001010	0.063
-82	125	3.26641	117.950	-620.7123147	0.0002432	0.153
-82	128	3.26641	115.466	-620.7121101	0.0004478	0.281
-82	131	3.26641	112.995	-620.7118552	0.0007027	0.441
-82	134	3.26641	110.537	-620.7115629	0.0009950	0.624
-82	137	3.26641	108.094	-620.7112405	0.0013174	0.827
-82	140	3.26641	105.668	-620.7108834	0.0016745	1.051
-82	143	3.26641	103.260	-620.7104817	0.0020762	1.303
-82	146	3.26641	100.872	-620.7100420	0.0025159	1.579
-82	149	3.26641	98.506	-620.7095855	0.0029724	1.865
-82	152	3.26641	96.164	-620.7091297	0.0034282	2.151
-82	155	3.26641	93.847	-620.7086809	0.0038770	2.433
-82	158	3.26641	91.559	-620.7082366	0.0043213	2.712
-82	161	3.26641	89.301	-620.7077968	0.0047611	2.988
-82	164	3.26641	87.077	-620.7073731	0.0051848	3.253
-82	167	3.26641	84.888	-620.7069735	0.0055844	3.504
-82	170	3.26641	82.739	-620.7066030	0.0059549	3.737
-82	173	3.26641	80.633	-620.7062681	0.0062898	3.947
-82	176	3.26641	78.573	-620.7059679	0.0065900	4.135
-85	110	3.31569	131.372	-620.7123164	0.0002415	0.152
-85	113	3.31570	128.893	-620.7124224	0.0001355	0.085
-85	116	3.31569	126.418	-620.7124718	0.0000861	0.054
-85	119	3.31569	123.947	-620.7124674	0.0000905	0.057
-85	122	3.31569	121.484	-620.7124042	0.0001537	0.096

-85	125	3.31570	119.028	-620.7122744	0.0002835	0.178
-85	128	3.31570	116.582	-620.7120787	0.0004792	0.301
-85	131	3.31569	114.148	-620.7118264	0.0007315	0.459
-85	134	3.31569	111.726	-620.7115320	0.0010259	0.644
-85	137	3.31570	109.319	-620.7112064	0.0013515	0.848
-85	140	3.31570	106.928	-620.7108496	0.0017083	1.072
-85	143	3.31569	104.555	-620.7104512	0.0021067	1.322
-85	146	3.31570	102.201	-620.7100108	0.0025471	1.598
-85	149	3.31569	99.869	-620.7095469	0.0030110	1.889
-85	152	3.31569	97.560	-620.7090803	0.0034776	2.182
-85	155	3.31570	95.277	-620.7086225	0.0039354	2.470
-85	158	3.31569	93.022	-620.7081736	0.0043843	2.751
-85	161	3.31569	90.797	-620.7077303	0.0048276	3.029
-85	164	3.31570	88.605	-620.7073029	0.0052550	3.298
-85	167	3.31570	86.448	-620.7069041	0.0056538	3.548
-85	170	3.31569	84.331	-620.7065362	0.0060217	3.779
-85	173	3.31570	82.255	-620.7062028	0.0063551	3.988
-85	176	3.31570	80.225	-620.7059075	0.0066504	4.173
-85	179	3.31569	78.244	-620.7056476	0.0069103	4.336

Table S5. Data used to generate Figure 3C.

ϕ (□)	ψ (□)	d (Å)	θ (□)	Energy (au)	Relative Energy (au)	Relative Energy (kcal/mol)
-67	100	3.03740	133.216	-521.4330290	0.0050866	3.192
-67	105	3.03741	128.806	-521.4334343	0.0046813	2.938
-67	110	3.03741	124.418	-521.4337222	0.0043934	2.757
-67	115	3.03740	120.057	-521.4339073	0.0042083	2.641
-67	120	3.03740	115.727	-521.4340021	0.0041135	2.581
-67	125	3.03741	111.430	-521.4340311	0.0040845	2.563
-67	130	3.03740	107.174	-521.4339971	0.0041185	2.584
-67	135	3.03741	102.962	-521.4339002	0.0042154	2.645
-67	140	3.03741	98.803	-521.4337571	0.0043585	2.735
-67	145	3.03740	94.702	-521.4335898	0.0045258	2.840
-67	150	3.03740	90.669	-521.4334013	0.0047143	2.958
-67	155	3.03741	86.714	-521.4331895	0.0049261	3.091
-67	160	3.03740	82.849	-521.4329952	0.0051204	3.213
-67	165	3.03741	79.087	-521.4328525	0.0052631	3.303
-67	170	3.03741	75.444	-521.4327708	0.0053448	3.354
-67	175	3.03740	71.938	-521.4327624	0.0053532	3.359
-67	180	3.03741	68.592	-521.4328265	0.0052891	3.319
-72	100	3.12027	135.643	-521.4354241	0.0026915	1.689
-72	105	3.12027	131.281	-521.4357236	0.0023920	1.501

-72	110	3.12027	126.943	-521.4359161	0.0021995	1.380
-72	115	3.12027	122.633	-521.4360267	0.0020889	1.311
-72	120	3.12027	118.354	-521.4360549	0.0020607	1.293
-72	125	3.12027	114.110	-521.4360158	0.0020998	1.318
-72	130	3.12027	109.907	-521.4359040	0.0022116	1.388
-72	135	3.12027	105.750	-521.4357255	0.0023901	1.500
-72	140	3.12027	101.646	-521.4355066	0.0026090	1.637
-72	145	3.12027	97.601	-521.4352626	0.0028530	1.790
-72	150	3.12027	93.624	-521.4350064	0.0031092	1.951
-72	155	3.12027	89.725	-521.4347469	0.0033687	2.114
-72	160	3.12027	85.915	-521.4345168	0.0035988	2.258
-72	165	3.12027	82.206	-521.4343512	0.0037644	2.362
-72	170	3.12027	78.615	-521.4342611	0.0038545	2.419
-72	175	3.12027	75.157	-521.4342472	0.0038684	2.427
-72	180	3.12027	71.853	-521.4342961	0.0038195	2.397
-77	100	3.20349	137.729	-521.4369394	0.0011762	0.738
-77	105	3.20349	133.437	-521.4371871	0.0009285	0.583
-77	110	3.20349	129.167	-521.4373277	0.0007879	0.494
-77	115	3.20350	124.923	-521.4374021	0.0007135	0.448
-77	120	3.20349	120.710	-521.4374002	0.0007154	0.449
-77	125	3.20349	116.533	-521.4373128	0.0008028	0.504
-77	130	3.20349	112.395	-521.4371409	0.0009747	0.612
-77	135	3.20349	108.304	-521.4369051	0.0012105	0.760
-77	140	3.20349	104.266	-521.4366220	0.0014936	0.937
-77	145	3.20349	100.287	-521.4363075	0.0018081	1.135
-77	150	3.20349	96.376	-521.4359971	0.0021185	1.329
-77	155	3.20349	92.542	-521.4357103	0.0024053	1.509
-77	160	3.20349	88.797	-521.4354586	0.0026570	1.667
-77	165	3.20349	85.152	-521.4352645	0.0028511	1.789
-77	170	3.20349	81.622	-521.4351384	0.0029772	1.868
-77	175	3.20349	78.223	-521.4350806	0.0030350	1.905
-77	180	3.20349	74.972	-521.4350807	0.0030349	1.904
-82	100	3.28644	139.455	-521.4376025	0.0005131	0.322
-82	105	3.28644	135.257	-521.4378358	0.0002798	0.176
-82	110	3.28644	131.077	-521.4379755	0.0001401	0.088
-82	115	3.28644	126.919	-521.4380491	0.0000665	0.042
-82	120	3.28644	122.789	-521.4380367	0.0000789	0.050
-82	125	3.28644	118.692	-521.4379144	0.0002012	0.126
-82	130	3.28644	114.634	-521.4377006	0.0004150	0.260
-82	135	3.28644	110.622	-521.4374231	0.0006925	0.435
-82	140	3.28644	106.661	-521.4370958	0.0010198	0.640
-82	145	3.28644	102.759	-521.4367385	0.0013771	0.864
-82	150	3.28644	98.925	-521.4363953	0.0017203	1.080

-82	155	3.28644	95.167	-521.4360900	0.0020256	1.271
-82	160	3.28644	91.496	-521.4358144	0.0023012	1.444
-82	165	3.28644	87.925	-521.4355760	0.0025396	1.594
-82	170	3.28644	84.466	-521.4353932	0.0027224	1.708
-82	175	3.28644	81.135	-521.4352740	0.0028416	1.783
-82	180	3.28644	77.948	-521.4352209	0.0028947	1.816
-87	100	3.36852	140.803	-521.4374640	0.0006516	0.409
-87	105	3.36852	136.729	-521.4377275	0.0003881	0.244
-87	110	3.36852	132.662	-521.4379056	0.0002100	0.132
-87	115	3.36852	128.611	-521.4379842	0.0001314	0.082
-87	120	3.36852	124.583	-521.4379612	0.0001544	0.097
-87	125	3.36852	120.583	-521.4378297	0.0002859	0.179
-87	130	3.36852	116.620	-521.4375986	0.0005170	0.324
-87	135	3.36852	112.700	-521.4372946	0.0008210	0.515
-87	140	3.36852	108.830	-521.4369475	0.0011681	0.733
-87	145	3.36852	105.017	-521.4365748	0.0015408	0.967
-87	150	3.36852	101.270	-521.4362022	0.0019134	1.201
-87	155	3.36852	97.599	-521.4358586	0.0022570	1.416
-87	160	3.36852	94.014	-521.4355414	0.0025742	1.615
-87	165	3.36852	90.525	-521.4352457	0.0028699	1.801
-87	170	3.36852	87.147	-521.4350002	0.0031154	1.955
-87	175	3.36852	83.894	-521.4348329	0.0032827	2.060
-87	180	3.36852	80.781	-521.4347417	0.0033739	2.117

Atomic Coordinates of **1a** (cis, endo, distal)

C	0.201318000	1.841644000	-0.918965000
C	-0.624036000	2.387946000	0.253758000
C	-1.745887000	1.357368000	0.423412000
N	-1.164737000	0.114497000	-0.108266000
C	0.144675000	0.310624000	-0.706735000
C	-1.861606000	-1.057288000	-0.032770000
O	-2.978795000	-1.093179000	0.462348000
C	-1.194563000	-2.298834000	-0.594898000
C	1.291269000	-0.146320000	0.199635000
O	1.223161000	-0.318830000	1.388417000
O	2.418761000	-0.303424000	-0.522207000
C	3.593649000	-0.675161000	0.224819000
H	4.391498000	-0.754200000	-0.508713000
H	3.435657000	-1.628818000	0.727088000
H	3.826931000	0.086966000	0.967696000
H	-1.873935000	-3.135786000	-0.454819000
H	-0.254731000	-2.512136000	-0.080567000
H	-0.979177000	-2.189993000	-1.660985000
H	-2.640957000	1.618520000	-0.148266000
H	-2.049719000	1.217489000	1.460480000
H	0.242366000	-0.217984000	-1.655448000
H	-1.009022000	3.389770000	0.062602000
H	-0.013144000	2.430111000	1.157503000
H	1.222373000	2.220335000	-0.955534000
H	-0.278906000	2.077836000	-1.871190000

Atomic coordinates of **1b** (cis, endo, proximal)

C	0.186817000	1.994710000	-0.892351000
C	-0.328913000	2.368503000	0.504399000
C	-1.428087000	1.335842000	0.779992000
N	-1.048776000	0.183845000	-0.052921000
C	0.100133000	0.451002000	-0.905526000
C	-1.776179000	-0.969885000	-0.001161000
O	-2.742095000	-1.071667000	0.742132000
C	-1.342594000	-2.104503000	-0.910572000
C	1.427437000	-0.163451000	-0.450104000
O	2.367404000	-0.300195000	-1.193520000
O	1.441111000	-0.496331000	0.849573000
C	2.678738000	-1.050649000	1.338940000
H	2.501868000	-1.270992000	2.388071000
H	3.487154000	-0.329186000	1.225178000
H	2.928539000	-1.958030000	0.790456000
H	-1.984542000	-2.958469000	-0.709777000
H	-0.302236000	-2.389358000	-0.738981000
H	-1.441444000	-1.826144000	-1.963100000
H	-2.418006000	1.692619000	0.482514000
H	-1.490987000	1.041336000	1.827567000
H	-0.052784000	0.082560000	-1.920099000
H	-0.703908000	3.391046000	0.550574000
H	0.471247000	2.274551000	1.241279000
H	1.192291000	2.354950000	-1.106777000
H	-0.481233000	2.384330000	-1.663633000

Atomic coordinates of **1c** (trans, endo, distal)

C	-1.825179000	1.248034000	0.363705000
H	-2.190052000	1.032486000	1.368815000
H	-2.684194000	1.525490000	-0.257688000
C	-0.758854000	2.350538000	0.363079000
H	-0.207180000	2.329927000	1.303943000
H	-1.192866000	3.343732000	0.244173000
C	0.166227000	1.960872000	-0.798912000
H	1.161459000	2.398790000	-0.724943000
H	-0.263564000	2.269030000	-1.754902000
C	0.189820000	0.419011000	-0.738453000
H	0.335732000	-0.035378000	-1.717133000
C	1.304207000	-0.079915000	0.181513000
O	1.218864000	-0.191440000	1.378176000
O	2.424052000	-0.320943000	-0.521308000
C	3.556432000	-0.773256000	0.243926000
H	3.835609000	-0.027795000	0.988227000
H	3.318596000	-1.711081000	0.744452000
H	4.356557000	-0.915456000	-0.477679000
N	-1.126543000	0.089660000	-0.208807000
C	-1.555043000	-1.204887000	-0.212769000
O	-0.858412000	-2.099717000	-0.673576000
C	-2.924177000	-1.471558000	0.378450000
H	-2.907408000	-1.317444000	1.460659000
H	-3.686034000	-0.809870000	-0.039756000
H	-3.187469000	-2.506295000	0.173906000

Atomic coordinates of **1d** (trans, endo, proximal)

C	-1.518135000	1.246684000	0.745673000
H	-1.705323000	0.858886000	1.748231000
H	-2.456843000	1.664305000	0.364313000
C	-0.399013000	2.295073000	0.729374000
H	0.324764000	2.076668000	1.516856000
H	-0.777797000	3.304563000	0.891118000
C	0.247177000	2.111452000	-0.650768000
H	1.264468000	2.495278000	-0.713867000
H	-0.346477000	2.610410000	-1.420181000
C	0.180506000	0.587171000	-0.881077000
H	0.083741000	0.335723000	-1.936700000
C	1.467794000	-0.102356000	-0.427403000
O	2.459514000	-0.138169000	-1.110789000
O	1.393157000	-0.604265000	0.816814000
C	2.578045000	-1.276942000	1.282981000
H	2.807582000	-2.121575000	0.634637000
H	3.425093000	-0.591572000	1.295377000
H	2.342654000	-1.617793000	2.287869000
N	-1.018358000	0.194188000	-0.149446000
C	-1.559460000	-1.044257000	-0.332629000
O	-1.045754000	-1.853898000	-1.092924000
C	-2.815890000	-1.360846000	0.453562000
H	-2.597230000	-1.413060000	1.523492000
H	-3.587147000	-0.600535000	0.310384000
H	-3.190465000	-2.325840000	0.121518000

Atomic coordinates of **1e** (cis, exo, distal)

N	-1.152178000	0.003084000	-0.013504000
C	-0.670488000	-2.316479000	-0.698104000
C	-1.601090000	-1.287352000	-0.086372000
C	-2.022639000	1.069663000	0.494850000
C	-1.487402000	2.313740000	-0.211887000
C	0.020678000	2.048702000	-0.289146000
C	0.119760000	0.513360000	-0.511081000
C	1.337381000	-0.032827000	0.227731000
C	3.677198000	-0.314043000	0.068349000
O	-2.708820000	-1.595801000	0.328938000
O	1.343403000	-0.474492000	1.346522000
O	2.436436000	0.091802000	-0.541904000
H	0.118639000	-2.572584000	0.012331000
H	-0.198413000	-1.965959000	-1.618598000
H	-1.254231000	-3.209177000	-0.909160000
H	-1.931482000	1.152617000	1.583179000
H	-3.059099000	0.832655000	0.264208000
H	-1.721812000	3.235498000	0.321528000
H	-1.914454000	2.385577000	-1.215545000
H	0.491886000	2.312692000	0.660626000
H	0.528067000	2.599000000	-1.080253000
H	0.246657000	0.295897000	-1.574907000
H	3.637966000	-1.368613000	0.338608000
H	3.871350000	0.278496000	0.961757000
H	4.441621000	-0.138337000	-0.683746000

Atomic coordinates of **1g** (trans, exo, distal)

N	-1.102077000	-0.025542000	-0.099939000
C	-2.531300000	-1.991447000	0.254391000
C	-1.232749000	-1.375807000	-0.226309000
C	-2.084460000	0.921235000	0.433056000
C	-1.636093000	2.252119000	-0.174905000
C	-0.107243000	2.120539000	-0.212146000
C	0.134259000	0.625947000	-0.529782000
C	1.345888000	0.092932000	0.229255000
C	3.629991000	-0.447270000	0.049636000
O	-0.333482000	-2.050054000	-0.712084000
O	1.355316000	-0.170476000	1.404401000
O	2.422523000	0.031154000	-0.570424000
H	-3.375498000	-1.652789000	-0.351995000
H	-2.738330000	-1.725294000	1.293378000
H	-2.444811000	-3.071581000	0.167661000
H	-2.042384000	0.954086000	1.528016000
H	-3.096481000	0.644764000	0.138324000
H	-1.972320000	3.111556000	0.406082000
H	-2.035958000	2.350139000	-1.187350000
H	0.309080000	2.357201000	0.769425000
H	0.365682000	2.770676000	-0.947197000
H	0.298313000	0.455980000	-1.595186000
H	3.481525000	-1.461291000	0.418783000
H	3.916453000	0.200878000	0.877592000
H	4.384654000	-0.430009000	-0.732287000

Atomic coordinates of **1f** (cis, exo, proximal)

N	-1.038724000	-0.067438000	0.013555000
C	-0.494255000	-2.260696000	-0.966137000
C	-1.344914000	-1.398422000	-0.053216000
C	-1.869409000	0.856141000	0.795054000
C	-1.662661000	2.189924000	0.079243000
C	-0.199547000	2.118855000	-0.374259000
C	0.009727000	0.622466000	-0.735413000
C	1.444529000	0.215234000	-0.417751000
C	2.958278000	-0.470549000	1.254553000
O	-2.265444000	-1.870567000	0.598925000
O	2.336276000	0.265333000	-1.228019000
O	1.610119000	-0.143084000	0.865208000
H	0.498935000	-2.410469000	-0.535814000
H	-0.364272000	-1.821518000	-1.957345000
H	-0.981085000	-3.228329000	-1.059153000
H	-1.524121000	0.898324000	1.833795000
H	-2.898346000	0.502588000	0.800135000
H	-1.858595000	3.048285000	0.722576000
H	-2.328221000	2.256673000	-0.785228000
H	0.458645000	2.392405000	0.453416000
H	0.036302000	2.766172000	-1.217640000
H	-0.107829000	0.473754000	-1.811244000
H	3.611329000	0.390727000	1.116961000
H	3.332794000	-1.302504000	0.659230000
H	2.897431000	-0.745212000	2.304079000

Atomic coordinates of **1h** (trans, exo, proximal)

N	-1.007581000	-0.024541000	-0.069668000
C	-2.293038000	-2.082307000	0.315980000
C	-1.137302000	-1.353750000	-0.341212000
C	-1.896652000	0.804821000	0.749150000
C	-1.625712000	2.217793000	0.226573000
C	-0.136042000	2.176584000	-0.137199000
C	0.072669000	0.745854000	-0.687187000
C	1.479102000	0.244442000	-0.387662000
C	2.891082000	-0.796471000	1.179819000
O	-0.348800000	-1.923732000	-1.083771000
O	2.405041000	0.401776000	-1.141564000
O	1.584285000	-0.301993000	0.835499000
H	-3.251078000	-1.728830000	-0.074390000
H	-2.299305000	-1.934045000	1.398199000
H	-2.192728000	-3.141946000	0.094922000
H	-1.640921000	0.722299000	1.812378000
H	-2.937223000	0.505191000	0.627423000
H	-1.861926000	2.987694000	0.961821000
H	-2.229954000	2.404895000	-0.664751000
H	0.470971000	2.321811000	0.759580000
H	0.156899000	2.931522000	-0.865055000
H	-0.018662000	0.718263000	-1.774687000
H	3.621881000	0.011739000	1.162238000
H	3.193400000	-1.571776000	0.476882000
H	2.792868000	-1.205226000	2.182250000

Atomic coordinates of **2a** (cis, endo, distal 1)

C	0.005709000	0.008883000	-0.001987000
C	0.004961000	0.008861000	1.532663000
C	1.491894000	0.006935000	1.903209000
N	2.159610000	0.603601000	0.734764000
C	1.239771000	0.859642000	-0.385472000
C	3.522158000	0.697502000	0.716848000
C	4.175434000	1.213345000	-0.551191000
C	0.918111000	2.316196000	-0.575429000
C	1.039813000	3.033907000	-1.683435000
F	0.414432000	2.894664000	0.553815000
C	0.671320000	4.478408000	-1.852072000
C	1.866579000	5.351159000	-2.261416000
O	4.185652000	0.363604000	1.689313000
H	1.555116000	6.386782000	-2.414191000
H	2.316223000	4.997235000	-3.192907000
H	2.641112000	5.341329000	-1.491607000
H	5.240915000	1.313948000	-0.360090000
H	3.763588000	2.175636000	-0.858137000
H	4.031172000	0.509607000	-1.376126000
H	0.233053000	4.856117000	-0.927276000
H	-0.104812000	4.556423000	-2.622281000
H	1.454733000	2.518213000	-2.544155000
H	1.880116000	-1.002559000	2.064766000
H	1.710908000	0.584419000	2.801491000
H	-0.518506000	-0.852715000	1.948164000
H	-0.479507000	0.909821000	1.909327000
H	-0.913686000	0.398795000	-0.438312000
H	0.154491000	-1.005085000	-0.381469000
H	1.669852000	0.507185000	-1.324221000

Atomic coordinates of **2b** (cis, endo, distal 2)

C	0.003945000	0.010032000	-0.003613000
C	0.003166000	0.007754000	1.531072000
C	1.489963000	0.003105000	1.900543000
N	2.156464000	0.609171000	0.736387000
C	1.238906000	0.859826000	-0.387142000
C	3.517991000	0.719941000	0.726660000
C	4.172682000	1.252897000	-0.533584000
C	0.918152000	2.315407000	-0.583412000
C	1.042923000	3.029006000	-1.693681000
F	0.420034000	2.899984000	0.544954000
C	0.661880000	4.469012000	-1.870930000
C	-0.414439000	4.668287000	-2.947947000
O	4.179726000	0.388260000	1.701057000
H	-0.642786000	5.728782000	-3.075047000
H	-1.338761000	4.152810000	-2.678260000
H	-0.085483000	4.279618000	-3.915319000
H	5.236626000	1.358602000	-0.336746000
H	3.755716000	2.215928000	-0.831541000
H	4.036506000	0.557566000	-1.366920000
H	1.554894000	5.038842000	-2.152543000
H	0.318196000	4.877435000	-0.919510000
H	1.447919000	2.506617000	-2.554999000
H	1.878081000	-1.007812000	2.054198000
H	1.709896000	0.573563000	2.803012000
H	-0.521617000	-0.853771000	1.945124000
H	-0.479782000	0.908942000	1.909618000
H	-0.914975000	0.401419000	-0.439551000
H	0.151513000	-1.003703000	-0.384266000
H	1.670217000	0.502754000	-1.323756000

Atomic coordinates of **2c** (cis, endo, proximal 1)

C	0.004769000	0.009249000	0.000234000
C	0.004664000	-0.003531000	1.533969000
C	1.493304000	-0.003577000	1.898404000
N	2.141085000	0.649006000	0.746869000
C	1.204919000	0.920745000	-0.343356000
C	3.504657000	0.722274000	0.688220000
C	4.123224000	1.259242000	-0.588587000
C	0.801459000	2.370597000	-0.440736000
C	1.076081000	3.387409000	0.360840000
F	0.027898000	2.563117000	-1.553254000
C	0.619808000	4.805346000	0.177211000
C	1.789783000	5.793485000	0.067202000
O	4.192006000	0.355070000	1.631270000
H	1.423428000	6.818668000	-0.021611000
H	2.404987000	5.577665000	-0.809149000
H	2.434982000	5.744116000	0.948049000
H	5.176413000	1.449019000	-0.396276000
H	3.640117000	2.175013000	-0.931594000
H	4.045175000	0.516472000	-1.387773000
H	-0.002177000	5.088321000	1.034431000
H	-0.015271000	4.878589000	-0.706901000
H	1.701775000	3.162520000	1.217520000
H	1.894150000	-1.014281000	2.013853000
H	1.712846000	0.536025000	2.820241000
H	-0.519413000	-0.864569000	1.948887000
H	-0.480024000	0.897160000	1.916142000
H	-0.925057000	0.370404000	-0.437344000
H	0.197155000	-0.992504000	-0.391835000
H	1.632964000	0.635852000	-1.308059000

Atomic coordinates of **2d** (cis, endo, proximal 2)

C	0.629400000	2.108623000	0.674992000
C	0.813831000	2.246169000	-0.841539000
C	1.667859000	1.030039000	-1.217272000
N	1.355001000	0.039167000	-0.172539000
C	0.493168000	0.582289000	0.876571000
C	2.029564000	-1.148980000	-0.140595000
C	1.778932000	-2.065594000	1.042070000
C	-0.940105000	0.124715000	0.770979000
C	-1.538187000	-0.593502000	-0.166151000
F	-1.651715000	0.571934000	1.851219000
C	-2.986931000	-0.984210000	-0.189434000
C	-3.717356000	-0.467224000	-1.437244000
O	2.813231000	-1.447578000	-1.031324000
H	-4.756722000	-0.802968000	-1.444576000

H	-3.242657000	-0.829618000	-2.352678000
H	-3.714379000	0.624557000	-1.469218000
H	2.215815000	-3.034525000	0.812874000
H	0.716637000	-2.182486000	1.260424000
H	2.265893000	-1.669194000	1.937718000
H	-3.483001000	-0.619847000	0.711310000
H	-3.057292000	-2.077857000	-0.166835000
H	-0.912097000	-0.917501000	-0.990155000
H	2.738650000	1.250240000	-1.197852000
H	1.440548000	0.631016000	-2.206386000
H	1.290273000	3.184843000	-1.124622000
H	-0.154868000	2.200658000	-1.343234000
H	-0.228712000	2.653904000	1.065861000
H	1.520915000	2.456820000	1.202382000
H	0.854534000	0.297052000	1.868111000

Atomic coordinates of **2e** (trans, endo, distal 1)

C	-1.112665000	-1.933300000	0.932986000
C	-1.992186000	-2.021501000	-0.322592000
C	-2.430661000	-0.572053000	-0.569267000
N	-1.365642000	0.235719000	0.042871000
C	-0.395671000	-0.572280000	0.807113000
C	-1.371405000	1.596666000	0.160701000
C	-2.458794000	2.335106000	-0.597029000
C	0.944629000	-0.650048000	0.137895000
C	2.102629000	-0.199426000	0.593154000
F	0.890190000	-1.286056000	-1.076968000
C	3.429537000	-0.300656000	-0.097630000
C	4.039637000	1.075775000	-0.401407000
O	-0.541289000	2.188970000	0.837170000
H	5.019509000	0.969486000	-0.872802000
H	4.167944000	1.662172000	0.511850000
H	3.397227000	1.648048000	-1.073546000
H	-2.319265000	3.401163000	-0.436709000
H	-3.452954000	2.046233000	-0.246425000
H	-2.411808000	2.119514000	-1.667102000
H	3.323535000	-0.874049000	-1.019918000
H	4.120401000	-0.860935000	0.543391000
H	2.065500000	0.323674000	1.542765000
H	-3.392428000	-0.364475000	-0.087380000
H	-2.535003000	-0.351105000	-1.633354000
H	-2.847216000	-2.685915000	-0.193115000
H	-1.406496000	-2.384768000	-1.166853000
H	-0.412044000	-2.762875000	1.021637000
H	-1.733750000	-1.920733000	1.832083000
H	-0.235355000	-0.102423000	1.777183000

Atomic coordinates of **2f** (trans, endo, distal 2)

C	-0.645947000	1.905835000	-1.023577000
C	-1.597039000	2.267852000	0.126166000
C	-2.377326000	0.971902000	0.378923000
N	-1.463874000	-0.089571000	-0.068724000
C	-0.269176000	0.432363000	-0.761443000
C	-1.761969000	-1.421694000	-0.120429000
C	-3.053268000	-1.850889000	0.550677000
C	0.985386000	0.258737000	0.042832000
C	2.035105000	-0.491632000	-0.250817000
F	0.975435000	0.994866000	1.201170000
C	3.285241000	-0.632612000	0.564224000
C	4.552461000	-0.291432000	-0.232669000
O	-1.024910000	-2.226506000	-0.674053000
H	5.446712000	-0.440867000	0.376721000
H	4.539132000	0.749147000	-0.564850000
H	4.643427000	-0.923475000	-1.119842000
H	-3.133009000	-2.932113000	0.471510000
H	-3.920867000	-1.391263000	0.070152000
H	-3.068462000	-1.561544000	1.604043000
H	3.356605000	-1.668322000	0.916644000
H	3.221341000	-0.003864000	1.453702000
H	1.961097000	-1.069888000	-1.165597000
H	-3.303750000	0.950944000	-0.205700000
H	-2.642521000	0.850865000	1.430992000
H	-2.260015000	3.098399000	-0.118610000
H	-1.025721000	2.539337000	1.013600000
H	0.228576000	2.553622000	-1.074228000
H	-1.167031000	1.969612000	-1.982129000
H	-0.128834000	-0.125919000	-1.686759000

Atomic coordinates of **2g** (trans, endo, proximal 1)

C	-1.050965000	-2.150494000	0.386554000
C	-1.533606000	-1.962120000	-1.056805000
C	-2.087930000	-0.532613000	-1.064422000
N	-1.300565000	0.155825000	-0.027011000
C	-0.464643000	-0.768785000	0.744557000
C	-1.534631000	1.425314000	0.429568000
C	-2.533587000	2.251459000	-0.359234000
C	0.999735000	-0.665919000	0.408763000
C	1.619240000	0.059502000	-0.507035000
F	1.719286000	-1.488666000	1.232578000
C	3.100610000	0.107977000	-0.741651000
C	3.685338000	1.509653000	-0.512909000
O	-0.965572000	1.870450000	1.414671000
H	4.758223000	1.520694000	-0.719050000
H	3.532054000	1.832280000	0.518712000
H	3.211370000	2.248000000	-1.164941000
H	-2.553751000	3.252354000	0.064220000
H	-3.535530000	1.818172000	-0.298742000
H	-2.263973000	2.308494000	-1.416305000
H	3.308388000	-0.199629000	-1.773280000
H	3.600542000	-0.613642000	-0.093758000
H	0.989115000	0.702770000	-1.110595000
H	-3.152203000	-0.524879000	-0.806147000
H	-1.976331000	-0.048911000	-2.037016000
H	-2.284319000	-2.693183000	-1.357885000
H	-0.691919000	-2.041769000	-1.747602000
H	-0.321636000	-2.951060000	0.500427000
H	-1.894657000	-2.364853000	1.047350000
H	-0.567779000	-0.545054000	1.808808000

Atomic coordinates of **2h** (trans, endo, proximal 2)

C	-0.594057000	2.204741000	-0.337511000
C	-0.864772000	2.066327000	1.165763000
C	-1.735125000	0.807177000	1.258794000
N	-1.322487000	0.006180000	0.093472000
C	-0.426020000	0.743065000	-0.801833000
C	-1.927194000	-1.148793000	-0.324776000
C	-2.949344000	-1.753905000	0.619681000
C	1.004717000	0.279197000	-0.722015000
C	1.567929000	-0.628250000	0.057815000
F	1.759961000	0.954814000	-1.642034000
C	3.014356000	-1.026753000	0.046570000
C	3.694502000	-0.837146000	1.409741000
O	-1.652948000	-1.667959000	-1.396062000
H	4.732922000	-1.174825000	1.376205000
H	3.183905000	-1.407427000	2.190439000
H	3.690503000	0.213842000	1.707903000
H	-3.296373000	-2.689178000	0.188022000
H	-3.802875000	-1.085227000	0.758461000
H	-2.519636000	-1.946220000	1.605640000
H	3.547422000	-0.459826000	-0.718089000
H	3.084770000	-2.082266000	-0.240756000
H	0.907939000	-1.134515000	0.752893000
H	-2.798419000	1.060940000	1.192364000
H	-1.579353000	0.262913000	2.192561000
H	-1.360279000	2.937650000	1.594650000
H	0.072741000	1.915229000	1.704400000
H	0.278370000	2.814277000	-0.567850000
H	-1.457089000	2.645244000	-0.843091000
H	-0.753154000	0.602522000	-1.834632000

Atomic coordinates of **2i** (cis, exo, distal 1)

C	1.126569000	-2.002548000	-0.592709000
C	2.609328000	-1.713181000	-0.334147000
C	2.566961000	-0.479938000	0.566602000
N	1.424013000	0.273870000	0.038845000
C	0.446654000	-0.604761000	-0.631887000
C	1.443335000	1.642305000	0.029621000
C	0.314219000	2.355467000	-0.688479000
C	-0.903578000	-0.630740000	0.022864000
C	-2.086476000	-0.443506000	-0.544858000
F	-0.827096000	-0.944059000	1.348451000
C	-3.422019000	-0.549886000	0.129778000
C	-4.224820000	0.757916000	0.070473000
O	2.342871000	2.267729000	0.574559000
H	-5.204961000	0.631277000	0.535442000
H	-4.384480000	1.080037000	-0.961866000
H	-3.704193000	1.562134000	0.594712000
H	0.535544000	3.419736000	-0.676529000
H	-0.641718000	2.178107000	-0.193410000
H	0.215591000	2.019249000	-1.723688000
H	-3.285779000	-0.856380000	1.167875000
H	-4.000375000	-1.342824000	-0.358518000
H	-2.073864000	-0.179887000	-1.597966000
H	3.457998000	0.142223000	0.523787000
H	2.396063000	-0.754254000	1.613076000
H	3.126505000	-2.554977000	0.127816000
H	3.124150000	-1.471770000	-1.267877000
H	0.710150000	-2.583814000	0.231451000
H	0.940999000	-2.552679000	-1.515157000
H	0.300131000	-0.285341000	-1.667138000

Atomic coordinates of **2j** (cis, exo, distal 2)

C	0.574546000	-2.039307000	-0.546335000
C	2.093019000	-2.164829000	-0.381816000
C	2.445242000	-0.958536000	0.486757000
N	1.517218000	0.073819000	0.010165000
C	0.302738000	-0.510051000	-0.591162000
C	1.899891000	1.387561000	-0.015677000
C	0.962144000	2.380652000	-0.674565000
C	-0.967513000	-0.154325000	0.124237000
C	-2.080702000	0.343422000	-0.394754000
F	-0.910321000	-0.450593000	1.454506000
C	-3.361866000	0.608525000	0.338934000
C	-4.548106000	-0.174990000	-0.241669000
O	2.963612000	1.747483000	0.470397000
H	-5.469944000	0.066708000	0.291909000
H	-4.383026000	-1.251643000	-0.162063000
H	-4.701802000	0.062109000	-1.297696000
H	1.474465000	3.338543000	-0.718174000
H	0.040881000	2.489918000	-0.099930000
H	0.684674000	2.072112000	-1.685409000
H	-3.585176000	1.680438000	0.285440000
H	-3.236904000	0.368224000	1.395714000
H	-2.054420000	0.566276000	-1.457017000
H	3.466902000	-0.603008000	0.373545000
H	2.275954000	-1.166424000	1.548680000
H	2.388720000	-3.111271000	0.072389000
H	2.594723000	-2.084004000	-1.349845000
H	0.068917000	-2.470871000	0.319046000
H	0.186882000	-2.531115000	-1.438409000
H	0.196259000	-0.175993000	-1.626780000

Atomic coordinates of **2k** (cis, exo, proximal 1)

C	0.709664000	2.141778000	0.324251000
C	1.935340000	2.108898000	-0.600067000
C	1.822535000	0.749533000	-1.289717000
N	1.287321000	-0.112173000	-0.228824000
C	0.470526000	0.651309000	0.719282000
C	1.802896000	-1.365301000	-0.017926000
C	1.393104000	-2.079502000	1.256325000
C	-0.992279000	0.299706000	0.680695000
C	-1.658680000	-0.488375000	-0.147054000
F	-1.650716000	0.965391000	1.678607000
C	-3.137905000	-0.741768000	-0.126682000
C	-3.824233000	-0.336376000	-1.439031000
O	2.570182000	-1.881004000	-0.818185000
H	-4.890821000	-0.569816000	-1.406483000

H	-3.392155000	-0.865849000	-2.292053000
H	-3.717723000	0.735054000	-1.622525000
H	1.743467000	-3.106450000	1.190142000
H	0.313807000	-2.067021000	1.411235000
H	1.861711000	-1.606409000	2.124108000
H	-3.592455000	-0.211474000	0.711490000
H	-3.310394000	-1.810312000	0.046585000
H	-1.069289000	-0.980415000	-0.913058000
H	2.765499000	0.337811000	-1.641095000
H	1.131143000	0.789508000	-2.138661000
H	1.948311000	2.940973000	-1.305201000
H	2.859012000	2.147993000	-0.017052000
H	-0.162006000	2.518954000	-0.213581000
H	0.849778000	2.770360000	1.202797000
H	0.820039000	0.482404000	1.742694000

Atomic coordinates of **2l** (cis, exo, proximal 2)

C	-1.244852000	-2.059424000	0.200444000
C	-2.538888000	-1.631590000	-0.505812000
C	-2.164493000	-0.298709000	-1.153602000
N	-1.262236000	0.304133000	-0.164604000
C	-0.556834000	-0.720662000	0.611071000
C	-1.383827000	1.627151000	0.175895000
C	-0.616427000	2.105031000	1.394209000
C	0.925438000	-0.764946000	0.355043000
C	1.657162000	-0.118338000	-0.537618000
F	1.510707000	-1.663156000	1.205416000
C	3.138493000	-0.259082000	-0.734186000
C	3.890315000	1.065625000	-0.540405000
O	-2.091093000	2.387830000	-0.469304000
H	4.957810000	0.937014000	-0.733065000
H	3.773886000	1.437316000	0.480050000
H	3.518398000	1.836103000	-1.220628000
H	-0.680216000	3.189850000	1.423782000
H	0.429342000	1.797176000	1.374002000
H	-1.066607000	1.704374000	2.307045000
H	3.324764000	-0.625633000	-1.750358000
H	3.532375000	-1.014591000	-0.052703000
H	1.124384000	0.580455000	-1.173409000
H	-3.000977000	0.373545000	-1.327970000
H	-1.645230000	-0.450420000	-2.106291000
H	-2.883094000	-2.371367000	-1.229704000
H	-3.340527000	-1.473698000	0.220228000
H	-0.597370000	-2.603105000	-0.489863000
H	-1.416111000	-2.701154000	1.063811000
H	-0.699318000	-0.549376000	1.682758000

Atomic coordinates of **2m** (trans, exo, distal 1)

C	1.099839000	-2.055007000	-0.563686000
C	2.569314000	-1.739994000	-0.254604000
C	2.478464000	-0.486069000	0.618832000
N	1.348926000	0.240557000	0.032801000
C	0.401073000	-0.672441000	-0.640333000
C	1.263236000	1.588286000	-0.171564000
C	2.303534000	2.459007000	0.511215000
C	-0.954744000	-0.674264000	-0.003280000
C	-2.116567000	-0.375197000	-0.560977000
F	-0.905381000	-1.066413000	1.309625000
C	-3.458936000	-0.412508000	0.105571000
C	-4.140737000	0.963715000	0.127728000
O	0.383362000	2.074461000	-0.869064000
H	-5.128240000	0.899163000	0.590784000
H	-4.269033000	1.357904000	-0.883447000
H	-3.545126000	1.685256000	0.690187000
H	1.978910000	3.493193000	0.425734000
H	3.275977000	2.358962000	0.021193000
H	2.429914000	2.200070000	1.564149000
H	-3.356206000	-0.794365000	1.122562000
H	-4.102591000	-1.118684000	-0.432229000
H	-2.072775000	-0.034506000	-1.589992000
H	3.386776000	0.112739000	0.593581000
H	2.271658000	-0.749972000	1.662414000
H	3.083463000	-2.562121000	0.245016000
H	3.114985000	-1.507526000	-1.172833000
H	0.665093000	-2.641986000	0.246458000
H	0.966104000	-2.614280000	-1.489265000
H	0.273283000	-0.338882000	-1.671440000

Atomic coordinates of **2n** (trans, exo, distal 2)

C	-0.577337000	2.060586000	-0.580082000
C	-2.092781000	2.145083000	-0.353430000
C	-2.378861000	0.928726000	0.531034000
N	-1.448732000	-0.078422000	0.014097000
C	-0.257820000	0.542910000	-0.602427000
C	-1.707088000	-1.405157000	-0.182174000
C	-2.977703000	-1.961212000	0.436593000
C	1.010549000	0.210387000	0.122183000
C	2.087943000	-0.391045000	-0.355011000
F	0.981644000	0.629372000	1.427287000
C	3.356615000	-0.667849000	0.393816000
C	4.589741000	-0.047822000	-0.278972000
O	-0.945887000	-2.116382000	-0.823846000
H	5.500003000	-0.301458000	0.269279000
H	4.510055000	1.041000000	-0.317332000
H	4.705688000	-0.409790000	-1.303930000
H	-2.931333000	-3.045629000	0.372673000
H	-3.859004000	-1.618374000	-0.112607000
H	-3.093515000	-1.659709000	1.479317000
H	3.494866000	-1.753520000	0.456410000
H	3.267816000	-0.304696000	1.418887000
H	2.025565000	-0.725828000	-1.384934000
H	-3.409184000	0.586230000	0.458593000
H	-2.165328000	1.151207000	1.582845000
H	-2.400097000	3.082703000	0.111645000
H	-2.630732000	2.044614000	-1.299746000
H	-0.049279000	2.534909000	0.248215000
H	-0.253713000	2.543599000	-1.501678000
H	-0.157923000	0.162767000	-1.620311000

Atomic coordinates of **2o** (trans, exo, proximal 1)

C	-0.681179000	2.187610000	-0.040929000
C	-1.975176000	2.023630000	0.766588000
C	-1.888292000	0.581609000	1.271307000
N	-1.257300000	-0.126599000	0.150819000
C	-0.413590000	0.778921000	-0.642065000
C	-1.679512000	-1.311480000	-0.393599000
C	-2.663388000	-2.137265000	0.416897000
C	1.046378000	0.425940000	-0.613591000
C	1.687143000	-0.520659000	0.049666000
F	1.736737000	1.285316000	-1.425198000
C	3.165296000	-0.776045000	0.015654000
C	3.813199000	-0.703107000	1.405475000
O	-1.270625000	-1.695339000	-1.478629000
H	4.879545000	-0.934475000	1.350161000
H	3.353013000	-1.415853000	2.095195000
H	3.705788000	0.294786000	1.837067000
H	-2.709376000	-3.127937000	-0.028797000
H	-3.662746000	-1.694841000	0.378909000
H	-2.372770000	-2.220141000	1.465780000
H	3.647578000	-0.066080000	-0.657925000
H	3.339200000	-1.773475000	-0.404545000
H	1.074398000	-1.173196000	0.660873000
H	-2.859777000	0.154441000	1.508336000
H	-1.261783000	0.518816000	2.168760000
H	-2.063307000	2.747787000	1.577684000
H	-2.849859000	2.132764000	0.120095000
H	0.142478000	2.467655000	0.618901000
H	-0.754253000	2.948158000	-0.816926000
H	-0.737938000	0.727718000	-1.685900000

Atomic coordinates of **2p** (trans, exo, proximal 2)

C	-1.140451000	-2.126056000	0.101462000
C	-2.489793000	-1.696658000	-0.489023000
C	-2.187619000	-0.316276000	-1.076462000
N	-1.237578000	0.255026000	-0.113853000
C	-0.480545000	-0.800025000	0.574562000
C	-1.300993000	1.510134000	0.433482000
C	-2.211589000	2.519044000	-0.244570000
C	0.993422000	-0.772393000	0.286102000
C	1.691875000	-0.010170000	-0.537139000
F	1.618991000	-1.738427000	1.027415000
C	3.176814000	-0.068030000	-0.746879000
C	3.874482000	1.247958000	-0.373392000
O	-0.641728000	1.810192000	1.416917000
H	4.948630000	1.185128000	-0.563552000
H	3.727082000	1.481340000	0.682850000
H	3.479587000	2.084635000	-0.955587000
H	-1.966173000	3.502514000	0.148845000
H	-3.259986000	2.307905000	-0.016107000
H	-2.098007000	2.519479000	-1.330130000
H	3.379677000	-0.290969000	-1.801117000
H	3.599037000	-0.890230000	-0.167017000
H	1.132369000	0.744069000	-1.078566000
H	-3.072464000	0.308373000	-1.173022000
H	-1.725654000	-0.406041000	-2.066595000
H	-2.868067000	-2.396977000	-1.235030000
H	-3.242607000	-1.602414000	0.297943000
H	-0.521619000	-2.590415000	-0.668990000
H	-1.238364000	-2.839169000	0.918665000
H	-0.601106000	-0.663261000	1.653453000

Atomic coordinates of **3a** (cis, endo, distal 1)

C	0.420025000	2.241110000	0.971776000
C	1.299730000	2.517247000	-0.253539000
C	2.053780000	1.201982000	-0.471852000
N	1.215374000	0.170700000	0.166179000
C	0.028043000	0.754109000	0.831916000
C	1.585195000	-1.122669000	0.207655000
C	0.685637000	-2.067960000	0.967591000
C	-1.245348000	0.546245000	0.059922000
C	-2.392940000	0.061886000	0.512674000
F	-1.149588000	0.969608000	-1.233639000
C	-3.666196000	-0.078632000	-0.267938000
C	-4.162880000	-1.529952000	-0.335928000
H	-5.109359000	-1.588771000	-0.877553000
H	-4.324259000	-1.941881000	0.663629000
H	-3.440206000	-2.168351000	-0.848400000
H	1.074189000	-3.077331000	0.879281000
H	-0.337811000	-2.039975000	0.587154000
H	0.651458000	-1.801607000	2.029345000
H	-3.524807000	0.315300000	-1.275304000
H	-4.438185000	0.539091000	0.205482000
H	-2.398874000	-0.267906000	1.547102000
H	3.038151000	1.194403000	0.003509000
H	2.207081000	0.958321000	-1.523146000
H	1.983469000	3.351172000	-0.093762000
H	0.681419000	2.751784000	-1.119977000
H	-0.453720000	2.888912000	1.038082000
H	0.999139000	2.360810000	1.890763000
H	-0.114637000	0.299700000	1.811996000
S	2.982209000	-1.677202000	-0.519523000

Atomic coordinates of **3b** (cis, endo, distal 2)

C	0.003590000	2.053705000	1.043775000
C	0.866022000	2.575678000	-0.111773000
C	1.878889000	1.452513000	-0.356320000
N	1.239452000	0.238003000	0.181786000
C	-0.071644000	0.530208000	0.805999000
C	1.861157000	-0.955757000	0.179074000
C	1.136359000	-2.107385000	0.833748000
C	-1.238245000	0.118044000	-0.047994000
C	-2.269369000	-0.636780000	0.303664000
F	-1.181968000	0.647634000	-1.304386000
C	-3.452428000	-0.975442000	-0.553859000
C	-4.779105000	-0.495683000	0.052482000
H	-5.620624000	-0.789915000	-0.578355000
H	-4.794344000	0.591858000	0.151523000

H	-4.940488000	-0.924017000	1.045164000
H	1.734041000	-3.007382000	0.732310000
H	0.156471000	-2.271958000	0.379808000
H	0.978984000	-1.913805000	1.900017000
H	-3.493888000	-2.063049000	-0.683256000
H	-3.319363000	-0.547215000	-1.548209000
H	-2.252126000	-1.031508000	1.314879000
H	2.823639000	1.612301000	0.169941000
H	2.122786000	1.308418000	-1.408874000
H	1.359939000	3.516517000	0.131866000
H	0.254260000	2.738219000	-0.999072000
H	-0.985577000	2.508504000	1.090482000
H	0.501160000	2.230361000	2.000528000
H	-0.163836000	-0.003733000	1.751319000
S	3.374323000	-1.175184000	-0.492242000

Atomic coordinates of **3c** (cis, endo, proximal 1)

C	0.337259000	2.497484000	0.353742000
C	0.820672000	2.358390000	-1.094272000
C	1.655884000	1.073793000	-1.079481000
N	1.118149000	0.295347000	0.052817000
C	0.073014000	1.037077000	0.773087000
C	1.636477000	-0.890113000	0.424727000
C	1.071868000	-1.518337000	1.676952000
C	-1.321287000	0.590125000	0.411738000
C	-1.729572000	-0.272341000	-0.505260000
F	-2.231913000	1.240987000	1.198277000
C	-3.154571000	-0.643155000	-0.794824000
C	-3.421537000	-2.145106000	-0.619974000
H	-4.454594000	-2.386535000	-0.879468000
H	-3.251052000	-2.456712000	0.412848000
H	-2.767323000	-2.741642000	-1.260681000
H	1.478473000	-2.518258000	1.789436000
H	-0.018830000	-1.572379000	1.650063000
H	1.355653000	-0.931452000	2.556789000
H	-3.386537000	-0.360733000	-1.828298000
H	-3.824535000	-0.066660000	-0.155367000
H	-0.953663000	-0.762137000	-1.083528000
H	2.718034000	1.261422000	-0.901748000
H	1.588099000	0.494872000	-2.000898000
H	1.402240000	3.217032000	-1.429255000
H	-0.032347000	2.250937000	-1.766751000
H	-0.548126000	3.121858000	0.465502000
H	1.126786000	2.910983000	0.985922000
H	0.191445000	0.918368000	1.851950000
S	2.864200000	-1.633886000	-0.427459000

Atomic coordinates of **3d** (cis, endo, proximal 2)

C	-0.036557000	2.407362000	0.275652000
C	0.259964000	2.227423000	-1.217417000
C	1.319514000	1.121542000	-1.248970000
N	1.096944000	0.360386000	-0.004402000
C	0.043770000	0.967687000	0.822709000
C	1.873725000	-0.678574000	0.355479000
C	1.610287000	-1.288231000	1.712148000
C	-1.277357000	0.247973000	0.719129000
C	-1.646128000	-0.750024000	-0.067808000
F	-2.164157000	0.785742000	1.610765000
C	-3.003480000	-1.389122000	-0.107271000
C	-3.655388000	-1.301580000	-1.494733000
H	-4.621773000	-1.810379000	-1.500366000
H	-3.027605000	-1.768748000	-2.257754000
H	-3.818996000	-0.261955000	-1.786884000
H	2.198342000	-2.194366000	1.816630000
H	0.553401000	-1.524012000	1.855687000
H	1.908152000	-0.593290000	2.504233000
H	-3.651966000	-0.930358000	0.640509000
H	-2.901939000	-2.444819000	0.169318000
H	-0.889323000	-1.132883000	-0.743781000
H	2.340197000	1.513023000	-1.242136000
H	1.240917000	0.461382000	-2.113142000
H	0.614555000	3.142970000	-1.690480000
H	-0.640836000	1.907783000	-1.744591000
H	-1.000541000	2.870820000	0.481302000
H	0.739376000	3.011582000	0.751863000
H	0.336377000	0.972009000	1.874692000
S	3.093148000	-1.262493000	-0.623418000

Atomic coordinates of **3e** (trans, endo, distal 1)

C	0.951835000	-2.036933000	-1.142933000
C	1.780189000	-2.376870000	0.103277000
C	2.294433000	-1.016663000	0.589557000
N	1.347396000	-0.029030000	0.031348000
C	0.320555000	-0.668442000	-0.822142000
C	1.505945000	1.304253000	0.123642000
C	2.627097000	1.767313000	1.023612000
C	-1.013726000	-0.761133000	-0.142514000
C	-2.162610000	-0.244138000	-0.546168000
F	-0.966161000	-1.503665000	1.011550000
C	-3.487683000	-0.377121000	0.142281000
C	-4.064055000	0.981194000	0.569308000
H	-5.044065000	0.855746000	1.035415000
H	-4.182218000	1.647577000	-0.288556000
H	-3.405536000	1.477257000	1.284777000
H	2.641270000	2.851824000	1.054459000
H	3.596366000	1.412528000	0.659708000
H	2.499636000	1.381628000	2.039502000
H	-3.390445000	-1.031822000	1.009637000
H	-4.193393000	-0.862959000	-0.541759000
H	-2.116477000	0.362753000	-1.443889000
H	3.299607000	-0.813126000	0.209484000
H	2.327983000	-0.952670000	1.678313000
H	2.601556000	-3.061312000	-0.111108000
H	1.148693000	-2.834939000	0.863445000
H	0.200913000	-2.790870000	-1.376111000
H	1.601074000	-1.926917000	-2.015141000
H	0.184799000	-0.053847000	-1.711129000
S	0.561378000	2.415413000	-0.691122000

Atomic coordinates of **3f** (trans, endo, distal 2)

C	-0.362678000	1.987130000	-1.219994000
C	-1.205777000	2.609533000	-0.099189000
C	-2.104080000	1.459373000	0.370853000
N	-1.385853000	0.229306000	-0.023110000
C	-0.143913000	0.529421000	-0.770964000
C	-1.886278000	-1.012936000	0.110045000
C	-3.180650000	-1.116215000	0.881530000
C	1.088604000	0.331113000	0.061053000
C	2.097503000	-0.490876000	-0.176202000
F	1.111237000	1.140503000	1.169844000
C	3.337654000	-0.640773000	0.651783000
C	4.620070000	-0.381870000	-0.152044000
H	5.505084000	-0.540230000	0.468330000
H	4.648503000	0.643837000	-0.526703000
H	4.690537000	-1.053045000	-1.011901000
H	-3.472952000	-2.158275000	0.958819000
H	-3.981320000	-0.561776000	0.382308000
H	-3.073411000	-0.698930000	1.887215000
H	3.367890000	-1.662056000	1.048736000
H	3.293273000	0.028394000	1.512416000
H	1.993765000	-1.124724000	-1.050104000
H	-3.078474000	1.488024000	-0.125339000
H	-2.275472000	1.482152000	1.448178000
H	-1.793411000	3.463006000	-0.438712000
H	-0.563972000	2.943366000	0.715131000
H	0.578173000	2.509814000	-1.388264000
H	-0.919075000	1.984582000	-2.160652000
H	-0.076243000	-0.159310000	-1.612031000
S	-1.169111000	-2.381119000	-0.525968000

Atomic coordinates of **3g** (trans, endo, proximal 1)

C	0.784021000	2.311804000	0.695972000
C	1.175965000	2.465102000	-0.777513000
C	1.851634000	1.130832000	-1.107580000
N	1.238909000	0.165245000	-0.168444000
C	0.350843000	0.836092000	0.790927000
C	1.624662000	-1.121924000	-0.044889000
C	2.627366000	-1.602038000	-1.067301000
C	-1.109437000	0.651731000	0.472765000
C	-1.696206000	0.085175000	-0.567783000
F	-1.864377000	1.196841000	1.473676000
C	-3.175193000	-0.062938000	-0.774356000
C	-3.610454000	-1.532966000	-0.863005000
H	-4.685575000	-1.607965000	-1.042050000
H	-3.379628000	-2.064648000	0.061961000
H	-3.098161000	-2.049545000	-1.678789000
H	2.836020000	-2.653913000	-0.902230000
H	3.564120000	-1.041063000	-0.991053000
H	2.250894000	-1.468077000	-2.085909000
H	-3.457880000	0.448200000	-1.702250000
H	-3.712314000	0.436534000	0.033325000
H	-1.037465000	-0.348872000	-1.311553000
H	2.930575000	1.180953000	-0.933484000
H	1.694043000	0.824324000	-2.142900000
H	1.838883000	3.311129000	-0.959869000
H	0.284358000	2.598879000	-1.392631000
H	-0.005857000	2.992681000	1.009055000
H	1.648871000	2.475145000	1.343904000
H	0.524002000	0.416215000	1.784066000
S	1.060809000	-2.146468000	1.142689000

Atomic coordinates of **3h** (trans, endo, proximal 2)

C	-0.206735000	2.227844000	-0.926665000
C	-0.318995000	2.588713000	0.558405000
C	-1.314694000	1.558967000	1.100545000
N	-1.162078000	0.391806000	0.203360000
C	-0.257990000	0.688103000	-0.916458000
C	-1.929950000	-0.715983000	0.263023000
C	-2.870070000	-0.793100000	1.442657000
C	1.108292000	0.076854000	-0.747864000
C	1.624574000	-0.603492000	0.261359000
F	1.855230000	0.314674000	-1.868064000
C	3.006763000	-1.183930000	0.319019000
C	3.803151000	-0.704496000	1.540514000
H	4.787055000	-1.177919000	1.572570000
H	3.285699000	-0.949052000	2.472104000
H	3.950176000	0.377755000	1.514500000
H	-3.409693000	-1.733938000	1.413686000
H	-3.592529000	0.028813000	1.423536000
H	-2.324532000	-0.723903000	2.388678000
H	3.547136000	-0.942908000	-0.597534000
H	2.924696000	-2.276419000	0.355419000
H	0.970819000	-0.774350000	1.109074000
H	-2.340790000	1.934741000	1.045274000
H	-1.114010000	1.285046000	2.137510000
H	-0.659171000	3.610421000	0.728270000
H	0.649103000	2.471016000	1.048540000
H	0.698681000	2.604932000	-1.399360000
H	-1.065257000	2.612722000	-1.482705000
H	-0.687891000	0.280509000	-1.834034000
S	-1.878005000	-1.939941000	-0.867105000

Atomic coordinates of **3i** (cis, exo, distal 1)

C	-0.456104000	2.397267000	-0.447691000
C	-1.978145000	2.385099000	-0.289341000
C	-2.240820000	1.074114000	0.445453000
N	-1.239407000	0.160636000	-0.124176000
C	-0.062617000	0.908202000	-0.637765000
C	-1.440016000	-1.168006000	-0.225320000
C	-0.401249000	-1.963847000	-0.977579000
C	1.221351000	0.592028000	0.071408000
C	2.394158000	0.293829000	-0.468099000
F	1.104407000	0.722944000	1.423633000
C	3.682064000	0.081431000	0.270866000
C	4.277728000	-1.314781000	0.038705000
H	5.233384000	-1.417357000	0.557168000
H	4.453047000	-1.500416000	-1.024174000

H	3.608331000	-2.094315000	0.408377000
H	-0.773977000	-2.971071000	-1.133556000
H	0.531807000	-2.017489000	-0.412667000
H	-0.169429000	-1.513923000	-1.947620000
H	3.525480000	0.248030000	1.337518000
H	4.405293000	0.834993000	-0.061950000
H	2.410038000	0.187455000	-1.548480000
H	-3.233182000	0.658713000	0.287147000
H	-2.088947000	1.170154000	1.525444000
H	-2.350828000	3.250980000	0.258531000
H	-2.470116000	2.367071000	-1.265380000
H	0.011680000	2.781997000	0.459794000
H	-0.105300000	3.000796000	-1.284635000
H	0.080198000	0.685106000	-1.697489000
S	-2.769337000	-1.938356000	0.432168000

Atomic coordinates of **3j** (cis, exo, distal 2)

C	0.029145000	2.258988000	-0.430534000
C	-1.458685000	2.597283000	-0.314540000
C	-2.032914000	1.386102000	0.414108000
N	-1.252826000	0.263766000	-0.128099000
C	0.073993000	0.719933000	-0.618236000
C	-1.748824000	-0.985004000	-0.228867000
C	-0.902313000	-2.006201000	-0.949434000
C	1.237149000	0.116856000	0.112491000
C	2.310239000	-0.460995000	-0.406890000
F	1.135914000	0.282986000	1.462169000
C	3.504903000	-0.958595000	0.350861000
C	4.809078000	-0.280602000	-0.093552000
H	5.662505000	-0.690047000	0.451096000
H	4.774076000	0.795267000	0.091028000
H	4.991017000	-0.430814000	-1.160910000
H	-1.502865000	-2.890504000	-1.137436000
H	-0.039656000	-2.291906000	-0.343138000
H	-0.520668000	-1.623100000	-1.900322000
H	3.596262000	-2.039877000	0.195464000
H	3.350787000	-0.808753000	1.420316000
H	2.318567000	-0.570878000	-1.486959000
H	-3.089760000	1.207526000	0.230514000
H	-1.890350000	1.451983000	1.497624000
H	-1.637913000	3.529337000	0.222046000
H	-1.915121000	2.684686000	-1.304012000
H	0.545446000	2.524850000	0.493120000
H	0.533859000	2.765308000	-1.253120000
H	0.180260000	0.468769000	-1.676000000
S	-3.233782000	-1.425104000	0.399089000

Atomic coordinates of **3k** (cis, exo, proximal 1)

C	0.504845000	2.512095000	0.079472000
C	1.860928000	2.330334000	-0.616995000
C	1.839402000	0.876992000	-1.084344000
N	1.124450000	0.194385000	0.002225000
C	0.143569000	1.098237000	0.627009000
C	1.429461000	-1.046218000	0.433976000
C	0.757077000	-1.502512000	1.707299000
C	-1.284170000	0.740418000	0.309097000
C	-1.773919000	-0.146503000	-0.541468000
F	-2.123656000	1.543138000	1.031307000
C	-3.228240000	-0.394829000	-0.818004000
C	-3.649058000	-1.840352000	-0.516951000
H	-4.699547000	-1.997793000	-0.771147000
H	-3.519078000	-2.074892000	0.541842000
H	-3.054633000	-2.554394000	-1.092307000
H	1.054594000	-2.523615000	1.921758000
H	-0.331077000	-1.453642000	1.630381000
H	1.058822000	-0.867991000	2.547115000
H	-3.423740000	-0.182337000	-1.875448000
H	-3.839485000	0.300979000	-0.241412000
H	-1.048836000	-0.752488000	-1.074118000
H	2.819722000	0.423504000	-1.205298000
H	1.295824000	0.758380000	-2.027989000
H	2.004513000	3.030871000	-1.440112000
H	2.680934000	2.472732000	0.090952000
H	-0.254340000	2.829186000	-0.636838000
H	0.531053000	3.252561000	0.877873000
H	0.258706000	1.077530000	1.713906000
S	2.506810000	-2.047094000	-0.358190000

Atomic coordinates of **3l** (cis, exo, proximal 2)

C	0.005145000	2.436589000	0.020442000
C	1.245730000	2.478015000	-0.883360000
C	1.467248000	1.016715000	-1.266429000
N	1.090683000	0.296849000	-0.042589000
C	0.045124000	1.030225000	0.690785000
C	1.717060000	-0.814821000	0.394239000
C	1.356658000	-1.291590000	1.781490000
C	-1.302221000	0.359854000	0.636542000
C	-1.712257000	-0.676325000	-0.076173000
F	-2.171354000	1.021710000	1.459075000
C	-3.103916000	-1.238179000	-0.098094000
C	-3.727508000	-1.209327000	-1.500952000
H	-4.722128000	-1.660486000	-1.491297000
H	-3.116142000	-1.763399000	-2.217714000
H	-3.824341000	-0.184534000	-1.866216000
H	1.905701000	-2.201454000	2.000330000
H	0.286170000	-1.486459000	1.875509000
H	1.621970000	-0.535763000	2.527974000
H	-3.736112000	-0.691823000	0.603396000
H	-3.069151000	-2.276125000	0.252170000
H	-0.966885000	-1.151237000	-0.705115000
H	2.491825000	0.764265000	-1.526778000
H	0.824034000	0.710411000	-2.098722000
H	1.106828000	3.120881000	-1.753007000
H	2.113960000	2.845001000	-0.330782000
H	-0.905074000	2.530968000	-0.573359000
H	-0.006200000	3.231381000	0.765190000
H	0.326698000	1.125576000	1.742738000
S	2.851867000	-1.637342000	-0.514301000

Atomic coordinates of **3m** (trans, exo, distal 1)

C	0.990035000	-2.168007000	-0.835932000
C	2.440521000	-2.006464000	-0.361096000
C	2.347063000	-0.888735000	0.677101000
N	1.337698000	0.012110000	0.099557000
C	0.351695000	-0.759153000	-0.696705000
C	1.381925000	1.356470000	0.118668000
C	2.442209000	1.978470000	0.999433000
C	-0.994269000	-0.813047000	-0.041972000
C	-2.159709000	-0.426386000	-0.533364000
F	-0.930113000	-1.384916000	1.204086000
C	-3.492204000	-0.546268000	0.142680000
C	-4.152823000	0.819465000	0.383396000
H	-5.135100000	0.696869000	0.845560000
H	-4.288007000	1.364754000	-0.553948000
H	-3.539913000	1.439249000	1.040427000
H	2.270173000	3.048232000	1.061378000
H	3.439857000	1.817428000	0.578662000
H	2.432101000	1.551240000	2.005939000
H	-3.381113000	-1.079102000	1.088318000
H	-4.153023000	-1.154459000	-0.486163000
H	-2.125248000	0.057336000	-1.503543000
H	3.290005000	-0.371799000	0.831134000
H	2.000456000	-1.273291000	1.642414000
H	2.854757000	-2.925892000	0.054161000
H	3.084592000	-1.686192000	-1.183670000
H	0.462596000	-2.877459000	-0.197888000
H	0.916848000	-2.526880000	-1.861982000
H	0.234265000	-0.260300000	-1.658831000
S	0.357327000	2.330105000	-0.771806000

Atomic coordinates of **3n** (trans, exo, distal 2)

C	-0.372418000	2.160228000	-0.875683000
C	-1.850237000	2.411555000	-0.547538000
C	-2.156146000	1.359028000	0.517295000
N	-1.378232000	0.196132000	0.062545000
C	-0.153989000	0.639666000	-0.648502000
C	-1.786283000	-1.085230000	0.102842000
C	-3.049617000	-1.359969000	0.887512000
C	1.092379000	0.359017000	0.133013000
C	2.142293000	-0.356701000	-0.233544000
F	1.077480000	0.981494000	1.355928000
C	3.397472000	-0.565504000	0.557931000
C	4.658873000	-0.158575000	-0.217127000
H	5.557211000	-0.360112000	0.370700000
H	4.644862000	0.906549000	-0.459335000
H	4.742308000	-0.712967000	-1.155434000
H	-3.178220000	-2.432724000	0.989898000
H	-3.925001000	-0.959655000	0.366226000
H	-3.015026000	-0.903140000	1.880336000
H	3.469326000	-1.627403000	0.820612000
H	3.340161000	-0.014539000	1.497931000
H	2.062468000	-0.851964000	-1.195115000
H	-3.213278000	1.118910000	0.586689000
H	-1.808424000	1.682302000	1.504423000
H	-2.039030000	3.426310000	-0.195350000
H	-2.477811000	2.235507000	-1.424596000
H	0.264680000	2.730386000	-0.199073000
H	-0.109673000	2.441442000	-1.894895000
H	-0.091380000	0.085445000	-1.585145000
S	-0.987927000	-2.336988000	-0.662889000

Atomic coordinates of **3o** (trans, exo, proximal 1)

C	-0.351107000	2.334967000	-0.553758000
C	-1.528650000	2.548333000	0.406393000
C	-1.521153000	1.279307000	1.257558000
N	-1.152015000	0.233323000	0.288066000
C	-0.270596000	0.793600000	-0.749866000
C	-1.738986000	-0.977383000	0.179128000
C	-2.672922000	-1.372548000	1.301208000
C	1.146218000	0.300020000	-0.662189000
C	1.728840000	-0.490651000	0.221578000
F	1.868304000	0.825584000	-1.698018000
C	3.170790000	-0.905022000	0.216976000
C	3.895092000	-0.552088000	1.523489000
H	4.929424000	-0.902883000	1.501193000
H	3.405487000	-1.013673000	2.385227000
H	3.908205000	0.528130000	1.686352000
H	-2.937627000	-2.419141000	1.190524000
H	-3.594376000	-0.782591000	1.265545000
H	-2.217026000	-1.217808000	2.283138000
H	3.683530000	-0.446649000	-0.629840000
H	3.221982000	-1.989241000	0.064133000
H	1.092380000	-0.888218000	1.003830000
H	-2.480980000	1.066419000	1.717958000
H	-0.765772000	1.340643000	2.049308000
H	-1.427330000	3.453576000	1.006235000
H	-2.470755000	2.611133000	-0.143611000
H	0.575319000	2.699417000	-0.106920000
H	-0.481205000	2.850144000	-1.504246000
H	-0.664151000	0.491319000	-1.724452000
S	-1.479556000	-2.012207000	-1.101361000

Atomic coordinates of **3p** (trans, exo, proximal 2)

C	-0.993668000	-2.310695000	0.406374000
C	-2.294502000	-2.089276000	-0.377405000
C	-2.012771000	-0.816860000	-1.175050000
N	-1.215735000	-0.007522000	-0.237566000
C	-0.417545000	-0.883477000	0.635893000
C	-1.378680000	1.311899000	-0.004138000
C	-2.286819000	2.053331000	-0.959460000
C	1.056817000	-0.829932000	0.348570000
C	1.722880000	-0.215672000	-0.613275000
F	1.720309000	-1.595110000	1.267246000
C	3.210601000	-0.238667000	-0.809139000
C	3.837268000	1.159910000	-0.711195000
H	4.914469000	1.114262000	-0.887937000
H	3.670276000	1.593988000	0.276323000

H	3.405021000	1.840414000	-1.449330000
H	-2.206224000	3.119016000	-0.771218000
H	-3.330629000	1.758572000	-0.811496000
H	-2.029627000	1.851391000	-2.003137000
H	3.433213000	-0.659497000	-1.796828000
H	3.668625000	-0.903949000	-0.075668000
H	1.134005000	0.390422000	-1.292287000
H	-2.914279000	-0.292614000	-1.477136000
H	-1.425783000	-1.036730000	-2.074218000
H	-2.552174000	-2.933983000	-1.017394000
H	-3.131287000	-1.913633000	0.302935000
H	-0.290527000	-2.902663000	-0.181689000
H	-1.152385000	-2.831588000	1.349415000
H	-0.562702000	-0.552702000	1.667907000
S	-0.641507000	2.120285000	1.253278000

Atomic coordinates of **4a** (cis, endo, distal 1)

C	-1.072321000	-1.974802000	0.815800000
C	-1.958425000	-2.062326000	-0.433501000
C	-2.433124000	-0.620652000	-0.640356000
N	-1.369517000	0.194486000	-0.033109000
C	-0.349742000	-0.617340000	0.664348000
C	-1.487721000	1.552863000	-0.025593000
C	-0.423349000	2.345241000	0.709071000
C	0.939402000	-0.726360000	-0.109965000
C	2.143836000	-0.466400000	0.389616000
C	3.443151000	-0.595935000	-0.350446000
C	4.226628000	0.722713000	-0.419420000
O	-2.428857000	2.105608000	-0.582365000
H	5.182198000	0.583021000	-0.929784000
H	4.437155000	1.109906000	0.581060000
H	3.662492000	1.485983000	-0.960086000
H	-0.595062000	3.400391000	0.510672000
H	0.582587000	2.067310000	0.392201000
H	-0.492582000	2.174727000	1.787312000
H	3.253686000	-0.970686000	-1.360352000
H	4.065062000	-1.348576000	0.149313000
H	2.217533000	-0.121541000	1.421530000
H	-3.382268000	-0.421021000	-0.134157000
H	-2.568533000	-0.354353000	-1.689011000
H	-2.791038000	-2.755925000	-0.313366000
H	-1.373313000	-2.399417000	-1.292584000
H	-0.370322000	-2.802828000	0.913038000
H	-1.693616000	-1.950129000	1.715199000
H	-0.136097000	-0.188469000	1.645669000
H	0.849587000	-1.056667000	-1.143296000

Atomic coordinates of **4b** (cis, endo, distal 2)

C	0.519263000	1.955979000	0.865866000
C	1.421235000	2.334937000	-0.315906000
C	2.289331000	1.089657000	-0.518175000
N	1.453590000	-0.010932000	-0.013702000
C	0.209441000	0.460206000	0.631682000
C	1.934158000	-1.286720000	-0.046283000
C	1.080516000	-2.374043000	0.577630000
C	-1.010581000	0.245649000	-0.227435000
C	-2.114818000	-0.378151000	0.171634000
C	-3.354786000	-0.572603000	-0.651307000
C	-4.600147000	0.060311000	-0.014080000
O	3.022146000	-1.536254000	-0.551515000
H	-5.488589000	-0.130207000	-0.620300000
H	-4.482724000	1.141768000	0.085632000
H	-4.783901000	-0.347792000	0.983303000
H	1.550256000	-3.331259000	0.364938000
H	0.062540000	-2.365546000	0.185998000
H	1.021862000	-2.243845000	1.662008000
H	-3.534096000	-1.646959000	-0.779835000
H	-3.198136000	-0.161444000	-1.652556000
H	-2.148636000	-0.782607000	1.183833000
H	3.219855000	1.137091000	0.055456000
H	2.564317000	0.915589000	-1.558772000
H	2.018683000	3.226463000	-0.123566000
H	0.819256000	2.529666000	-1.206858000
H	-0.388517000	2.555334000	0.933923000
H	1.067704000	2.063872000	1.805614000
H	0.064192000	-0.051586000	1.585513000
H	-0.958021000	0.646682000	-1.238060000

Atomic coordinates of **4c** (cis, endo, proximal 1)

C	-1.310558000	-1.964665000	0.844179000
C	-1.603031000	-2.054434000	-0.658937000
C	-1.905451000	-0.604721000	-1.055979000
N	-1.178089000	0.196682000	-0.058389000
C	-0.539745000	-0.630468000	0.973482000
C	-1.313716000	1.553004000	-0.052073000
C	-0.656551000	2.316979000	1.083064000
C	0.950064000	-0.820750000	0.795238000
C	1.694359000	-0.371525000	-0.209328000
C	3.171284000	-0.595111000	-0.361019000
C	3.972571000	0.714046000	-0.403101000
O	-1.955121000	2.127134000	-0.923901000
H	5.036194000	0.516510000	-0.554908000
H	3.861057000	1.271366000	0.529785000
H	3.633364000	1.358605000	-1.218078000
H	-0.660268000	3.372788000	0.822788000
H	0.365499000	1.985942000	1.270898000
H	-1.229274000	2.186279000	2.005896000
H	3.353799000	-1.147511000	-1.290753000
H	3.534902000	-1.228565000	0.453298000
H	1.217001000	0.218062000	-0.989900000
H	-2.972376000	-0.371290000	-1.000644000
H	-1.575679000	-0.356885000	-2.065909000
H	-2.431148000	-2.724934000	-0.889643000
H	-0.721089000	-2.417923000	-1.190185000
H	-0.740807000	-2.812020000	1.226837000
H	-2.243729000	-1.899581000	1.410103000
H	-0.716029000	-0.195022000	1.961174000
H	1.420816000	-1.403800000	1.586014000

Atomic coordinates of **4d** (cis, endo, proximal 2)

C	0.650530000	2.056587000	0.994569000
C	0.672408000	2.330808000	-0.514347000
C	1.431041000	1.129164000	-1.089610000
N	1.199432000	0.058641000	-0.106489000
C	0.455779000	0.524276000	1.071106000
C	1.823534000	-1.143788000	-0.257514000
C	1.661540000	-2.161631000	0.856745000
C	-1.006984000	0.140202000	1.084666000
C	-1.670955000	-0.496210000	0.125962000
C	-3.131877000	-0.840252000	0.165666000
C	-3.925562000	-0.204336000	-0.984720000
O	2.500008000	-1.383353000	-1.250539000
H	-4.974724000	-0.506627000	-0.949698000
H	-3.523840000	-0.506389000	-1.955368000
H	-3.884929000	0.886125000	-0.932479000
H	2.016416000	-3.121184000	0.488190000
H	0.627147000	-2.253016000	1.190175000
H	2.270762000	-1.875649000	1.719200000
H	-3.558091000	-0.534506000	1.125600000
H	-3.243328000	-1.929719000	0.107369000
H	-1.132849000	-0.796569000	-0.771207000
H	2.504982000	1.316653000	-1.175583000
H	1.078299000	0.829787000	-2.077581000
H	1.150844000	3.277643000	-0.765748000
H	-0.347129000	2.358053000	-0.904212000
H	-0.132252000	2.601244000	1.523409000
H	1.611415000	2.321855000	1.443563000
H	0.921512000	0.137072000	1.981856000
H	-1.537044000	0.442640000	1.987104000

Atomic coordinates of **4e** (cis, endo, distal 1)

C	-1.093232000	-2.065617000	0.709656000
C	-1.954144000	-2.026150000	-0.560151000
C	-2.379442000	-0.556248000	-0.656967000
N	-1.284040000	0.169096000	0.000646000
C	-0.319554000	-0.732680000	0.673640000
C	-1.241161000	1.516761000	0.210075000
C	-2.319869000	2.340415000	-0.471591000
C	0.986035000	-0.825449000	-0.071747000
C	2.154726000	-0.422971000	0.414746000
C	3.471220000	-0.505751000	-0.299664000
C	4.127338000	0.868765000	-0.495730000
O	-0.379557000	2.038245000	0.905534000
H	5.097772000	0.771837000	-0.988513000
H	4.286535000	1.369406000	0.462650000
H	3.496767000	1.518991000	-1.105681000
H	-2.152446000	3.386181000	-0.226347000
H	-3.317763000	2.047557000	-0.134967000
H	-2.288519000	2.214266000	-1.556634000
H	3.334712000	-0.995846000	-1.268392000
H	4.153385000	-1.141848000	0.277918000
H	2.174526000	0.032616000	1.403676000
H	-3.326004000	-0.388959000	-0.130203000
H	-2.512879000	-0.231082000	-1.690916000
H	-2.811449000	-2.698936000	-0.519912000
H	-1.358357000	-2.303365000	-1.433026000
H	-0.425863000	-2.926392000	0.750407000
H	-1.732609000	-2.092702000	1.596348000
H	-0.126387000	-0.344159000	1.673823000
H	0.941815000	-1.253657000	-1.072633000

Atomic coordinates of **4f** (cis, endo, distal 2)

C	-0.586607000	2.038212000	-0.802320000
C	-1.513249000	2.293719000	0.393910000
C	-2.296684000	0.981728000	0.523781000
N	-1.375602000	-0.030284000	-0.011194000
C	-0.170788000	0.563566000	-0.637751000
C	-1.652797000	-1.358371000	-0.153995000
C	-2.947427000	-1.849300000	0.469690000
C	1.058081000	0.384975000	0.215229000
C	2.104143000	-0.358775000	-0.127411000
C	3.343463000	-0.550271000	0.695466000
C	4.619553000	-0.096654000	-0.028195000
O	-0.899882000	-2.117653000	-0.749861000
H	5.505061000	-0.285847000	0.583211000
H	4.583762000	0.972099000	-0.252216000
H	4.747134000	-0.630220000	-0.973642000
H	-3.026094000	-2.918213000	0.288098000
H	-3.815139000	-1.346355000	0.034996000
H	-2.964617000	-1.663499000	1.546414000
H	3.440302000	-1.613582000	0.945814000
H	3.243084000	-0.014338000	1.644001000
H	2.072412000	-0.890687000	-1.076935000
H	-3.218017000	1.018486000	-0.068785000
H	-2.574993000	0.765896000	1.557425000
H	-2.171390000	3.151735000	0.253349000
H	-0.927225000	2.472460000	1.298511000
H	0.273727000	2.706834000	-0.831656000
H	-1.139522000	2.159224000	-1.737895000
H	-0.006938000	0.073654000	-1.597727000
H	1.060601000	0.902597000	1.173858000

Atomic coordinates of **4g** (cis, endo, proximal 1)

C	-1.190812000	-2.086560000	0.725050000
C	-1.545258000	-2.045812000	-0.766393000
C	-1.916693000	-0.576440000	-1.003344000
N	-1.141016000	0.152319000	0.012975000
C	-0.448272000	-0.751512000	0.944904000
C	-1.255615000	1.485910000	0.283599000
C	-2.100738000	2.299947000	-0.680465000
C	1.036806000	-0.878064000	0.701118000
C	1.745935000	-0.278552000	-0.247057000
C	3.227312000	-0.425398000	-0.443164000
C	3.979390000	0.906987000	-0.313631000
O	-0.704754000	2.002508000	1.245968000
H	5.048756000	0.771565000	-0.492915000
H	3.850711000	1.332750000	0.683652000

H	3.609801000	1.639895000	-1.035574000
H	-2.049113000	3.342583000	-0.377291000
H	-3.144049000	1.973889000	-0.663075000
H	-1.743770000	2.202765000	-1.708526000
H	3.419627000	-0.841543000	-1.439934000
H	3.624004000	-1.147704000	0.276435000
H	1.238401000	0.400760000	-0.929017000
H	-2.990081000	-0.416420000	-0.855275000
H	-1.666525000	-0.244772000	-2.013705000
H	-2.357232000	-2.721845000	-1.035960000
H	-0.671831000	-2.312472000	-1.364665000
H	-0.583921000	-2.950300000	0.997293000
H	-2.099897000	-2.105914000	1.332448000
H	-0.595372000	-0.374257000	1.959768000
H	1.543297000	-1.538322000	1.404068000

Atomic coordinates of **4h** (cis, endo, proximal 2)

C	-0.648787000	2.169774000	-0.778769000
C	-0.755249000	2.241786000	0.749490000
C	-1.508783000	0.956406000	1.114435000
N	-1.161952000	0.023723000	0.030266000
C	-0.390562000	0.671145000	-1.042824000
C	-1.715652000	-1.211352000	-0.152146000
C	-2.604710000	-1.723879000	0.967201000
C	1.081347000	0.333748000	-1.041819000
C	1.718859000	-0.456156000	-0.186874000
C	3.185300000	-0.774437000	-0.229982000
C	3.921055000	-0.397791000	1.063563000
O	-1.506297000	-1.873842000	-1.158924000
H	4.975385000	-0.679696000	1.011565000
H	3.483757000	-0.905129000	1.927774000
H	3.866777000	0.678035000	1.246983000
H	-2.916042000	-2.734580000	0.715826000
H	-3.491506000	-1.095302000	1.083952000
H	-2.080633000	-1.732844000	1.925794000
H	3.647437000	-0.267418000	-1.082092000
H	3.309312000	-1.850202000	-0.403810000
H	1.149005000	-0.932388000	0.608443000
H	-2.589910000	1.130885000	1.140478000
H	-1.211035000	0.565845000	2.090245000
H	-1.272355000	3.133785000	1.104408000
H	0.241418000	2.230913000	1.194949000
H	0.138730000	2.805861000	-1.183443000
H	-1.594517000	2.466401000	-1.240573000
H	-0.809434000	0.356675000	-2.001832000
H	1.640749000	0.798361000	-1.852787000

Atomic coordinates of **4i** (cis, exo, distal 1)

C	-1.047032000	-2.095156000	0.255178000
C	-2.545624000	-1.784903000	0.217738000
C	-2.596676000	-0.462618000	-0.546404000
N	-1.373241000	0.224257000	-0.111002000
C	-0.358926000	-0.716106000	0.421210000
C	-1.358519000	1.588309000	-0.017561000
C	-0.154797000	2.236412000	0.637810000
C	0.960329000	-0.667190000	-0.298396000
C	2.149262000	-0.622310000	0.294066000
C	3.475731000	-0.646625000	-0.407811000
C	4.339074000	0.585819000	-0.103030000
O	-2.288657000	2.263338000	-0.441921000
H	5.310572000	0.513955000	-0.597178000
H	4.518339000	0.686842000	0.970636000
H	3.852317000	1.501379000	-0.446485000
H	-0.365221000	3.298376000	0.738206000
H	0.742392000	2.098578000	0.032965000
H	0.049731000	1.810407000	1.622886000
H	3.317850000	-0.734714000	-1.486495000
H	4.025197000	-1.544696000	-0.100248000
H	2.188094000	-0.556851000	1.381794000
H	-3.460878000	0.158077000	-0.318560000
H	-2.584725000	-0.626668000	-1.629887000
H	-3.130176000	-2.571025000	-0.261980000
H	-2.935300000	-1.645385000	1.229825000
H	-0.734280000	-2.541859000	-0.692588000
H	-0.753271000	-2.779461000	1.051448000
H	-0.193981000	-0.515640000	1.485646000
H	0.898344000	-0.721610000	-1.384408000

Atomic coordinates of **4j** (cis, exo, distal 2)

C	0.487716000	2.085776000	0.257738000
C	2.014145000	2.203716000	0.240760000
C	2.440395000	0.951405000	-0.523802000
N	1.448227000	-0.049797000	-0.108961000
C	0.207645000	0.569921000	0.413830000
C	1.808847000	-1.365914000	-0.022053000
C	0.821501000	-2.328326000	0.608987000
C	-1.038473000	0.157650000	-0.319195000
C	-2.165213000	-0.243360000	0.260497000
C	-3.438016000	-0.591338000	-0.454351000
C	-4.622245000	0.289929000	-0.031445000
O	2.895234000	-1.754257000	-0.434234000
H	-5.537932000	-0.014949000	-0.543045000
H	-4.433821000	1.339331000	-0.269062000
H	-4.802679000	0.219334000	1.044445000
H	1.323701000	-3.285511000	0.726544000
H	-0.058633000	-2.455688000	-0.022894000
H	0.473464000	-1.976410000	1.582864000
H	-3.689138000	-1.638894000	-0.247887000
H	-3.284375000	-0.514661000	-1.534484000
H	-2.192181000	-0.325457000	1.347365000
H	3.438933000	0.592364000	-0.282799000
H	2.399758000	1.111234000	-1.607157000
H	2.363832000	3.123383000	-0.230089000
H	2.413713000	2.173040000	1.258077000
H	0.075666000	2.433081000	-0.693885000
H	0.005653000	2.658353000	1.050473000
H	0.094737000	0.326773000	1.476295000
H	-0.987974000	0.240555000	-1.403961000

Atomic coordinates of **4k** (cis, exo, proximal 1)

C	-0.746087000	2.111733000	-0.711961000
C	-1.915898000	2.126790000	0.281070000
C	-1.659249000	0.886971000	1.137910000
N	-1.124019000	-0.074714000	0.168869000
C	-0.425146000	0.601953000	-0.936952000
C	-1.548361000	-1.375363000	0.176123000
C	-1.171522000	-2.236197000	-1.015593000
C	1.064085000	0.359281000	-0.998497000
C	1.800742000	-0.295051000	-0.107626000
C	3.289974000	-0.472444000	-0.178822000
C	4.019340000	0.129023000	1.031157000
O	-2.219054000	-1.826210000	1.096186000
H	5.094880000	-0.052086000	0.969207000
H	3.660671000	-0.309946000	1.965759000
H	3.859609000	1.208267000	1.087887000
H	-1.412724000	-3.267924000	-0.771936000
H	-0.115673000	-2.152529000	-1.273250000
H	-1.754892000	-1.940259000	-1.892557000
H	3.671670000	-0.027483000	-1.102386000
H	3.521048000	-1.543402000	-0.229346000
H	1.306960000	-0.735404000	0.756580000
H	-2.545686000	0.466605000	1.606950000
H	-0.924327000	1.092676000	1.924466000
H	-1.957075000	3.045983000	0.867196000
H	-2.869140000	2.018447000	-0.242944000
H	0.125207000	2.602767000	-0.273910000
H	-0.972382000	2.618289000	-1.650941000
H	-0.864893000	0.282482000	-1.888027000
H	1.550037000	0.806023000	-1.865170000

Atomic coordinates of **4l** (cis, exo, proximal 2)

C	-1.346522000	-2.029924000	0.518679000
C	-2.579403000	-1.562520000	-0.264902000
C	-2.048050000	-0.375255000	-1.067902000
N	-1.101793000	0.251563000	-0.138151000
C	-0.533284000	-0.730216000	0.802094000
C	-1.080045000	1.611768000	0.011801000
C	-0.300433000	2.170158000	1.187977000
C	0.951010000	-0.969892000	0.663935000
C	1.750758000	-0.488363000	-0.280932000
C	3.217110000	-0.785334000	-0.408618000
C	4.090193000	0.476416000	-0.354144000
O	-1.678577000	2.351307000	-0.759069000
H	5.145105000	0.228433000	-0.492274000
H	3.985041000	0.984857000	0.607070000
H	3.808742000	1.184811000	-1.137492000
H	-0.219926000	3.246173000	1.054638000
H	0.693318000	1.731490000	1.276701000
H	-0.837722000	1.974865000	2.120810000
H	3.394824000	-1.293085000	-1.364527000
H	3.522487000	-1.484345000	0.375485000
H	1.331241000	0.182049000	-1.028844000
H	-2.801972000	0.353577000	-1.355763000
H	-1.534111000	-0.709127000	-1.976311000
H	-2.998171000	-2.347545000	-0.896262000
H	-3.364694000	-1.223205000	0.415818000
H	-0.744668000	-2.703372000	-0.095122000
H	-1.594634000	-2.557062000	1.440657000
H	-0.734300000	-0.402252000	1.828003000
H	1.362602000	-1.638680000	1.419087000

Atomic coordinates of **4m** (trans, exo, distal 1)

C	1.062271000	-2.149164000	-0.237476000
C	2.543449000	-1.770624000	-0.134437000
C	2.499534000	-0.442864000	0.625937000
N	1.274800000	0.189814000	0.122972000
C	0.317693000	-0.806081000	-0.423153000
C	1.126200000	1.515299000	-0.173909000
C	2.177977000	2.468235000	0.370737000
C	-1.013378000	-0.782416000	0.273397000
C	-2.178682000	-0.577328000	-0.328919000
C	-3.518012000	-0.571402000	0.346696000
C	-4.249217000	0.770760000	0.198366000
O	0.186712000	1.924088000	-0.841953000
H	-5.231108000	0.735843000	0.676623000
H	-4.398118000	1.023406000	-0.854500000
H	-3.674117000	1.580110000	0.652624000
H	1.789449000	3.479638000	0.277450000
H	3.100277000	2.398790000	-0.213003000
H	2.425057000	2.264192000	1.414249000
H	-3.395952000	-0.814986000	1.406389000
H	-4.143079000	-1.363061000	-0.084757000
H	-2.179864000	-0.364675000	-1.396910000
H	3.372192000	0.179963000	0.437588000
H	2.437185000	-0.615655000	1.707444000
H	3.145738000	-2.524938000	0.374063000
H	2.969522000	-1.611048000	-1.128523000
H	0.733324000	-2.625071000	0.690563000
H	0.844491000	-2.839677000	-1.052206000
H	0.166213000	-0.583578000	-1.482659000
H	-0.985523000	-0.967151000	1.346949000

Atomic coordinates of **4n** (trans, exo, distal 2)

C	-0.531878000	2.139543000	-0.267450000
C	-2.062801000	2.167208000	-0.200059000
C	-2.389603000	0.890964000	0.579530000
N	-1.365333000	-0.052607000	0.119027000
C	-0.161656000	0.643544000	-0.402679000
C	-1.564644000	-1.375335000	-0.159235000
C	-2.847736000	-2.005211000	0.358283000
C	1.090183000	0.287687000	0.348675000
C	2.169216000	-0.261637000	-0.195898000
C	3.436309000	-0.599044000	0.531804000
C	4.670751000	0.100317000	-0.055186000
O	-0.747410000	-2.030489000	-0.790932000
H	5.578888000	-0.198065000	0.474037000
H	4.577351000	1.186564000	0.016697000

H	4.802094000	-0.152861000	-1.110537000
H	-2.742760000	-3.084696000	0.279407000
H	-3.702229000	-1.696649000	-0.250730000
H	-3.057518000	-1.731228000	1.393969000
H	3.591112000	-1.683788000	0.484768000
H	3.332308000	-0.344263000	1.590633000
H	2.146800000	-0.507247000	-1.256494000
H	-3.391404000	0.516987000	0.376034000
H	-2.308543000	1.063196000	1.659932000
H	-2.455149000	3.064257000	0.281298000
H	-2.493518000	2.105765000	-1.203016000
H	-0.110798000	2.539579000	0.659203000
H	-0.122277000	2.725942000	-1.089939000
H	-0.037081000	0.361456000	-1.451269000
H	1.080477000	0.518999000	1.413559000

Atomic coordinates of **4o** (trans, exo, proximal 1)

C	-0.773252000	2.209355000	-0.442131000
C	-2.024279000	2.035894000	0.426726000
C	-1.764309000	0.702508000	1.132111000
N	-1.090492000	-0.094059000	0.100752000
C	-0.377481000	0.767188000	-0.863715000
C	-1.390572000	-1.386054000	-0.232446000
C	-2.237883000	-2.179683000	0.748937000
C	1.116901000	0.581024000	-0.903896000
C	1.842408000	-0.247362000	-0.164152000
C	3.335555000	-0.385732000	-0.236031000
C	4.030061000	-0.106610000	1.104271000
O	-0.984182000	-1.891992000	-1.268815000
H	5.109997000	-0.253061000	1.025129000
H	3.660427000	-0.775320000	1.886371000
H	3.850165000	0.919903000	1.432727000
H	-2.181646000	-3.227028000	0.462227000
H	-3.284066000	-1.864705000	0.700982000
H	-1.899781000	-2.063278000	1.780360000
H	3.730923000	0.283529000	-1.005879000
H	3.582613000	-1.405888000	-0.553972000
H	1.336990000	-0.893195000	0.550460000
H	-2.676141000	0.217651000	1.472952000
H	-1.110350000	0.843862000	2.000845000
H	-2.176014000	2.859420000	1.126164000
H	-2.918685000	1.951436000	-0.196245000
H	0.033411000	2.651722000	0.147067000
H	-0.939801000	2.850859000	-1.308028000
H	-0.771180000	0.539246000	-1.859782000
H	1.617145000	1.216026000	-1.634158000

Atomic coordinates of **4p** (trans, exo, proximal 2)

C	-1.278403000	-2.120649000	0.379955000
C	-2.565774000	-1.592609000	-0.263661000
C	-2.088805000	-0.333343000	-0.991231000
N	-1.076726000	0.213598000	-0.080601000
C	-0.461103000	-0.848642000	0.739309000
C	-0.977313000	1.520136000	0.310579000
C	-1.738188000	2.551758000	-0.506516000
C	1.016474000	-1.047245000	0.522093000
C	1.795530000	-0.398853000	-0.333983000
C	3.267347000	-0.637401000	-0.510650000
C	4.112056000	0.604962000	-0.192730000
O	-0.293480000	1.852897000	1.268218000
H	5.174365000	0.408983000	-0.358028000
H	3.977291000	0.912008000	0.846437000
H	3.825115000	1.448905000	-0.825417000
H	-1.373145000	3.534899000	-0.219331000
H	-2.809360000	2.505156000	-0.291393000
H	-1.605635000	2.411202000	-1.580952000
H	3.463221000	-0.940426000	-1.546729000
H	3.582856000	-1.472561000	0.121930000
H	1.361887000	0.390075000	-0.944319000
H	-2.887467000	0.382828000	-1.170456000
H	-1.640531000	-0.589732000	-1.958593000
H	-3.034536000	-2.314149000	-0.934573000
H	-3.296385000	-1.317969000	0.501828000
H	-0.719500000	-2.721963000	-0.340765000
H	-1.462492000	-2.742159000	1.256771000
H	-0.613615000	-0.580992000	1.790043000
H	1.451924000	-1.821149000	1.153028000

Atomic coordinates of **5a** (cis, endo)

C	0.327939000	1.760928000	0.922803000
C	1.187941000	2.365830000	-0.196358000
C	2.217742000	1.270735000	-0.497480000
N	1.554361000	0.028194000	-0.070573000
C	0.237383000	0.269531000	0.549091000
C	2.263922000	-1.134668000	-0.065140000
C	1.607858000	-2.361932000	0.544149000
C	-0.931039000	-0.056566000	-0.398860000
C	-2.301637000	-0.052420000	0.283241000
C	-3.449489000	-0.405345000	-0.666992000
C	-4.819226000	-0.398168000	0.012803000
O	3.401352000	-1.184106000	-0.519003000
H	-5.614341000	-0.655006000	-0.690872000
H	-5.049755000	0.586940000	0.428049000
H	-4.857579000	-1.119328000	0.834044000
H	2.236031000	-3.220605000	0.319879000
H	0.602384000	-2.537717000	0.159292000
H	1.535257000	-2.256402000	1.630340000
H	-3.263923000	-1.392213000	-1.105232000
H	-3.453950000	0.301208000	-1.504511000
H	-2.498108000	0.929528000	0.727958000
H	-2.293503000	-0.765003000	1.117519000
H	-0.756186000	-1.040758000	-0.843379000
H	-0.928498000	0.652416000	-1.234021000
H	3.141942000	1.401178000	0.072124000
H	2.497146000	1.218730000	-1.550579000
H	1.660963000	3.303729000	0.095671000
H	0.577086000	2.570104000	-1.078611000
H	-0.651442000	2.231181000	1.013676000
H	0.836687000	1.865806000	1.884596000

H	0.140093000	-0.345837000	1.446554000

Atomic coordinates of **5b** (trans, endo)

C	-0.302674000	1.890471000	-0.742097000
C	-1.289499000	2.329840000	0.348980000
C	-2.309703000	1.188800000	0.380930000
N	-1.522966000	0.012959000	-0.012660000
C	-0.192760000	0.366470000	-0.554363000
C	-2.001875000	-1.258147000	-0.116163000
C	-3.416781000	-1.494939000	0.381160000
C	0.944995000	-0.075311000	0.378568000
C	2.325369000	-0.011737000	-0.279640000
C	3.456926000	-0.471302000	0.643625000
C	4.833239000	-0.426889000	-0.021637000
O	-1.324604000	-2.168482000	-0.580064000
H	5.617864000	-0.761103000	0.661345000
H	5.084866000	0.587419000	-0.344667000
H	4.865620000	-1.071338000	-0.904531000
H	-3.655077000	-2.545566000	0.235613000
H	-4.139537000	-0.882744000	-0.164378000
H	-3.510696000	-1.247917000	1.441547000
H	3.248646000	-1.491206000	0.984571000
H	3.466031000	0.153813000	1.543928000
H	2.537454000	1.008534000	-0.621405000
H	2.319151000	-0.638896000	-1.178965000
H	0.743946000	-1.103448000	0.687036000
H	0.934199000	0.539377000	1.286853000
H	-3.120412000	1.372100000	-0.334416000
H	-2.759355000	1.058170000	1.367043000
H	-1.756449000	3.293812000	0.144091000
H	-0.782457000	2.405669000	1.313680000
H	0.663389000	2.389729000	-0.665751000
H	-0.713408000	2.116899000	-1.729789000
H	-0.069611000	-0.149703000	-1.508852000

Atomic coordinates of **5c** (cis, exo)

C	0.237207000	1.932617000	0.360511000
C	1.718582000	2.313467000	0.261186000
C	2.305889000	1.178789000	-0.575383000
N	1.546613000	0.007604000	-0.119629000
C	0.218056000	0.385848000	0.415523000
C	2.169902000	-1.202468000	-0.017175000
C	1.425229000	-2.348440000	0.645257000
C	-0.951201000	-0.223507000	-0.368939000
C	-2.322656000	0.118420000	0.220713000
C	-3.483391000	-0.531479000	-0.537584000
C	-4.853052000	-0.193064000	0.052236000
O	3.303271000	-1.376976000	-0.450770000
H	-5.658281000	-0.671215000	-0.510166000
H	-5.034285000	0.885335000	0.038449000
H	-4.930383000	-0.527059000	1.090754000
H	2.170412000	-3.006781000	1.087859000
H	0.884652000	-2.919763000	-0.113046000
H	0.712681000	-2.035958000	1.408642000
H	-3.346197000	-1.618473000	-0.543625000
H	-3.449341000	-0.216308000	-1.586420000
H	-2.466532000	1.204445000	0.230207000
H	-2.355601000	-0.200847000	1.270074000
H	-0.842469000	-1.310251000	-0.402600000
H	-0.891376000	0.124170000	-1.406507000
H	3.367849000	1.001804000	-0.420946000
H	2.148762000	1.349673000	-1.646632000
H	2.182161000	2.319442000	1.251374000
H	1.874613000	3.295189000	-0.188169000
H	-0.292324000	2.271056000	-0.535086000
H	-0.263367000	2.376106000	1.221512000
H	0.149168000	0.060919000	1.459804000

Atomic coordinates of **5d** (trans, exo)

C	-0.211404000	1.957540000	-0.263240000
C	-1.701421000	2.315122000	-0.212592000
C	-2.308858000	1.137991000	0.553676000
N	-1.503495000	-0.002339000	0.103781000
C	-0.173190000	0.420596000	-0.396891000
C	-1.969458000	-1.258557000	-0.145842000
C	-3.371703000	-1.589059000	0.338519000
C	0.979929000	-0.241723000	0.363354000
C	2.356328000	0.101735000	-0.212440000
C	3.504852000	-0.599995000	0.517433000
C	4.880750000	-0.265399000	-0.060088000
O	-1.289031000	-2.094315000	-0.729622000
H	5.677267000	-0.782058000	0.480711000
H	5.084025000	0.807917000	-0.003506000
H	4.949749000	-0.558734000	-1.111409000
H	-3.498960000	-2.667223000	0.277165000
H	-4.122857000	-1.115171000	-0.299724000
H	-3.545815000	-1.256711000	1.363684000
H	3.344783000	-1.682825000	0.478876000
H	3.477992000	-0.327057000	1.578558000
H	2.522157000	1.185126000	-0.178597000
H	2.381717000	-0.178032000	-1.272717000
H	0.833434000	-1.322805000	0.331985000
H	0.929352000	0.063355000	1.415817000
H	-3.364087000	0.989729000	0.331405000
H	-2.210272000	1.285190000	1.636390000
H	-2.121406000	2.351744000	-1.221326000
H	-1.897325000	3.274498000	0.268539000
H	0.274041000	2.257251000	0.670748000
H	0.315347000	2.453114000	-1.078637000
H	-0.107370000	0.124080000	-1.448775000

Atomic coordinates of **6a** (cis, endo, distal 1)

C	-0.810376000	1.890071000	-1.056874000
C	-1.625971000	2.332694000	0.164885000
C	-2.390077000	1.066292000	0.564160000
N	-1.532065000	-0.029533000	0.088117000
C	-0.385100000	0.444788000	-0.712949000
C	-1.916482000	-1.323183000	0.284914000

C	-1.041989000	-2.409643000	-0.310557000
O	-2.934741000	-1.588003000	0.912650000
C	0.910681000	0.387909000	0.056616000
C	2.042519000	-0.141532000	-0.385439000
F	2.069085000	-0.700743000	-1.635220000
C	3.379028000	-0.250291000	0.270735000
C	3.466644000	0.338652000	1.676954000
H	4.475396000	0.211611000	2.072823000
H	2.775569000	-0.155718000	2.362652000
H	3.241177000	1.407109000	1.678373000
H	-1.435446000	-3.370425000	0.012030000
H	-0.002633000	-2.311862000	0.006909000
H	-1.057477000	-2.368685000	-1.402894000
H	4.111814000	0.231070000	-0.386949000
H	3.654103000	-1.311164000	0.288049000
H	0.917820000	0.818799000	1.049861000
H	-3.368281000	1.004537000	0.078056000
H	-2.560788000	0.981216000	1.637724000
H	-2.294859000	3.165848000	-0.051992000
H	-0.961181000	2.648727000	0.972889000
H	0.046226000	2.529958000	-1.267484000
H	-1.446204000	1.871679000	-1.946023000
H	-0.287882000	-0.149798000	-1.619733000

Atomic coordinates of **6a′** (cis, endo, distal 2)

C	0.711670000	1.938661000	0.899342000
C	1.670342000	2.364616000	-0.220128000
C	2.522684000	1.114287000	-0.457396000
N	1.644167000	0.005148000	-0.054909000
C	0.385060000	0.465640000	0.565078000
C	2.095773000	-1.279080000	-0.139996000
C	1.186078000	-2.375380000	0.379635000
O	3.198977000	-1.527298000	-0.611363000
C	-0.793260000	0.324945000	-0.364458000
C	-1.957102000	-0.229813000	-0.053634000
F	-2.138047000	-0.732103000	1.207002000
C	-3.169514000	-0.406742000	-0.903690000
C	-4.400370000	0.345828000	-0.377033000
H	-5.261670000	0.163237000	-1.022402000
H	-4.218306000	1.422262000	-0.349235000
H	-4.658994000	0.019167000	0.631060000
H	1.646221000	-3.331812000	0.144074000
H	0.192281000	-2.324252000	-0.067775000
H	1.063942000	-2.298569000	1.463362000
H	-3.396180000	-1.477365000	-0.961778000
H	-2.925882000	-0.077212000	-1.915689000
H	-0.685112000	0.705380000	-1.373543000
H	3.427126000	1.108612000	0.158264000
H	2.840975000	0.994914000	-1.493412000
H	2.275982000	3.230667000	0.047905000
H	1.111124000	2.623419000	-1.122898000
H	-0.186041000	2.552869000	0.966185000
H	1.221853000	1.978462000	1.865471000
H	0.185955000	-0.096281000	1.476347000

Atomic coordinates of **6b** (cis, endo, distal 3)

C	-1.185612000	-1.983065000	0.730760000
C	-2.151485000	-2.064890000	-0.458153000
C	-2.663840000	-0.628705000	-0.603572000
N	-1.569293000	0.193805000	-0.065374000
C	-0.495870000	-0.611651000	0.552047000
C	-1.698221000	1.551205000	-0.033132000
C	-0.586647000	2.342791000	0.628238000
O	-2.681885000	2.100809000	-0.513899000
C	0.733081000	-0.688052000	-0.317970000
C	1.978345000	-0.476474000	0.086198000
F	2.204755000	-0.142159000	1.394397000
C	3.244132000	-0.544528000	-0.699531000
C	3.990590000	0.795846000	-0.773312000
H	4.919386000	0.681967000	-1.335421000
H	4.242289000	1.161033000	0.223237000
H	3.383701000	1.555070000	-1.271072000
H	-0.782154000	3.399098000	0.460737000
H	0.393878000	2.080755000	0.228185000
H	-0.564717000	2.154157000	1.705012000
H	3.002250000	-0.900572000	-1.702909000
H	3.894800000	-1.297687000	-0.241015000
H	0.593606000	-0.943624000	-1.362086000
H	-3.573923000	-0.454907000	-0.021778000
H	-2.884547000	-0.347453000	-1.633663000
H	-2.961845000	-2.776289000	-0.297211000
H	-1.619076000	-2.374703000	-1.360976000
H	-0.466864000	-2.801294000	0.769354000
H	-1.745439000	-1.979383000	1.669793000
H	-0.220833000	-0.194705000	1.519609000

Atomic coordinates of **6b′** (cis, endo, distal 4)

C	-0.810443000	1.890097000	-1.056837000
C	-1.626056000	2.332667000	0.164905000
C	-2.390216000	1.066267000	0.564023000
N	-1.531999000	-0.029538000	0.088259000
C	-0.385084000	0.444826000	-0.712888000
C	-1.916431000	-1.323184000	0.285011000
C	-1.041916000	-2.409675000	-0.310391000
O	-2.934829000	-1.588005000	0.912538000
C	0.910726000	0.387992000	0.056598000
C	2.042530000	-0.141527000	-0.385478000
F	2.069006000	-0.700884000	-1.635141000
C	3.379072000	-0.250266000	0.270660000
C	3.466844000	0.338754000	1.676834000
H	4.475663000	0.211786000	2.072564000
H	2.775918000	-0.155670000	2.362652000
H	3.241277000	1.407191000	1.678263000
H	-1.434463000	-3.370406000	0.013454000
H	-0.002195000	-2.311020000	0.005559000
H	-1.058961000	-2.369656000	-1.402761000
H	4.111852000	0.230991000	-0.387118000
H	3.654077000	-1.311163000	0.288027000
H	0.917979000	0.818997000	1.049794000

H	-3.368277000	1.004424000	0.077630000
H	-2.561253000	0.981198000	1.637539000
H	-2.294890000	3.165886000	-0.051917000
H	-0.961262000	2.648576000	0.972959000
H	0.046135000	2.530027000	-1.267440000
H	-1.446258000	1.871645000	-1.945996000
H	-0.287920000	-0.149766000	-1.619684000

Atomic coordinates of **6c** (cis, endo, proximal 1)

C	0.672693000	2.025778000	1.086576000
C	1.092022000	2.316787000	-0.360206000
C	1.907551000	1.080430000	-0.757034000
N	1.384716000	0.018152000	0.114171000
C	0.387240000	0.505591000	1.071494000
C	1.887242000	-1.243973000	0.027854000
C	1.332623000	-2.281337000	0.987654000
O	2.761625000	-1.523227000	-0.783138000
C	-1.060698000	0.192877000	0.752156000
C	-1.631982000	-0.094473000	-0.410010000
F	-0.885896000	-0.151289000	-1.550330000
C	-3.065097000	-0.397766000	-0.710981000
C	-4.014886000	-0.370360000	0.483824000
H	-5.029760000	-0.605902000	0.159489000
H	-4.037779000	0.614014000	0.956153000
H	-3.729476000	-1.104284000	1.240340000
H	1.734177000	-3.250479000	0.702113000
H	0.241908000	-2.314671000	0.966600000
H	1.641686000	-2.062107000	2.013727000
H	-3.096983000	-1.380387000	-1.195481000
H	-3.399357000	0.314299000	-1.474128000
H	-1.728312000	0.230325000	1.605168000
H	2.977393000	1.210915000	-0.571939000
H	1.788678000	0.805583000	-1.805181000
H	1.667263000	3.238210000	-0.454364000
H	0.209618000	2.408249000	-0.996640000
H	-0.188129000	2.606969000	1.417359000
H	1.502751000	2.225625000	1.769777000
H	0.593129000	0.082668000	2.057932000

Atomic coordinates of **6c′** (cis, endo, proximal 2)

C	-1.301437000	-2.008974000	0.901252000
C	-1.502942000	-2.112484000	-0.616264000
C	-1.925073000	-0.695928000	-1.024477000
N	-1.345869000	0.160008000	0.020866000
C	-0.676921000	-0.604856000	1.077433000
C	-1.530928000	1.508050000	-0.020680000
C	-0.947866000	2.326613000	1.117383000
O	-2.156566000	2.033263000	-0.933265000
C	0.836432000	-0.636869000	1.028343000
C	1.665295000	-0.425036000	0.013396000
F	1.182397000	-0.110084000	-1.222076000
C	3.158188000	-0.474174000	0.023511000
C	3.811733000	0.879125000	-0.293224000
H	4.899034000	0.782036000	-0.306867000
H	3.546603000	1.626754000	0.457366000
H	3.493382000	1.250077000	-1.268231000
H	-1.056932000	3.378185000	0.863687000
H	0.105254000	2.097138000	1.288545000
H	-1.488907000	2.133027000	2.048157000
H	3.482406000	-1.214772000	-0.716145000
H	3.484514000	-0.834505000	1.001022000
H	1.314705000	-0.894687000	1.967594000
H	-3.011447000	-0.572135000	-1.037193000
H	-1.551955000	-0.403121000	-2.006024000
H	-2.246868000	-2.860331000	-0.892015000
H	-0.563300000	-2.382186000	-1.102461000
H	-0.672793000	-2.798689000	1.312815000
H	-2.265993000	-2.036890000	1.415491000
H	-0.954549000	-0.198105000	2.052957000

Atomic coordinates of **6d** (cis, endo, proximal 3)

C	0.643809000	2.075244000	1.051412000
C	0.695438000	2.342808000	-0.458265000
C	1.560832000	1.199399000	-1.001126000
N	1.389596000	0.126229000	-0.011465000
C	0.569443000	0.532105000	1.133609000
C	2.024487000	-1.065956000	-0.182393000
C	1.838259000	-2.115861000	0.898108000
O	2.727680000	-1.273087000	-1.163566000
C	-0.857003000	0.023539000	1.151841000
C	-1.623496000	-0.412292000	0.159617000
F	-1.146558000	-0.456271000	-1.116718000
C	-3.032586000	-0.901834000	0.236861000
C	-4.018289000	-0.048440000	-0.574450000
H	-5.026341000	-0.461507000	-0.503650000
H	-3.738393000	-0.021323000	-1.628307000
H	-4.044693000	0.978269000	-0.202779000
H	2.301823000	-3.036867000	0.553359000
H	0.783578000	-2.294386000	1.115058000
H	2.323711000	-1.805102000	1.827681000
H	-3.329996000	-0.931646000	1.286837000
H	-3.057606000	-1.933314000	-0.132407000
H	-1.329262000	0.033503000	2.128701000
H	2.617907000	1.471832000	-1.065562000
H	1.251321000	0.858297000	-1.989211000
H	1.109243000	3.322762000	-0.697560000
H	-0.308788000	2.292786000	-0.883890000
H	-0.195029000	2.559023000	1.551990000
H	1.567462000	2.413361000	1.529095000
H	1.040097000	0.189564000	2.058601000

Atomic coordinates of **6d′** (cis, endo, proximal 4)

C	0.672669000	2.026179000	1.086105000
C	1.092397000	2.316632000	-0.360686000
C	1.907985000	1.080105000	-0.756878000
N	1.385048000	0.018188000	0.114676000
C	0.387386000	0.505946000	1.071616000
C	1.886658000	-1.244295000	0.028029000

C	1.331747000	-2.281314000	0.988018000
O	2.760578000	-1.524063000	-0.783273000
C	-1.060529000	0.193033000	0.752227000
C	-1.631702000	-0.094420000	-0.409970000
F	-0.885463000	-0.151323000	-1.550221000
C	-3.064745000	-0.397929000	-0.711046000
C	-4.014769000	-0.369685000	0.483575000
H	-5.029615000	-0.605277000	0.159185000
H	-4.037582000	0.614965000	0.955326000
H	-3.729617000	-1.103224000	1.240562000
H	1.733533000	-3.250532000	0.703060000
H	0.241042000	-2.314798000	0.966331000
H	1.640145000	-2.061629000	2.014186000
H	-3.096581000	-1.380899000	-1.194840000
H	-3.398854000	0.313613000	-1.474741000
H	-1.728181000	0.230482000	1.605204000
H	2.977784000	1.210771000	-0.571632000
H	1.789319000	0.804788000	-1.804923000
H	1.667767000	3.237968000	-0.454965000
H	0.210193000	2.407997000	-0.997400000
H	-0.188359000	2.607361000	1.416374000
H	1.502474000	2.226494000	1.769473000
H	0.593162000	0.083500000	2.058290000

Atomic coordinates of **6e** (trans, endo, distal 1)

C	-0.647021000	2.057215000	-0.681053000
C	-1.515156000	2.284163000	0.562305000
C	-2.366024000	1.011477000	0.631771000
N	-1.503947000	-0.016092000	0.030982000
C	-0.306818000	0.551752000	-0.625155000
C	-1.825503000	-1.334021000	-0.120202000
C	-3.124220000	-1.790926000	0.520955000
O	-1.104479000	-2.108315000	-0.733808000
C	0.950089000	0.244531000	0.148553000
C	2.119531000	-0.051260000	-0.398346000
F	2.225079000	-0.071898000	-1.760983000
C	3.423814000	-0.395972000	0.240555000
C	3.417339000	-0.419799000	1.767184000
H	4.407118000	-0.685782000	2.142019000
H	2.706838000	-1.154673000	2.150684000
H	3.155902000	0.555992000	2.182411000
H	-3.260624000	-2.845065000	0.293108000
H	-3.979132000	-1.225765000	0.141385000
H	-3.097371000	-1.658184000	1.605507000
H	4.175378000	0.314081000	-0.123545000
H	3.729267000	-1.373620000	-0.149481000
H	0.891610000	0.255151000	1.229418000
H	-3.290221000	1.130111000	0.054127000
H	-2.644692000	0.751985000	1.655005000
H	-2.127883000	3.184227000	0.502485000
H	-0.889093000	2.368581000	1.454066000
H	0.247568000	2.678022000	-0.705808000
H	-1.226926000	2.262172000	-1.585267000
H	-0.216173000	0.126044000	-1.623077000

Atomic coordinates of **6e′** (trans, endo, distal 2)

C	0.577498000	1.984106000	0.781156000
C	1.559641000	2.365134000	-0.333273000
C	2.478022000	1.142007000	-0.422142000
N	1.609040000	0.026455000	-0.022549000
C	0.322102000	0.478647000	0.550395000
C	1.977695000	-1.286634000	0.035429000
C	3.354405000	-1.626530000	-0.508630000
O	1.238102000	-2.145477000	0.494630000
C	-0.829405000	0.200045000	-0.379396000
C	-2.002904000	-0.292611000	-0.009673000
F	-2.223709000	-0.564143000	1.310285000
C	-3.186332000	-0.623976000	-0.854019000
C	-4.442682000	0.182663000	-0.495195000
H	-5.282716000	-0.120626000	-1.123333000
H	-4.276998000	1.252285000	-0.642468000
H	-4.725920000	0.024081000	0.546214000
H	3.514457000	-2.693907000	-0.378926000
H	4.139892000	-1.077222000	0.016547000
H	3.431956000	-1.377703000	-1.570052000
H	-3.395738000	-1.693587000	-0.740244000
H	-2.915165000	-0.462362000	-1.899296000
H	-0.690925000	0.403917000	-1.434938000
H	3.324944000	1.241507000	0.267059000
H	2.881708000	0.995764000	-1.425895000
H	2.114011000	3.281091000	-0.126429000
H	1.027602000	2.505281000	-1.277525000
H	-0.344921000	2.563205000	0.763497000
H	1.046718000	2.124857000	1.758861000
H	0.148139000	-0.047760000	1.487269000

Atomic coordinates of **6f** (trans, endo, distal 3)

C	-0.994710000	-2.076587000	0.585015000
C	-2.024296000	-2.113729000	-0.550901000
C	-2.638631000	-0.710774000	-0.511660000
N	-1.543625000	0.133664000	-0.014439000
C	-0.402345000	-0.652389000	0.503070000
C	-1.605309000	1.484202000	0.174250000
C	-2.862611000	2.179004000	-0.318870000
O	-0.695319000	2.104057000	0.706716000
C	0.798923000	-0.547337000	-0.399359000
C	2.050231000	-0.411062000	0.015317000
F	2.304240000	-0.375611000	1.357214000
C	3.294502000	-0.264380000	-0.793450000
C	3.990113000	1.089292000	-0.584336000
H	4.901271000	1.144664000	-1.183564000
H	4.263358000	1.230885000	0.462002000
H	3.335181000	1.912475000	-0.875719000
H	-2.774813000	3.238094000	-0.090031000
H	-3.757029000	1.778468000	0.164992000
H	-2.987623000	2.053126000	-1.397294000
H	3.034628000	-0.399441000	-1.845487000
H	3.983685000	-1.073510000	-0.526240000
H	0.633636000	-0.570977000	-1.470208000

H	-3.494938000	-0.680431000	0.172484000
H	-2.985488000	-0.380056000	-1.492547000
H	-2.775570000	-2.894447000	-0.427398000
H	-1.527568000	-2.280715000	-1.509919000
H	-0.226883000	-2.844523000	0.500304000
H	-1.495554000	-2.203652000	1.548794000
H	-0.131737000	-0.275006000	1.487782000

Atomic coordinates of **6f′** (trans, endo, distal 4)

C	-0.644966000	2.057899000	-0.677547000
C	-1.513277000	2.283355000	0.565923000
C	-2.365934000	1.011701000	0.632201000
N	-1.504778000	-0.015738000	0.029891000
C	-0.306611000	0.551884000	-0.624522000
C	-1.826799000	-1.333372000	-0.122228000
C	-3.125994000	-1.790188000	0.518026000
O	-1.105804000	-2.107591000	-0.736031000
C	0.949602000	0.241515000	0.149063000
C	2.119801000	-0.050626000	-0.398151000
F	2.226783000	-0.064134000	-1.760770000
C	3.423474000	-0.398378000	0.240103000
C	3.416839000	-0.425136000	1.766632000
H	4.406605000	-0.691744000	2.141007000
H	2.706353000	-1.160737000	2.148770000
H	3.155333000	0.549895000	2.183614000
H	-3.263885000	-2.843503000	0.287345000
H	-3.980317000	-1.222719000	0.140650000
H	-3.098292000	-1.660583000	1.602955000
H	4.175921000	0.311384000	-0.122699000
H	3.727640000	-1.375697000	-0.151823000
H	0.889932000	0.246270000	1.229898000
H	-3.289551000	1.132763000	0.054136000
H	-2.645682000	0.750439000	1.654680000
H	-2.124709000	3.184412000	0.507859000
H	-0.887443000	2.364862000	1.458104000
H	0.250413000	2.677610000	-0.700676000
H	-1.224225000	2.265375000	-1.581586000
H	-0.216074000	0.128146000	-1.623300000

Atomic coordinates of **6g** (trans, endo, proximal 1)

C	0.431374000	1.924013000	0.932552000
C	0.943363000	2.263874000	-0.472227000
C	1.960093000	1.151256000	-0.759703000
N	1.480967000	0.019845000	0.047018000
C	0.349273000	0.390070000	0.933710000
C	2.050338000	-1.212920000	0.119882000
C	3.248342000	-1.463369000	-0.777220000
O	1.614467000	-2.081428000	0.868819000
C	-0.928291000	-0.275707000	0.473185000
C	-2.052475000	0.229500000	-0.011869000
F	-2.201218000	1.582940000	-0.186879000
C	-3.298606000	-0.477419000	-0.440748000
C	-3.279120000	-1.997243000	-0.298652000
H	-4.229244000	-2.415361000	-0.635667000
H	-3.129914000	-2.300538000	0.739383000
H	-2.485061000	-2.446592000	-0.898111000
H	3.618483000	-2.465656000	-0.576689000
H	4.045454000	-0.738755000	-0.594002000
H	2.971004000	-1.387503000	-1.831706000
H	-3.494463000	-0.198935000	-1.482880000
H	-4.130716000	-0.056161000	0.135285000
H	-0.898194000	-1.354044000	0.562707000
H	2.966204000	1.448343000	-0.443592000
H	2.005855000	0.894687000	-1.820188000
H	1.395536000	3.254133000	-0.536437000
H	0.121431000	2.222665000	-1.188693000
H	-0.512164000	2.404010000	1.175152000
H	1.170280000	2.227383000	1.679677000
H	0.568224000	-0.013965000	1.924544000

Atomic coordinates of **6g′** (trans, endo, proximal 2)

C	-0.323427000	1.913695000	-0.856453000
C	-0.610561000	2.178821000	0.626101000
C	-1.738026000	1.190871000	0.952337000
N	-1.526527000	0.089593000	0.001820000
C	-0.464607000	0.389963000	-0.990701000
C	-2.276228000	-1.040930000	-0.096632000
C	-3.384629000	-1.212522000	0.925397000
O	-2.063728000	-1.882031000	-0.963949000
C	0.749265000	-0.477453000	-0.746404000
C	1.990449000	-0.171470000	-0.395941000
F	2.363747000	1.130248000	-0.171526000
C	3.138237000	-1.104292000	-0.187972000
C	3.670896000	-1.104173000	1.252260000
H	4.523750000	-1.779895000	1.342939000
H	2.900849000	-1.433757000	1.953211000
H	3.998116000	-0.107045000	1.550424000
H	-3.907665000	-2.140050000	0.706504000
H	-4.092866000	-0.380915000	0.890968000
H	-2.980419000	-1.258078000	1.939820000
H	3.944274000	-0.817435000	-0.872854000
H	2.818344000	-2.107618000	-0.474321000
H	0.555099000	-1.533915000	-0.889642000
H	-2.719890000	1.650457000	0.793472000
H	-1.697448000	0.840171000	1.985689000
H	-0.902093000	3.209842000	0.829143000
H	0.275055000	1.956759000	1.223948000
H	0.644276000	2.284152000	-1.181149000
H	-1.094128000	2.384597000	-1.473204000
H	-0.851670000	0.114536000	-1.974319000

Atomic coordinates of **6h** (trans, endo, proximal 3)

C	0.274220000	1.744740000	1.010708000
C	0.803577000	2.248038000	-0.337736000
C	1.963332000	1.291203000	-0.645010000
N	1.597566000	0.055466000	0.061771000
C	0.383687000	0.216759000	0.900288000
C	2.317507000	-1.098153000	0.087145000

C	3.581762000	-1.128478000	-0.751473000
O	1.961293000	-2.066138000	0.751173000
C	-0.773715000	-0.556114000	0.309645000
C	-1.937776000	-0.155989000	-0.182189000
F	-2.269347000	1.174951000	-0.227372000
C	-3.036088000	-1.002822000	-0.736445000
C	-4.337939000	-0.917961000	0.073750000
H	-5.114387000	-1.531421000	-0.387728000
H	-4.704119000	0.108571000	0.122873000
H	-4.185427000	-1.273774000	1.094904000
H	4.053773000	-2.098796000	-0.619266000
H	4.279210000	-0.342956000	-0.449913000
H	3.356474000	-0.978744000	-1.810329000
H	-2.683038000	-2.034582000	-0.779739000
H	-3.229669000	-0.685931000	-1.767658000
H	-0.607231000	-1.626799000	0.292540000
H	2.910038000	1.686356000	-0.260496000
H	2.085164000	1.117237000	-1.716214000
H	1.130956000	3.287822000	-0.309168000
H	0.026604000	2.161843000	-1.099182000
H	-0.731459000	2.087887000	1.234445000
H	0.935402000	2.077402000	1.815877000
H	0.597116000	-0.235169000	1.871519000

Atomic coordinates of **6h′** (trans, endo, proximal 4)

C	0.431605000	1.924001000	0.932956000
C	0.944035000	2.263940000	-0.471649000
C	1.960659000	1.151203000	-0.758978000
N	1.481013000	0.019716000	0.047315000
C	0.349360000	0.390049000	0.934023000
C	2.049725000	-1.213386000	0.119608000
C	3.247514000	-1.464138000	-0.777702000
O	1.613383000	-2.082005000	0.868142000
C	-0.928350000	-0.275550000	0.473621000
C	-2.052108000	0.229803000	-0.012281000
F	-2.200126000	1.583171000	-0.188469000
C	-3.298410000	-0.476864000	-0.441073000
C	-3.279729000	-1.996575000	-0.297661000
H	-4.229924000	-2.414518000	-0.634693000
H	-3.131079000	-2.299049000	0.740692000
H	-2.485654000	-2.446826000	-0.896421000
H	3.618347000	-2.465967000	-0.576156000
H	4.044285000	-0.738800000	-0.595952000
H	2.969442000	-1.389844000	-1.832117000
H	-3.493687000	-0.199187000	-1.483530000
H	-4.130555000	-0.054693000	0.134241000
H	-0.898793000	-1.353828000	0.563973000
H	2.966699000	1.448050000	-0.442393000
H	2.006802000	0.894834000	-1.819492000
H	1.396398000	3.254130000	-0.535591000
H	0.122289000	2.222960000	-1.188338000
H	-0.511984000	2.404039000	1.175288000
H	1.170286000	2.227300000	1.680332000
H	0.568300000	-0.014005000	1.924851000

Atomic coordinates of **6i** (cis, exo, distal 1)

C	0.715811000	2.103676000	0.216168000
C	2.244092000	2.176295000	0.279066000
C	2.673662000	0.934988000	-0.501900000
N	1.635822000	-0.049383000	-0.166896000
C	0.390683000	0.592301000	0.318317000
C	1.956865000	-1.376342000	-0.083823000
C	0.909480000	-2.321389000	0.472057000
O	3.052915000	-1.786895000	-0.445361000
C	-0.822286000	0.224891000	-0.487334000
C	-1.991032000	-0.166510000	0.001441000
F	-2.136824000	-0.291397000	1.356671000
C	-3.242975000	-0.514791000	-0.729523000
C	-4.421643000	0.412468000	-0.398024000
H	-5.316814000	0.096389000	-0.936934000
H	-4.199726000	1.443402000	-0.681799000
H	-4.646339000	0.394908000	0.669230000
H	1.384277000	-3.288039000	0.621726000
H	0.079358000	-2.434503000	-0.227647000
H	0.492656000	-1.967962000	1.417411000
H	-3.511873000	-1.547259000	-0.478870000
H	-3.029716000	-0.491221000	-1.800086000
H	-0.739687000	0.311489000	-1.565177000
H	3.648610000	0.540281000	-0.223180000
H	2.691414000	1.127992000	-1.580535000
H	2.589735000	2.103580000	1.313733000
H	2.642686000	3.098954000	-0.144670000
H	0.363370000	2.488050000	-0.744956000
H	0.210945000	2.668359000	1.000192000
H	0.222491000	0.325480000	1.364016000

Atomic coordinates of **6i′** (cis, exo, distal 2)

C	0.865950000	-2.113354000	-0.243844000
C	2.388598000	-2.028644000	-0.104848000
C	2.584365000	-0.737184000	0.688134000
N	1.510013000	0.129949000	0.187083000
C	0.404994000	-0.644940000	-0.426610000
C	1.707382000	1.480280000	0.098335000
C	0.652717000	2.299866000	-0.619311000
O	2.701041000	2.009300000	0.581566000
C	-0.927121000	-0.392797000	0.221006000
C	-2.059084000	-0.118722000	-0.411275000
F	-2.048456000	-0.012187000	-1.775931000
C	-3.431816000	0.113613000	0.127650000
C	-3.563930000	0.016828000	1.645782000
H	-4.596878000	0.203873000	1.943302000
H	-2.934417000	0.751612000	2.151690000
H	-3.287682000	-0.975017000	2.009435000
H	1.047336000	3.304778000	-0.748432000
H	-0.265051000	2.348571000	-0.030373000
H	0.392319000	1.880189000	-1.593087000
H	-4.104201000	-0.603799000	-0.356482000
H	-3.760138000	1.100803000	-0.217895000
H	-0.962430000	-0.469336000	1.301070000

H	3.544559000	-0.250167000	0.530572000
H	2.473856000	-0.909328000	1.764913000
H	2.860197000	-1.937797000	-1.087054000
H	2.817449000	-2.898364000	0.394643000
H	0.429862000	-2.520380000	0.672475000
H	0.529193000	-2.737140000	-1.072044000
H	0.341390000	-0.412532000	-1.491578000

Atomic coordinates of **6j** (cis, exo, distal 3)

C	0.866431000	-2.113405000	-0.243891000
C	2.389063000	-2.028285000	-0.104875000
C	2.584444000	-0.736834000	0.688215000
N	1.509881000	0.130055000	0.187181000
C	0.405107000	-0.645119000	-0.426623000
C	1.706975000	1.480430000	0.098328000
C	0.652081000	2.299772000	-0.619248000
O	2.700547000	2.009682000	0.581474000
C	-0.927079000	-0.393278000	0.220942000
C	-2.059014000	-0.118995000	-0.411285000
F	-2.048299000	-0.012002000	-1.775942000
C	-3.431761000	0.113225000	0.127639000
C	-3.563780000	0.016692000	1.645801000
H	-4.596740000	0.203635000	1.943345000
H	-2.934331000	0.751668000	2.151512000
H	-3.287379000	-0.975041000	2.009641000
H	1.046682000	3.304631000	-0.748865000
H	-0.265438000	2.348735000	-0.029940000
H	0.391260000	1.879798000	-1.592777000
H	-4.104120000	-0.604314000	-0.356331000
H	-3.760169000	1.100336000	-0.218050000
H	-0.962446000	-0.470172000	1.300983000
H	3.544514000	-0.249550000	0.530737000
H	2.473900000	-0.909098000	1.764970000
H	2.860632000	-1.937207000	-1.087075000
H	2.818162000	-2.897929000	0.394535000
H	0.430454000	-2.520586000	0.672414000
H	0.529864000	-2.737265000	-1.072113000
H	0.341515000	-0.412688000	-1.491585000

Atomic coordinates of **6j′** (cis, exo, distal 4)

C	-1.185253000	-2.088554000	0.102601000
C	-2.688010000	-1.799144000	0.156012000
C	-2.797960000	-0.450522000	-0.554129000
N	-1.564375000	0.240307000	-0.156226000
C	-0.511313000	-0.704463000	0.285746000
C	-1.567107000	1.597574000	0.012435000
C	-0.335943000	2.231281000	0.630044000
O	-2.530097000	2.276501000	-0.322473000
C	0.759819000	-0.594286000	-0.507145000
C	1.986862000	-0.550451000	-0.006500000
F	2.150450000	-0.561022000	1.352564000
C	3.291300000	-0.485734000	-0.726635000
C	4.090883000	0.791649000	-0.430420000
H	5.047063000	0.770724000	-0.956659000
H	4.295158000	0.888943000	0.636594000
H	3.545061000	1.680075000	-0.754721000
H	-0.564716000	3.276144000	0.825133000
H	0.514511000	2.170390000	-0.051142000
H	-0.043210000	1.740626000	1.560699000
H	3.092867000	-0.570808000	-1.796923000
H	3.886473000	-1.360607000	-0.441626000
H	0.663900000	-0.584238000	-1.587303000
H	-3.657572000	0.147536000	-0.258548000
H	-2.840229000	-0.574447000	-1.642257000
H	-3.024581000	-1.703008000	1.191818000
H	-3.286423000	-2.576312000	-0.321139000
H	-0.917911000	-2.495993000	-0.876086000
H	-0.841217000	-2.795895000	0.857380000
H	-0.291500000	-0.542189000	1.343023000

Atomic coordinates of **6k** (cis, exo, proximal 1)

C	-1.061677000	-2.041610000	0.620112000
C	-2.330899000	-1.872981000	-0.221479000
C	-2.053372000	-0.590295000	-1.004948000
N	-1.299610000	0.226731000	-0.047655000
C	-0.643840000	-0.594238000	0.994402000
C	-1.420446000	1.585468000	-0.055402000
C	-0.756180000	2.354731000	1.071842000
O	-2.042964000	2.167965000	-0.935647000
C	0.853615000	-0.416652000	1.119560000
C	1.745288000	-0.522236000	0.142521000
F	1.312804000	-0.797623000	-1.122401000
C	3.227920000	-0.373748000	0.207918000
C	3.762359000	0.788289000	-0.642542000
H	4.851544000	0.831490000	-0.583653000
H	3.364843000	1.744201000	-0.295400000
H	3.484852000	0.667337000	-1.690300000
H	-1.092427000	3.386988000	1.011587000
H	0.330344000	2.325948000	0.970891000
H	-1.007663000	1.947486000	2.054046000
H	3.682137000	-1.311055000	-0.133097000
H	3.512556000	-0.243704000	1.253958000
H	1.248780000	-0.199706000	2.104487000
H	-2.945091000	-0.049976000	-1.315872000
H	-1.450639000	-0.788496000	-1.897306000
H	-3.205498000	-1.735495000	0.420460000
H	-2.521539000	-2.729084000	-0.870066000
H	-0.275338000	-2.503613000	0.022275000
H	-1.205141000	-2.653281000	1.511573000
H	-1.082576000	-0.341645000	1.964894000

Atomic coordinates of **6k′** (cis, exo, proximal 2)

C	0.744563000	-1.977062000	-0.848649000
C	2.170040000	-2.017802000	-0.288081000
C	2.194973000	-0.824627000	0.666806000
N	1.351992000	0.163699000	-0.015064000
C	0.414965000	-0.465555000	-0.972408000
C	1.613513000	1.496565000	0.109271000

C	0.815857000	2.450921000	-0.760749000
O	2.461176000	1.913130000	0.890056000
C	-1.049509000	-0.148726000	-0.756202000
C	-1.728224000	-0.307865000	0.371980000
F	-1.078586000	-0.790458000	1.471534000
C	-3.162053000	-0.029677000	0.681591000
C	-3.994560000	0.503604000	-0.481858000
H	-5.023376000	0.670753000	-0.159265000
H	-4.017575000	-0.201907000	-1.315001000
H	-3.604543000	1.454021000	-0.851962000
H	1.249392000	3.441799000	-0.649462000
H	-0.229200000	2.479138000	-0.446697000
H	0.837035000	2.162451000	-1.814623000
H	-3.187732000	0.676481000	1.519610000
H	-3.602034000	-0.956523000	1.067344000
H	-1.603106000	0.233561000	-1.603610000
H	3.183380000	-0.401620000	0.834010000
H	1.769223000	-1.083449000	1.641762000
H	2.903595000	-1.871582000	-1.085829000
H	2.398841000	-2.960685000	0.210480000
H	0.053501000	-2.442734000	-0.145366000
H	0.636545000	-2.484153000	-1.808154000
H	0.672585000	-0.131008000	-1.982256000

Atomic coordinates of **6l** (cis, exo, proximal 3)

C	0.747414000	-1.978664000	-0.844962000
C	2.173666000	-2.016072000	-0.286170000
C	2.198230000	-0.820465000	0.665679000
N	1.352855000	0.164853000	-0.017537000
C	0.416011000	-0.467927000	-0.972711000
C	1.609154000	1.498592000	0.107624000
C	0.808532000	2.450685000	-0.762151000
O	2.454721000	1.917865000	0.889257000
C	-1.048685000	-0.152120000	-0.756592000
C	-1.726675000	-0.309061000	0.372332000
F	-1.076028000	-0.788165000	1.472805000
C	-3.160646000	-0.031547000	0.681908000
C	-3.994039000	0.498640000	-0.482316000
H	-5.022690000	0.666340000	-0.159485000
H	-4.017404000	-0.208943000	-1.313688000
H	-3.604479000	1.448223000	-0.855025000
H	1.245732000	3.440837000	-0.658821000
H	-0.233956000	2.483837000	-0.440063000
H	0.820563000	2.157052000	-1.814676000
H	-3.186661000	0.676256000	1.518526000
H	-3.599661000	-0.958012000	1.069677000
H	-1.603069000	0.227539000	-1.604666000
H	3.186309000	-0.395674000	0.830368000
H	1.774368000	-1.077377000	1.641972000
H	2.905963000	-1.870878000	-1.085254000
H	2.404422000	-2.957364000	0.214482000
H	0.057846000	-2.442976000	-0.139315000
H	0.638655000	-2.488737000	-1.802798000
H	0.672793000	-0.135905000	-1.983632000

Atomic coordinates of **6l′** (cis, exo, proximal 4)

C	0.024587000	-0.004723000	0.007760000
C	0.106245000	0.016761000	1.537683000
C	1.611095000	0.073288000	1.798683000
N	2.167558000	-0.746404000	0.716266000
C	1.244832000	-0.853884000	-0.436009000
C	3.306036000	-1.470822000	0.916852000
C	3.729694000	-2.430868000	-0.179675000
O	3.965448000	-1.354971000	1.943202000
C	1.819394000	-0.434031000	-1.771160000
C	2.401203000	0.724993000	-2.052173000
F	2.524130000	1.662104000	-1.067695000
C	2.982015000	1.190853000	-3.344456000
C	2.289959000	2.440966000	-3.907383000
H	2.769505000	2.754299000	-4.836611000
H	2.346525000	3.271230000	-3.202262000
H	1.236464000	2.244349000	-4.117668000
H	4.528206000	-3.053877000	0.216030000
H	4.101435000	-1.883142000	-1.047762000
H	2.906229000	-3.065122000	-0.516365000
H	2.925887000	0.368641000	-4.060563000
H	4.045028000	1.405352000	-3.185933000
H	1.744861000	-1.140059000	-2.589231000
H	1.917672000	-0.339407000	2.757679000
H	1.990690000	1.098425000	1.736473000
H	-0.310578000	-0.901921000	1.959845000
H	-0.428680000	0.860593000	1.975515000
H	0.123471000	1.007225000	-0.386228000
H	-0.906797000	-0.422879000	-0.375728000
H	0.928495000	-1.897470000	-0.533723000

Atomic coordinates of **6m** (trans, exo, distal 1)

C	0.571996000	2.104290000	0.065121000
C	2.090838000	2.263000000	0.175678000
C	2.612904000	0.987628000	-0.490887000
N	1.603720000	-0.018691000	-0.136103000
C	0.324110000	0.596181000	0.294397000
C	1.843850000	-1.345248000	0.082419000
C	3.206472000	-1.875591000	-0.332653000
O	1.001714000	-2.077711000	0.582004000
C	-0.857508000	0.074627000	-0.468701000
C	-2.036791000	-0.223658000	0.054978000
F	-2.227271000	-0.063368000	1.399278000
C	-3.254946000	-0.749407000	-0.624354000
C	-4.470509000	0.182662000	-0.517711000
H	-5.338315000	-0.264346000	-1.006995000
H	-4.269117000	1.144629000	-0.994396000
H	-4.730490000	0.369379000	0.525175000
H	3.159904000	-2.961811000	-0.316068000
H	3.977182000	-1.551138000	0.372244000
H	3.499988000	-1.535336000	-1.327775000
H	-3.499536000	-1.720097000	-0.178422000
H	-3.007070000	-0.934641000	-1.671470000
H	-0.738252000	-0.060701000	-1.537782000

H	3.599807000	0.700697000	-0.130414000
H	2.676557000	1.114481000	-1.578659000
H	2.397536000	2.284208000	1.224714000
H	2.466020000	3.167904000	-0.304152000
H	0.237469000	2.383741000	-0.937859000
H	0.013879000	2.709877000	0.778855000
H	0.177628000	0.389089000	1.356453000

Atomic coordinates of **6m′** (trans, exo, distal 2)

C	-0.696894000	2.122234000	0.174401000
C	-2.227509000	2.126083000	0.197529000
C	-2.560660000	0.717587000	0.696121000
N	-1.489922000	-0.108662000	0.122515000
C	-0.323529000	0.701322000	-0.304854000
C	-1.613633000	-1.409655000	-0.272740000
C	-2.874739000	-2.142205000	0.155066000
O	-0.748588000	-1.966120000	-0.934476000
C	0.971393000	0.207712000	0.272530000
C	2.133344000	0.209447000	-0.361155000
F	2.184849000	0.681246000	-1.645174000
C	3.478621000	-0.251918000	0.090242000
C	3.530997000	-0.819383000	1.506816000
H	4.547056000	-1.138250000	1.745495000
H	2.875381000	-1.685938000	1.611876000
H	3.233539000	-0.074730000	2.248488000
H	-2.717702000	-3.204353000	-0.017026000
H	-3.729839000	-1.817663000	-0.444627000
H	-3.119482000	-1.971970000	1.205368000
H	4.175689000	0.588488000	-0.006981000
H	3.822214000	-1.004975000	-0.628285000
H	0.949145000	-0.165411000	1.288745000
H	-3.541575000	0.378097000	0.366033000
H	-2.542878000	0.678103000	1.792255000
H	-2.624923000	2.265443000	-0.811344000
H	-2.647581000	2.904348000	0.836071000
H	-0.305978000	2.284095000	1.182839000
H	-0.263985000	2.884284000	-0.473248000
H	-0.258911000	0.671472000	-1.394624000

Atomic coordinates of **6n** (trans, exo, distal 3)

C	-0.698400000	2.122910000	0.172154000
C	-2.229037000	2.125501000	0.195389000
C	-2.560962000	0.717283000	0.695615000
N	-1.489514000	-0.108708000	0.122976000
C	-0.323848000	0.701752000	-0.305408000
C	-1.612359000	-1.410181000	-0.271241000
C	-2.872834000	-2.143242000	0.157532000
O	-0.747098000	-1.966524000	-0.932710000
C	0.971493000	0.210181000	0.272760000
C	2.132834000	0.208383000	-0.362051000
F	2.183555000	0.674281000	-1.648158000
C	3.478289000	-0.251468000	0.090360000
C	3.531639000	-0.812834000	1.509329000
H	4.547733000	-1.131232000	1.748454000
H	2.875722000	-1.678628000	1.618672000
H	3.235197000	-0.064869000	2.248054000
H	-2.715090000	-3.205439000	-0.013591000
H	-3.728316000	-1.819881000	-0.442235000
H	-3.117421000	-1.972212000	1.207738000
H	4.175524000	0.588312000	-0.011010000
H	3.821127000	-1.007690000	-0.625183000
H	0.950021000	-0.158120000	1.290754000
H	-3.541584000	0.376605000	0.365896000
H	-2.543209000	0.679065000	1.791791000
H	-2.626625000	2.263376000	-0.813613000
H	-2.649710000	2.904132000	0.833072000
H	-0.307582000	2.286348000	1.180374000
H	-0.266196000	2.884564000	-0.476423000
H	-0.259093000	0.670578000	-1.395114000

Atomic coordinates of **6n′** (trans, exo, distal 4)

C	-1.010489000	-2.131308000	-0.039805000
C	-2.521668000	-1.949998000	0.125692000
C	-2.762165000	-0.558688000	-0.466467000
N	-1.540057000	0.176385000	-0.115436000
C	-0.420692000	-0.730251000	0.238276000
C	-1.465851000	1.511353000	0.162475000
C	-2.685239000	2.353500000	-0.175219000
O	-0.463960000	2.011523000	0.653971000
C	0.824811000	-0.452756000	-0.550635000
C	2.057373000	-0.472691000	-0.066678000
F	2.245635000	-0.750115000	1.259373000
C	3.343423000	-0.205737000	-0.771721000
C	4.077144000	1.032497000	-0.234349000
H	5.016349000	1.180627000	-0.771468000
H	4.307437000	0.920716000	0.825937000
H	3.465813000	1.928781000	-0.353763000
H	-2.391813000	3.399386000	-0.125708000
H	-3.483870000	2.183547000	0.552443000
H	-3.083821000	2.130093000	-1.166831000
H	3.129161000	-0.087512000	-1.835990000
H	3.989391000	-1.085332000	-0.670317000
H	0.706089000	-0.231185000	-1.605227000
H	-3.645967000	-0.074872000	-0.052795000
H	-2.888200000	-0.615012000	-1.554732000
H	-2.793881000	-1.953961000	1.184496000
H	-3.106122000	-2.722744000	-0.375489000
H	-0.778248000	-2.431623000	-1.065488000
H	-0.582244000	-2.879793000	0.626561000
H	-0.198583000	-0.612481000	1.300896000

Atomic coordinates of **6o** (trans, exo, proximal 1)

C	-0.961875000	-2.124207000	0.474611000
C	-2.244519000	-1.913883000	-0.339360000
C	-2.014340000	-0.551210000	-0.999023000
N	-1.271994000	0.189205000	0.024359000
C	-0.587287000	-0.710456000	0.981713000
C	-1.340341000	1.523325000	0.279500000

C	-2.100629000	2.381169000	-0.716776000
O	-0.807169000	2.013272000	1.268947000
C	0.895269000	-0.456514000	1.111238000
C	1.787627000	-0.498796000	0.132835000
F	1.367797000	-0.794513000	-1.140525000
C	3.253157000	-0.232109000	0.188454000
C	3.676223000	1.003077000	-0.620993000
H	4.757480000	1.143868000	-0.562967000
H	3.192384000	1.903095000	-0.236777000
H	3.406263000	0.894174000	-1.672471000
H	-1.894235000	3.423692000	-0.486846000
H	-3.177664000	2.212348000	-0.630613000
H	-1.810167000	2.168370000	-1.747510000
H	3.783106000	-1.114546000	-0.188093000
H	3.535410000	-0.112364000	1.236228000
H	1.267309000	-0.186240000	2.090410000
H	-2.944639000	-0.045487000	-1.253822000
H	-1.418037000	-0.655277000	-1.912602000
H	-3.114987000	-1.860831000	0.320191000
H	-2.421444000	-2.706006000	-1.068273000
H	-0.170191000	-2.511333000	-0.167080000
H	-1.089409000	-2.820207000	1.304090000
H	-1.029745000	-0.535633000	1.965579000

Atomic coordinates of **6o′** (trans, exo, proximal 2)

C	0.681762000	-2.041549000	-0.758359000
C	2.109148000	-2.058343000	-0.197142000
C	2.152651000	-0.798757000	0.672569000
N	1.315095000	0.144832000	-0.072073000
C	0.367407000	-0.542238000	-0.980083000
C	1.475147000	1.492762000	-0.153479000
C	2.496645000	2.126261000	0.774885000
O	0.819626000	2.168529000	-0.939080000
C	-1.077042000	-0.156168000	-0.764236000
C	-1.762176000	-0.292151000	0.360788000
F	-1.138777000	-0.834174000	1.458131000
C	-3.170323000	0.080794000	0.684992000
C	-3.960011000	0.704009000	-0.463998000
H	-4.971876000	0.945600000	-0.134178000
H	-4.040324000	0.020423000	-1.311817000
H	-3.492658000	1.626270000	-0.813905000
H	2.366405000	3.204809000	0.729739000
H	3.514163000	1.884545000	0.455364000
H	2.380216000	1.785536000	1.805672000
H	-3.141691000	0.769748000	1.537250000
H	-3.679758000	-0.818513000	1.050572000
H	-1.590814000	0.305299000	-1.595310000
H	3.162581000	-0.412140000	0.801662000
H	1.730204000	-0.994246000	1.664766000
H	2.841939000	-1.973489000	-1.004185000
H	2.333487000	-2.963919000	0.368229000
H	-0.011339000	-2.462613000	-0.030296000
H	0.578987000	-2.607922000	-1.684304000
H	0.627549000	-0.251598000	-2.000908000

Atomic coordinates of **6p** (trans, exo, proximal 3)

C	0.681655000	-2.041705000	-0.757941000
C	2.109148000	-2.058463000	-0.197037000
C	2.152939000	-0.798707000	0.672420000
N	1.315106000	0.144748000	-0.072106000
C	0.367375000	-0.542421000	-0.979963000
C	1.475127000	1.492675000	-0.153657000
C	2.496701000	2.126286000	0.774560000
O	0.819599000	2.168357000	-0.939319000
C	-1.077076000	-0.156301000	-0.764186000
C	-1.762134000	-0.291781000	0.360954000
F	-1.138642000	-0.833238000	1.458494000
C	-3.170280000	0.081233000	0.685100000
C	-3.960380000	0.703176000	-0.464295000
H	-4.972198000	0.944918000	-0.134441000
H	-4.040802000	0.018707000	-1.311396000
H	-3.493294000	1.625168000	-0.815274000
H	2.365488000	3.204758000	0.730388000
H	3.514158000	1.885775000	0.453883000
H	2.381511000	1.784558000	1.805142000
H	-3.141613000	0.770998000	1.536710000
H	-3.679426000	-0.817846000	1.051649000
H	-1.590935000	0.304704000	-1.595466000
H	3.162920000	-0.412046000	0.801058000
H	1.730871000	-0.993993000	1.664822000
H	2.841770000	-1.973829000	-1.004257000
H	2.333551000	-2.963937000	0.368480000
H	-0.011335000	-2.462505000	-0.029614000
H	0.578617000	-2.608320000	-1.683716000
H	0.627508000	-0.252011000	-2.000862000

Atomic coordinates of **6p′** (trans, exo, proximal 4)

C	0.357215000	2.040025000	0.713144000
C	1.656644000	2.335108000	-0.046700000
C	1.871086000	1.062568000	-0.870883000
N	1.374290000	0.007253000	0.015737000
C	0.425508000	0.526143000	1.028417000
C	1.852055000	-1.261774000	0.123440000
C	2.862284000	-1.711995000	-0.917415000
O	1.479705000	-2.011260000	1.019317000
C	-0.908013000	-0.182371000	1.036910000
C	-1.755763000	-0.273681000	0.022680000
F	-1.434727000	0.321857000	-1.171893000
C	-3.067982000	-0.977806000	-0.042652000
C	-4.250521000	-0.044743000	-0.340965000
H	-5.179309000	-0.615230000	-0.404173000
H	-4.110309000	0.476313000	-1.289188000
H	-4.365166000	0.705307000	0.444727000
H	2.991640000	-2.786773000	-0.815518000
H	3.828968000	-1.227506000	-0.754101000
H	2.537641000	-1.476216000	-1.932882000
H	-3.220976000	-1.496689000	0.905430000
H	-3.007320000	-1.748035000	-0.820123000
H	-1.189789000	-0.695566000	1.946518000

H	2.916713000	0.900235000	-1.128635000
H	1.289884000	1.095738000	-1.799515000
H	2.489124000	2.467331000	0.649825000
H	1.592231000	3.229214000	-0.668354000
H	-0.503379000	2.249061000	0.077883000
H	0.250965000	2.628894000	1.624537000
H	0.878887000	0.367674000	2.010062000