Understanding the Torquoselectivity in 8π -Electrocyclic Cascade Reactions: Synthesis of Fenestradienes versus Cyclooctatrienes

Catherine Hulot,[‡] Shadi Amiri,[§] Gaëlle Blond,[‡] Peter R. Schreiner,^{*,§} and Jean Suffert^{*,‡}

Faculté de Pharmacie, Université de Strasbourg (UMR 7200 CNRS/UDS), 74 Route du Rhin, 67401 Illkirch/Strasbourg, France; Institut für Organische Chemie, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 58, D-35392 Giessen, Germany

[‡] Université de Strasbourg

[§] Justus-Liebig-Universität Giessen

Supporting Information

Contents

General Methods: S1

Characterization data for **5-34**: S2-S16

Computational Section : S17-S80

References of Supporting Information : S80

Then NMR spectra

General Methods. Reactions were run under an atmosphere of argon in oven-dried glassware using a standard syringe and septa apparatus. Et₂O and THF were distilled from sodium / benzophenone. Crude products were purified by flash column chromatography on Merck silica gel Si 60 (40-63 μ m). For some compounds, 5% Et₃N treated silica gel was used to avoid decomposition. Analytical TLC was carried out on Merck aluminium sheets silica gel 60 F₂₅₄. ¹H NMR spectra were recorded at 200, 300 or 500 MHz using the residual solvent signal as internal reference (CDCl₃, 7.26 ppm). Chemical shifts are quoted in ppm, coupling constants (*J*) are given in Hz. The following abbreviations are used to describe peak patterns when appropriate: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintuplet), m (multiplet), ap (apparent), br (broad). ¹³C NMR spectra were recorded at 50 or 75 MHz at ambient temperature in CDCl₃ with δ (CDCl₃) at 77.16 as internal standard. Multiplicities were determined in some cases by DEPT pulse sequence and are given as follow: + = CH or CH₃, - = CH₂, and C_{quat} = C. Melting points were determined with a glass capillary apparatus Gallenkamp and are uncorrected. I.R were determined with a Nicolet 380 FT-IR apparatus. We thank Pr. Van Dorsselaer (LSMBO, Cronenbourg, France) to lend us the spectrometers for mass spectra. Gas Chromatography Mass Spectrometry (GCMS) were performed using an Agilent 5975 GCMS spectrometer (EI Quad, positive ion 70 eV). High Resolution Mass Spectral analysis (HRMS) were performed using a Bruker MicroTOF-Q (ESI Q-TOF, positive ion: solution of lithium formate in isopropanol, 10 mM). *n*-BuLi was titrated using *N*-pivaloyl *o*-toluidine following the Suffert's procedure.¹ X-ray Cristallographic Study were done by the X-Ray Central Service of the Chemistry Institute of Strasbourg (France). Microwave irradiations have been performed using BIOTAGE Smith Creator. The program NameiPro (ACD/Name version 5.5.5.5) was used to name the different compounds.

Compounds **1**, **2**, **3**, **4**, **6**, **13**, **14**, **21**, **25**, **26**, **28**, **30**, **32** have already been described.²

• **Synthesis of trienynes 5a-f**

{[(4*S,5*S**)-6-bromo-2,2-dimethyl-1,3-dioxaspiro[4.6]undec-6-en-4-yl]ethynyl}(trimethyl) silane (**34**)**

A solution of diol *anti* **3** (2 g, 6.30 mmol, 1 eq), 2,2-dimethoxypropane (20 mL, 162.8 mmol, 26 eq), and *p*-TsOH (200 mg, 1.05 mmol, 0.17 eq) in acetone (50 mL) was stirred for 7 h at room temperature. Then the mixture was quenched by addition of a saturated solution of NaHCO₃ (50 mL). After extraction with Et₂O, the combined organic layers were washed with water, brine, dried over MgSO₄ and concentrated *in vacuo*. The crude product was purified by chromatography on silica gel (elution with pentane/Et₂O 98:2) to give 2.1 g (93%) of the product as a white powder.

C₁₆H₂₅BrO₂Si, MW = 357.36 g·mol⁻¹

R_f = 0.16 (Pentane/Et₂O 98:2)

Mp = 44 °C

¹H NMR (200 MHz, CDCl₃) δ 6.54 (t, *J* = 6.8 Hz, 1H), 4.82 (s, 1H), 2.28-1.58 (m, 8H), 1.70 (s, 3H), 1.39 (s, 3H), 0.17 (s, 9H). ¹³C NMR (50 MHz, CDCl₃) δ 135.4, 129.7, 110.8, 100.2, 94.2,

88.9, 73.8, 37.6, 27.4, 26.4 (2C), 24.5, 21.7, -0.5 (3C). **IR** (CHCl₃) ν 3053, 2938, 2857, 1457, 1379, 1249, 1208, 1188, 1163, 1096, 1069, 1042, 980, 939, 893, 843, 760, 738, 704, 654, 559, 524, 407. **MS** (GCMS) : 356.1, 358.1 [M⁺].

(4*S,5*S**)-6-bromo-4-ethynyl-2,2-dimethyl-1,3-dioxaspiro[4.6]undec-6-ene (27)**

A solution of diol *anti* **34** (2.89 g, 8.09 mmol, 1 eq) and K₂CO₃ (1.12 g, 8.09 mmol, 1 eq) in MeOH (40 mL) was stirred for 20 min at room temperature. The mixture was quenched by addition of a saturated solution of NH₄Cl (40 mL). After extraction with AcOEt, the combined organic layers were washed with water, brine, dried over MgSO₄ and concentrated *in vacuo*. 2.25 g (97%) of product were obtained as a white powder, and used without purification.

C₁₃H₁₇BrO₂, MW = 285.18 g.mol⁻¹

R_f = 0,58 (Heptane/Et₂O 7:3)

Mp = 78 °C

¹H NMR (200 MHz, CDCl₃) δ 6.59 (t, *J* = 6.6 Hz, 1H), 4.87 (d, *J* = 2.3 Hz, 1H), 2.65 (d, *J* = 2.3 Hz, 1H), 2.30-1.54 (m, 8H), 1.72 (s, 3H), 1.41 (s, 3H). ¹³C NMR (50 MHz, CDCl₃) δ 136.3, 129.2, 111.0, 88.6, 78.7, 77.2, 73.4, 37.7, 27.4, 26.5, 26.4, 24.6, 21.7. **IR** (CHCl₃) ν 3853, 3751, 3648, 3283, 2938, 2360, 1684, 1653, 1558, 1541, 1507, 1457, 1375, 1261, 1209, 1163, 1068, 1040, 866, 669, 518, 419. **MS** (GCMS) : 284.1, 286.1 [M⁺].

3-[(4*S,5*S**)-6-bromo-2,2-dimethyl-1,3-dioxaspiro[4.6]undec-6-en-4-yl]prop-2-yn-1-ol (29)**

To a solution of compound **27** (2.14 g, 7.50 mmol, 1 eq) in THF (63 mL) was added dropwise *n*-BuLi (5.1 mL, 8.25 mmol, 1.1 eq, 1.6 M in hexane) at -78 °C. The resulting solution was stirred for 30 min at -78 °C and paraformaldehyde (356 mg, 11.25 mmol, 1.5 eq) was then added. The reaction mixture was kept at -78 °C for 1 h and then allowed to warm up to room temperature for 18 h before addition of a saturated solution of NaHCO₃ (70 mL). After extraction with Et₂O, the combined organic layers were washed with water, brine, dried over MgSO₄ and concentrated *in vacuo*. The crude product was purified by chromatography on silica gel (elution with pentane/AcOEt 8:2) to afford 1.715 g (73%) of the product as a white solid.

C₁₄H₁₉BrO₃, MW = 315.2 g.mol⁻¹

R_f = 0.24 (pentane/AcOEt 8:2)

Mp = 72 °C

¹H NMR (200 MHz, CDCl₃) δ 6.57 (t, J = 6.8 Hz, 1H), 4.88 (t, J = 2.1 Hz, 1H), 4.34 (d, J = 2.1 Hz, 2H), 2.29-1.64 (m, 9H), 1.71 (s, 3H), 1.41 (s, 3H). **¹³C NMR** (50 MHz, CDCl₃) δ 136.3, 129.3, 110.9, 88.7, 87.3, 80.6, 73.6, 51.1, 37.6, 27.4, 26.5 (2C), 24.7, 21.6. **IR** (CHCl₃) ν 3414, 2986, 2937, 2864, 2183, 2144, 1457, 1380, 1275, 1261, 1209, 1162, 1043, 898, 867, 764, 750, 559, 430. **MS** (GCMS) : 314.1, 316.1 [M⁺].

(2Z)-2-[(3aS*,9aR*)-2,2-dimethyl-6,7,8,9-tetrahydrocyclohepta[1,4]cyclobuta[1,2-*d*][1,3]dioxol-4(3aH)-ylidene]-4-(trimethylsilyl)but-3-yn-1-ol (31)

The reaction was carried out in a BIOTAGE sealed tube, under argon atmosphere. To a solution of the protected diol **29** (1.182 g, 3.75 mmol, 1 eq) in benzene (15 mL) were added Pd(PPh₃)₄ (433 mg, 0.375 mmol, 0.1 eq) and the stannylated reagent (2.178 g, 5.63 mmol, 1.5 eq). The yellow mixture was purged 10 min with argon and heated at 130 °C under microwave irradiation for 20 min. The resulted black solution was then cooled and concentrated. The reaction mixture was purified by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 92:8) to give 1.233 g (99%) of the product as a yellow solid.

C₁₉H₂₈O₃Si, MW = 332.51 g.mol⁻¹

Rf = 0.23 (pentane/AcOEt 92:8)

Mp = 36 °C

¹H NMR (300 MHz, CDCl₃) δ 6.66 (dd, J = 7.5 Hz, J = 4.5 Hz, 1H), 4.84 (s, 1H), 4.25 (m, 2H), 2.44 (m, 1H), 2.25 (m, 2H), 1.92 (m, 4H), 1.75 (m, 2H), 1.47 (s, 3H), 1.42 (s, 3H), 0.21 (s, 9H). **¹³C NMR** (75 MHz, CDCl₃) δ 146.8, 144.6, 131.0, 117.2, 114.5, 103.8, 103.0, 90.1, 81.8, 62.7, 34.5, 29.5, 28.8 (2C), 27.7, 26.7, -0.0 (3C). **IR** (CHCl₃) ν 3438, 2926, 2855, 2132, 1443, 1370, 1250, 1230, 1208, 1192, 1148, 1106, 1054, 1010, 899, 922, 875, 841, 759, 698, 636, 555 cm⁻¹. **MS** (GCMS) : 332.2 [M⁺]. **COSY**, **NOESY**, **HSQC**, **HMBC**.

(2Z,5E)-2-[(3aS*,9aR*)-2,2-dimethyl-6,7,8,9-tetrahydrocyclohepta[1,4]cyclobuta[1,2-*d*][1,3]dioxol-4(3aH)-ylidene]-7-methyloct-5-en-3-yne-1,7-diol (5a)

A solution of compound **31** (150 mg, 0.45 mmol, 1 eq) and K₂CO₃ (62 mg, 0.45 mmol, 1 eq) in MeOH (2.25 mL) was stirred at room temperature under argon for 1 h. Then the mixture was

quenched by addition of water (3 mL). After extraction with Et₂O, the combined organic layers were washed with water, brine, dried over MgSO₄ and concentrated. It is important to note that this terminal alkyne **33** should not be dried, in order to avoid polymerization. Before the total evaporation of Et₂O was added MeCN (4.5 mL). When the residual Et₂O was evaporated, the product was then engaged in the Sonogashira reaction. To the mixture were added the vinyl iodide (115 mg, 0.54 mmol, 1.2 eq), Pd(PPh₃)₄ (26 mg, 0.023 mmol, 0.05 eq), CuI (13 mg, 0.07 mmol, 0.15 eq) and Et₃N (1.1 mL, MeCN/Et₃N 8:2). According to the TLC, the reaction was completed after 20 min of stirring at room temperature under argon. The opaque yellow solution became a clear orange solution. Ethanolamine (41 μL, 0.68 mmol, 10 eq/CuI) was then added. The mixture was stirred for 1 h at room temperature, and became green, with the formation of precipitate. Then the mixture was quenched by addition of water (5 mL). After extraction with Et₂O, the combined organic layers were washed with water, brine, dried over MgSO₄ and concentrated. The crude product was purified by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 7:3) to give 126 mg (81%) of the product as an orange oil.

C₂₁H₂₈O₄, MW = 344.44 g.mol⁻¹

R_f = 0.14 (pentane/AcOEt 7:3)

¹H NMR (300 MHz, CDCl₃) δ 6.61 (dd, *J* = 7.9 Hz, *J* = 4.5 Hz, 1H), 6.29 (d, *J* = 16.0 Hz, 1H), 5.95 (d, *J* = 16.0 Hz, 1H), 4.86 (s, 1H), 4.32 (d, *J* = 13.6 Hz, 1H), 4.24 (d, *J* = 13.6 Hz, 1H), 2.44 (m, 1H), 2.25 (m, 2H), 1.98-1.35 (m, 7H), 1.47 (s, 3H), 1.43 (s, 3H), 1.35 (s, 6H). ¹³C NMR (50 MHz, CDCl₃) δ 151.2, 145.5, 144.6, 130.7, 117.4, 114.5, 106.9, 96.5, 90.0, 88.1, 81.7, 71.0, 62.9, 34.5, 29.5 (2C), 28.8 (2C), 27.8, 26.8. IR (CHCl₃) ν 3382, 2975, 2930, 2858, 1652, 1457, 1371, 1307, 1261, 1230, 1209, 1192, 1148, 1087, 1054, 1006, 957, 928, 844 cm⁻¹. MS (GCMS) : 344.2 [M⁺].

(2*Z*,5*E*)-2-[(3*aS**,9*aR**)-2,2-dimethyl-6,7,8,9-tetrahydrocyclohepta[1,4]cyclobuta[1,2-*d*][1,3]dioxol-4(3*aH*)-ylidene]dodec-5-en-3-yn-1-ol (**5b**)

Compound **5b** was prepared following the same procedure than for the preparation of **5a**, starting from compound **31** (180 mg, 0.54 mmol, 1 eq) and K₂CO₃ (75 mg, 0.54 mmol, 1 eq) in MeOH (2.7 mL). After 10 min of reaction and extraction, the alkyne **33** was reacted with the vinyl iodide (154 mg, 0.65 mmol, 1.2 eq), Pd(PPh₃)₄ (31 mg, 0.027 mmol, 0.05 eq), CuI (15 mg, 0.08 mmol, 0.15 eq), in MeCN/Et₃N 8:2 (6.8 mL). The mixture was stirred for 20 min at room temperature. Ethanolamine (50 μL, 0.81 mmol, 10 eq/CuI) was then added, and the solution was stirred for 1 hour. After extraction and purification by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 93:7), 168 mg (84%) of the product were obtained as an orange oil.

C₂₄H₃₄O₃, MW = 370.52 g.mol⁻¹

R_f = 0.29 (pentane/AcOEt 92:8)

¹H NMR (300 MHz, CDCl₃) δ 6.61 (dd, *J* = 7.6 Hz, *J* = 4.9 Hz, 1H), 6.20 (dt, *J* = 15.9 Hz, *J* = 7.0 Hz, 1H), 5.68 (dt, *J* = 15.9 Hz, *J* = 1.4 Hz, 1H), 4.86 (s, 1H), 4.32 (d, *J* = 14.2 Hz, 1H), 4.23 (d, *J* =

14.2 Hz, 1H), 2.53-1.56 (m, 11H), 1.48 (s, 3H), 1.43 (s, 3H), 1.28 (m, 8H), 0.88 (t, $J = 6.7$ Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 146.2, 145.3, 144.7, 130.6, 117.6, 114.6, 109.6, 97.6, 90.2, 86.1, 81.8, 63.3, 34.7, 33.4, 31.8, 29.7, 28.9, 28.8 (2C), 27.9, 26.9, 22.7, 14.2. IR (CHCl_3) ν 3433, 2925, 2855, 2360, 1651, 1612, 1456, 1379, 1370, 1306, 1259, 1230, 1209, 1192, 1150, 1087, 1054, 1007, 951, 928, 894, 841, 691, 556 cm^{-1} . MS (GCMS) : 370.3 $[\text{M}^+]$.

1-{(1*E*,5*Z*)-5-[(3*aS,9*aR**)-2,2-dimethyl-6,7,8,9-tetrahydrocyclohepta[1,4]cyclobuta[1,2-*d*][1,3]dioxol-4(3*aH*)-ylidene]-6-hydroxyhex-1-en-3-ynyl}cyclohexanol (5c)**

Compound **5c** was prepared following the same procedure than for the preparation of **5a**, starting from compound **31** (220 mg, 0.66 mmol, 1 eq) and K_2CO_3 (91 mg, 0.66 mmol, 1 eq) in MeOH (3.3 mL). After 20 min of reaction and extraction, the alkyne **33** was reacted with the vinyl iodide (200 mg, 0.79 mmol, 1.2 eq), $\text{Pd}(\text{PPh}_3)_4$ (38 mg, 0.033 mmol, 0.05 eq), CuI (19 mg, 0.10 mmol, 0.15 eq), in MeCN/ Et_3N 8:2 (8.3 mL). The mixture was stirred for 20 min at room temperature. Ethanamine (60 μL , 0.99 mmol, 10 eq/ CuI) was then added, and the solution was stirred for 1 hour. After extraction and purification by chromatography on 5% Et_3N treated silica gel (elution with pentane/ AcOEt 7:3), 216 mg (85%) of the product were obtained as a yellow solid.

$\text{C}_{24}\text{H}_{32}\text{O}_4$, MW = 384.51 $\text{g}\cdot\text{mol}^{-1}$

Rf = 0.26 (pentane/ AcOEt 7:3)

Mp = 64 $^\circ\text{C}$

^1H NMR (300 MHz, CDCl_3) δ 6.62 (dd, $J = 7.8$ Hz, $J = 4.7$ Hz, 1H), 6.30 (d, $J = 15.9$ Hz, 1H), 5.99 (d, $J = 15.9$ Hz, 1H), 4.86 (s, 1H), 4.32 (dd, $J = 13.6$ Hz, $J = 6.6$ Hz, 1H), 4.24 (dd, $J = 13.6$ Hz, $J = 6.6$ Hz, 1H), 2.45 (m, 1H), 2.29 (m, 1H), 2.17 (t, $J = 6.6$ Hz, 1H : OH), 2.04 (s, 1H : OH), 1.93 (m, 4H), 1.79-1.36 (m, 12H), 1.47 (s, 3H), 1.43 (s, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 151.3, 145.8, 144.6, 130.9, 117.4, 114.6, 107.5, 96.9, 90.1, 88.2, 81.8, 72.1, 63.2, 37.6 (2C), 34.7, 29.7, 28.9 (2C), 27.9, 26.8, 25.4, 21.9 (2C). IR (CHCl_3) ν 3396, 2986, 2930, 2856, 1448, 1380, 1370, 1261, 1231, 1209, 1191, 1150, 1088, 1054, 1006, 957, 909, 845, 833, 733, 417, 405 cm^{-1} . MS (GCMS) : 384.3 $[\text{M}^+]$.

1-{(1*E*,5*Z*)-5-[(3*aS,9*aR**)-2,2-dimethyl-6,7,8,9-tetrahydrocyclohepta[1,4]cyclobuta[1,2-*d*][1,3]dioxol-4(3*aH*)-ylidene]-6-hydroxyhex-1-en-3-ynyl}cyclopentanol (5d)**

Compound **5d** was prepared following the same procedure than for the preparation of **5a**, starting from compound **31** (150 mg, 0.45 mmol, 1 eq) and K_2CO_3 (62 mg, 0.45 mmol, 1 eq) in MeOH (2.3 mL). After 20 min of reaction and extraction, the alkyne **33** was reacted with the vinyl iodide (129 mg, 0.54 mmol, 1.2 eq), $\text{Pd(PPh}_3)_4$ (26 mg, 0.023 mmol, 0.05 eq), CuI (13 mg, 0.068 mmol, 0.15 eq), in MeCN/ Et_3N 8:2 (5.6 mL). The mixture was stirred for 25 min at room temperature. Ethanolamine (40 μL , 0.68 mmol, 10 eq/CuI) was then added, and the solution was stirred for 1 hour. After extraction and purification by chromatography on 5% Et_3N treated silica gel (elution with pentane/AcOEt 75:25), 143 mg (86%) of the product were obtained as an orange solid.

$\text{C}_{23}\text{H}_{30}\text{O}_4$, MW = 370.48 $\text{g}\cdot\text{mol}^{-1}$

Rf = 0.18 (pentane/AcOEt 75:25)

Mp = 44 $^\circ\text{C}$

^1H NMR (300 MHz, CDCl_3) δ 6.62 (dd, $J = 7.8$ Hz, $J = 4.7$ Hz, 1H), 6.33 (d, $J = 15.9$ Hz, 1H), 6.03 (d, $J = 15.9$ Hz, 1H), 4.87 (s, 1H), 4.32 (dd, $J = 13.4$ Hz, $J = 5.9$ Hz, 1H), 4.24 (dd, $J = 13.4$ Hz, $J = 5.9$ Hz, 1H), 2.50-2.17 (m, 3H), 1.98-1.62 (m, 15H), 1.48 (s, 3H), 1.43 (s, 3H). **^{13}C NMR** (75 MHz, CDCl_3) δ 150.1, 145.5, 144.6, 130.7, 117.4, 114.5, 107.1, 96.8, 90.0, 88.1, 82.2, 81.7, 63.0, 40.7 (2C), 34.6, 29.6, 28.9, 28.8, 27.8, 26.8, 23.9 (2C). **IR** (CHCl_3) ν 3392, 2931, 2858, 2156, 1653, 1436, 1370, 1261, 1231, 1210, 1192, 1149, 1088, 1054, 1007, 957, 845, 555, 409 cm^{-1} . **MS** (GCMS) : 370.2 [M^+].

(2Z,5E)-2-[(3aS*,9aR*)-2,2-dimethyl-6,7,8,9-tetrahydrocyclohepta[1,4]cyclobuta[1,2-d][1,3]dioxol-4(3aH)-ylidene]-8-phenyloct-5-en-3-yn-1-ol (5e)

Compound **5e** was prepared following the same procedure than for the preparation of **5a**, starting from compound **31** (140 mg, 0.42 mmol, 1 eq) and K_2CO_3 (58 mg, 0.42 mmol, 1 eq) in MeOH (2.1 mL). After 20 min of reaction and extraction, the alkyne **33** was reacted with the vinyl iodide (163 mg, 0.63 mmol, 1.5 eq), $\text{Pd(PPh}_3)_4$ (24 mg, 0.02 mmol, 0.05 eq), CuI (12 mg, 0.06 mmol, 0.15 eq), in MeCN/ Et_3N 8:2 (5.3 mL). The mixture was stirred for 30 min at room temperature. Ethanolamine (0.04 mL, 0.60 mmol, 10 eq/CuI) was then added, and the solution was stirred for 1 hour. After extraction and purification by chromatography on 5% Et_3N treated silica gel (elution with pentane/AcOEt 9:1), 130 mg (79%) of the product were obtained as an orange oil.

$\text{C}_{26}\text{H}_{30}\text{O}_3$, MW = 390.51 $\text{g}\cdot\text{mol}^{-1}$

R_f = 0.26 (pentane/AcOEt 85:15)

¹H NMR (300 MHz, CDCl₃) δ 7.32-7.17 (m, 5H), 6.59 (dd, *J* = 7.9 Hz, *J* = 4.5 Hz, 1H), 6.22 (dt, *J* = 15.8 Hz, *J* = 7.2 Hz, 1H), 5.72 (d, *J* = 15.8 Hz, 1H), 4.86 (s, 1H), 4.31 (dd, *J* = 13.6 Hz, *J* = 6.4 Hz, 1H), 4.23 (dd, *J* = 13.6 Hz, *J* = 6.4 Hz, 1H), 2.74 (t, *J* = 7.2 Hz, 2H), 2.48 (m, 3H), 2.30 (m, 1H), 2.13 (t, *J* = 6.4 Hz, 1H : OH), 1.93 (m, 4H), 1.80-1.58 (m, 2H), 1.48 (s, 3H), 1.43 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 145.5, 144.63, 144.57, 141.2, 130.6, 128.53 (2C), 128.50 (2C), 126.2, 117.5, 114.6, 110.4, 97.2, 90.1, 86.5, 81.8, 63.3, 35.2, 35.1, 34.7, 29.7, 28.94, 28.92, 27.9, 26.8. IR (CHCl₃) ν 3448, 3026, 2987, 2929, 2855, 2331, 1605, 1497, 1454, 1379, 1370, 1306, 1260, 1231, 1209, 1192, 1149, 1087, 1054, 1007, 952, 842, 747, 699, 556 cm⁻¹. MS (GCMS) : 390.2 [M⁺].

(2*Z*,5*E*)-2-[(3*aS**,9*aR**)-2,2-dimethyl-6,7,8,9-tetrahydrocyclohepta[1,4]cyclobuta[1,2-*d*][1,3]dioxol-4(3*aH*)-ylidene]-7-isobutyl-9-methyldec-5-en-3-yne-1,7-diol (**5f**)

Compound **5f** was prepared following the same procedure than for the preparation of **5a**, starting from compound **31** (180 mg, 0.54 mmol, 1 eq) and K₂CO₃ (75 mg, 0.54 mmol, 1 eq) in MeOH (2.7 mL). After 20 min of reaction and extraction, the alkyne **33** was reacted with the vinyl iodide (193 mg, 0.65 mmol, 1.2 eq), Pd(PPh₃)₄ (31 mg, 0.027 mmol, 0.05 eq), CuI (15 mg, 0.08 mmol, 0.15 eq), in MeCN/Et₃N 8:2 (6.8 mL). The mixture was stirred for 20 min at room temperature. Ethanamine (50 μL, 0.81 mmol, 10 eq/CuI) was then added, and the solution was stirred for 1 hour. After extraction and purification by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 8:2), 187 mg (81%) of the product were obtained as an orange oil.

C₂₇H₄₀O₄, MW = 428.6 g.mol⁻¹

R_f = 0.22 (pentane/AcOEt 8:2)

¹H NMR (300 MHz, CDCl₃) δ 6.61 (dd, *J* = 7.5 Hz, *J* = 4.4 Hz, 1H), 6.16 (d, *J* = 15.9 Hz, 1H), 5.97 (d, *J* = 15.9 Hz, 1H), 4.87 (s, 1H), 4.33 (dd, *J* = 13.4 Hz, *J* = 6.1 Hz, 1H), 4.25 (dd, *J* = 13.4 Hz, *J* = 6.1 Hz, 1H), 2.43 (m, 1H), 2.23 (m, 2H), 1.97 (m, 4H), 1.74 (m, 3H), 1.59 (s, 1H : OH), 1.49 (s, 3H), 1.46 (d, *J* = 5.9 Hz, 4H), 1.43 (s, 3H), 1.34 (s, 1H : OH), 0.94 (d, *J* = 6.7 Hz, 6H), 0.91 (d, *J* = 6.7 Hz, 6H). ¹³C NMR (75 MHz, CDCl₃) δ 150.3, 145.3, 144.7, 130.5, 117.6, 114.5, 107.6, 97.1, 90.0, 87.8, 81.7, 76.9, 62.9, 51.0 (2C), 34.6, 29.5, 28.8 (2C), 27.8, 26.8, 24.7 (2C), 24.6 (2C), 24.0 (2C). IR (CHCl₃) ν 3431, 2951, 2927, 2868, 1651, 1467, 1380, 1370, 1304, 1260, 1231, 1210, 1192, 1150, 1087, 1054, 1008, 963, 894, 845, 555 cm⁻¹. MS (GCMS) : 428.3 [M⁺].

• **Synthesis of cyclooctatrienes 16a and 18a-f**

2-[(3a*R**,4*S**,5*R**,9b*S**)-9-(hydroxymethyl)-2,2-dimethyl-4,9b-dihydro-5*H*-3a,4-propanocycloocta[3,4]cyclobuta[1,2-*d*][1,3]dioxol-5-yl]propan-2-ol

- **Path A : semihydrogenation of trienynone 4a at 70 °C**

To a solution of Ni(OAc)₂·4H₂O (68 mg, 0.27 mmol, 1 eq) in EtOH (0.68 mL) at room temperature under argon was added a solution of NaBH₄ (10 mg, 0.27 mmol, 1 eq) in EtOH (0.22 mL). After stirring 1 h under one atmosphere of H₂, a solution of trienynone **4a** (90 mg, 0.27 mmol, 1 eq) and ethylenediamine (0.06 mL, 0.95 mmol, 3.5 eq) in EtOH (0.56 mL) was added. The black mixture was stirred at 70 °C for 23 h and after a complete conversion, was filtrated on 5% Et₃N treated silica gel with AcOEt, and concentrated. The crude product was purified by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 5:5) to give 39 mg (43%) of the product as a white solid.

- **Path B : heating of fenestradiene 21a**

The reaction was carried out in a BIOTAGE sealed tube, under argon atmosphere. A solution of the fenestradiene **21a** (70 mg, 0.21 mmol, 1 eq) in benzene (5 mL) was purged 5 min with argon and heated at 110 °C under microwave irradiation for 30 min. The resulted solution was then cooled and concentrated. According to the ¹H NMR, the conversion of fenestradiene in cyclooctatriene was complete. The reaction mixture was then purified by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 5:5) to give 44 mg (63%) of the product as a white solid.

C₂₀H₂₈O₄, MW = 332.42 g.mol⁻¹

R_f = 0.37 (heptane/Et₂O 1:9)

Mp = 180 °C

¹H NMR (200 MHz, CDCl₃) δ 6.07 (d, *J* = 4.4 Hz, 1H), 5.98 (dd, *J* = 11.0 Hz, *J* = 4.6 Hz, 1H), 5.64 (dd, *J* = 11.0 Hz, *J* = 9.0 Hz, 1H), 4.93 (s, 1H), 4.27 (br s, 2H), 2.64 (m, 2H), 2.17 -1.61 (m, 8H), 1.36 (s, 3H), 1.33 (s, 3H), 1.27 (s, 3H), 1.16 (s, 3H). ¹³C NMR (50 MHz, CDCl₃) δ 157.2 (C_{quat}), 140.7 (+), 137.2 (C_{quat}), 134.6 (C_{quat}), 127.2 (+), 127.1 (+), 114.7 (C_{quat}), 85.4 (C_{quat}), 83.9 (+), 72.8 (C_{quat}), 64.9 (-), 51.8 (+), 41.2 (+), 34.1 (-), 33.3 (-), 30.8 (+), 29.7 (+), 28.7 (+), 24.2 (+), 23.8 (-). IR (CHCl₃) ν 3676, 3649, 3630, 3399, 2927, 2854, 2031, 2024, 2008, 1995, 1970, 1918, 1458, 1369, 1261, 1234, 1206, 1184, 1143, 1075, 1057, 1017, 929, 840, 775, 711, 572. HRMS (ESI, positive ion): calc'd for (C₂₀H₂₈O₄Li)⁺ 339.2143 ; found 339.2137. X-Ray analysis : see Table 1

Single crystals of compound **16a** were obtained at room temperature in a crystallisation tube (height = 15 cm, diameter = 0.4 cm), upon slow diffusion of *n*-hexane (0.19 mL) into a chloroform solution (0.06 mL) containing compound **16a** (5 mg).

CCDC 707562 for **16a** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (from the Cambridge

Crystallographic Data Center, 12, Union Road, Cambridge CB21EZ, UK ; fax : (+44) 1223-336-033 ; or deposit@ccdc.cam.ac.uk).

The majority of H are omitted for clarity. The crystal data were collected at 173 K for complex on a Kappa CCD diffractometer, using monochromated Mo K α radiation ($\lambda = 0.71073$ Å). Details of data collection parameters and refinements results are listed in the following Table. The structures were solved using direct methods. After refinement of the non hydrogen atoms, difference-Fourier maps revealed maxima of residual electron density close to positions expected for hydrogen atoms. Hydrogen atoms were introduced as fixed contributors at calculated positions (C-H = 0.95 Å, B(H) = 1.3 Beqv). Final difference maps revealed no significant maxima. All calculations were done using the Nonius OpenMoleN package (OpenMoleN, Interactive Structure Solutions, Nonius B.V., Delft, The Netherlands, 1997). Neutral atom scattering factor coefficients and anomalous dispersion coefficients were taken from a standard source (D. T. Cromer, J. T. Waber, International Tables for X-Ray Crystallography, 1974, Vol IV, The Kynoch Press, Birmingham).

Table 1 : X-Ray experimental data

Formula	C ₂₀ H ₂₈ O ₄
Molecular weight M_r	332.42
Crystal system	Monoclinic
Space group	P 2 ₁ /c
a (Å)	8.1351 (2)
b (Å)	21.0319 (10)
c (Å)	10.6795 (5)
α (deg)	90.00
β (deg)	98.594 (2)
γ (deg)	90.00
V (Å ³)	1806.71(13)
Z	4
Color	Colorless
Crystal dim (mm)	0.45*0.40*0.35
ρ_{calcd} (g.cm ⁻³)	1.222
F000	720
μ (mm ⁻¹)	0.084
Temperature (K)	173(2)
Wavelength (Å)	0.71073
Radiation	MoK α graphite monochromated
Diffractometer	KappaCCD
Scan mode	phi and omega scans
Hkl limits	-10,10/-27,25/-13,9
Theta limits (deg)	1.94/27.48
Number of data meas.	13039

Number of data with $I > 2\sigma(I)$	4132
R	0.0523
R _w	0.1314

2-[(3a*R,4*S**,5*R**,9b*S**)-9-(hydroxymethyl)-2,2-dimethyl-4,9b-dihydro-5*H*-3a,4-butano cycloocta[3,4]cyclobuta[1,2-*d*][1,3]dioxol-5-yl]propan-2-ol (18a)**

To a solution of $\text{Ni(OAc)}_2 \cdot 4\text{H}_2\text{O}$ (72 mg, 0.29 mmol, 1 eq) in EtOH (0.73 mL) at room temperature under argon was added a solution of NaBH_4 (11 mg, 0.29 mmol, 1 eq) in EtOH (0.23 mL). After stirring 1 h under one atmosphere of H_2 , a solution of trienynone **5a** (100 mg, 0.29 mmol, 1 eq) and ethylenediamine (69 μL , 1.02 mmol, 3.5 eq) in EtOH (0.60 mL) was added. The black mixture was stirred overnight and after a complete conversion, was filtrated on 5% Et_3N treated silica gel with AcOEt, and concentrated. The crude product was purified by chromatography on 5% Et_3N treated silica gel (elution with pentane/AcOEt 6:4) to give 77 mg (77%) of the product as a yellow solid.

$\text{C}_{21}\text{H}_{30}\text{O}_4$, $M = 346.46 \text{ g} \cdot \text{mol}^{-1}$

R_f = 0.16 (pentane/AcOEt 6:4)

Mp = 118 °C

^1H NMR (300 MHz, CDCl_3) δ 6.10 (d, $J = 4.0$ Hz, 1H), 5.97 (dd, $J = 10.7$ Hz, $J = 4.0$ Hz, 1H), 5.64 (t, $J = 10.7$ Hz, 1H), 4.83 (s, 1H), 4.31 (d, $J = 12.8$ Hz, 1H), 4.24 (d, $J = 12.8$ Hz, 1H), 2.64 (t, $J = 10.7$ Hz, 1H), 2.51 (m, 2H), 2.32 (m, 1H), 2.10 (m, 2H), 1.97 (m, 2H), 1.77 (m, 3H), 1.57 (m, 1H), 1.35 (s, 3H), 1.27 (s, 3H), 1.22 (s, 3H), 1.11 (s, 3H). **^{13}C NMR** (75 MHz, CDCl_3) δ 158.0 (C_{quat}), 141.1 (C_{quat}), 139.5 (+), 137.0 (C_{quat}), 127.5 (+), 127.1 (+), 114.7 (C_{quat}), 91.3 (C_{quat}), 82.0 (+), 73.5 (C_{quat}), 64.9 (-), 52.2 (+), 41.0 (+), 36.9 (-), 35.2 (-), 32.0 (+), 30.2 (+), 29.7 (-), 28.7 (+), 24.7 (-), 23.7 (+). **IR** (CHCl_3) ν 3649, 3503, 3412, 2975, 2924, 2852, 1647, 1559, 1541, 1507, 1458, 1449, 1396, 1368, 1314, 1278, 1244, 1207, 1139, 1112, 1042, 1025, 920, 861, 838, 561, 554, 548, 541, 407, 401 cm^{-1} . **HRMS** (ESI, positive ion): calc'd for $(\text{C}_{21}\text{H}_{30}\text{O}_4\text{Li})^+$ 353.2299 ; found 353.2292. **COSY, NOESY, HSQC, HMBC**. **X-Ray analysis** : see Table 2

Single crystals of compound **18a** were obtained at room temperature in a crystallisation tube (height = 15 cm, diameter = 0.4 cm), upon slow diffusion and slow evaporation of *n*-heptane (0.5 mL) into a benzene solution (0.17 mL) containing compound **18a** (8 mg).

CCDC 653647 for **18a** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (from the Cambridge Crystallographic Data Center, 12, Union Road, Cambridge CB21EZ, UK ; fax : (+44) 1223-336-033 ; or deposit@ccdc.cam.ac.uk).

The majority of H are omitted for clarity. The crystal data were collected at 173 K for complex on a Kappa CCD diffractometer, using monochromated Mo K α radiation ($\lambda = 0.71073$ Å). Details of data collection parameters and refinements results are listed in the following Table. The structures were solved using direct methods. After refinement of the non hydrogen atoms, difference-Fourier maps revealed maxima of residual electron density close to positions expected for hydrogen atoms. Hydrogen atoms were introduced as fixed contributors at calculated positions (C-H = 0.95 Å, B(H) = 1.3 Beqv). Final difference maps revealed no significant maxima. All calculations were done using the Nonius OpenMoleN package (OpenMoleN, Interactive Structure Solutions, Nonius B.V., Delft, The Netherlands, 1997). Neutral atom scattering factor coefficients and anomalous dispersion coefficients were taken from a standard source (D. T. Cromer, J. T. Waber, International Tables for X-Ray Crystallography, 1974, Vol IV, The Kynoch Press, Birmingham).

Table 2 : X-Ray experimental data

Formula	C ₂₁ H ₃₀ O ₄
Molecular weight M_r	346.45
Crystal system	Monoclinic
Space group	P 21/c
a (Å)	8.2890(3)
b (Å)	21.1559(7)
c (Å)	10.7607(4)
α (deg)	90.00
β (deg)	100.360(2)
γ (deg)	90.00
V (Å ³)	1856.25(11)
Z	4
Color	colorless
Crystal dim (mm)	0.40*0.20*0.15
ρ_{calcd} (g.cm ⁻³)	1.240
F000	752
μ (mm ⁻¹)	0.084
Temperature (K)	173
Wavelength (Å)	0.71073
Radiation	MoK α graphite monochromated
Diffractometer	KappaCCD
Scan mode	phi and omega scans
Hkl limits	-10,10/-27,24/-13,13
Theta limits (deg)	1.93/27.48
Number of data meas.	4242
Number of data with $I > 2\sigma(I)$	3164
R	0.0444

Rw	0.0995
----	--------

[(3a*R,4*S**,5*R**,9b*S**)-5-hexyl-2,2-dimethyl-4,9b-dihydro-5*H*-3a,4-butanocycloocta[3,4]cyclobuta[1,2-*d*][1,3]dioxol-9-yl]methanol (18b)**

To a solution of $\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (80 mg, 0.32 mmol, 1 eq) in EtOH (0.80 mL) at room temperature under argon was added a solution of NaBH_4 (12 mg, 0.32 mmol, 1 eq) in EtOH (0.26 mL). After stirring 1 h under one atmosphere of H_2 , a solution of trienyne **5b** (120 mg, 0.32 mmol, 1 eq) and ethylenediamine (0.08 mL, 1.12 mmol, 3.5 eq) in EtOH (0.67 mL) was added. The black mixture was stirred overnight and after a complete conversion, was filtrated on 5% Et_3N treated silica gel with AcOEt, and concentrated. The crude product was purified by chromatography on 5% Et_3N treated silica gel (elution with pentane/ Et_2O 8:2) to give 75 mg (63%) of the product as a colorless oil.

$\text{C}_{24}\text{H}_{36}\text{O}_3$, $M = 372.54 \text{ g} \cdot \text{mol}^{-1}$

Rf = 0.15 (pentane/ Et_2O 8:2)

^1H NMR (300 MHz, CDCl_3) δ 6.06 (d, $J = 4.3 \text{ Hz}$, 1H), 5.94 (dd, $J = 11.1 \text{ Hz}$, $J = 4.3 \text{ Hz}$, 1H), 5.70 (dd, $J = 11.1 \text{ Hz}$, $J = 9.4 \text{ Hz}$, 1H), 4.83 (s, 1H), 4.26 (s, 2H), 2.38-1.93 (m, 7H), 1.76 (m, 2H), 1.51-1.06 (m, 12H), 1.35 (s, 3H), 1.31 (s, 3H), 0.84 (t, $J = 6.8 \text{ Hz}$, 3H). **^{13}C NMR** (75 MHz, CDCl_3) δ 157.7 (C_{quat}), 142.8 (+), 141.3 (C_{quat}), 136.0 (C_{quat}), 127.5 (+), 127.4 (+), 114.4 (C_{quat}), 91.0 (C_{quat}), 82.2 (+), 65.3 (-), 42.4 (+), 42.1 (+), 36.7 (-), 35.3 (-), 33.1 (-), 31.9 (-), 30.2 (+), 29.8 (-), 29.4 (-), 28.7 (+), 26.9 (-), 24.9 (-), 22.7 (-), 14.2 (+). **IR** (CHCl_3) ν 3448, 2924, 2853, 2160, 1448, 1378, 1368, 1316, 1278, 1244, 1210, 1174, 1141, 1114, 1055, 1029, 861, 832, 774, 748, 707 cm^{-1} . **HRMS** (ESI, positive ion): calc'd for $(\text{C}_{24}\text{H}_{36}\text{O}_3\text{Li})^+$ 379.2820 ; found 379.2811. **COSY**, **NOESY**, **HSQC**, **HMBC**.

1-[(3a*R,4*S**,5*R**,9b*S**)-9-(hydroxymethyl)-2,2-dimethyl-4,9b-dihydro-5*H*-3a,4-butanocycloocta[3,4]cyclobuta[1,2-*d*][1,3]dioxol-5-yl]cyclohexanol (18c)**

To a solution of $\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (113 mg, 0.46 mmol, 1 eq) in EtOH (1.14 mL) at room temperature under argon was added a solution of NaBH_4 (17 mg, 0.46 mmol, 1 eq) in EtOH (0.37

mL). After stirring 1 h under one atmosphere of H₂, a solution of trienyne **5c** (175 mg, 0.46 mmol, 1 eq) and ethylenediamine (0.11 mL, 1.59 mmol, 3.5 eq) in EtOH (0.95 mL) was added. The black mixture was stirred overnight and after a complete conversion, was filtrated on 5% Et₃N treated silica gel with AcOEt, and concentrated. The crude product was purified by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 75:25) to give 142 mg (81%) of the product as a white solid.

C₂₄H₃₄O₄, M = 386.52 g.mol⁻¹

R_f = 0.24 (pentane/AcOEt 7:3)

Mp = 87 °C

¹H NMR (300 MHz, CDCl₃) δ 6.10 (d, *J* = 4.0 Hz, 1H), 5.98 (dd, *J* = 11.3 Hz, *J* = 4.0 Hz, 1H), 5.75 (m, 1H), 4.83 (s, 1H), 4.28 (s, 2H), 2.57 (m, 3H), 2.10 (m, 1H), 1.97-1.07 (m, 18H), 1.36 (s, 3H), 1.29 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 158.0 (C_{quat}), 140.9 (C_{quat}), 139.3 (+), 136.8 (C_{quat}), 127.3 (+), 126.9 (+), 114.7 (C_{quat}), 91.2 (C_{quat}), 82.0 (+), 73.9 (C_{quat}), 64.8 (-), 52.4 (+), 40.3 (+), 38.4 (2C, (-)), 37.2 (-), 35.1 (-), 30.6 (-), 30.2 (+), 29.8 (-), 28.7 (+), 25.8 (-), 24.7 (-), 21.5 (-). IR (CHCl₃) ν 3648, 3416, 2926, 2853, 2248, 1725, 1448, 1378, 1369, 1317, 1277, 1244, 1206, 1138, 1112, 1030, 959, 922, 864, 838, 773, 734, 710, 419 cm⁻¹. HRMS (ESI, positive ion): calc'd for (C₂₄H₃₄O₄Li)⁺ 393.2612 ; found 393.2602. COSY, NOESY, HSQC, HMBC.

1-[(3a*R,4*S**,5*R**,9b*S**)-9-(hydroxymethyl)-2,2-dimethyl-4,9b-dihydro-5*H*-3a,4-butano cycloocta[3,4]cyclobuta[1,2-*d*][1,3]dioxol-5-yl]cyclopentanol (**18d**)**

To a solution of Ni(OAc)₂.4H₂O (96 mg, 0.39 mmol, 1 eq) in EtOH (0.98 mL) at room temperature under argon was added a solution of NaBH₄ (15 mg, 0.39 mmol, 1 eq) in EtOH (0.31 mL). After stirring 1 h under one atmosphere of H₂, a solution of trienyne **5d** (143 mg, 0.39 mmol, 1 eq) and ethylenediamine (0.09 mL, 1.37 mmol, 3.5 eq) in EtOH (0.81 mL) was added. The black mixture was stirred overnight and after a complete conversion, was filtrated on 5% Et₃N treated silica gel with AcOEt, and concentrated. The crude product was purified by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 8:2) to give 78 mg of a compound **18d'** (54%) as a white solid, and 39 mg (27%) of the desired compound **18d** as a white solid. The compound **18d'** rapidly rearranged at room temperature to give the desired compound **18d**. When the compound **18d'** was heated at 80°C in benzene for 5 min under microwave irradiation, this product was totally rearranged in the desired compound **18d** (final yield : 81%).

Compound 18d' : (contaminated with traces of compound **18d**)

C₂₃H₃₂O₄, M = 372.50 g.mol⁻¹

R_f = 0.56 (pentane/AcOEt 7:3)

Mp = 48 °C

¹H NMR (300 MHz, CDCl₃) δ 6.02 (d, *J* = 3.1 Hz, 1H), 5.83 (m, 2H), 4.91 (d, *J* = 2.2 Hz, 1H), 4.5 (d, *J* = 11.4 Hz, 1H), 4.02 (t, *J* = 11.4 Hz, 1H), 3.49 (m, 1H : OH), 2.57 (m, 1H), 2.36-1.37 (m, 18H), 1.54 (s, 3H), 1.42 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 159.5 (C_{quat}), 141.3 (+), 138.2

(C_{quat}), 133.2 (C_{quat}), 127.6 (+), 123.0 (+), 114.7 (C_{quat}), 89.8 (C_{quat}), 83.4 (C_{quat}), 82.4 (+), 68.0 (-), 55.1 (+), 50.8 (+), 42.7 (-), 41.0 (-), 34.8 (-), 32.0 (-), 30.7 (-), 30.3 (+), 29.1 (+), 25.3 (-), 25.0 (-), 23.8 (-). **IR** (CHCl₃) ν 3691, 3675, 3614, 3587, 2987, 2361, 2340, 2014, 1982, 1967, 1949, 1560, 1507, 1457, 1394, 1242, 1066, 669 cm⁻¹. **HRMS** (ESI, positive ion): calc'd for (C₂₃H₃₂O₄Li)⁺ 379.2456; found 379.2451. **COSY, NOESY, HSQC, HMBC**.

Compound 18d :

C₂₃H₃₂O₄, M = 372.50 g.mol⁻¹

Rf = 0.20 (pentane/AcOEt 7:3)

Mp = 152 °C

¹H NMR (300 MHz, CDCl₃) δ 6.11 (d, *J* = 4.0 Hz, 1H), 5.97 (dd, *J* = 11.1 Hz, *J* = 4.0 Hz, 1H), 5.86 (m, 1H), 4.84 (s, 1H), 4.30 (s, 2H), 2.64 (m, 2H), 2.34 (m, 1H), 2.17-1.09 (m, 17H), 1.37 (s, 3H), 1.30 (s, 3H). **¹³C NMR** (75 MHz, CDCl₃) δ 158.3 (C_{quat}), 140.9 (C_{quat}), 139.9 (+), 136.4 (C_{quat}), 127.2 (+), 126.6 (+), 114.7 (C_{quat}), 91.0 (C_{quat}), 84.3 (C_{quat}), 82.2 (+), 65.0 (-), 51.2 (+), 41.7 (-), 41.4 (+), 39.4 (-), 36.3 (-), 34.9 (-), 30.2 (+), 29.4 (-), 28.7 (+), 24.6 (-), 24.5 (-), 23.1 (-). **IR** (CHCl₃) ν 3417, 2930, 2852, 2365, 2357, 2334, 2210, 2164, 2148, 1998, 1447, 1379, 1369, 1318, 1275, 1243, 1206, 1140, 1113, 1025, 921, 841, 774, 733, 547, 418, 409 cm⁻¹. **HRMS** (ESI, positive ion): calc'd for (C₂₃H₃₂O₄Li)⁺ 379.2456; found 379.2452. **COSY, NOESY, HSQC, HMBC**.

[(3a*R,4*S**,5*R**,9b*S**)-2,2-dimethyl-5-(2-phenylethyl)-4,9b-dihydro-5*H*-3a,4-butano cycloocta[3,4]cyclobuta[1,2-*d*][1,3]dioxol-9-yl]methanol (18e)**

To a solution of Ni(OAc)₂·4H₂O (64 mg, 0.26 mmol, 1 eq) in EtOH (0.65 mL) at room temperature under argon was added a solution of NaBH₄ (10 mg, 0.26 mmol, 1 eq) in EtOH (0.21 mL). After stirring 1 h under one atmosphere of H₂, a solution of trienynone **5e** (100 mg, 0.26 mmol, 1 eq) and ethylenediamine (0.06 mL, 0.91 mmol, 3.5 eq) in EtOH (0.54 mL) was added. The black mixture was stirred overnight and after a complete conversion, was filtrated on 5% Et₃N treated silica gel with AcOEt, and concentrated. The crude product was purified by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 9:1) to give 76 mg (76%) of the product as a white oil.

C₂₆H₃₂O₃, M = 392.53 g.mol⁻¹

Rf = 0.17 (pentane/AcOEt 9:1)

¹H NMR (300 MHz, CDCl₃) δ 7.29-7.12 (m, 5H), 6.11 (d, *J* = 4.4 Hz, 1H), 6.05 (dd, *J* = 11.1 Hz, *J* = 4.4 Hz, 1H), 5.81 (dd, *J* = 11.1 Hz, *J* = 9.4 Hz, 1H), 4.84 (s, 1H), 4.28 (d, *J* = 5.0 Hz, 2H), 2.68 (m, 1H), 2.40 (m, 2H), 2.27-1.49 (m, 12H), 1.38 (s, 3H), 1.34 (s, 3H). **¹³C NMR** (75 MHz, CDCl₃) δ 157.6 (C_{quat}), 142.5 (C_{quat}), 142.3 (+), 141.4 (C_{quat}), 136.2 (C_{quat}), 128.5 (2C, (+)), 128.4 (2C, (+)), 128.1 (+), 127.4 (+), 125.8 (+), 114.5 (C_{quat}), 90.9 (C_{quat}), 82.2 (+), 65.3 (-), 42.4 (+), 41.9 (+), 36.6 (-), 35.3 (-), 35.1 (-), 33.4 (-), 30.2 (+), 29.7 (-), 28.8 (+), 24.9 (-). **IR** (CHCl₃) ν 3460, 3025, 2924, 2852, 2365, 1727, 1603, 1496, 1454, 1378, 1368, 1316, 1278, 1244, 1210, 1174, 1140, 1112, 1077, 1032, 922, 861, 833, 775, 747, 699, 628, 511 cm⁻¹. **HRMS** (ESI, positive ion): calc'd for

(C₂₆H₃₂O₃Li)⁺ 399.2507 ; found 399.2498. **COSY, NOESY, HSQC, HMBC.**

4-[(3a*R,4*S**,5*R**,9b*S**)-9-(hydroxymethyl)-2,2-dimethyl-4,9b-dihydro-5*H*-3a,4-butano cycloocta[3,4]cyclobuta[1,2-*d*][1,3]dioxol-5-yl]-2,6-dimethylheptan-4-ol (18f)**

To a solution of Ni(OAc)₂·4H₂O (70 mg, 0.28 mmol, 1 eq) in EtOH (0.70 mL) at room temperature under argon was added a solution of NaBH₄ (11 mg, 0.28 mmol, 1 eq) in EtOH (0.23 mL). After stirring 1 h under one atmosphere of H₂, a solution of trienyl **5f** (120 mg, 0.28 mmol, 1 eq) and ethylenediamine (0.07 mL, 0.98 mmol, 3.5 eq) in EtOH (0.58 mL) was added. The black mixture was stirred overnight and after a complete conversion, was filtrated on 5% Et₃N treated silica gel with AcOEt, and concentrated. The crude product was purified by chromatography on 5% Et₃N treated silica gel (elution with pentane/AcOEt 8:2) to give 105 mg (88%) of the product as a white solid.

C₂₇H₄₂O₄, M = 430.62 g.mol⁻¹

R_f = 0.26 (pentane/AcOEt 8:2)

Mp = 45 °C

¹H NMR (300 MHz, CDCl₃) δ 6.12 (d, *J* = 4.1 Hz, 1H), 5.96 (dd, *J* = 10.6 Hz, *J* = 4.1 Hz, 1H), 5.68 (t, *J* = 10.6 Hz, 1H), 4.84 (s, 1H), 4.32 (s, 2H), 2.78 (t, *J* = 10.6 Hz, 1H), 2.57 (m, 2H), 2.17-1.18 (m, 9H), 1.45 (s, 1H : OH), 1.37 (s, 3H), 1.28 (s, 3H), 1.14 (s, 1H : OH), 1.00 (d, *J* = 6.8 Hz, 6H), 0.97 (d, *J* = 6.4 Hz, 2H), 0.96 (d, *J* = 6.8 Hz, 6H), 0.84 (d, *J* = 6.7 Hz, 2H). **¹³C NMR** (50 MHz, CDCl₃) δ 158.3 (C_{quat}), 140.8 (C_{quat}), 139.4 (+), 137.5 (C_{quat}), 127.6 (+), 126.8 (+), 114.8 (C_{quat}), 91.3 (C_{quat}), 82.1 (+), 78.7 (C_{quat}), 65.1 (-), 49.7 (+), 47.8 (-), 44.1 (-), 40.5 (+), 36.7 (-), 35.2 (-), 30.3 (+), 29.7 (-), 28.8 (+), 25.6 (+), 25.5 (+), 25.0 (+), 24.7 (-), 24.6 (+), 23.6 (+), 22.8 (+). **IR** (CHCl₃) ν 3419, 2951, 2925, 2867, 2359, 1449, 1368, 1316, 1276, 1243, 1206, 1137, 1112, 1065, 1023, 997, 920, 851, 831, 774, 734, 628 cm⁻¹. **HRMS** (ESI, positive ion): calc'd for (C₂₇H₄₂O₄Li)⁺ 437.3238 ; found 437.3250. **COSY, NOESY, HSQC, HMBC.**

The stannane derivative (2-(tributylstannyl)ethynyl)trimethylsilane is commercially available.

The following products were prepared by literature methods:

- The vinyl stannanes ((*E*)-4-(tributylstannyl)-2-methylbut-3-en-2-ol, 1-((*E*)-2-(tributylstannyl)vinyl)cyclohexanol)^{3,4}
- The vinyl iodides ((*E*)-4-iodo-2-methylbut-3-en-2-ol, (*E*)-1-iodooct-1-ene, (*E*)-1-iodo-4-phenylbut-1-ene).^{5,6,7} The 1-((*E*)-2-iodovinyl)cyclohexanol has already been described in literature.⁸
- These vinyl stannanes (1-[(*E*)-2-(tributylstannyl)vinyl]cyclopentanol, 4-[(*E*)-2-(tributylstannyl)vinyl]-2,6-dimethylheptan-4-ol) and these vinyl iodides ((1-[(*E*)-2-iodovinyl]cyclopentanol, 4-[(*E*)-2-iodovinyl]-2,6-dimethylheptan-4-ol, 1-[(*E*)-2-iodovinyl]cyclohexanol) have already been described in our preceding paper.^{2c}

Computational Section

Pathway IIa: TS¹ (9a to 15a)

HOMO

HOMO-1

DFT

CASSCF(8,8)

Pathway I.

X = 6 (r,r)

Table S2. B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	ZPVE	$E^0 + \text{ZPVE}$	$\langle S^2 \rangle$	Dipl.
8	-1636.00622	0.51387	-1635.49235	0.00	2.79
TS¹ (8→14')	-1635.99570	0.51459	-1635.48111	0.00	4.63
14'	-1636.03676	0.51775	-1635.51901	0.00	3.81
TS² (14'→20')	-1636.00478	0.51711	-1635.48767	0.00	2.81
20'	-1636.03255	0.51798	-1635.51456	0.00	4.12

X = 6 (r,s)

Table S3. B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	ZPVE	$E^0 + \text{ZPVE}$	$\langle S^2 \rangle$	Dipl.
8	-1636.00622	0.51387	-1635.49235	0.00	2.79
TS¹ (8→14)	-1635.99023	0.51438	-1635.47585	0.00	3.94
14	-1636.04605	0.51786	-1635.52819	0.00	2.91
TS² (14→20)	-1636.00880	0.51678	-1635.49202	0.00	4.31
20	-1636.02304	0.51851	-1635.50453	0.00	4.72

8

SiC23H32O6

C1

6	3.755520000	-0.228286000	-0.376721000
6	2.268401000	0.071109000	-0.069896000
8	3.907858000	-1.898543000	1.371804000
8	4.763789000	0.393223000	0.363219000
6	1.588033000	1.201365000	0.219394000
6	-0.271415000	0.369584000	-2.403176000
6	-1.167052000	0.476226000	-1.411916000
6	0.182272000	1.178641000	0.662066000
6	-0.951272000	0.887795000	-0.010151000
1	0.035212000	1.529856000	1.688196000
1	3.977237000	-0.110318000	-1.444285000
1	0.778593000	0.588379000	-2.251778000
6	1.993727000	-1.376958000	-0.089088000
6	1.042812000	-2.250090000	-0.455236000
6	1.399418000	-3.687309000	-0.722279000
6	2.866322000	-4.053098000	-0.433572000
6	3.848053000	-2.929594000	-0.804553000
6	3.460386000	-1.716615000	0.014334000
1	0.727307000	-4.353705000	-0.164639000
1	1.164563000	-3.880999000	-1.780744000
1	2.989632000	-4.257861000	0.636579000
1	3.120457000	-4.979021000	-0.960426000
1	3.773733000	-2.687601000	-1.872197000
1	4.881050000	-3.229200000	-0.598715000
1	0.026092000	-1.934806000	-0.671480000

1	4.806902000	-0.134895000	1.180084000
1	3.137894000	-1.795780000	1.943585000
14	2.410112000	2.928649000	0.256307000
6	1.044854000	4.200243000	-0.058382000
1	1.466469000	5.211603000	-0.078021000
1	0.553890000	4.024230000	-1.021203000
1	0.270968000	4.178312000	0.715489000
6	3.720466000	3.121761000	-1.085473000
1	4.064821000	4.162125000	-1.112309000
1	4.584551000	2.482751000	-0.889241000
1	3.321496000	2.881779000	-2.076574000
6	3.161295000	3.239046000	1.962964000
1	3.549743000	4.261083000	2.036306000
1	2.424042000	3.106053000	2.761990000
1	3.989064000	2.546633000	2.139926000
1	-0.580066000	0.060446000	-3.398083000
6	-2.648954000	0.196768000	-1.598362000
1	-3.139761000	1.061326000	-2.061432000
1	-2.840516000	-0.685029000	-2.212801000
6	-2.316080000	0.997060000	0.646244000
1	-2.719987000	2.008321000	0.519062000
1	-2.309294000	0.768240000	1.713947000
6	-3.199859000	0.022609000	-0.165116000
6	-4.696127000	0.301432000	-0.110431000
8	-5.552273000	-0.552209000	-0.055452000
6	-2.992080000	-1.420535000	0.306716000
8	-2.630080000	-2.340980000	-0.390046000
8	-4.964204000	1.616945000	-0.187532000
8	-3.251360000	-1.535919000	1.617417000
6	-6.356865000	1.950851000	-0.210785000
1	-6.397917000	3.037929000	-0.272887000
1	-6.846370000	1.497296000	-1.076016000
1	-6.850407000	1.598320000	0.697912000
6	-3.149439000	-2.862062000	2.144817000
1	-3.399586000	-2.779364000	3.202157000
1	-3.850483000	-3.527889000	1.636217000
1	-2.135233000	-3.249086000	2.019405000

TS¹ (8→14)
SiC23H32O6
C1

6	3.925348000	-0.315414000	-0.132020000
6	2.433298000	0.021454000	0.136726000
8	4.160759000	-2.382501000	1.192003000
8	4.806961000	0.153770000	0.857266000
6	1.748992000	1.206531000	0.148339000
6	0.110584000	-1.313480000	-1.471214000
6	-0.861190000	-0.592222000	-0.803006000
6	0.366245000	1.384044000	0.243652000
6	-0.726356000	0.600801000	-0.070472000
1	0.070854000	2.380926000	0.651170000
1	4.278345000	-0.027643000	-1.149560000
1	1.015542000	-0.806101000	-1.839658000
6	2.103832000	-1.351135000	0.243244000
6	1.031838000	-2.215108000	0.164977000
6	1.403388000	-3.604635000	-0.260143000

6	2.424208000	-3.592974000	-1.388360000
6	3.710204000	-2.835442000	-1.084096000
6	3.543534000	-1.841942000	0.043484000
1	1.828330000	-4.155015000	0.622962000
1	0.486788000	-4.154961000	-0.597708000
1	2.682612000	-4.652913000	-1.648616000
1	1.941676000	-3.136253000	-2.294197000
1	4.050577000	-2.293198000	-2.004040000
1	4.516839000	-3.565208000	-0.803077000
1	0.125190000	-2.107812000	0.779827000
1	5.506976000	-0.510720000	0.936517000
1	3.869165000	-1.854027000	1.948127000
14	2.621205000	2.820111000	0.140889000
6	1.496783000	4.192449000	-0.321615000
1	2.081892000	5.066370000	-0.691928000
1	0.789050000	3.902051000	-1.131250000
1	0.889368000	4.546007000	0.542847000
6	3.991147000	2.805905000	-1.074845000
1	4.377126000	3.834870000	-1.257738000
1	4.843730000	2.187790000	-0.705548000
1	3.675373000	2.388990000	-2.057793000
6	3.299155000	3.139481000	1.807422000
1	3.838485000	4.112900000	1.853549000
1	2.503277000	3.161752000	2.585904000
1	4.024386000	2.339702000	2.092249000
1	-0.180518000	-2.219249000	-2.025754000
6	-2.274573000	-1.098626000	-0.752627000
1	-2.673082000	-1.275686000	-1.785900000
1	-2.326426000	-2.068530000	-0.193777000
6	-2.082134000	1.070543000	0.399774000
1	-2.342166000	2.059661000	-0.056022000
1	-2.089385000	1.193499000	1.514799000
6	-3.097910000	-0.010028000	-0.030497000
6	-4.129860000	0.587664000	-0.962575000
8	-4.344371000	0.318821000	-2.144050000
6	-3.797391000	-0.603472000	1.172855000
8	-3.605880000	-0.370289000	2.365663000
8	-4.883968000	1.562938000	-0.370453000
8	-4.742011000	-1.534048000	0.836715000
6	-5.883854000	2.181252000	-1.183759000
1	-6.362435000	2.918733000	-0.493392000
1	-5.404390000	2.685839000	-2.056610000
1	-6.614164000	1.414312000	-1.536989000
6	-5.455900000	-2.140692000	1.916380000
1	-6.164321000	-2.836348000	1.402853000
1	-4.745834000	-2.691588000	2.578707000
1	-5.997973000	-1.358973000	2.500702000

14

SiC23H32O6

C1

6	3.496718000	-0.367436000	1.006583000
6	2.211690000	-0.017925000	0.266986000
8	3.069518000	-2.747818000	1.620754000
8	3.399325000	-0.193388000	2.412138000
6	1.594337000	1.289783000	0.051240000
6	0.157981000	-1.184550000	-1.806607000
6	-0.875845000	-0.657020000	-0.863987000

6	0.252101000	1.472764000	-0.094124000
6	-0.813691000	0.481202000	-0.141046000
1	-0.109008000	2.502132000	-0.133070000
1	4.416851000	0.096656000	0.618445000
1	0.690318000	-0.349135000	-2.277602000
6	1.997172000	-1.306979000	-0.112877000
6	1.190923000	-2.074090000	-1.096652000
6	2.183598000	-2.752970000	-2.070532000
6	3.340685000	-3.464202000	-1.354045000
6	4.160910000	-2.503773000	-0.479533000
6	3.244704000	-1.849049000	0.546153000
1	1.638441000	-3.464102000	-2.703365000
1	2.591756000	-1.982962000	-2.741022000
1	2.943369000	-4.266591000	-0.719785000
1	3.990137000	-3.942320000	-2.096695000
1	4.607964000	-1.724833000	-1.111698000
1	4.975888000	-3.030763000	0.029340000
1	0.660579000	-2.874471000	-0.558308000
1	4.220221000	-0.527240000	2.796591000
1	2.597592000	-2.243274000	2.300006000
14	2.704817000	2.837110000	0.056797000
6	4.102701000	2.609226000	-1.200385000
1	4.721262000	3.512575000	-1.249498000
1	4.763770000	1.772075000	-0.955514000
1	3.698246000	2.429358000	-2.202241000
6	3.409695000	3.156400000	1.779270000
1	4.204090000	3.910413000	1.745765000
1	2.623520000	3.528030000	2.445369000
1	3.806072000	2.242108000	2.228968000
6	1.701462000	4.349188000	-0.474829000
1	2.363232000	5.221309000	-0.526062000
1	1.248832000	4.220033000	-1.463274000
1	0.903723000	4.590824000	0.235331000
1	-0.325822000	-1.756948000	-2.608057000
6	-2.159322000	-1.402799000	-0.601108000
1	-2.626178000	-1.811170000	-1.502602000
1	-1.998019000	-2.239226000	0.092227000
6	-2.074943000	0.677986000	0.673949000
1	-2.466473000	1.697491000	0.641485000
1	-1.876343000	0.441370000	1.728260000
6	-3.070948000	-0.348527000	0.064818000
6	-3.994714000	0.253420000	-1.003670000
8	-4.541092000	-0.408764000	-1.857837000
6	-3.934259000	-0.959717000	1.168123000
8	-3.659100000	-1.960008000	1.788608000
8	-4.154050000	1.579705000	-0.888539000
8	-5.023333000	-0.209870000	1.411069000
6	-5.052834000	2.163027000	-1.836839000
1	-5.064242000	3.229871000	-1.614789000
1	-4.703769000	1.985784000	-2.856952000
1	-6.052886000	1.736608000	-1.727406000
6	-5.866958000	-0.684629000	2.466595000
1	-6.693899000	0.022578000	2.523341000
1	-6.234296000	-1.688574000	2.241386000
1	-5.319496000	-0.711984000	3.411822000

TS² (14→20)
 SiC23H32O6
 C1

6	-2.634231000	0.923790000	0.888840000
6	-1.804584000	0.268038000	-0.208123000
8	-0.797343000	1.710984000	2.256496000
8	-2.941537000	0.209902000	2.051799000
6	-1.760055000	-1.037479000	-0.671537000
6	-0.011804000	1.324855000	-2.325238000
6	0.729429000	0.543822000	-1.243926000
6	-0.512055000	-1.590363000	-1.085141000
6	0.665892000	-0.874627000	-1.132835000
1	-0.443336000	-2.677675000	-1.132776000
1	-3.554517000	1.381659000	0.506478000
1	-0.768862000	0.690242000	-2.797248000
6	-0.871935000	1.365238000	-0.242972000
6	-0.650813000	2.332469000	-1.385990000
6	-1.910419000	3.126760000	-1.714849000
6	-2.503691000	3.803071000	-0.440785000
6	-1.791577000	3.453752000	0.884190000
6	-1.466176000	1.972738000	1.036479000
1	-1.696385000	3.880304000	-2.482081000
1	-2.645770000	2.438715000	-2.149855000
1	-2.483467000	4.891993000	-0.554914000
1	-3.563902000	3.540478000	-0.356928000
1	-2.399372000	3.784506000	1.734232000
1	-0.842864000	4.001727000	0.956119000
1	0.133867000	3.036030000	-1.070024000
1	-2.144871000	0.327820000	2.601037000
1	0.129499000	1.485717000	2.073167000
14	-3.201100000	-2.251677000	-0.405673000
6	-3.270916000	-3.363111000	-1.938612000
1	-4.080984000	-4.094702000	-1.841406000
1	-3.458908000	-2.777480000	-2.844740000
1	-2.342245000	-3.922532000	-2.092592000
6	-4.850831000	-1.353707000	-0.242761000
1	-5.672536000	-2.078766000	-0.250451000
1	-4.901636000	-0.797994000	0.697237000
1	-5.017420000	-0.656850000	-1.070923000
6	-2.893801000	-3.317680000	1.123371000
1	-3.691364000	-4.057804000	1.253088000
1	-1.943691000	-3.858432000	1.056616000
1	-2.866208000	-2.683536000	2.014187000
1	0.646144000	1.724799000	-3.106950000
6	2.142841000	0.985428000	-0.894942000
1	2.713317000	1.173242000	-1.814662000
1	2.189644000	1.885729000	-0.277722000
6	2.045675000	-1.433240000	-0.853537000
1	2.584588000	-1.649670000	-1.783927000
1	2.055788000	-2.334476000	-0.236975000
6	2.742041000	-0.234844000	-0.157046000
6	4.263550000	-0.238736000	-0.225760000
8	4.991537000	0.065841000	0.692206000
6	2.361444000	-0.174079000	1.325745000
8	1.884499000	0.793335000	1.884226000

8	4.708751000	-0.575440000	-1.447959000
8	2.617594000	-1.325133000	1.946316000
6	6.132920000	-0.544297000	-1.603677000
1	6.322054000	-0.835571000	-2.636372000
1	6.518487000	0.459452000	-1.409725000
1	6.608903000	-1.244318000	-0.913075000
6	2.334660000	-1.346755000	3.351995000
1	2.601640000	-2.347538000	3.688814000
1	2.933197000	-0.593548000	3.868707000
1	1.275223000	-1.150207000	3.531076000

20

SiC₂₃H₃₂O₆

C1

6	-2.650586000	1.005388000	0.852803000
6	-1.865924000	0.392100000	-0.289590000
8	-0.780298000	1.157476000	2.403411000
8	-3.151384000	0.168173000	1.853160000
6	-1.816140000	-0.874629000	-0.772155000
6	0.120254000	1.746637000	-2.081914000
6	0.578921000	0.828989000	-0.894858000
6	-0.520409000	-1.378380000	-1.241307000
6	0.602089000	-0.635828000	-1.195439000
1	-0.443677000	-2.436172000	-1.488884000
1	-3.446192000	1.691734000	0.543263000
1	-0.567304000	1.199153000	-2.733507000
6	-0.731887000	1.370626000	-0.151134000
6	-0.616038000	2.609666000	-1.051941000
6	-1.865292000	3.451630000	-1.165756000
6	-2.196363000	3.991439000	0.261637000
6	-1.467020000	3.271499000	1.427557000
6	-1.315764000	1.761218000	1.249567000
1	-1.734354000	4.285315000	-1.865045000
1	-2.689233000	2.839859000	-1.553613000
1	-1.933411000	5.053434000	0.316739000
1	-3.278225000	3.949530000	0.424980000
1	-2.008993000	3.449186000	2.363276000
1	-0.466269000	3.698090000	1.572930000
1	0.158017000	3.235229000	-0.580068000
1	-2.380102000	0.028510000	2.434151000
1	0.066693000	0.726719000	2.196492000
14	-3.262808000	-2.096081000	-0.641897000
6	-3.231717000	-3.147059000	-2.220596000
1	-4.070864000	-3.852010000	-2.219758000
1	-3.323894000	-2.523742000	-3.116405000
1	-2.313859000	-3.736279000	-2.318742000
6	-4.921668000	-1.205127000	-0.562466000
1	-5.741987000	-1.928322000	-0.633462000
1	-5.027060000	-0.663366000	0.380753000
1	-5.033210000	-0.494891000	-1.388505000

6	-3.053033000	-3.241234000	0.847319000
1	-3.839555000	-4.003952000	0.868072000
1	-2.087836000	-3.758602000	0.825679000
1	-3.112476000	-2.663787000	1.774000000
1	0.905613000	2.212911000	-2.687213000
6	1.983716000	1.151367000	-0.331290000
1	2.559876000	1.742612000	-1.050966000
1	1.961720000	1.696970000	0.614344000
6	2.031507000	-1.091332000	-1.267259000
1	2.503048000	-0.818186000	-2.219301000
1	2.175128000	-2.162885000	-1.110882000
6	2.675989000	-0.226262000	-0.150951000
6	4.188515000	-0.070162000	-0.202289000
8	4.887499000	0.082732000	0.774246000
6	2.316442000	-0.823284000	1.210506000
8	1.608863000	-0.302158000	2.049717000
8	4.654296000	-0.055008000	-1.462047000
8	2.856123000	-2.031790000	1.366538000
6	6.064883000	0.167335000	-1.582373000
1	6.275919000	0.145544000	-2.651046000
1	6.338713000	1.134998000	-1.155205000
1	6.620796000	-0.617088000	-1.063730000
6	2.591075000	-2.674301000	2.621087000
1	3.103080000	-3.634360000	2.571320000
1	2.982381000	-2.072164000	3.443802000
1	1.516729000	-2.816023000	2.757945000

TS¹ (8→14')
SiC23H32O6
C1

6	-3.747912000	-0.453982000	0.407519000
6	-2.286525000	-0.029435000	0.112358000
8	-3.738063000	-2.150046000	-1.330103000
8	-4.817532000	0.053313000	-0.336117000
6	-1.675042000	1.210207000	-0.068839000
6	0.068085000	-1.497179000	-1.722041000
6	1.010393000	-0.592421000	-1.273374000
6	-0.304396000	1.451832000	-0.360123000
6	0.813735000	0.712553000	-0.758106000
1	-0.027623000	2.493103000	-0.193485000
1	-3.986610000	-0.350077000	1.472155000
1	-0.897015000	-1.137645000	-2.047688000
6	-1.892416000	-1.387789000	0.136445000
6	-0.770112000	-2.174117000	0.301673000
6	-0.988145000	-3.651407000	0.559818000
6	-2.423457000	-4.165568000	0.333607000
6	-3.509230000	-3.183423000	0.810201000
6	-3.295210000	-1.907680000	0.024014000
1	-0.279293000	-4.255299000	-0.020232000
1	-0.703698000	-3.817415000	1.610340000
1	-2.589683000	-4.344298000	-0.734716000
1	-2.533334000	-5.133557000	0.834561000
1	-3.405038000	-2.975190000	1.882484000

1	-4.508730000	-3.598380000	0.642558000
1	0.137470000	-1.757790000	0.721241000
1	-3.058079000	-1.811518000	-1.923995000
1	-4.840883000	-0.513344000	-1.127276000
14	-2.752323000	2.788392000	0.111800000
6	-1.636388000	4.283797000	0.447629000
1	-0.980388000	4.528607000	-0.394045000
1	-2.269901000	5.160222000	0.626760000
1	-1.011875000	4.146245000	1.337023000
6	-3.965013000	2.665655000	1.555505000
1	-4.416080000	3.648206000	1.736323000
1	-4.774601000	1.964156000	1.339721000
1	-3.468160000	2.355843000	2.480984000
6	-3.696649000	3.094814000	-1.494314000
1	-3.018050000	3.169271000	-2.350579000
1	-4.393281000	2.270890000	-1.670921000
1	-4.272072000	4.025773000	-1.438438000
1	0.395956000	-2.436968000	-2.160167000
6	2.185487000	1.364911000	-0.623108000
1	2.491749000	1.868237000	-1.549087000
1	2.247109000	2.099147000	0.183234000
6	2.486399000	-0.945366000	-1.246317000
1	2.900126000	-0.932260000	-2.263496000
1	2.675805000	-1.933634000	-0.818565000
6	3.132709000	0.169738000	-0.398303000
6	3.118879000	-0.231336000	1.077681000
8	2.633770000	-1.242191000	1.533536000
6	4.558415000	0.461170000	-0.849288000
8	4.901304000	1.389436000	-1.543020000
8	3.698113000	0.718353000	1.830802000
8	5.396370000	-0.499371000	-0.418061000
6	6.761991000	-0.344892000	-0.819898000
1	7.294691000	-1.190314000	-0.385489000
1	6.845818000	-0.357598000	-1.909338000
1	7.167138000	0.598312000	-0.445631000
6	3.723348000	0.454214000	3.237744000
1	4.222065000	1.311132000	3.689536000
1	2.707481000	0.352177000	3.626898000
1	4.276146000	-0.465255000	3.444936000

14'
SiC23H32O6
C1

6	3.640851000	-0.472601000	0.974223000
6	2.403105000	0.039123000	0.209762000
8	2.580696000	-2.581585000	1.685122000
8	3.784091000	-0.265055000	2.347389000
6	1.764675000	1.299126000	-0.096297000
6	-0.041762000	-2.077137000	-1.030639000
6	-0.852510000	-0.977068000	-0.403193000
6	0.425433000	1.331978000	-0.359418000
6	-0.656577000	0.350436000	-0.183291000
1	0.017136000	2.315134000	-0.600768000
1	4.577029000	-0.180297000	0.480320000

1	-0.610577000	-2.454269000	-1.895331000
6	2.141346000	-1.184567000	-0.299274000
6	1.380151000	-1.707269000	-1.459111000
6	2.177998000	-2.879893000	-2.089691000
6	2.969497000	-3.743056000	-1.088968000
6	3.957269000	-2.918151000	-0.244180000
6	3.143644000	-1.909712000	0.544020000
1	1.498778000	-3.515203000	-2.671322000
1	2.890486000	-2.455775000	-2.809054000
1	2.284807000	-4.262235000	-0.406500000
1	3.505159000	-4.522231000	-1.643030000
1	4.661161000	-2.388208000	-0.898776000
1	4.541331000	-3.560412000	0.423487000
1	1.286782000	-0.901396000	-2.199679000
1	3.342948000	-1.028774000	2.756247000
1	1.689587000	-2.226141000	1.799586000
14	2.780799000	2.902974000	-0.069127000
6	4.295671000	2.712031000	-1.185774000
1	4.881547000	3.637937000	-1.197505000
1	4.957269000	1.910352000	-0.842704000
1	4.005172000	2.487979000	-2.217603000
6	3.322727000	3.238196000	1.706721000
1	2.465325000	3.530612000	2.322344000
1	3.764694000	2.346731000	2.162617000
1	4.057351000	4.050177000	1.747940000
6	1.737324000	4.343761000	-0.706246000
1	2.341689000	5.257751000	-0.713756000
1	1.382173000	4.176635000	-1.728517000
1	0.866792000	4.535081000	-0.070269000
1	0.002259000	-2.924568000	-0.329473000
6	-2.242757000	-1.399803000	0.024724000
1	-2.729446000	-2.047588000	-0.711120000
1	-2.192447000	-1.958882000	0.970456000
6	-1.918482000	0.968359000	0.411235000
1	-2.171431000	1.931375000	-0.044492000
1	-1.797011000	1.154047000	1.485475000
6	-3.024841000	-0.081596000	0.198477000
6	-3.813024000	0.220538000	-1.079002000
8	-3.835602000	-0.458091000	-2.078579000
6	-3.985143000	-0.160198000	1.381233000
8	-3.794322000	0.309389000	2.478455000
8	-4.480616000	1.382349000	-0.952873000
8	-5.070871000	-0.886866000	1.059808000
6	-5.258862000	1.764693000	-2.091405000
1	-5.730713000	2.709468000	-1.822732000
1	-4.620352000	1.890999000	-2.969169000
1	-6.014618000	1.006592000	-2.310955000
6	-6.024160000	-1.061360000	2.113752000
1	-6.831818000	-1.654179000	1.685436000
1	-5.571005000	-1.584864000	2.959131000
1	-6.397664000	-0.093592000	2.456965000

TS² (14'→20')
 SiC23H32O6
 C1

6	-2.430073000	0.765997000	1.275365000
6	-1.914772000	0.248787000	-0.062491000
8	-0.383131000	1.983667000	1.931636000
8	-2.171509000	0.043497000	2.449588000
6	-1.862423000	-0.944514000	-0.759558000
6	0.216913000	2.170929000	-1.989832000
6	0.675908000	0.954884000	-1.186374000
6	-0.710463000	-1.168844000	-1.565017000
6	0.460760000	-0.413809000	-1.553431000
1	-0.603343000	-2.173242000	-1.975615000
1	-3.494171000	1.036020000	1.245267000
1	0.465073000	2.105102000	-3.058570000
6	-1.212797000	1.442388000	-0.345248000
6	-1.257036000	2.236330000	-1.640731000
6	-1.856939000	3.640325000	-1.462384000
6	-1.523909000	4.263378000	-0.099738000
6	-2.095971000	3.422259000	1.047182000
6	-1.493541000	2.022376000	1.039279000
1	-1.506094000	4.286896000	-2.276743000
1	-2.949498000	3.586603000	-1.559807000
1	-0.436518000	4.354037000	0.025939000
1	-1.926112000	5.281647000	-0.053622000
1	-3.184929000	3.352207000	0.929448000
1	-1.904237000	3.889450000	2.019013000
1	-1.841874000	1.667177000	-2.372954000
1	-1.381673000	0.479624000	2.814437000
1	0.273616000	1.377700000	1.553016000
14	-3.002527000	-2.412012000	-0.367847000
6	-4.653954000	-1.789165000	0.299663000
1	-5.350962000	-2.625656000	0.422752000
1	-4.534431000	-1.314006000	1.277985000
1	-5.119299000	-1.066662000	-0.378915000
6	-2.185083000	-3.533384000	0.911612000
1	-1.205708000	-3.885248000	0.571382000
1	-2.038881000	-2.983257000	1.846457000
1	-2.805025000	-4.411353000	1.124879000
6	-3.305521000	-3.371119000	-1.969996000
1	-3.989162000	-4.207040000	-1.784047000
1	-3.758425000	-2.734982000	-2.737483000
1	-2.384257000	-3.792143000	-2.385707000
1	0.733726000	3.054430000	-1.593560000
6	2.105350000	1.064531000	-0.658948000
1	2.728387000	1.554228000	-1.423382000
1	2.194424000	1.662304000	0.251499000
6	1.808440000	-1.118850000	-1.600632000
1	2.342027000	-0.937687000	-2.542418000
1	1.763022000	-2.195904000	-1.428976000
6	2.578402000	-0.393410000	-0.480475000
6	4.090128000	-0.491179000	-0.663849000

8	4.649068000	-0.709453000	-1.712802000
6	2.199600000	-1.027922000	0.860199000
8	2.290412000	-2.212984000	1.077473000
8	4.731815000	-0.239650000	0.489761000
8	1.761826000	-0.142168000	1.778382000
6	6.162237000	-0.273988000	0.415058000
1	6.515003000	-0.045232000	1.420129000
1	6.504628000	-1.263699000	0.104131000
1	6.526652000	0.468296000	-0.299061000
6	1.428309000	-0.710341000	3.056026000
1	1.248599000	0.139338000	3.714131000
1	0.531371000	-1.327413000	2.969006000
1	2.254207000	-1.320610000	3.424854000

20'
SiC₂₃H₃₂O₆
C1

6	-2.920011000	1.253705000	0.775862000
6	-2.146087000	0.378285000	-0.186485000
8	-1.088858000	1.305727000	2.278108000
8	-3.621814000	0.701917000	1.849512000
6	-2.143965000	-0.890096000	-0.638519000
6	0.695679000	1.810400000	-1.522830000
6	0.422459000	0.698167000	-0.469178000
6	-0.852009000	-1.372531000	-1.172398000
6	0.297471000	-0.681105000	-1.069878000
1	-0.807492000	-2.390060000	-1.556726000
1	-3.598413000	1.947286000	0.262640000
1	1.042948000	1.480198000	-2.506797000
6	-0.982463000	1.324209000	-0.205006000
6	-0.781534000	2.260071000	-1.440831000
6	-1.041796000	3.748459000	-1.218430000
6	-0.657421000	4.189525000	0.194476000
6	-1.528478000	3.494469000	1.243850000
6	-1.551728000	1.964313000	1.104942000
1	-0.483919000	4.325168000	-1.967557000
1	-2.104882000	3.974275000	-1.383207000
1	0.402768000	3.965574000	0.377116000
1	-0.759274000	5.276089000	0.294597000
1	-2.554233000	3.876775000	1.165122000
1	-1.192590000	3.748846000	2.256184000
1	-1.357372000	1.895005000	-2.297778000
1	-2.941659000	0.338851000	2.436571000
1	-0.185620000	1.592184000	2.451256000
14	-3.606207000	-2.082296000	-0.470403000
6	-5.239135000	-1.142183000	-0.523098000
1	-6.083437000	-1.839204000	-0.476564000
1	-5.318234000	-0.457092000	0.325697000
1	-5.336245000	-0.562818000	-1.447310000
6	-3.474259000	-3.062495000	1.141150000
1	-2.509197000	-3.573659000	1.221399000
1	-3.578066000	-2.398296000	2.004575000

1	-4.262438000	-3.821185000	1.204330000
6	-3.545354000	-3.290524000	-1.927677000
1	-4.420460000	-3.949729000	-1.905916000
1	-3.552440000	-2.763050000	-2.887458000
1	-2.656813000	-3.930120000	-1.903676000
1	1.399949000	2.561199000	-1.150151000
6	1.507630000	0.452406000	0.587014000
1	2.031790000	1.355695000	0.910740000
1	1.054445000	-0.034668000	1.456051000
6	1.693712000	-1.204472000	-1.263722000
1	2.113852000	-0.895721000	-2.229041000
1	1.761888000	-2.292397000	-1.202867000
6	2.497754000	-0.539199000	-0.098064000
6	3.719624000	0.200793000	-0.636783000
8	3.887234000	1.398683000	-0.637568000
6	2.968748000	-1.587004000	0.909560000
8	2.688394000	-2.761776000	0.904724000
8	4.600957000	-0.672456000	-1.156565000
8	3.727829000	-1.006174000	1.858695000
6	5.784976000	-0.090792000	-1.712663000
1	6.378885000	-0.926788000	-2.080902000
1	5.532230000	0.589229000	-2.529820000
1	6.334891000	0.464214000	-0.948746000
6	4.207796000	-1.887766000	2.879660000
1	4.807735000	-1.268475000	3.545992000
1	3.373083000	-2.337842000	3.422698000
1	4.815638000	-2.684536000	2.444242000

Pathway II.

X = 6 (r,r) IIa

Table S4. B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	ZPVE	$E^0 + \text{ZPVE}$	$\langle S^2 \rangle$	Dipl.
9a	-1079.41179	0.44672	-1078.96507	0.00	3.96
TS¹ (9a→15a)	-1079.39974	0.44751	-1078.95223	0.00	3.69
15a	-1079.42852	0.45087	-1078.97764	0.00	3.68
TS² (15a→21a)	-1079.40124	0.44871	-1078.95252	0.00	2.59
21a	-1079.43884	0.45044	-1078.98841	0.00	2.00

X = 6 (r,s) IIb

Table S5. B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	ZPVE	$E^0 + \text{ZPVE}$	$\langle S^2 \rangle$	Dipl.
10a	-1079.41179	0.446723	-1078.96507	0.00	3.96
TS¹ (10a→16a)	-1079.39829	0.447415	-1078.95087	0.00	4.71
16a	-1079.44178	0.450663	-1078.99111	0.00	4.03
TS² (16a→22a)	-1079.40776	0.448784	-1078.95897	0.00	3.65
22a	-1079.42685	0.450544	-1078.97631	0.00	3.45

X = 7 (r,r) IIc

Table S6. B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	ZPVE	$E^0 + \text{ZPVE}$	$\langle S^2 \rangle$	Dipl.
11a	-1118.71159	0.47570	-1118.23590	0.00	3.80
TS¹ (11a→17a)	-1118.69694	0.47648	-1118.22046	0.00	3.32
17a	-1118.72626	0.47989	-1118.24638	0.00	4.33
TS² (17a→23a)	-1118.69421	0.47763	-1118.21658	0.00	4.05
23a	-1118.73047	0.47916	-1118.25131	0.00	4.04

X = 7 (r,s) IIe**Table S7.** B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	郑VE	$E^0 + \text{郑VE}$	$\langle S^2 \rangle$	Dipl.
12a	-1118.71159	0.47569	-1118.23589	0.00	3.80
TS ¹ (12a→18a)	-1118.70216	0.47681	-1118.22535	0.00	4.53
18a	-1118.74121	0.47929	-1118.26192	0.00	3.64
TS ² (18a→24a)	-1118.71303	0.47749	-1118.23554	0.00	3.06
24a	-1118.73248	0.47942	-1118.25306	0.00	3.17

X = 4 (r,r)**Table S8.** B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	郑VE	$E^0 + \text{郑VE}$	$\langle S^2 \rangle$	Dipl.
t4	-1000.72533	0.38677	-1000.33856	0.00	3.37
TS ¹	-1000.71092	0.38694	-1000.32398	0.00	3.65
c4	-1000.74322	0.39027	-1000.35296	0.00	3.55
TS ²	-1000.73115	0.38891	-1000.34225	0.00	2.70
f4	-1000.79724	0.39148	-1000.40576	0.00	2.34

X = 4 (r,s)**Table S9.** B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	郑VE	$E^0 + \text{郑VE}$	$\langle S^2 \rangle$	Dipl.
t4	-1000.72533	0.38677	-1000.3385	0.00	3.37
TS ¹	-1000.71092	0.38694	-1000.3234	0.00	3.65
c4	-1000.77067	0.39074	-1000.3799	0.00	3.08
TS ²	-1000.73390	0.38913	-1000.3448	0.00	2.66
f4	— ^a	— ^a	— ^a	— ^a	— ^a

^aThe data are not available because of bond dissociation upon optimization.**X = 5 (r,r)****Table S10.** B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	郑VE	$E^0 + \text{郑VE}$	$\langle S^2 \rangle$	Dipl.
t5	-1040.08857	0.41679	-1039.67178	0.00	3.91
TS ¹	-1040.07429	0.41781	-1039.65648	0.00	3.71
c5	-1040.11114	0.42066	-1039.69048	0.00	3.77
TS ²	-1040.08763	0.41900	-1039.66863	0.00	2.59
f5	-1040.13559	0.42124	-1039.71435	0.00	1.97

X = 8 (r,r)**Table S11.** B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	郑VE	$E^0 + \text{郑VE}$	$\langle S^2 \rangle$	Dipl.
t8	-1158.01153	0.50431	-1157.50721	0.00	3.42
TS ¹	-1157.99641	0.50526	-1157.49114	0.00	3.17
c8	-1158.02453	0.50910	-1157.51542	0.00	2.64
TS ²	-1157.99497	0.50701	-1157.48795	0.00	3.17
f8	-1158.02862	0.50854	-1157.52007	0.00	1.90

X = 8 (r,s)**Table S12.** B3PW 91/6-31g(d,p) Absolute energies [hartree], zero point vibrational energies [hartree], spin contaminations, and dipole moments [D].

	E^0	ZPVE	$E^0 + \text{ZPVE}$	$\langle S^2 \rangle$	Dipl.
t8	-1158.01152	0.50431	-1157.50721	0.00	3.42
TS¹	-1157.99022	0.50562	-1157.48460	0.00	3.64
c8	-1158.03331	0.50886	-1157.52444	0.00	4.14
TS²	-1158.00108	0.50608	-1157.49500	0.00	3.62
f8	-1158.02397	0.50829	-1157.51567	0.00	3.73

IIa.

9a

C₂₀H₂₈O₄

C1

6	1.593092000	0.214521000	-1.066658000
6	0.653637000	0.764761000	0.029102000
8	2.871058000	-1.293637000	0.176010000
8	2.940907000	0.616115000	-1.084230000
6	3.634342000	-0.117621000	-0.069474000
6	4.985495000	-0.526753000	-0.633601000
1	5.583696000	0.358339000	-0.865679000
1	5.527973000	-1.136609000	0.093425000
1	4.838118000	-1.107160000	-1.546733000
6	3.767644000	0.708877000	1.207634000
1	4.334317000	1.622998000	1.008102000
1	2.784827000	0.980509000	1.596582000
1	4.294303000	0.129017000	1.970957000
6	0.219141000	2.027939000	0.265755000
6	-2.709990000	0.322116000	0.024501000
6	-2.838551000	1.058717000	1.142862000
6	-0.678370000	2.451871000	1.336552000
6	-1.909154000	2.024249000	1.713753000
6	-3.754437000	-0.590076000	-0.570005000
6	-4.877759000	-0.966333000	0.396440000
1	-4.470164000	-1.437984000	1.294265000
1	-5.472058000	-0.096527000	0.692118000
1	-5.559226000	-1.676661000	-0.085327000
6	-4.327466000	0.067458000	-1.836731000
1	-3.523858000	0.296479000	-2.542456000
1	-5.035867000	-0.608257000	-2.333109000
1	-4.856863000	0.994512000	-1.598259000
8	-3.026981000	-1.771116000	-0.943877000
1	-3.641416000	-2.343628000	-1.419849000
6	0.820129000	3.169483000	-0.528749000
1	1.531151000	3.715386000	0.105606000
1	1.396247000	2.778149000	-1.378203000
8	-0.134721000	4.136727000	-0.932031000
1	-0.842108000	3.666785000	-1.388362000
1	-0.316676000	3.331616000	1.872696000
1	-2.323848000	2.553211000	2.571208000
1	1.196799000	0.276010000	-2.085476000

1	-1.802078000	0.384266000	-0.568108000
6	0.509757000	-0.574652000	0.597925000
6	-0.339078000	-1.309454000	1.334820000
6	-0.302858000	-2.810008000	1.250298000
6	0.799712000	-3.383166000	0.338805000
6	1.090283000	-2.497350000	-0.886858000
6	1.547346000	-1.159942000	-0.343367000
1	-0.228699000	-3.254034000	2.252688000
1	-1.291665000	-3.105855000	0.869140000
1	1.731840000	-3.482124000	0.906104000
1	0.514748000	-4.392307000	0.021387000
1	0.178186000	-2.359463000	-1.480253000
1	1.857488000	-2.950052000	-1.523608000
1	-3.765870000	0.965235000	1.706472000
1	-1.138891000	-0.854376000	1.909667000

TS¹ (9a→15a)

C₂₀H₂₈O₄

C1

6	2.205755000	-0.587670000	-0.738798000
6	1.280832000	0.642860000	-0.646782000
8	0.829719000	-2.039415000	0.445363000
8	2.898338000	-1.034474000	0.399482000
6	1.964230000	-1.706530000	1.247076000
6	2.615210000	-2.992990000	1.733206000
1	3.508370000	-2.769083000	2.322969000
1	1.915753000	-3.558320000	2.354749000
1	2.901835000	-3.604055000	0.874490000
6	1.539038000	-0.803573000	2.401017000
1	2.399578000	-0.568945000	3.034406000
1	1.121077000	0.130348000	2.020241000
1	0.782256000	-1.307265000	3.009076000
6	1.534504000	1.966489000	-0.293263000
6	-1.893496000	0.861138000	0.404949000
6	-1.863311000	2.221925000	0.087635000
6	0.607121000	3.005999000	-0.110752000
6	-0.790022000	3.108603000	-0.060314000
6	-3.200345000	0.190007000	0.800111000
6	-3.508222000	0.551880000	2.264001000
1	-2.679971000	0.248789000	2.910344000
1	-3.667819000	1.626982000	2.383941000
1	-4.415809000	0.034468000	2.602203000
6	-4.386534000	0.558129000	-0.097063000
1	-4.163169000	0.357657000	-1.147690000
1	-5.260885000	-0.038554000	0.187142000
1	-4.670313000	1.609721000	0.002345000
8	-2.948352000	-1.214922000	0.715464000
1	-3.710364000	-1.665326000	1.099042000
6	3.003109000	2.329490000	-0.068293000
1	3.244567000	2.246315000	0.997508000
1	3.646793000	1.607203000	-0.589306000
8	3.336407000	3.658529000	-0.425290000
1	3.134919000	3.760183000	-1.363260000

1	1.102846000	3.972126000	-0.018233000
1	-1.122476000	4.144848000	-0.137537000
1	2.893026000	-0.593955000	-1.591039000
1	-1.048216000	0.427590000	0.924989000
6	0.172698000	-0.132468000	-1.016898000
6	-1.110358000	0.016161000	-1.521562000
6	-1.742902000	-1.220507000	-2.134875000
6	-1.033307000	-2.547085000	-1.813602000
6	0.500964000	-2.453363000	-1.900301000
6	0.911277000	-1.441050000	-0.851557000
1	-2.794031000	-1.302769000	-1.844277000
1	-1.739035000	-1.058587000	-3.224707000
1	-1.298881000	-2.850908000	-0.795786000
1	-1.409424000	-3.320936000	-2.492446000
1	0.808954000	-2.104869000	-2.895016000
1	0.967434000	-3.427091000	-1.719811000
1	-2.831437000	2.684514000	-0.104467000
1	-1.381908000	0.957500000	-1.983621000

15a

C20H28O4

C1

6	2.378816000	-0.194519000	-0.776218000
6	1.267853000	0.831924000	-0.506808000
8	1.498511000	-2.080555000	0.312196000
8	3.238359000	-0.576858000	0.266257000
6	2.552580000	-1.518911000	1.099008000
6	3.529448000	-2.632288000	1.441266000
1	4.371586000	-2.233879000	2.013331000
1	3.031819000	-3.401601000	2.037621000
1	3.905481000	-3.082589000	0.520177000
6	1.996919000	-0.836625000	2.345452000
1	2.814029000	-0.393809000	2.922508000
1	1.286627000	-0.052737000	2.078924000
1	1.484933000	-1.572224000	2.973114000
6	1.137767000	2.248804000	-0.269566000
6	-1.911435000	-0.176302000	0.503915000
6	-1.480014000	0.888176000	1.491324000
6	0.150000000	2.728296000	0.528335000
6	-0.747870000	2.027265000	1.447792000
6	-3.475320000	-0.222945000	0.419484000
6	-4.135931000	-0.196979000	1.804776000
1	-3.691971000	-0.949132000	2.464467000
1	-4.074241000	0.782050000	2.286854000
1	-5.200622000	-0.436500000	1.695664000
6	-4.040680000	0.908911000	-0.442143000
1	-3.721526000	0.814098000	-1.482909000
1	-5.137236000	0.893623000	-0.423808000
1	-3.715373000	1.884039000	-0.065686000
8	-3.770043000	-1.497329000	-0.167516000
1	-4.729169000	-1.556719000	-0.254757000
6	2.154370000	3.176921000	-0.901876000

1	3.124522000	3.031036000	-0.410090000
1	2.299809000	2.887808000	-1.956292000
8	1.858525000	4.550634000	-0.785120000
1	1.044309000	4.710112000	-1.277210000
1	0.161130000	3.808380000	0.675296000
1	-0.817519000	2.593360000	2.380494000
1	2.972867000	-0.041319000	-1.683864000
1	-1.638053000	-1.149795000	0.936601000
6	0.288983000	-0.086977000	-0.619359000
6	-1.177124000	-0.028725000	-0.849696000
6	-1.492192000	-1.043104000	-1.985382000
6	-0.686712000	-2.351147000	-1.922821000
6	0.830501000	-2.111438000	-2.003728000
6	1.233872000	-1.256013000	-0.816876000
1	-2.557645000	-1.272755000	-1.995977000
1	-1.251264000	-0.544182000	-2.934856000
1	-0.918423000	-2.891475000	-0.996479000
1	-1.005667000	-3.000470000	-2.746485000
1	1.066026000	-1.578499000	-2.934669000
1	1.390794000	-3.051990000	-2.003699000
1	-1.932719000	0.730349000	2.468253000
1	-1.408323000	0.981742000	-1.214349000

TS² (15a→21a)

C₂₀H₂₈O₄

C1

6	2.172855000	-0.141390000	-0.993726000
6	1.001043000	0.790403000	-0.711013000
8	1.830008000	-1.805607000	0.616518000
8	3.273222000	-0.171500000	-0.117597000
6	2.916006000	-0.963305000	1.018860000
6	4.100502000	-1.852973000	1.359545000
1	4.964876000	-1.243840000	1.636835000
1	3.849977000	-2.509559000	2.196881000
1	4.358406000	-2.464193000	0.492112000
6	2.507497000	-0.071213000	2.186517000
1	3.354180000	0.550028000	2.493095000
1	1.676829000	0.578858000	1.906847000
1	2.199115000	-0.686824000	3.036543000
6	0.777496000	2.141941000	-0.524553000
6	-2.006748000	-0.521233000	0.405472000
6	-1.054176000	0.273490000	1.303287000
6	-0.200740000	2.527686000	0.417570000
6	-0.823653000	1.671782000	1.327424000
6	-3.509613000	-0.173724000	0.514562000
6	-3.960001000	-0.209755000	1.978428000
1	-3.710560000	-1.173905000	2.432163000
1	-3.493678000	0.586178000	2.566787000
1	-5.046564000	-0.075775000	2.043093000
6	-3.876288000	1.166256000	-0.123864000
1	-3.688987000	1.148544000	-1.200703000

1	-4.942158000	1.377607000	0.028593000
1	-3.306791000	1.989899000	0.315284000
8	-4.154990000	-1.237588000	-0.200017000
1	-5.099532000	-1.041245000	-0.216241000
6	1.752680000	3.189681000	-1.029169000
1	2.595664000	3.278706000	-0.334004000
1	2.173846000	2.865110000	-1.992763000
8	1.193429000	4.485649000	-1.120754000
1	0.446888000	4.432078000	-1.729304000
1	-0.217675000	3.590710000	0.651825000
1	-0.973901000	2.139163000	2.305314000
1	2.542073000	-0.149626000	-2.025023000
1	-1.937535000	-1.563267000	0.744420000
6	0.117430000	-0.264908000	-0.422721000
6	-1.301620000	-0.432378000	-0.937630000
6	-1.455234000	-1.627243000	-1.892344000
6	-0.581436000	-2.821714000	-1.492510000
6	0.907651000	-2.462334000	-1.530321000
6	1.236409000	-1.318305000	-0.573875000
1	-2.511181000	-1.911509000	-1.923066000
1	-1.171743000	-1.317405000	-2.908023000
1	-0.850203000	-3.172461000	-0.487317000
1	-0.775450000	-3.660885000	-2.170313000
1	1.169597000	-2.161486000	-2.553570000
1	1.535017000	-3.321961000	-1.274369000
1	-1.010638000	-0.149554000	2.312351000
1	-1.583592000	0.494389000	-1.452275000

21a

C20H28O4

C1

6	1.903675000	-0.331702000	-1.083102000
6	0.915455000	0.753259000	-0.706021000
8	1.751094000	-1.400802000	0.962994000
8	3.178937000	-0.322852000	-0.492810000
6	3.075838000	-0.878108000	0.823434000
6	4.091293000	-2.008109000	0.932849000
1	5.105644000	-1.622086000	0.799069000
1	4.022946000	-2.485262000	1.914126000
1	3.896890000	-2.755894000	0.160272000
6	3.284623000	0.200731000	1.876748000
1	4.277826000	0.645438000	1.769977000
1	2.528286000	0.979700000	1.764960000
1	3.199528000	-0.230539000	2.878165000
6	0.935290000	2.054741000	-0.386848000
6	-2.172454000	-0.484746000	0.370566000
6	-0.932837000	0.195998000	1.040362000
6	-0.142459000	2.533635000	0.493075000
6	-0.944601000	1.695997000	1.177947000
6	-3.611479000	0.043063000	0.454184000
6	-4.052181000	0.148958000	1.918254000
1	-3.902346000	-0.806034000	2.430644000

1	-3.500520000	0.924090000	2.458576000
1	-5.117792000	0.401298000	1.978439000
6	-3.854764000	1.360028000	-0.284995000
1	-3.674262000	1.237317000	-1.356013000
1	-4.897940000	1.674670000	-0.154913000
1	-3.213983000	2.165151000	0.082341000
8	-4.371371000	-0.995077000	-0.187107000
1	-5.287153000	-0.693821000	-0.231465000
6	2.042889000	3.006484000	-0.751186000
1	2.556392000	3.357678000	0.151785000
1	2.791100000	2.493280000	-1.370918000
8	1.548468000	4.183140000	-1.377780000
1	1.057221000	3.899536000	-2.157882000
1	-0.206250000	3.605997000	0.661712000
1	-1.618309000	2.117893000	1.922085000
1	2.005089000	-0.549682000	-2.152035000
1	-2.229718000	-1.504085000	0.769501000
6	-0.097185000	-0.225744000	-0.200550000
6	-1.412526000	-0.521620000	-0.979833000
6	-1.468962000	-1.809725000	-1.794774000
6	-0.786315000	-2.971202000	-1.071454000
6	0.703538000	-2.709552000	-0.827171000
6	1.026667000	-1.320657000	-0.255811000
1	-2.519269000	-2.048995000	-1.994884000
1	-0.983621000	-1.655370000	-2.769553000
1	-1.290085000	-3.156042000	-0.114651000
1	-0.899755000	-3.894348000	-1.651239000
1	1.248233000	-2.836789000	-1.772254000
1	1.105722000	-3.453938000	-0.132804000
1	-0.657448000	-0.255617000	2.002965000
1	-1.674483000	0.340784000	-1.602423000

lib.

10a
C20H28O4
C1

6	1.593092000	0.214521000	-1.066658000
6	0.653637000	0.764761000	0.029102000
8	2.871058000	-1.293637000	0.176010000
8	2.940907000	0.616115000	-1.084230000
6	3.634342000	-0.117621000	-0.069474000
6	4.985495000	-0.526753000	-0.633601000
1	5.583696000	0.358339000	-0.865679000
1	5.527973000	-1.136609000	0.093425000
1	4.838118000	-1.107160000	-1.546733000
6	3.767644000	0.708877000	1.207634000
1	4.334317000	1.622998000	1.008102000
1	2.784827000	0.980509000	1.596582000
1	4.294303000	0.129017000	1.970957000
6	0.219141000	2.027939000	0.265755000
6	-2.709990000	0.322116000	0.024501000
6	-2.838551000	1.058717000	1.142862000

6	-0.678370000	2.451871000	1.336552000
6	-1.909154000	2.024249000	1.713753000
6	-3.754437000	-0.590076000	-0.570005000
6	-4.877759000	-0.966333000	0.396440000
1	-4.470164000	-1.437984000	1.294265000
1	-5.472058000	-0.096527000	0.692118000
1	-5.559226000	-1.676661000	-0.085327000
6	-4.327466000	0.067458000	-1.836731000
1	-3.523858000	0.296479000	-2.542456000
1	-5.035867000	-0.608257000	-2.333109000
1	-4.856863000	0.994512000	-1.598259000
8	-3.026981000	-1.771116000	-0.943877000
1	-3.641416000	-2.343628000	-1.419849000
6	0.820129000	3.169483000	-0.528749000
1	1.531151000	3.715386000	0.105606000
1	1.396247000	2.778149000	-1.378203000
8	-0.134721000	4.136727000	-0.932031000
1	-0.842108000	3.666785000	-1.388362000
1	-0.316676000	3.331616000	1.872696000
1	-2.323848000	2.553211000	2.571208000
1	1.196799000	0.276010000	-2.085476000
1	-1.802078000	0.384266000	-0.568108000
6	0.509757000	-0.574652000	0.597925000
6	-0.339078000	-1.309454000	1.334820000
6	-0.302858000	-2.810008000	1.250298000
6	0.799712000	-3.383166000	0.338805000
6	1.090283000	-2.497350000	-0.886858000
6	1.547346000	-1.159942000	-0.343367000
1	-0.228699000	-3.254034000	2.252688000
1	-1.291665000	-3.105855000	0.869140000
1	1.731840000	-3.482124000	0.906104000
1	0.514748000	-4.392307000	0.021387000
1	0.178186000	-2.359463000	-1.480253000
1	1.857488000	-2.950052000	-1.523608000
1	-3.765870000	0.965235000	1.706472000
1	-1.138891000	-0.854376000	1.909667000

TS¹ (10a→16a)

C₂₀H₂₈O₄

C1

6	1.737405000	0.123340000	-1.049651000
6	0.795975000	0.865802000	-0.084888000
8	2.302354000	-1.796627000	0.168635000
8	3.124894000	0.108753000	-0.801074000
6	3.390661000	-0.877561000	0.201321000
6	4.653369000	-1.622508000	-0.199782000
1	4.515203000	-2.064487000	-1.188698000
1	5.504142000	-0.936691000	-0.230592000
1	4.868039000	-2.416911000	0.519832000
6	3.516371000	-0.231014000	1.579712000
1	4.342687000	0.485901000	1.582950000
1	2.596679000	0.291051000	1.848084000
1	3.715218000	-0.997853000	2.334145000
6	0.573562000	2.241979000	0.046241000

6	-2.354050000	0.388417000	0.057208000
6	-2.516071000	1.412257000	0.991678000
6	-0.431602000	2.897867000	0.768892000
6	-1.678166000	2.497691000	1.264987000
6	-3.537718000	-0.455880000	-0.381771000
6	-4.425140000	-0.934541000	0.771742000
1	-3.842613000	-1.470377000	1.524821000
1	-4.944062000	-0.105205000	1.260372000
1	-5.195135000	-1.613614000	0.388111000
6	-4.370975000	0.361930000	-1.385328000
1	-3.750423000	0.667560000	-2.232395000
1	-5.204630000	-0.240755000	-1.769504000
1	-4.788476000	1.258489000	-0.919134000
8	-2.975547000	-1.581529000	-1.064336000
1	-3.705422000	-2.063812000	-1.470959000
6	1.640742000	3.128341000	-0.589876000
1	2.519739000	3.174520000	0.063374000
1	1.985393000	2.660673000	-1.525074000
8	1.252615000	4.470692000	-0.798020000
1	0.459057000	4.457623000	-1.346746000
1	-0.201576000	3.946871000	0.955493000
1	-2.115900000	3.219361000	1.955229000
1	1.580711000	0.332271000	-2.114170000
1	-1.638711000	0.545000000	-0.743127000
6	0.284733000	-0.341359000	0.423193000
6	-0.787307000	-0.861145000	1.142763000
6	-0.961418000	-2.366700000	1.106714000
6	-0.265405000	-3.136417000	-0.052252000
6	0.356385000	-2.258048000	-1.155223000
6	1.173519000	-1.194790000	-0.461680000
1	-0.590976000	-2.755912000	2.066068000
1	-2.031536000	-2.588120000	1.095493000
1	0.537487000	-3.749355000	0.368793000
1	-0.984039000	-3.825350000	-0.506403000
1	-0.435613000	-1.779582000	-1.740919000
1	0.970401000	-2.869020000	-1.826028000
1	-3.405701000	1.365472000	1.619497000
1	-1.163688000	-0.364034000	2.025839000

16a

C20H28O4

C1

6	2.141826000	0.174253000	-0.967647000
6	0.810639000	0.774498000	-0.492801000
8	2.363245000	-1.695355000	0.435669000
8	3.280058000	0.326823000	-0.152169000
6	3.224625000	-0.650283000	0.894165000
6	4.618889000	-1.230977000	1.063560000
1	5.318081000	-0.450223000	1.374477000
1	4.610672000	-2.017859000	1.822352000
1	4.955327000	-1.653437000	0.114472000
6	2.697604000	-0.034847000	2.188291000
1	3.359895000	0.773092000	2.512761000

1	1.693948000	0.369014000	2.049699000
1	2.664227000	-0.795991000	2.973476000
6	0.414068000	2.171470000	-0.420636000
6	-2.114865000	0.043005000	0.210348000
6	-1.783309000	0.804944000	1.465875000
6	-0.418870000	2.691638000	0.512970000
6	-1.107559000	1.962357000	1.566207000
6	1.145747000	3.092033000	-1.381974000
1	2.207652000	3.123030000	-1.108496000
1	1.102504000	2.661052000	-2.396794000
8	0.699448000	4.428997000	-1.377014000
1	-0.224196000	4.422033000	-1.655793000
1	-0.475456000	3.779236000	0.551913000
1	-1.059260000	2.427915000	2.552236000
1	2.430402000	0.363019000	-2.007970000
6	0.284771000	-0.443511000	-0.198444000
6	-1.039647000	-1.073615000	0.071260000
6	-1.231843000	-2.171224000	-1.005482000
6	-0.001193000	-3.080314000	-1.153490000
6	1.240958000	-2.305961000	-1.613318000
6	1.534352000	-1.205363000	-0.608579000
1	-2.101129000	-2.777104000	-0.735324000
1	-1.437835000	-1.701215000	-1.977239000
1	0.214197000	-3.567832000	-0.193573000
1	-0.229041000	-3.881598000	-1.866172000
1	1.042883000	-1.852375000	-2.593614000
1	2.112112000	-2.960819000	-1.717872000
1	-2.164070000	0.357253000	2.383299000
1	-0.992188000	-1.603064000	1.032800000
6	-3.602048000	-0.425124000	0.235086000
6	-4.136240000	-0.773377000	-1.162226000
1	-4.100376000	0.099930000	-1.821906000
1	-3.584467000	-1.583595000	-1.634818000
1	-5.186282000	-1.081778000	-1.088691000
6	-4.514974000	0.669109000	0.810622000
1	-4.427523000	1.599561000	0.240901000
1	-5.562177000	0.345985000	0.757772000
1	-4.277947000	0.887018000	1.853374000
8	-3.630863000	-1.573379000	1.086583000
1	-4.554157000	-1.828829000	1.200085000
1	-2.008480000	0.718630000	-0.648635000

TS² (16a→22a)

C₂₀H₂₈O₄

C1

6	-1.938391000	-0.326738000	0.974931000
6	-0.720172000	0.537630000	0.673319000
8	-2.132506000	-1.648481000	-0.949078000
8	-3.155300000	-0.034443000	0.324318000

6	-3.105938000	-0.601395000	-0.990761000
6	-4.460613000	-1.224698000	-1.280817000
1	-5.238150000	-0.456290000	-1.280860000
1	-4.449091000	-1.712720000	-2.258836000
1	-4.692885000	-1.966906000	-0.514291000
6	-2.716035000	0.449388000	-2.025012000
1	-3.456425000	1.254582000	-2.038502000
1	-1.736899000	0.876260000	-1.799723000
1	-2.676980000	-0.006491000	-3.018664000
6	-0.586416000	1.916598000	0.664034000
6	2.153457000	0.088199000	-0.075585000
6	1.257238000	0.540502000	-1.228553000
6	0.151416000	2.562218000	-0.355209000
6	0.809182000	1.872797000	-1.360165000
6	-1.556032000	2.753274000	1.486188000
1	-2.543100000	2.737268000	1.010827000
1	-1.681682000	2.300634000	2.481735000
8	-1.192496000	4.115742000	1.586130000
1	-0.326970000	4.151042000	2.010423000
1	-0.050664000	3.623885000	-0.480198000
1	0.853086000	2.346122000	-2.341699000
1	-2.146298000	-0.533594000	2.030248000
6	-0.032308000	-0.518930000	-0.002030000
6	1.318150000	-1.132995000	0.296613000
6	1.369063000	-1.826067000	1.663583000
6	0.042691000	-2.564887000	1.997354000
6	-0.899147000	-2.775098000	0.800192000
6	-1.262745000	-1.452980000	0.143775000
1	2.201434000	-2.538301000	1.680538000
1	1.577212000	-1.083757000	2.443848000
1	0.262558000	-3.536377000	2.452235000
1	-0.500855000	-2.000372000	2.764459000
1	-1.814064000	-3.287019000	1.120021000
1	-0.426822000	-3.416197000	0.044774000
1	1.476142000	0.002002000	-2.151607000
1	1.504127000	-1.883546000	-0.482638000
6	3.632081000	-0.112675000	-0.461740000
6	4.455678000	-0.580793000	0.742890000
1	4.412404000	0.141815000	1.564435000
1	4.098161000	-1.545558000	1.108714000
1	5.509545000	-0.696044000	0.461177000
6	4.226684000	1.179608000	-1.029426000
1	4.182224000	1.993112000	-0.298218000
1	5.280281000	1.030396000	-1.296830000
1	3.685720000	1.494663000	-1.924830000
8	3.633020000	-1.129150000	-1.468433000
1	4.544016000	-1.247506000	-1.761279000
1	2.105180000	0.831801000	0.729753000

22a

C20H28O4

C1

6	-1.793068000	-0.479290000	0.984890000
---	--------------	--------------	-------------

6	-0.735705000	0.576024000	0.719785000
8	-1.900964000	-1.545898000	-1.101636000
8	-3.072187000	-0.279989000	0.423195000
6	-3.060623000	-0.723733000	-0.937945000
6	-4.296240000	-1.582936000	-1.157002000
1	-5.202243000	-0.987386000	-1.016102000
1	-4.298171000	-1.990848000	-2.171200000
1	-4.299446000	-2.407938000	-0.441298000
6	-2.995893000	0.455658000	-1.901296000
1	-3.858604000	1.111280000	-1.751879000
1	-2.081508000	1.031390000	-1.746827000
1	-3.008496000	0.092392000	-2.932912000
6	-0.859696000	1.907977000	0.543194000
6	2.234384000	0.229064000	0.017141000
6	1.101868000	0.442571000	-1.054996000
6	-0.033584000	2.572494000	-0.463202000
6	0.758282000	1.871965000	-1.299371000
6	-1.989640000	2.705491000	1.146101000
1	-2.697370000	3.010562000	0.366506000
1	-2.548726000	2.092499000	1.865603000
8	-1.529839000	3.917980000	1.728938000
1	-0.867897000	3.679058000	2.388438000
1	-0.195910000	3.636719000	-0.614009000
1	1.215915000	2.371149000	-2.151049000
1	-1.915226000	-0.838304000	2.011535000
6	0.154568000	-0.352696000	-0.056190000
6	1.429184000	-0.975315000	0.532299000
6	1.283272000	-1.550136000	1.923936000
6	0.213912000	-2.686122000	1.854129000
6	-0.580209000	-2.760901000	0.526507000
6	-1.030656000	-1.403509000	-0.006774000
1	2.228444000	-1.946682000	2.310234000
1	0.962773000	-0.763021000	2.618314000
1	0.697648000	-3.657252000	2.003995000
1	-0.489562000	-2.577762000	2.687019000
1	-1.471784000	-3.381232000	0.670825000
1	0.016362000	-3.256517000	-0.248571000
1	1.348962000	-0.107467000	-1.967929000
1	1.695621000	-1.793691000	-0.151006000
6	3.675451000	0.021607000	-0.456582000
6	4.577919000	-0.341571000	0.727587000
1	4.583271000	0.449684000	1.484190000
1	4.240358000	-1.269495000	1.196148000
1	5.612606000	-0.486759000	0.393218000
6	4.202133000	1.272885000	-1.165759000
1	4.177399000	2.147643000	-0.508210000
1	5.241625000	1.125768000	-1.484703000
1	3.603870000	1.491245000	-2.054109000
8	3.632985000	-1.069905000	-1.380549000
1	4.530771000	-1.213684000	-1.701478000
1	2.205395000	1.063986000	0.726946000

lld.

11a
C21H30O4
C1

6	-1.661297000	-1.153253000	-0.276530000
6	-1.375184000	-2.499191000	-0.946866000
6	-0.572011000	-0.528311000	0.601671000
6	0.100015000	-2.915684000	-0.926467000
6	0.252914000	-1.145359000	1.464055000
6	0.119142000	-2.627656000	1.663192000
1	-1.748795000	-2.464254000	-1.978084000
1	-1.983484000	-3.251747000	-0.430478000
1	0.729585000	-2.076865000	-1.241708000
1	0.258753000	-3.705334000	-1.670985000
1	0.673076000	-2.956501000	2.548593000
1	-0.935660000	-2.865993000	1.848133000
1	1.050186000	-0.600815000	1.958794000
6	-1.698209000	0.187465000	-1.065965000
6	-0.723255000	0.777988000	-0.035707000
8	-2.962863000	-1.208686000	0.308996000
8	-3.037717000	0.617455000	-1.069845000
6	-3.717048000	-0.038571000	0.004869000
1	-1.331900000	0.173336000	-2.098369000
6	-0.340078000	2.062481000	0.174856000
6	0.500218000	2.548554000	1.266004000
6	1.734826000	2.197166000	1.701635000
6	2.749228000	1.293834000	1.175082000
6	2.718607000	0.542522000	0.060220000
1	3.663645000	1.280694000	1.766820000
1	1.828032000	0.520526000	-0.562429000
6	-0.972760000	3.162784000	-0.653266000
1	-1.500172000	2.734567000	-1.516208000
1	-1.730085000	3.681493000	-0.050660000
8	-0.051869000	4.169641000	-1.038493000
1	0.690611000	3.728678000	-1.467277000
6	-3.809109000	0.867919000	1.229702000
1	-4.374825000	1.772551000	0.988360000
1	-4.318485000	0.342321000	2.042363000
1	-2.813389000	1.154083000	1.572336000
6	-5.086336000	-0.463420000	-0.501645000
1	-5.676107000	0.413108000	-0.782771000
1	-4.966940000	-1.108107000	-1.374893000
1	-5.622402000	-1.012686000	0.276649000
6	3.870312000	-0.255385000	-0.500773000
6	4.961230000	-0.578663000	0.520948000
1	4.539491000	-1.119715000	1.371771000
1	5.728092000	-1.210013000	0.057889000
1	5.461911000	0.322796000	0.886788000
6	4.459515000	0.504323000	-1.701672000
1	3.683192000	0.696531000	-2.447823000
1	4.890741000	1.460891000	-1.392957000
1	5.252898000	-0.086513000	-2.177656000
8	3.274997000	-1.475173000	-0.965784000
1	3.954542000	-1.960524000	-1.449484000
1	0.066295000	3.410868000	1.776820000
1	2.079405000	2.757667000	2.569965000
6	0.603685000	-3.431803000	0.432477000
1	1.698721000	-3.429789000	0.409078000

1 0.286251000 -4.473589000 0.573493000

TS¹ (11a→17a)

C21H30O4

C1

6	-1.026027000	-1.480178000	-0.556122000
6	-1.067995000	-2.729183000	-1.441145000
6	-0.218286000	-0.246999000	-0.980195000
6	0.150652000	-2.912912000	-2.351267000
6	1.082698000	-0.047213000	-1.453301000
6	1.976131000	-1.173122000	-1.924570000
1	-1.980852000	-2.719289000	-2.049966000
1	-1.152338000	-3.586920000	-0.765835000
1	0.048637000	-2.275142000	-3.239696000
1	0.146552000	-3.943983000	-2.724174000
1	2.107660000	-1.043652000	-3.010326000
1	2.971064000	-1.056635000	-1.487786000
1	1.227946000	0.883117000	-1.989132000
6	-2.244910000	-0.528234000	-0.454421000
6	-1.271789000	0.631044000	-0.671380000
8	-0.815485000	-1.850916000	0.811049000
8	-2.823898000	-0.723646000	0.812653000
6	-1.863636000	-1.364847000	1.653663000
1	-3.025530000	-0.646584000	-1.213746000
6	-1.492273000	2.006540000	-0.536475000
6	-0.576339000	3.068273000	-0.573700000
6	0.819979000	3.195912000	-0.533858000
6	1.867503000	2.342196000	-0.186660000
6	1.817207000	1.045559000	0.337789000
1	2.857825000	2.744528000	-0.396651000
6	-2.955847000	2.409828000	-0.319002000
1	-3.619854000	1.628234000	-0.712356000
1	-3.161607000	2.477842000	0.755070000
8	-3.300099000	3.676051000	-0.849876000
1	-3.153339000	3.634741000	-1.802524000
6	-1.295635000	-0.372892000	2.662319000
1	-2.081011000	-0.035097000	3.344610000
1	-0.500661000	-0.845889000	3.245522000
1	-0.887819000	0.497456000	2.144912000
6	-2.545008000	-2.546429000	2.330515000
1	-3.375074000	-2.201984000	2.953606000
1	-2.932817000	-3.228866000	1.570850000
1	-1.831411000	-3.084258000	2.960465000
1	-1.083792000	4.029831000	-0.649612000
1	1.155297000	4.200550000	-0.793482000
6	1.487731000	-2.598040000	-1.661386000
1	2.262808000	-3.283794000	-2.024019000
1	1.411722000	-2.761321000	-0.580226000
6	3.059206000	0.426913000	0.963658000
6	4.361441000	0.722234000	0.209248000
1	4.648091000	1.775306000	0.280571000
1	5.177396000	0.136902000	0.648092000
1	4.284929000	0.457446000	-0.848114000

6	3.169309000	0.940912000	2.410867000
1	2.266612000	0.686001000	2.972514000
1	4.029533000	0.479308000	2.913658000
1	3.303403000	2.025845000	2.440738000
8	2.819864000	-0.981679000	0.992980000
1	3.522794000	-1.380706000	1.519607000
1	0.916115000	0.742360000	0.855512000

17a

C21H30O4

C1

6	1.638888000	0.577493000	-0.703056000
6	1.756615000	1.672290000	-1.749408000
6	0.253807000	0.360341000	-0.100864000
6	1.300505000	3.073058000	-1.245704000
6	-0.760393000	1.414652000	0.185913000
6	-0.159128000	2.653347000	0.882473000
1	1.159503000	1.380239000	-2.621399000
1	2.800556000	1.708665000	-2.077248000
1	0.356184000	3.351774000	-1.731100000
1	2.029977000	3.815768000	-1.586292000
1	-0.931925000	3.433706000	0.851181000
1	0.007227000	2.429749000	1.943911000
1	-1.073351000	1.753911000	-0.815099000
6	1.613429000	-0.938324000	-1.036155000
6	0.280570000	-0.980626000	-0.291420000
8	2.724105000	0.683645000	0.222085000
8	2.756709000	-1.508969000	-0.444909000
6	3.226415000	-0.613102000	0.560419000
1	1.569307000	-1.237079000	-2.087620000
6	-0.576347000	-2.121482000	-0.022037000
6	-1.326548000	-2.264347000	1.092065000
6	-1.465493000	-1.301382000	2.174871000
6	-1.733127000	0.014690000	2.099372000
6	-2.038599000	0.923172000	0.919158000
1	-1.785870000	0.527717000	3.059263000
6	-0.609102000	-3.160545000	-1.112634000
1	0.395234000	-3.551398000	-1.318550000
1	-1.239088000	-4.009827000	-0.804616000
8	-1.077785000	-2.569565000	-2.315665000
1	-1.700231000	-1.880326000	-2.037631000
6	2.741925000	-1.034483000	1.946258000
1	3.117393000	-2.034178000	2.183459000
1	3.114806000	-0.333200000	2.698900000
1	1.652266000	-1.046340000	1.991182000
6	4.743924000	-0.567318000	0.476806000
1	5.164726000	-1.551074000	0.701680000
1	5.044507000	-0.273684000	-0.531097000
1	5.140771000	0.156495000	1.193578000
1	-1.840171000	-3.217519000	1.230957000

1	-1.394930000	-1.720928000	3.180363000
6	1.147450000	3.212876000	0.279417000
1	1.200553000	4.277106000	0.539051000
1	2.005556000	2.737162000	0.760286000
6	-3.190212000	0.521774000	-0.071307000
6	-4.242853000	-0.377865000	0.575127000
1	-4.643634000	0.069850000	1.490298000
1	-5.078969000	-0.530430000	-0.117473000
1	-3.819429000	-1.351069000	0.825236000
6	-3.860132000	1.812630000	-0.566410000
1	-3.130800000	2.496268000	-1.011315000
1	-4.617066000	1.582571000	-1.327012000
1	-4.369640000	2.334030000	0.249564000
8	-2.631657000	-0.142863000	-1.220873000
1	-3.305195000	-0.099534000	-1.910577000
1	-2.448806000	1.822508000	1.395711000

TS² (17a→23a)

C21H30O4

C1

6	1.465456000	1.009550000	-0.430731000
6	1.602992000	2.256831000	-1.282103000
6	0.061303000	0.349889000	-0.268081000
6	0.992609000	3.513377000	-0.660690000
6	-1.297239000	0.929948000	-0.697323000
6	-1.304298000	2.426190000	-1.069889000
1	1.134740000	2.054659000	-2.253506000
1	2.669645000	2.417243000	-1.479578000
1	1.009658000	4.311475000	-1.414078000
1	1.623704000	3.853019000	0.167821000
1	-0.995010000	2.563303000	-2.113637000
1	-2.347723000	2.759708000	-1.031994000
1	-1.666614000	0.347542000	-1.549590000
6	1.952087000	-0.341419000	-1.016277000
6	0.589448000	-0.905237000	-0.660375000
8	2.216891000	1.147177000	0.764215000
8	3.083576000	-0.721675000	-0.266125000
6	3.080104000	0.017803000	0.955625000
1	2.212779000	-0.352003000	-2.078688000
6	0.150284000	-2.200529000	-0.428059000
6	-0.666216000	-2.458980000	0.689118000
6	-0.991718000	-1.498477000	1.639756000
6	-1.099706000	-0.102906000	1.454129000
6	-2.121190000	0.622935000	0.553717000
1	-0.913960000	0.455303000	2.375462000
6	0.847194000	-3.346993000	-1.125378000
1	1.909101000	-3.356636000	-0.854326000
1	0.412716000	-4.302802000	-0.790612000
8	0.820906000	-3.231431000	-2.538990000
1	-0.097942000	-3.077885000	-2.789064000
6	2.570080000	-0.840855000	2.106140000
1	3.234229000	-1.697300000	2.255359000

1	2.543931000	-0.253337000	3.028581000
1	1.563841000	-1.207232000	1.894872000
6	4.492941000	0.526749000	1.198299000
1	5.182403000	-0.313224000	1.318669000
1	4.816504000	1.131501000	0.348451000
1	4.523617000	1.138833000	2.103635000
1	-0.770599000	-3.505992000	0.974984000
1	-0.998034000	-1.854380000	2.672814000
6	-0.444814000	3.313811000	-0.154698000
1	-0.914410000	4.296975000	-0.034291000
1	-0.413163000	2.874203000	0.850567000
6	-3.494016000	-0.047902000	0.325057000
6	-4.150480000	-0.446546000	1.650600000
1	-4.279642000	0.419509000	2.308496000
1	-5.145655000	-0.870998000	1.467971000
1	-3.548210000	-1.193921000	2.170455000
6	-4.421807000	0.908332000	-0.439641000
1	-4.005361000	1.156613000	-1.419403000
1	-5.395515000	0.430838000	-0.603983000
1	-4.600423000	1.836414000	0.113433000
8	-3.266186000	-1.205268000	-0.478667000
1	-4.114666000	-1.651448000	-0.585128000
1	-2.349513000	1.566170000	1.067688000

23a

C₂₁H₃₀O₄

C1

6	-1.009596000	-1.299228000	-0.251870000
6	-0.673699000	-2.681021000	-0.816197000
6	0.042532000	-0.122069000	-0.235484000
6	0.698834000	-3.215598000	-0.403233000
6	1.426488000	-0.227514000	-0.954995000
6	1.705768000	-1.363118000	-1.934071000
1	-0.747149000	-2.659091000	-1.910697000
1	-1.464760000	-3.353685000	-0.469410000
1	0.676869000	-4.311400000	-0.377514000
1	0.896017000	-2.904316000	0.629594000
1	0.910838000	-1.356302000	-2.692219000
1	2.625280000	-1.143058000	-2.491294000
1	1.603306000	0.730545000	-1.457197000
6	-1.995260000	-0.389753000	-1.040137000
6	-1.054260000	0.761174000	-0.759235000
8	-1.649104000	-1.422230000	1.012590000
8	-3.223721000	-0.432339000	-0.350742000
6	-2.986947000	-0.909782000	0.975740000
1	-2.171761000	-0.647187000	-2.089841000
6	-1.170988000	2.069321000	-0.493181000
6	-0.139602000	2.651816000	0.377357000
6	0.697748000	1.897214000	1.113576000

6	0.787719000	0.395023000	1.032671000
6	2.113333000	-0.180005000	0.434413000
1	0.504135000	-0.048903000	1.996269000
6	-2.352290000	2.911314000	-0.900494000
1	-3.147469000	2.274595000	-1.294462000
1	-2.756745000	3.435953000	-0.018406000
8	-2.036481000	3.835703000	-1.935174000
1	-1.298015000	4.374817000	-1.629518000
6	-3.108674000	0.220681000	1.989946000
1	-4.114045000	0.649777000	1.956131000
1	-2.924394000	-0.159755000	2.998860000
1	-2.379206000	1.002088000	1.770217000
6	-3.973112000	-2.038323000	1.246256000
1	-4.999224000	-1.662189000	1.209343000
1	-3.859959000	-2.818556000	0.490059000
1	-3.792635000	-2.470493000	2.234110000
1	-0.139119000	3.731100000	0.527725000
1	1.341632000	2.391265000	1.835763000
6	1.836883000	-2.771514000	-1.339332000
1	1.901112000	-3.476399000	-2.178523000
1	2.793481000	-2.860109000	-0.809123000
6	3.468730000	0.509155000	0.622388000
6	3.827264000	0.581567000	2.112463000
1	3.913047000	-0.418685000	2.549799000
1	4.791602000	1.085764000	2.251112000
1	3.072477000	1.137047000	2.674543000
6	4.563824000	-0.250809000	-0.137173000
1	4.355478000	-0.253769000	-1.209909000
1	5.537444000	0.231455000	0.016330000
1	4.653490000	-1.286213000	0.206667000
8	3.352851000	1.824345000	0.080158000
1	4.214306000	2.249482000	0.168452000
1	2.227430000	-1.198799000	0.822032000

Ile.

12a
C₂₁H₃₀O₄
C1

6	-1.661297000	-1.153253000	-0.276530000
6	-1.375184000	-2.499191000	-0.946866000
6	-0.572011000	-0.528311000	0.601671000
6	0.100015000	-2.915684000	-0.926467000
6	0.252914000	-1.145359000	1.464055000
6	0.119142000	-2.627656000	1.663192000
1	-1.748795000	-2.464254000	-1.978084000
1	-1.983484000	-3.251747000	-0.430478000
1	0.729585000	-2.076865000	-1.241708000
1	0.258753000	-3.705334000	-1.670985000
1	0.673076000	-2.956501000	2.548593000
1	-0.935660000	-2.865993000	1.848133000
1	1.050186000	-0.600815000	1.958794000

6	-1.698209000	0.187465000	-1.065965000
6	-0.723255000	0.777988000	-0.035707000
8	-2.962863000	-1.208686000	0.308996000
8	-3.037717000	0.617455000	-1.069845000
6	-3.717048000	-0.038571000	0.004869000
1	-1.331900000	0.173336000	-2.098369000
6	-0.340078000	2.062481000	0.174856000
6	0.500218000	2.548554000	1.266004000
6	1.734826000	2.197166000	1.701635000
6	2.749228000	1.293834000	1.175082000
6	2.718607000	0.542522000	0.060220000
1	3.663645000	1.280694000	1.766820000
1	1.828032000	0.520526000	-0.562429000
6	-0.972760000	3.162784000	-0.653266000
1	-1.500172000	2.734567000	-1.516208000
1	-1.730085000	3.681493000	-0.050660000
8	-0.051869000	4.169641000	-1.038493000
1	0.690611000	3.728678000	-1.467277000
6	-3.809109000	0.867919000	1.229702000
1	-4.374825000	1.772551000	0.988360000
1	-4.318485000	0.342321000	2.042363000
1	-2.813389000	1.154083000	1.572336000
6	-5.086336000	-0.463420000	-0.501645000
1	-5.676107000	0.413108000	-0.782771000
1	-4.966940000	-1.108107000	-1.374893000
1	-5.622402000	-1.012686000	0.276649000
6	3.870312000	-0.255385000	-0.500773000
6	4.961230000	-0.578663000	0.520948000
1	4.539491000	-1.119715000	1.371771000
1	5.728092000	-1.210013000	0.057889000
1	5.461911000	0.322796000	0.886788000
6	4.459515000	0.504323000	-1.701672000
1	3.683192000	0.696531000	-2.447823000
1	4.890741000	1.460891000	-1.392957000
1	5.252898000	-0.086513000	-2.177656000
8	3.274997000	-1.475173000	-0.965784000
1	3.954542000	-1.960524000	-1.449484000
1	0.066295000	3.410868000	1.776820000
1	2.079405000	2.757667000	2.569965000
6	0.603685000	-3.431803000	0.432477000
1	1.698721000	-3.429789000	0.409078000
1	0.286251000	-4.473589000	0.573493000

TS¹ (12a→18a)

C21H30O4

C1

6	-1.214714000	-1.054928000	-0.515930000
6	-0.574223000	-2.141797000	-1.350186000
6	-0.251962000	-0.257284000	0.367985000

6	-0.271913000	-3.397195000	-0.505360000
6	0.828178000	-0.686621000	1.148843000
6	1.147948000	-2.162488000	1.315100000
1	0.358727000	-1.740315000	-1.760733000
1	-1.223756000	-2.406656000	-2.193193000
1	0.570128000	-3.931321000	-0.963068000
1	-1.132895000	-4.072883000	-0.556701000
1	2.014137000	-2.408540000	0.691610000
1	1.459926000	-2.322770000	2.355100000
1	1.103851000	-0.054212000	1.981353000
6	-1.702517000	0.306458000	-1.074268000
6	-0.729780000	0.979045000	-0.100751000
8	-2.379210000	-1.572760000	0.131164000
8	-3.091247000	0.371082000	-0.840991000
6	-3.417433000	-0.595475000	0.158504000
1	-1.524027000	0.516509000	-2.135143000
6	-0.483266000	2.349827000	0.079548000
6	0.532910000	2.986037000	0.802338000
6	1.796394000	2.591664000	1.268115000
6	2.622838000	1.511340000	0.961943000
6	2.395955000	0.488593000	0.035082000
1	3.536707000	1.452006000	1.552401000
1	1.661563000	0.678303000	-0.740206000
6	-1.556107000	3.263796000	-0.512217000
1	-1.905942000	2.835862000	-1.464022000
1	-2.431782000	3.281813000	0.146630000
8	-1.171348000	4.614078000	-0.667548000
1	-0.386502000	4.625687000	-1.228800000
6	-3.513087000	0.055105000	1.537198000
1	-4.301769000	0.813229000	1.539367000
1	-3.753072000	-0.700762000	2.290722000
1	-2.567915000	0.528530000	1.807335000
6	-4.717021000	-1.270496000	-0.248819000
1	-5.528914000	-0.539100000	-0.281804000
1	-4.599298000	-1.717693000	-1.238024000
1	-4.978056000	-2.052930000	0.468538000
6	3.549852000	-0.361809000	-0.468335000
6	4.463340000	-0.896080000	0.639402000
1	3.897246000	-1.458606000	1.384490000
1	5.219929000	-1.561116000	0.207155000
1	4.999235000	-0.089070000	1.147103000
6	4.367801000	0.475072000	-1.468631000
1	5.170477000	-0.133044000	-1.906266000
1	3.725983000	0.830181000	-2.279647000
1	4.825653000	1.341186000	-0.983084000
8	2.944440000	-1.450645000	-1.176791000
1	3.654542000	-1.950088000	-1.597701000
1	0.302921000	4.031299000	1.009262000
1	2.245775000	3.310464000	1.953426000
6	0.021940000	-3.155802000	0.983883000
1	0.295252000	-4.122894000	1.425415000
1	-0.899995000	-2.838867000	1.481133000

18a
C21H30O4
C1

6	1.595824000	-1.263951000	0.142891000
6	1.714446000	-2.645522000	0.761870000
6	0.260368000	-0.511754000	0.149962000
6	0.726104000	-2.941861000	1.888516000
6	-1.134464000	-1.012252000	-0.074165000
6	-1.551863000	-1.884534000	1.135237000
1	2.747554000	-2.773836000	1.108061000
1	1.571658000	-3.378718000	-0.042247000
1	0.765405000	-2.151914000	2.651999000
1	1.055659000	-3.859567000	2.390816000
1	-1.553341000	-1.240795000	2.025288000
1	-2.592094000	-2.184322000	0.994287000
1	-1.124609000	-1.646428000	-0.973043000
6	2.186388000	-0.003783000	0.825921000
6	0.809110000	0.632729000	0.633669000
8	2.264986000	-1.293928000	-1.116094000
8	3.261905000	0.429085000	0.030348000
6	3.120771000	-0.157624000	-1.266298000
1	2.537303000	-0.105957000	1.859021000
6	0.415031000	2.017216000	0.853188000
6	-0.322075000	2.736194000	-0.026891000
6	-0.889209000	2.221907000	-1.264132000
6	-1.570605000	1.073678000	-1.420530000
6	-2.090305000	0.191578000	-0.314094000
1	-1.846887000	0.790219000	-2.436354000
1	-2.090306000	0.781677000	0.611883000
6	1.063847000	2.696894000	2.044888000
1	0.939573000	2.057586000	2.935205000
1	2.144098000	2.771237000	1.868098000
8	0.615045000	4.010405000	2.290117000
1	-0.326249000	3.956062000	2.494909000
6	2.519224000	0.837690000	-2.252676000
1	3.166945000	1.714755000	-2.340960000
1	2.424341000	0.371640000	-3.238061000
1	1.530114000	1.158062000	-1.923217000
6	4.491251000	-0.646595000	-1.708522000
1	5.181979000	0.195958000	-1.800462000
1	4.883813000	-1.349770000	-0.970922000
1	4.418690000	-1.148916000	-2.676730000
6	-3.590498000	-0.149543000	-0.577824000
6	-3.777920000	-1.239468000	-1.637560000
1	-3.336775000	-2.185540000	-1.314103000
1	-4.845828000	-1.411247000	-1.817960000
1	-3.329352000	-0.959506000	-2.596269000
6	-4.365035000	1.114484000	-0.973953000
1	-4.222165000	1.897817000	-0.224092000
1	-4.061099000	1.509983000	-1.946105000
1	-5.436736000	0.885280000	-1.030275000
8	-4.115573000	-0.600064000	0.676964000

1	-5.056813000	-0.767518000	0.545778000
1	-0.380462000	3.810001000	0.147913000
1	-0.717732000	2.836776000	-2.149149000
6	-0.722752000	-3.139715000	1.422631000
1	-1.258323000	-3.695122000	2.203263000
1	-0.725093000	-3.796494000	0.539977000

TS² (18a→24)

C₂₁H₃₀O₄

C1

6	1.274443000	-1.349497000	-0.175115000
6	1.149877000	-2.841798000	0.104431000
6	0.014037000	-0.449406000	-0.081110000
6	0.489935000	-3.247294000	1.429547000
6	-1.383150000	-1.015343000	0.128179000
6	-1.640837000	-1.752061000	1.440986000
1	2.169792000	-3.243201000	0.075993000
1	0.619072000	-3.309348000	-0.736109000
1	0.925528000	-2.666319000	2.254238000
1	0.773305000	-4.288505000	1.627420000
1	-1.264795000	-1.141555000	2.273817000
1	-2.725709000	-1.822083000	1.572775000
1	-1.567982000	-1.711312000	-0.704072000
6	1.941145000	-0.409826000	0.868610000
6	0.720608000	0.490419000	0.734243000
8	2.071425000	-1.168503000	-1.335494000
8	3.164643000	0.011953000	0.311798000
6	3.125907000	-0.230125000	-1.098217000
1	2.133893000	-0.830474000	1.860809000
6	0.611867000	1.860443000	0.916097000
6	-0.067133000	2.662927000	-0.031193000
6	-0.675523000	2.137340000	-1.159324000
6	-1.157468000	0.810996000	-1.221445000
6	-2.125607000	0.280754000	-0.167960000
1	-1.318664000	0.400082000	-2.220393000
1	-2.064161000	0.929268000	0.714490000
6	1.567975000	2.549775000	1.880046000
1	1.627645000	1.971592000	2.814624000
1	2.575981000	2.552792000	1.450553000
8	1.245446000	3.901740000	2.135744000
1	0.368049000	3.916198000	2.536339000
6	2.853111000	1.056754000	-1.866183000
1	3.646966000	1.784989000	-1.676148000
1	2.819880000	0.847947000	-2.939429000
1	1.897157000	1.488181000	-1.564382000
6	4.446741000	-0.871557000	-1.496419000
1	5.275588000	-0.184466000	-1.305598000
1	4.602311000	-1.783817000	-0.916416000
1	4.437391000	-1.123494000	-2.560136000
6	-3.616828000	0.239333000	-0.564904000
6	-3.919580000	-0.741297000	-1.700514000

1	-3.657592000	-1.764281000	-1.417710000
1	-4.990556000	-0.722734000	-1.936246000
1	-3.383580000	-0.485006000	-2.619750000
6	-4.110829000	1.642791000	-0.927162000
1	-3.914637000	2.338603000	-0.106516000
1	-3.620799000	2.025761000	-1.826865000
1	-5.191603000	1.628275000	-1.115362000
8	-4.280948000	-0.198488000	0.628327000
1	-5.224743000	-0.242242000	0.432295000
1	0.161801000	3.725692000	0.008250000
1	-0.650618000	2.738718000	-2.068366000
6	-1.037640000	-3.157225000	1.497545000
1	-1.366371000	-3.639967000	2.426807000
1	-1.463376000	-3.759534000	0.681269000

24a

C₂₁H₃₀O₄

C1

6	1.036092000	-1.237328000	-0.287912000
6	0.751200000	-2.738405000	-0.167340000
6	-0.158733000	-0.233869000	-0.113473000
6	0.286646000	-3.265698000	1.205723000
6	-1.476622000	-0.870069000	0.371860000
6	-1.596201000	-1.530404000	1.732850000
1	1.692136000	-3.242009000	-0.416718000
1	0.040111000	-3.033515000	-0.950635000
1	0.977151000	-2.905753000	1.979206000
1	0.423826000	-4.354316000	1.189554000
1	-1.005596000	-0.979557000	2.477876000
1	-2.640637000	-1.484940000	2.060577000
1	-1.706572000	-1.633736000	-0.386567000
6	1.789275000	-0.522353000	0.874657000
6	0.750602000	0.577919000	0.764456000
8	1.853075000	-0.958650000	-1.410591000
8	3.087630000	-0.244682000	0.403892000
6	3.132187000	-0.458543000	-1.012000000
1	1.864463000	-1.053524000	1.827189000
6	0.914624000	1.916104000	0.731806000
6	0.123496000	2.710980000	-0.207396000
6	-0.655349000	2.127103000	-1.138477000
6	-1.035320000	0.687366000	-1.061743000
6	-2.213981000	0.401490000	-0.069300000
1	-1.220549000	0.244591000	-2.046965000
1	-2.164370000	1.149414000	0.730896000
6	2.052340000	2.612655000	1.437867000
1	2.583642000	1.909077000	2.092293000
1	2.781493000	2.986958000	0.710090000
8	1.606319000	3.761317000	2.146336000
1	0.930713000	3.464251000	2.767422000
6	3.381993000	0.853410000	-1.741296000
1	4.326436000	1.294344000	-1.410710000
1	3.436192000	0.679051000	-2.819643000
1	2.566276000	1.550474000	-1.541076000
6	4.213033000	-1.495200000	-1.296415000

1	5.192140000	-1.115825000	-0.990897000
1	4.007989000	-2.412452000	-0.739216000
1	4.243655000	-1.728002000	-2.364226000
6	-3.671138000	0.347113000	-0.542852000
6	-3.934881000	-0.720520000	-1.607391000
1	-3.725518000	-1.720989000	-1.220468000
1	-4.988032000	-0.693975000	-1.912388000
1	-3.333953000	-0.560512000	-2.508102000
6	-4.115675000	1.722279000	-1.052223000
1	-3.939585000	2.487363000	-0.290955000
1	-3.579870000	2.008298000	-1.962734000
1	-5.186699000	1.714585000	-1.289845000
8	-4.400194000	0.020704000	0.648403000
1	-5.334150000	-0.030438000	0.410806000
1	0.306102000	3.782290000	-0.227917000
1	-1.084280000	2.728495000	-1.937237000
6	-1.157036000	-2.998152000	1.655778000
1	-1.296614000	-3.475513000	2.634149000
1	-1.839859000	-3.518901000	0.968859000

X = 4 (r,r)

t4
C18H24O4
C1

6	1.680954000	-0.308795000	-0.982677000
6	0.676061000	0.407602000	-0.020397000
8	3.006260000	-1.603434000	0.464909000
8	3.010687000	0.133978000	-1.034093000
6	3.724660000	-0.435466000	0.074665000
6	5.096297000	-0.855271000	-0.421943000
1	5.656776000	0.016638000	-0.768806000
1	5.656812000	-1.335758000	0.383979000
1	4.984521000	-1.559986000	-1.248503000
6	3.795015000	0.553160000	1.233875000
1	4.320677000	1.460739000	0.923575000
1	2.792116000	0.825357000	1.567998000
1	4.333041000	0.103967000	2.073272000
6	0.310720000	1.696394000	0.113772000
6	-2.803261000	0.234192000	0.090413000
6	-2.631475000	0.762387000	1.311708000
6	-0.517128000	2.222504000	1.203460000
6	-1.684641000	1.795110000	1.729032000
6	-3.910247000	-0.705560000	-0.323518000
6	-4.701940000	-1.288442000	0.847203000
1	-4.039461000	-1.815150000	1.539217000
1	-5.244688000	-0.515066000	1.398760000
1	-5.444312000	-2.003055000	0.473875000
6	-4.847061000	0.026829000	-1.297857000
1	-4.282398000	0.406928000	-2.153936000
1	-5.619699000	-0.655776000	-1.674446000

1	-5.348849000	0.867715000	-0.810343000
8	-3.243554000	-1.766594000	-1.027553000
1	-3.928068000	-2.351105000	-1.376800000
6	0.925932000	2.748211000	-0.784726000
1	1.638135000	3.349966000	-0.205241000
1	1.497871000	2.273896000	-1.593562000
8	-0.025609000	3.677140000	-1.277660000
1	-0.718472000	3.170574000	-1.716664000
1	-0.106811000	3.129962000	1.650322000
1	-2.023317000	2.350629000	2.603732000
1	1.297005000	-0.440923000	-1.999376000
1	-2.136291000	0.512186000	-0.723429000
6	0.492298000	-0.896835000	0.631532000
6	-0.271468000	-2.011539000	0.482024000
6	0.878524000	-2.852996000	-0.081609000
6	1.695435000	-1.546286000	-0.019483000
1	0.682162000	-3.237895000	-1.090113000
1	1.274738000	-3.668155000	0.534562000
1	-3.332386000	0.472534000	2.093641000
1	-1.343428000	-2.158134000	0.400631000

TS¹
C18H24O4
C1

6	2.101289000	-0.415636000	-1.010419000
6	1.240718000	0.750088000	-0.407252000
8	1.041866000	-2.315684000	-0.097298000
8	3.010902000	-1.136972000	-0.232445000
6	2.273567000	-2.063419000	0.577653000
6	3.060824000	-3.360319000	0.633218000
1	4.029283000	-3.196111000	1.112558000
1	2.507817000	-4.110512000	1.204111000
1	3.221965000	-3.731111000	-0.381118000
6	2.011726000	-1.476479000	1.961093000
1	2.959308000	-1.284949000	2.473011000
1	1.461210000	-0.537192000	1.882668000
1	1.423482000	-2.179306000	2.557799000
6	1.356141000	2.057103000	0.041775000
6	-2.163630000	0.357689000	0.326363000
6	-2.150036000	1.755569000	0.180190000
6	0.250298000	2.872276000	0.351223000
6	-1.153280000	2.741336000	0.296801000
6	-3.471499000	-0.421574000	0.344493000
6	-4.173493000	-0.180711000	1.692021000
1	-3.508889000	-0.447692000	2.518316000
1	-4.468905000	0.865869000	1.807341000
1	-5.078545000	-0.797674000	1.765379000
6	-4.406122000	-0.088464000	-0.820010000
1	-3.919507000	-0.317412000	-1.771054000
1	-5.319375000	-0.690662000	-0.747743000
1	-4.712013000	0.961903000	-0.824392000
8	-3.075564000	-1.792461000	0.259914000
1	-3.869201000	-2.326645000	0.384479000

6	2.750440000	2.636044000	0.227166000
1	3.086943000	2.458067000	1.255477000
1	3.454119000	2.098263000	-0.426809000
8	2.837576000	4.035442000	0.042335000
1	2.521689000	4.225896000	-0.849053000
1	0.558105000	3.889326000	0.591012000
1	-1.613301000	3.731253000	0.326483000
1	2.566232000	-0.154776000	-1.965459000
1	-1.436037000	-0.109234000	0.980545000
6	0.120856000	-0.004767000	-0.721458000
6	-1.034433000	-0.191845000	-1.469494000
6	-0.452675000	-1.562765000	-1.970582000
6	0.763343000	-1.298732000	-1.024106000
1	-1.015228000	-2.458657000	-1.695601000
1	-0.249475000	-1.565600000	-3.047351000
1	-3.113741000	2.186940000	-0.093472000
1	-1.548370000	0.535037000	-2.089212000

c4

C18H24O4

C1

6	2.089956000	0.172746000	-0.837617000
6	1.085492000	1.001115000	0.030169000
8	2.047939000	-2.058997000	-0.092063000
8	3.371267000	-0.193695000	-0.411756000
6	3.264031000	-1.427444000	0.323336000
6	4.422446000	-2.317292000	-0.084038000
1	5.371968000	-1.845717000	0.181444000
1	4.353385000	-3.281550000	0.425997000
1	4.394081000	-2.481214000	-1.163279000
6	3.228359000	-1.141495000	1.820312000
1	4.148243000	-0.634409000	2.125346000
1	2.378664000	-0.502020000	2.066471000
1	3.138559000	-2.077658000	2.378773000
6	0.535316000	2.324557000	0.076660000
6	-2.089553000	-0.713917000	0.499759000
6	-2.180551000	0.491729000	1.416286000
6	-0.679538000	2.560912000	0.662252000
6	-1.633312000	1.739885000	1.418282000
6	-3.454994000	-1.094499000	-0.137205000
6	-4.472518000	-1.508187000	0.930790000
1	-4.061755000	-2.295956000	1.569584000
1	-4.779250000	-0.667808000	1.560444000
1	-5.378590000	-1.899070000	0.452063000
6	-4.029833000	0.019794000	-1.014495000
1	-3.366321000	0.235645000	-1.855667000
1	-5.001568000	-0.282581000	-1.423260000
1	-4.179009000	0.940522000	-0.442849000
8	-3.137146000	-2.234134000	-0.942226000
1	-3.951014000	-2.516473000	-1.376512000
6	1.347065000	3.475511000	-0.483862000
1	2.173682000	3.702035000	0.200539000
1	1.815624000	3.156616000	-1.430106000
8	0.636305000	4.682925000	-0.646215000
1	-0.086792000	4.507683000	-1.260608000

1	-0.940469000	3.618744000	0.706714000
1	-2.071718000	2.357147000	2.206707000
1	2.129234000	0.558903000	-1.864115000
1	-1.810453000	-1.580619000	1.116960000
6	0.325253000	-0.110505000	0.193068000
6	-0.969493000	-0.446771000	-0.482894000
6	-0.129168000	-1.514891000	-1.285659000
6	1.190009000	-1.070295000	-0.575689000
1	-0.183682000	-1.435144000	-2.374608000
1	-0.364310000	-2.538214000	-0.982992000
1	-2.901202000	0.348684000	2.221836000
1	-1.268028000	0.397937000	-1.117542000

TS2

C18H24O4

C1

6	2.028443000	0.196763000	-0.927576000
6	0.961589000	0.994722000	-0.142510000
8	2.103420000	-2.013782000	-0.126295000
8	3.307272000	-0.072017000	-0.413119000
6	3.243164000	-1.288592000	0.349500000
6	4.484602000	-2.102942000	0.041439000
1	5.379313000	-1.559108000	0.354634000
1	4.449543000	-3.057981000	0.571846000
1	4.539285000	-2.292237000	-1.032590000
6	3.086908000	-0.973684000	1.833084000
1	3.937101000	-0.379531000	2.179778000
1	2.169214000	-0.409397000	2.009856000
1	3.044444000	-1.901394000	2.410837000
6	0.438863000	2.270438000	0.019955000
6	-1.951246000	-0.947959000	0.283874000
6	-1.568189000	0.008287000	1.422557000
6	-0.727892000	2.402704000	0.794577000
6	-1.430337000	1.407871000	1.505726000
6	-3.453309000	-1.006048000	-0.080134000
6	-4.288796000	-1.413295000	1.137226000
1	-3.923899000	-2.356980000	1.554243000
1	-4.262181000	-0.649554000	1.920661000
1	-5.337870000	-1.552537000	0.849829000
6	-3.982526000	0.300054000	-0.674712000
1	-3.476473000	0.533972000	-1.614784000
1	-5.055485000	0.211201000	-0.885407000
1	-3.845976000	1.139509000	0.012696000
8	-3.501201000	-2.043697000	-1.065057000
1	-4.412269000	-2.104596000	-1.376544000
6	1.186151000	3.512446000	-0.420523000
1	1.924282000	3.793645000	0.339817000
1	1.755005000	3.288644000	-1.337215000
8	0.360367000	4.647861000	-0.585751000
1	-0.323050000	4.413362000	-1.224958000
1	-0.979404000	3.428025000	1.062073000
1	-1.850107000	1.811340000	2.432802000

1	2.110844000	0.532615000	-1.968977000
1	-1.704922000	-1.957391000	0.640033000
6	0.219231000	-0.166797000	0.059828000
6	-0.949956000	-0.588336000	-0.797245000
6	0.002483000	-1.618450000	-1.498650000
6	1.201079000	-1.099666000	-0.656738000
1	0.080864000	-1.545887000	-2.587529000
1	-0.221480000	-2.653877000	-1.224955000
1	-1.844446000	-0.408442000	2.396610000
1	-1.312757000	0.204580000	-1.459038000

f4

C₁₈H₂₄O₄

C1

6	-0.152521000	-0.106742000	-0.072646000
6	0.806326000	-1.271171000	-0.523811000
6	-0.310296000	-1.928732000	-1.346429000
6	-1.216944000	-0.703639000	-1.031284000
6	-1.168459000	0.116014000	1.036376000
6	-1.347443000	1.617046000	1.159125000
6	-0.455448000	2.513213000	0.683608000
6	0.760544000	2.170519000	-0.087225000
6	0.837977000	0.895166000	-0.489495000
1	-0.955911000	-0.300261000	2.032303000
1	-2.197612000	1.983513000	1.727479000
1	-0.627415000	3.568498000	0.891238000
6	1.738765000	-0.155942000	-1.123143000
8	3.001079000	-0.395988000	-0.523904000
8	1.636465000	-2.066477000	0.256582000
6	2.844082000	-1.354576000	0.534940000
6	2.750350000	-0.651780000	1.885432000
1	2.601977000	-1.387878000	2.680328000
1	3.673920000	-0.101506000	2.086826000
1	1.916864000	0.053456000	1.899130000
6	4.000162000	-2.333664000	0.458783000
1	3.893730000	-3.103884000	1.226989000
1	4.011386000	-2.808018000	-0.524512000
1	4.947654000	-1.811535000	0.613811000
6	-2.181237000	-0.756634000	0.203362000
1	-1.566244000	-0.126213000	-1.894086000
1	-2.187021000	-1.774150000	0.615318000
6	-3.645307000	-0.329706000	0.026494000
6	-4.328487000	-1.228433000	-1.011950000
1	-3.830212000	-1.156591000	-1.985157000
1	-4.315691000	-2.280075000	-0.706814000
1	-5.368768000	-0.916664000	-1.142136000
6	-4.383090000	-0.406415000	1.361993000
1	-3.890501000	0.212720000	2.116492000
1	-5.406782000	-0.040865000	1.240251000
1	-4.421916000	-1.436298000	1.729162000
6	1.835486000	3.195903000	-0.314918000

1	1.441785000	4.024553000	-0.919373000
1	-0.662400000	-2.859486000	-0.889208000
1	2.117233000	3.640160000	0.657759000
8	2.953437000	2.692615000	-1.006684000
1	-0.083745000	-2.122670000	-2.400020000
1	3.242516000	1.883622000	-0.560640000
8	-3.754496000	1.034407000	-0.378407000
1	-3.208776000	1.159864000	-1.163796000
1	1.877277000	-0.099314000	-2.207305000

X = 4 (r,s)

t4

C18H24O4

C1

6	1.680954000	-0.308795000	-0.982677000
6	0.676061000	0.407602000	-0.020397000
8	3.006260000	-1.603434000	0.464909000
8	3.010687000	0.133978000	-1.034093000
6	3.724660000	-0.435466000	0.074665000
6	5.096297000	-0.855271000	-0.421943000
1	5.656776000	0.016638000	-0.768806000
1	5.656812000	-1.335758000	0.383979000
1	4.984521000	-1.559986000	-1.248503000
6	3.795015000	0.553160000	1.233875000
1	4.320677000	1.460739000	0.923575000
1	2.792116000	0.825357000	1.567998000
1	4.333041000	0.103967000	2.073272000
6	0.310720000	1.696394000	0.113772000
6	-2.803261000	0.234192000	0.090413000
6	-2.631475000	0.762387000	1.311708000
6	-0.517128000	2.222504000	1.203460000
6	-1.684641000	1.795110000	1.729032000
6	-3.910247000	-0.705560000	-0.323518000
6	-4.701940000	-1.288442000	0.847203000
1	-4.039461000	-1.815150000	1.539217000
1	-5.244688000	-0.515066000	1.398760000
1	-5.444312000	-2.003055000	0.473875000
6	-4.847061000	0.026829000	-1.297857000
1	-4.282398000	0.406928000	-2.153936000
1	-5.619699000	-0.655776000	-1.674446000
1	-5.348849000	0.867715000	-0.810343000
8	-3.243554000	-1.766594000	-1.027553000
1	-3.928068000	-2.351105000	-1.376800000
6	0.925932000	2.748211000	-0.784726000
1	1.638135000	3.349966000	-0.205241000
1	1.497871000	2.273896000	-1.593562000
8	-0.025609000	3.677140000	-1.277660000
1	-0.718472000	3.170574000	-1.716664000
1	-0.106811000	3.129962000	1.650322000

1	-2.023317000	2.350629000	2.603732000
1	1.297005000	-0.440923000	-1.999376000
1	-2.136291000	0.512186000	-0.723429000
6	0.492298000	-0.896835000	0.631532000
6	-0.271468000	-2.011539000	0.482024000
6	0.878524000	-2.852996000	-0.081609000
6	1.695435000	-1.546286000	-0.019483000
1	0.682162000	-3.237895000	-1.090113000
1	1.274738000	-3.668155000	0.534562000
1	-3.332386000	0.472534000	2.093641000
1	-1.343428000	-2.158134000	0.400631000

TS¹

C18H24O4

C1

6	-1.500441000	-0.289885000	-0.986341000
6	-0.715853000	0.669513000	-0.033137000
8	-2.272322000	-2.013350000	0.413285000
8	-2.906318000	-0.315100000	-0.994955000
6	-3.345145000	-1.126783000	0.104743000
6	-3.685036000	-0.254708000	1.310491000
1	-4.487181000	0.443151000	1.052582000
1	-4.017687000	-0.880854000	2.143245000
1	-2.811087000	0.315434000	1.631497000
6	-4.525493000	-1.955679000	-0.368406000
1	-5.354787000	-1.304037000	-0.655266000
1	-4.226209000	-2.553878000	-1.231446000
1	-4.861685000	-2.622593000	0.429645000
6	-0.424396000	2.017831000	-0.137763000
6	2.399853000	0.144630000	0.041019000
6	2.473308000	1.090884000	1.045517000
6	0.518559000	2.703100000	0.663438000
6	1.669839000	2.236049000	1.273933000
6	3.589234000	-0.712054000	-0.355970000
6	4.504723000	0.126777000	-1.265923000
1	3.943623000	0.500377000	-2.126891000
1	4.923661000	0.981173000	-0.727412000
1	5.338355000	-0.483787000	-1.637151000
6	4.386334000	-1.274307000	0.824054000
1	3.755073000	-1.900473000	1.459519000
1	5.208404000	-1.895683000	0.450532000
1	4.832626000	-0.486562000	1.437018000
8	3.043304000	-1.792937000	-1.119399000
1	3.785888000	-2.291381000	-1.480981000
6	-1.269524000	2.863489000	-1.081945000
1	-0.646970000	3.274551000	-1.884662000
1	-2.046358000	2.241634000	-1.545371000
8	-1.835609000	3.995153000	-0.437155000
1	-2.404838000	3.660757000	0.266289000
1	0.304074000	3.762448000	0.803063000
1	2.108533000	2.928876000	1.992983000

1	-1.140339000	-0.264790000	-2.020236000
6	-0.265486000	-0.449169000	0.725614000
6	0.808273000	-1.323045000	0.950325000
6	0.165687000	-2.407602000	0.071892000
6	-1.066674000	-1.452095000	-0.045612000
1	-0.067840000	-3.374166000	0.534900000
1	0.724172000	-2.569862000	-0.853632000
1	3.306485000	0.996712000	1.742158000
1	1.591300000	-1.414421000	1.687674000
1	1.703764000	0.305567000	-0.777857000

c4

C18H24O4

C1

6	-1.807756000	0.074852000	-0.882618000
6	-0.795594000	0.828512000	0.026851000
8	-2.252906000	-2.037961000	0.058088000
8	-3.179596000	-0.020872000	-0.585433000
6	-3.391866000	-1.188209000	0.231873000
6	-3.533862000	-0.779033000	1.693936000
1	-4.386471000	-0.103713000	1.810431000
1	-3.695358000	-1.662349000	2.318626000
1	-2.633371000	-0.264738000	2.034843000
6	-4.610666000	-1.919148000	-0.298714000
1	-5.495136000	-1.281531000	-0.222940000
1	-4.449368000	-2.182859000	-1.346021000
1	-4.784566000	-2.832051000	0.277013000
6	-0.298510000	2.182545000	-0.049805000
6	2.131340000	-0.234433000	0.114042000
6	2.314822000	0.715093000	1.263618000
6	0.801661000	2.650142000	0.598253000
6	1.753048000	1.930963000	1.429798000
6	3.433011000	-0.984752000	-0.265115000
6	4.524471000	0.019493000	-0.647283000
1	4.175850000	0.666611000	-1.457427000
1	4.810315000	0.651778000	0.198442000
1	5.423890000	-0.506211000	-0.990958000
6	3.935690000	-1.934819000	0.826492000
1	3.193604000	-2.705962000	1.048457000
1	4.848625000	-2.438521000	0.486932000
1	4.186288000	-1.411691000	1.754255000
8	3.072315000	-1.749655000	-1.419914000
1	3.863572000	-2.215927000	-1.715015000
6	-1.156801000	3.135628000	-0.867589000
1	-0.993913000	2.945766000	-1.936345000
1	-2.217293000	2.910759000	-0.673818000
8	-0.874516000	4.505114000	-0.678466000
1	-1.112874000	4.721447000	0.230841000
1	0.962713000	3.726065000	0.534999000
1	2.099594000	2.498013000	2.296030000
1	-1.676371000	0.308352000	-1.947300000

1	1.854299000	0.351578000	-0.773031000
6	-0.333292000	-0.349657000	0.544584000
6	0.927034000	-1.148705000	0.409126000
6	0.151037000	-1.894609000	-0.758220000
6	-1.188406000	-1.223139000	-0.334253000
1	0.132299000	-2.984385000	-0.674977000
1	0.511385000	-1.607711000	-1.747645000
1	2.996029000	0.389935000	2.049448000
1	1.131730000	-1.830006000	1.241102000

TS²

C18H24O4

C1

6	-1.749690000	-0.035160000	-0.990629000
6	-0.620535000	0.739918000	-0.319516000
8	-2.204541000	-2.100281000	0.010971000
8	-3.048141000	0.005952000	-0.423014000
6	-3.266371000	-1.189389000	0.345216000
6	-3.216984000	-0.859261000	1.831509000
1	-3.976324000	-0.109522000	2.070367000
1	-3.407663000	-1.756557000	2.427028000
1	-2.235530000	-0.459906000	2.095761000
6	-4.577147000	-1.816897000	-0.088385000
1	-5.404824000	-1.132282000	0.113525000
1	-4.545212000	-2.029692000	-1.159081000
1	-4.751204000	-2.748968000	0.455785000
6	-0.292173000	2.079487000	-0.289679000
6	2.113108000	-0.250655000	-0.080458000
6	1.566231000	0.344499000	1.234061000
6	0.654280000	2.562981000	0.655181000
6	1.385815000	1.737437000	1.476421000
6	3.588698000	-0.684544000	-0.125457000
6	4.505445000	0.537508000	-0.018879000
1	4.274830000	1.254655000	-0.811804000
1	4.391397000	1.043064000	0.944808000
1	5.556893000	0.240647000	-0.118977000
6	3.958264000	-1.724678000	0.935062000
1	3.347049000	-2.625340000	0.832213000
1	5.007917000	-2.019268000	0.816764000
1	3.845757000	-1.337030000	1.952341000
8	3.710501000	-1.270542000	-1.426054000
1	4.631291000	-1.536878000	-1.536530000
6	-1.102167000	3.085393000	-1.080314000
1	-0.484150000	3.514782000	-1.877882000
1	-1.950501000	2.581701000	-1.564932000
8	-1.533873000	4.196225000	-0.310072000
1	-2.089584000	3.845926000	0.396500000
1	0.623928000	3.630637000	0.861889000
1	1.729653000	2.142051000	2.429099000

1	-1.816472000	0.072790000	-2.081731000
1	1.968968000	0.474761000	-0.888548000
6	-0.079688000	-0.402264000	0.361497000
6	1.002330000	-1.302742000	-0.137878000
6	0.056081000	-1.957177000	-1.182933000
6	-1.157871000	-1.329459000	-0.441376000
1	0.067250000	-3.049563000	-1.216738000
1	0.154062000	-1.562229000	-2.199045000
1	1.866031000	-0.239031000	2.107639000
1	1.199118000	-2.055553000	0.636252000

f4 (dissociation upon optimization)

C18H24O4

C1

6	-1.694997000	-0.057494000	-0.481348000
6	-0.650959000	0.887588000	0.014571000
8	-2.153726000	-2.302564000	-0.200886000
8	-2.858437000	-0.192737000	0.361570000
6	-3.333568000	-1.505212000	0.206860000
6	-3.808219000	-2.027852000	1.544910000
1	-4.653019000	-1.426593000	1.890375000
1	-4.127075000	-3.069687000	1.462020000
1	-3.000082000	-1.949406000	2.274753000
6	-4.358722000	-1.628512000	-0.910578000
1	-5.251098000	-1.054466000	-0.648757000
1	-3.956971000	-1.236616000	-1.848392000
1	-4.640768000	-2.673614000	-1.061750000
6	-0.681431000	2.278890000	-0.192202000
6	2.372712000	-0.216679000	-0.232705000
6	1.802947000	0.974358000	0.672770000
6	0.562992000	2.989998000	-0.046263000
6	1.753070000	2.413331000	0.278773000
6	3.774396000	-0.805209000	-0.041223000
6	4.831236000	0.218424000	-0.466078000
1	4.663346000	0.531805000	-1.500430000
1	4.808817000	1.106508000	0.173331000
1	5.837546000	-0.213618000	-0.397670000
6	4.047443000	-1.290835000	1.384591000
1	3.337486000	-2.067722000	1.680251000
1	5.055077000	-1.720067000	1.446149000
1	3.997183000	-0.475496000	2.112633000
8	3.791153000	-1.924533000	-0.937182000
1	4.665798000	-2.328606000	-0.878049000
6	-1.906648000	3.030792000	-0.614909000
1	-1.773576000	3.509620000	-1.594248000
1	-2.761248000	2.341981000	-0.706686000
8	-2.221237000	4.113809000	0.263419000
1	-2.180440000	3.750297000	1.156653000
1	0.538036000	4.057253000	-0.260160000
1	2.660171000	3.013005000	0.302532000
1	-2.029283000	0.269406000	-1.492117000
1	2.276027000	0.083681000	-1.282523000
6	0.483914000	0.282827000	0.511714000

6	1.092789000	-1.020342000	0.171612000
6	0.186702000	-1.854589000	-0.803900000
6	-1.179387000	-1.448424000	-0.483268000
1	0.315702000	-2.934890000	-0.698219000
1	0.469347000	-1.579527000	-1.829465000
1	2.229902000	0.849154000	1.684479000
1	1.291479000	-1.660561000	1.039967000

X = 5 (r,r)

t5

C₁₉H₂₆O₄

C1

6	1.626910000	-0.043329000	-1.044618000
6	0.693272000	0.619912000	0.003549000
8	2.815229000	-1.501713000	0.341748000
8	2.987936000	0.301276000	-1.064637000
6	3.635716000	-0.386248000	0.013126000
6	4.969963000	-0.901559000	-0.501933000
1	5.611067000	-0.067319000	-0.798891000
1	5.478167000	-1.475376000	0.277323000
1	4.801174000	-1.546481000	-1.366912000
6	3.795333000	0.530573000	1.222963000
1	4.410329000	1.396915000	0.962274000
1	2.821908000	0.880619000	1.570963000
1	4.280901000	-0.012652000	2.038597000
6	0.312364000	1.910722000	0.173594000
6	-2.668931000	0.268235000	0.059796000
6	-2.711334000	0.992534000	1.193050000
6	-0.561312000	2.413832000	1.226023000
6	-1.770980000	1.994526000	1.674453000
6	-3.748515000	-0.655361000	-0.449429000
6	-4.760862000	-1.078882000	0.615799000
1	-4.256724000	-1.569345000	1.452559000
1	-5.334348000	-0.228990000	0.997717000
1	-5.478047000	-1.786895000	0.185088000
6	-4.461476000	0.021346000	-1.632836000
1	-3.738649000	0.284865000	-2.410135000
1	-5.204089000	-0.657340000	-2.071868000
1	-4.981224000	0.930385000	-1.316686000
8	-3.041446000	-1.809984000	-0.926740000
1	-3.689868000	-2.378910000	-1.360021000
6	0.957556000	2.983921000	-0.678841000
1	1.716139000	3.509666000	-0.084051000
1	1.487173000	2.528034000	-1.526808000
8	0.050324000	3.989789000	-1.095523000
1	-0.691687000	3.547236000	-1.523387000
1	-0.191225000	3.330419000	1.688851000
1	-2.158955000	2.565220000	2.517785000
1	1.242258000	-0.034349000	-2.069446000
1	-1.825248000	0.362198000	-0.618463000

6	0.462757000	-0.680290000	0.622041000
6	-0.397496000	-1.558898000	1.167975000
6	-0.020883000	-2.960780000	0.722851000
6	0.895373000	-2.727132000	-0.515489000
6	1.513739000	-1.362621000	-0.219259000
1	0.503653000	-3.515834000	1.514161000
1	-0.918608000	-3.534291000	0.469786000
1	0.266483000	-2.670694000	-1.410335000
1	1.650231000	-3.503666000	-0.663170000
1	-3.582579000	0.872342000	1.835665000
1	-1.281736000	-1.343707000	1.753724000

TS¹

C₁₉H₂₆O₄

C1

6	-2.186349000	-0.539679000	0.866989000
6	-1.261106000	0.675869000	0.597122000
8	-0.858021000	-2.155908000	-0.167705000
8	-2.912855000	-1.120507000	-0.182661000
6	-2.004136000	-1.890663000	-0.976140000
6	-2.680135000	-3.212072000	-1.306938000
1	-3.582920000	-3.039856000	-1.899200000
1	-2.000823000	-3.850350000	-1.877956000
1	-2.953854000	-3.721816000	-0.380655000
6	-1.597183000	-1.120126000	-2.228577000
1	-2.472514000	-0.933938000	-2.857702000
1	-1.149837000	-0.161195000	-1.960467000
1	-0.868428000	-1.699781000	-2.802212000
6	-1.462855000	1.970988000	0.131639000
6	2.003379000	0.628068000	-0.358950000
6	1.981587000	2.005249000	-0.120604000
6	-0.466063000	2.928938000	-0.119539000
6	0.937786000	2.941869000	-0.105071000
6	3.320822000	-0.094910000	-0.601653000
6	3.880451000	0.338881000	-1.968046000
1	3.143765000	0.152491000	-2.754183000
1	4.136176000	1.402025000	-1.976348000
1	4.788926000	-0.230278000	-2.205291000
6	4.359147000	0.130363000	0.500634000
1	3.978439000	-0.223788000	1.461411000
1	5.276450000	-0.423497000	0.268463000
1	4.635823000	1.183997000	0.601078000
8	2.977651000	-1.481434000	-0.662710000
1	3.776732000	-1.963196000	-0.907583000
6	-2.907371000	2.384677000	-0.133695000
1	-3.160600000	2.180168000	-1.180484000
1	-3.582673000	1.765130000	0.474271000
8	-3.167750000	3.762760000	0.053825000
1	-2.959128000	3.969655000	0.972697000
1	-0.892579000	3.912209000	-0.315909000
1	1.321400000	3.963523000	-0.089620000
1	-2.841167000	-0.438640000	1.738050000

1	1.190772000	0.173611000	-0.912796000
6	-0.155070000	-0.065082000	1.014936000
6	1.105747000	-0.113634000	1.575800000
6	1.275090000	-1.545668000	2.102637000
6	-0.180717000	-2.122241000	2.172770000
6	-0.869109000	-1.380718000	1.026825000
1	1.885399000	-2.131118000	1.407145000
1	1.774874000	-1.560417000	3.077432000
1	-0.633832000	-1.845667000	3.131734000
1	-0.224304000	-3.209605000	2.067722000
1	2.951449000	2.452754000	0.101333000
1	1.586777000	0.717630000	2.072235000

c5

C19H26O4

C1

6	2.295858000	0.097078000	-0.872049000
6	1.098660000	0.908226000	-0.334237000
8	1.957492000	-2.057077000	0.018394000
8	3.368183000	-0.238723000	-0.030331000
6	2.996785000	-1.393099000	0.739313000
6	4.198148000	-2.320827000	0.793288000
1	5.031466000	-1.830683000	1.303432000
1	3.944113000	-3.236355000	1.333833000
1	4.503719000	-2.579135000	-0.222756000
6	2.518176000	-0.981588000	2.129274000
1	3.315210000	-0.447133000	2.654356000
1	1.644265000	-0.332169000	2.063617000
1	2.251512000	-1.870751000	2.708240000
6	0.743595000	2.282765000	-0.116183000
6	-2.051718000	-0.525620000	0.495901000
6	-1.842609000	0.613853000	1.470481000
6	-0.347631000	2.620871000	0.621006000
6	-1.229841000	1.823491000	1.470138000
6	-3.566547000	-0.662192000	0.136803000
6	-4.426939000	-0.867592000	1.389829000
1	-4.033867000	-1.685968000	2.001073000
1	-4.496993000	0.033256000	2.005447000
1	-5.448261000	-1.132749000	1.090928000
6	-4.087510000	0.533258000	-0.664585000
1	-3.591402000	0.601257000	-1.636136000
1	-5.163960000	0.427826000	-0.846718000
1	-3.929435000	1.471140000	-0.124401000
8	-3.638376000	-1.850195000	-0.655642000
1	-4.559238000	-1.962619000	-0.920150000
6	1.649725000	3.351357000	-0.694669000
1	2.597080000	3.354448000	-0.141295000
1	1.905095000	3.085006000	-1.734007000
8	1.145439000	4.665687000	-0.614894000

1	0.345939000	4.698942000	-1.153734000
1	-0.482607000	3.693403000	0.761147000
1	-1.462624000	2.392118000	2.374262000
1	2.687806000	0.429879000	-1.839948000
1	-1.816530000	-1.446675000	1.050540000
6	0.290115000	-0.174112000	-0.357852000
6	-1.116039000	-0.502414000	-0.718886000
6	-0.887062000	-1.836634000	-1.499978000
6	0.586434000	-1.811258000	-2.002085000
6	1.333790000	-1.134786000	-0.852602000
1	-1.018016000	-2.677251000	-0.809911000
1	-1.609988000	-1.974661000	-2.305422000
1	0.670098000	-1.201375000	-2.909985000
1	0.975174000	-2.808643000	-2.225744000
1	-2.392096000	0.435370000	2.394521000
1	-1.460703000	0.281316000	-1.408832000

TS²

C19H26O4

C1

6	2.070047000	0.124314000	-1.050668000
6	0.810874000	0.825779000	-0.546476000
8	2.237975000	-1.829134000	0.240539000
8	3.253058000	0.165497000	-0.288819000
6	3.178552000	-0.859353000	0.711336000
6	4.539052000	-1.528071000	0.798373000
1	5.295598000	-0.805076000	1.114078000
1	4.511336000	-2.346685000	1.522183000
1	4.812414000	-1.926052000	-0.181066000
6	2.728247000	-0.272612000	2.045800000
1	3.445024000	0.482923000	2.380277000
1	1.744528000	0.190888000	1.953500000
1	2.672705000	-1.062464000	2.800605000
6	0.383234000	2.116552000	-0.300895000
6	-2.025380000	-0.917127000	0.396840000
6	-1.229097000	-0.065702000	1.398361000
6	-0.606851000	2.320150000	0.681971000
6	-1.125821000	1.339012000	1.526781000
6	-3.520427000	-0.580644000	0.206930000
6	-4.256033000	-0.647929000	1.549076000
1	-4.112117000	-1.627377000	2.015452000
1	-3.905034000	0.124998000	2.239672000
1	-5.332364000	-0.497315000	1.402811000
6	-3.782437000	0.764004000	-0.472624000
1	-3.333978000	0.795383000	-1.468878000
1	-4.862995000	0.917696000	-0.586201000
1	-3.386432000	1.596762000	0.113332000
8	-3.973711000	-1.642171000	-0.642822000
1	-4.900148000	-1.469843000	-0.849708000
6	1.160686000	3.316539000	-0.809766000
1	2.008190000	3.521068000	-0.145324000
1	1.586524000	3.085948000	-1.798304000
8	0.402236000	4.509797000	-0.838861000
1	-0.358185000	4.351475000	-1.410900000

1	-0.746306000	3.356075000	0.986484000
1	-1.323547000	1.712855000	2.535654000
1	2.314820000	0.293637000	-2.105514000
1	-2.032728000	-1.930684000	0.816724000
6	0.159610000	-0.389094000	-0.257482000
6	-1.128159000	-0.950247000	-0.832393000
6	-0.691154000	-2.329256000	-1.376661000
6	0.806368000	-2.189769000	-1.736881000
6	1.376486000	-1.224426000	-0.692164000
1	-0.797312000	-3.077576000	-0.581897000
1	-1.304314000	-2.663395000	-2.217890000
1	0.919816000	-1.759174000	-2.739158000
1	1.337785000	-3.145310000	-1.724802000
1	-1.201193000	-0.546260000	2.381015000
1	-1.495333000	-0.317127000	-1.649190000

f5

C19H26O4

C1

6	1.883240000	-0.289433000	-1.131262000
6	0.960565000	0.796678000	-0.586929000
8	1.693061000	-1.876081000	0.580632000
8	3.140905000	-0.480369000	-0.530773000
6	2.960141000	-1.219174000	0.680835000
6	4.048160000	-2.278201000	0.747478000
1	5.033647000	-1.806811000	0.787596000
1	3.918154000	-2.896937000	1.639120000
1	3.993618000	-2.914031000	-0.138675000
6	2.973714000	-0.294484000	1.893909000
1	3.931155000	0.230673000	1.954791000
1	2.172437000	0.443353000	1.825815000
1	2.835793000	-0.878499000	2.808321000
6	0.947570000	2.070037000	-0.166762000
6	-2.122470000	-0.662499000	0.238563000
6	-0.984184000	0.078095000	1.021530000
6	-0.201145000	2.454979000	0.678523000
6	-1.059148000	1.571966000	1.231278000
6	-3.607284000	-0.289778000	0.308970000
6	-4.094668000	-0.355785000	1.760491000
1	-3.875299000	-1.337435000	2.190710000
1	-3.624598000	0.410806000	2.384490000
1	-5.179139000	-0.199335000	1.807298000
6	-3.952022000	1.062484000	-0.318384000
1	-3.724331000	1.059052000	-1.387367000
1	-5.024646000	1.264546000	-0.205016000
1	-3.406839000	1.886958000	0.147728000
8	-4.239924000	-1.330555000	-0.451084000
1	-5.179502000	-1.116926000	-0.504107000
6	2.035208000	3.078815000	-0.415075000
1	2.512271000	3.365277000	0.529815000
1	2.815424000	2.637076000	-1.051284000

8	1.529805000	4.291827000	-0.957043000
1	1.069602000	4.064218000	-1.773578000
1	-0.297988000	3.512316000	0.914559000
1	-1.800604000	1.946822000	1.935594000
1	2.005321000	-0.322942000	-2.219401000
1	-2.078965000	-1.717706000	0.538403000
6	-0.080526000	-0.184437000	-0.194111000
6	-1.314218000	-0.491648000	-1.077909000
6	-0.987298000	-1.710661000	-1.951528000
6	0.192244000	-2.422453000	-1.263155000
6	0.927469000	-1.343585000	-0.471907000
1	-1.856220000	-2.363399000	-2.079908000
1	-0.689261000	-1.373530000	-2.951886000
1	0.848242000	-2.948328000	-1.964698000
1	-0.161340000	-3.165424000	-0.538323000
1	-0.720707000	-0.409462000	1.971507000
1	-1.659082000	0.365600000	-1.662681000

X = 8 (r,r)

t8
C22H32O4
C1

6	1.851062000	0.779789000	-0.372951000
6	1.695425000	2.076566000	-1.162149000
6	0.886289000	0.443649000	0.769290000
6	0.299748000	2.727965000	-1.214017000
6	0.381874000	1.190960000	1.758329000
6	0.080562000	3.887224000	-0.224461000
6	0.716667000	2.636408000	1.978504000
1	2.049241000	1.865603000	-2.179293000
1	2.417036000	2.790795000	-0.747171000
1	-0.494272000	1.978667000	-1.111246000
1	0.174844000	3.148869000	-2.218953000
1	-0.730847000	4.517190000	-0.612669000
1	0.977805000	4.523173000	-0.240898000
1	0.669139000	2.852648000	3.052527000
1	1.744397000	2.847841000	1.662366000
1	-0.375296000	0.754081000	2.407066000
6	1.486260000	-0.594627000	-1.006403000
6	0.648143000	-0.905324000	0.236368000
8	3.237761000	0.628993000	-0.063866000
8	2.700732000	-1.277862000	-1.209615000
6	3.685936000	-0.692610000	-0.356067000
1	0.926577000	-0.583903000	-1.947175000
6	0.005962000	-2.026340000	0.613205000
6	-0.763156000	-2.166665000	1.867448000
6	-1.952759000	-1.613717000	2.178385000
6	-2.792505000	-0.727244000	1.366826000
6	-2.910705000	-0.760237000	0.032819000

1	-3.393578000	-0.019091000	1.936832000
1	-2.353385000	-1.500560000	-0.539139000
6	0.088148000	-3.286280000	-0.217651000
1	0.675153000	-3.114645000	-1.121842000
1	0.605368000	-4.071397000	0.361917000
8	-1.191008000	-3.743246000	-0.639571000
1	-1.735061000	-3.822878000	0.154839000
6	3.845585000	-1.497641000	0.931983000
1	4.167345000	-2.517417000	0.701435000
1	4.597701000	-1.028403000	1.572651000
1	2.902047000	-1.541191000	1.478264000
6	4.985004000	-0.599440000	-1.140360000
1	5.336351000	-1.598416000	-1.412163000
1	4.818772000	-0.019937000	-2.050764000
1	5.754504000	-0.107774000	-0.539599000
6	-3.788918000	0.125679000	-0.816694000
6	-4.428200000	1.285730000	-0.054769000
1	-3.660083000	1.907968000	0.411225000
1	-5.003438000	1.912340000	-0.745832000
1	-5.118937000	0.935155000	0.718502000
6	-4.863827000	-0.740142000	-1.492040000
1	-4.396249000	-1.545823000	-2.064764000
1	-5.539565000	-1.183081000	-0.754187000
1	-5.467650000	-0.134426000	-2.179810000
8	-2.896735000	0.637730000	-1.817815000
1	-3.432187000	1.129136000	-2.453094000
1	-0.330444000	-2.850260000	2.602914000
1	-2.342796000	-1.827970000	3.174316000
6	-0.265625000	3.569817000	1.235780000
1	-0.322904000	4.524936000	1.773978000
1	-1.271415000	3.132739000	1.288455000

TS¹
C22H32O4
C1

6	2.323938000	-0.061312000	-0.383467000
6	1.180495000	0.913620000	-0.650409000
8	1.209497000	-1.683869000	0.865452000
8	2.907368000	-0.137970000	0.897681000
6	2.058605000	-0.926043000	1.731590000
6	2.932053000	-1.892594000	2.516554000
1	3.626886000	-1.342052000	3.156491000
1	2.311756000	-2.537549000	3.144748000
1	3.503049000	-2.513422000	1.822927000
6	1.223219000	-0.035116000	2.645828000
1	1.869314000	0.482316000	3.360943000
1	0.687784000	0.714369000	2.061113000
1	0.496724000	-0.639422000	3.195634000
6	1.209455000	2.316160000	-0.648700000

6	-1.955583000	1.083935000	0.253930000
6	-2.168847000	2.278515000	-0.443168000
6	0.177969000	3.245182000	-0.843596000
6	-1.224071000	3.206168000	-0.877523000
6	-3.108384000	0.417555000	0.990887000
6	-3.293994000	1.149079000	2.333925000
1	-2.366519000	1.120163000	2.912163000
1	-3.578587000	2.194272000	2.183948000
1	-4.082328000	0.664014000	2.924653000
6	-4.434950000	0.406364000	0.223411000
1	-4.325579000	-0.047828000	-0.763632000
1	-5.174928000	-0.176310000	0.784047000
1	-4.847654000	1.411286000	0.098352000
8	-2.684811000	-0.920045000	1.251350000
1	-3.348814000	-1.326739000	1.820873000
6	2.598576000	2.926833000	-0.417696000
1	2.740701000	3.109474000	0.653397000
1	3.376836000	2.211263000	-0.714099000
8	2.805460000	4.179051000	-1.043903000
1	2.727343000	4.038625000	-1.995180000
1	0.573318000	4.247521000	-1.007761000
1	-1.663560000	4.120317000	-1.277523000
1	3.129391000	-0.065513000	-1.126758000
1	-1.024793000	0.990622000	0.799603000
6	0.272747000	-0.134523000	-0.886056000
6	-1.038265000	-0.142079000	-1.375852000
6	-1.801714000	-1.387054000	-1.754155000
6	-1.556480000	-2.698008000	-0.985345000
6	1.620853000	-2.369548000	-1.415908000
6	1.292086000	-1.212254000	-0.475388000
1	-2.865986000	-1.138824000	-1.707495000
1	-1.611721000	-1.556234000	-2.827245000
1	-1.220191000	-2.470810000	0.030065000
1	-2.531332000	-3.183702000	-0.867350000
1	1.506775000	-2.022488000	-2.451758000
1	2.688480000	-2.585185000	-1.275617000
1	-3.196502000	2.516599000	-0.715007000
1	-1.276715000	0.703939000	-2.009242000
6	-0.605425000	-3.702464000	-1.660167000
1	-0.646019000	-3.573556000	-2.751967000
1	-0.979058000	-4.717391000	-1.473422000
6	0.850099000	-3.672073000	-1.195984000
1	1.391129000	-4.472254000	-1.717680000
1	0.896408000	-3.914879000	-0.128131000

c8

C22H32O4

C1

6	-1.643535000	-0.453867000	-0.701692000
---	--------------	--------------	--------------

6	-1.963114000	-1.520768000	-1.752339000
6	-0.211698000	-0.304339000	-0.138862000
6	0.738535000	-1.385566000	0.279831000
6	0.140615000	-2.412713000	1.279200000
1	-1.642946000	-1.136710000	-2.729692000
1	-3.055682000	-1.599221000	-1.792926000
1	0.846034000	-3.254191000	1.307426000
1	0.164303000	-1.958136000	2.279495000
1	0.954173000	-1.952408000	-0.635078000
6	-1.524372000	1.036550000	-1.106299000
6	-0.173377000	1.033255000	-0.403360000
8	-2.694461000	-0.418220000	0.271059000
8	-2.597237000	1.727706000	-0.513700000
6	-3.086518000	0.927004000	0.561848000
1	-1.516741000	1.266311000	-2.177299000
6	0.670101000	2.192446000	-0.185675000
6	1.549816000	2.360062000	0.827747000
6	1.917115000	1.436682000	1.884776000
6	2.123294000	0.104715000	1.899673000
6	2.131980000	-0.959550000	0.821875000
1	2.397250000	-0.282949000	2.880224000
6	0.382328000	3.352902000	-1.125231000
1	0.385444000	2.982785000	-2.164392000
1	-0.633487000	3.719349000	-0.934726000
8	1.237190000	4.463881000	-0.979909000
1	2.124757000	4.179697000	-1.228876000
6	-2.511331000	1.385176000	1.899972000
1	-2.805698000	2.420315000	2.095938000
1	-2.898854000	0.754071000	2.705202000
1	-1.422602000	1.322836000	1.901164000
6	-4.605022000	0.990191000	0.541360000
1	-4.942605000	2.013597000	0.725761000
1	-4.970942000	0.665241000	-0.434803000
1	-5.021095000	0.338868000	1.314322000
1	1.965808000	3.362694000	0.924186000
1	2.097675000	1.936737000	2.838335000
6	-1.274541000	-2.952651000	1.050953000
1	-1.464875000	-3.675440000	1.856060000
1	-1.998215000	-2.150389000	1.200299000
6	3.242561000	-0.853423000	-0.271741000
6	2.968890000	0.106849000	-1.426876000
1	2.951553000	1.144440000	-1.090024000
1	3.764992000	0.010500000	-2.176923000
1	2.015703000	-0.117155000	-1.911622000
6	4.593978000	-0.533663000	0.374324000
1	4.824214000	-1.262560000	1.157300000
1	5.391129000	-0.582775000	-0.377150000
1	4.604485000	0.466982000	0.813891000
8	3.285496000	-2.193709000	-0.791043000
1	3.908809000	-2.195463000	-1.527089000
1	2.475904000	-1.859580000	1.345357000
6	-1.339674000	-2.915842000	-1.588954000
1	-1.735236000	-3.538336000	-2.402549000
1	-0.264769000	-2.852757000	-1.786204000
6	-1.578885000	-3.670516000	-0.272290000
1	-0.996967000	-4.601449000	-0.321854000
1	-2.632313000	-3.979778000	-0.234437000

TS²
C22H32O4
C1

6	-2.134844000	0.360592000	-0.910337000
6	-1.092737000	-0.735221000	-0.888797000
8	-1.666374000	1.334398000	1.157799000
8	-3.272724000	0.236972000	-0.079152000
6	-2.889351000	0.599534000	1.256115000
6	-3.963726000	1.518909000	1.815522000
1	-4.920316000	0.993108000	1.878438000
1	-3.683514000	1.858834000	2.815990000
1	-4.078545000	2.387833000	1.164183000
6	-2.688783000	-0.645869000	2.110642000
1	-3.628749000	-1.199593000	2.196028000
1	-1.930578000	-1.294918000	1.669007000
1	-2.362306000	-0.359074000	3.114345000
6	-1.106180000	-2.115046000	-1.002618000
6	2.013205000	-0.284643000	0.528469000
6	0.876991000	-1.036848000	1.224634000
6	-0.272843000	-2.863878000	-0.143703000
6	0.415501000	-2.346320000	0.954552000
6	3.406198000	-0.957471000	0.575389000
6	3.766185000	-1.337663000	2.015337000
1	3.696080000	-0.464064000	2.670861000
1	3.111822000	-2.122624000	2.405559000
1	4.795750000	-1.712980000	2.059866000
6	3.532821000	-2.170873000	-0.345934000
1	3.395886000	-1.882644000	-1.391568000
1	4.531944000	-2.613736000	-0.247723000
1	2.800307000	-2.944067000	-0.099881000
8	4.299472000	0.072346000	0.129994000
1	5.187080000	-0.305369000	0.110204000
6	-2.208774000	-2.830127000	-1.761036000
1	-1.834691000	-3.129053000	-2.749418000
1	-2.471380000	-3.762428000	-1.233702000
8	-3.344823000	-2.033772000	-2.006186000
1	-3.619122000	-1.629581000	-1.169860000
1	-0.452504000	-3.939036000	-0.126953000
1	0.408483000	-3.020312000	1.816282000
1	-2.454347000	0.707210000	-1.896312000
1	2.130829000	0.650206000	1.089881000
6	-0.088569000	0.096356000	-0.348893000
6	1.371903000	0.053878000	-0.805353000
6	1.975061000	1.196153000	-1.649996000
6	2.479620000	2.477116000	-0.958764000
6	-0.842024000	2.643182000	-0.677823000
6	-1.114730000	1.250119000	-0.151652000
1	2.847257000	0.749421000	-2.139260000
1	1.279308000	1.446616000	-2.462265000
1	2.926963000	2.215055000	0.005701000
1	3.321888000	2.846412000	-1.557404000
1	-0.600685000	2.571861000	-1.745245000

1	-1.793191000	3.184130000	-0.615092000
1	0.839058000	-0.811096000	2.294592000
1	1.411426000	-0.840210000	-1.442264000
6	1.521652000	3.658504000	-0.779145000
1	1.216072000	4.034702000	-1.766863000
1	2.099275000	4.472010000	-0.320556000
6	0.263604000	3.423078000	0.059596000
1	-0.135393000	4.398620000	0.359167000
1	0.520409000	2.914449000	0.997406000

f8

C22H32O4

C1

6	-1.062833000	1.134044000	-0.478572000
6	-0.863262000	2.650782000	-0.481555000
6	0.083890000	0.155227000	0.001619000
6	1.498413000	0.622835000	0.528058000
6	1.932854000	2.055952000	0.827581000
1	-1.667409000	3.058893000	-1.104056000
1	0.063193000	2.886064000	-1.012616000
1	3.022253000	2.015709000	0.948031000
1	1.779152000	2.675654000	-0.061495000
1	1.729815000	-0.013546000	1.393026000
6	-2.039710000	0.505460000	0.564148000
6	-0.955779000	-0.510661000	0.865191000
8	-1.613328000	0.724420000	-1.722398000
8	-3.167016000	0.062325000	-0.157633000
6	-2.850774000	0.025512000	-1.549598000
1	-2.393825000	1.139994000	1.380249000
6	-0.961976000	-1.814162000	1.185337000
6	0.120920000	-2.640578000	0.640648000
6	0.866428000	-2.216894000	-0.398698000
6	0.831152000	-0.823927000	-0.967981000
6	2.115791000	0.027829000	-0.755879000
1	0.485852000	-0.851867000	-2.009570000
6	-2.109428000	-2.509699000	1.869220000
1	-2.866384000	-1.775603000	2.177796000
1	-2.597769000	-3.206362000	1.177858000
8	-1.670843000	-3.309981000	2.959117000
1	-1.209009000	-2.723663000	3.570103000
6	-2.696384000	-1.412219000	-2.031570000
1	-3.633729000	-1.957596000	-1.889279000
1	-2.443867000	-1.425175000	-3.095821000
1	-1.905197000	-1.919983000	-1.476886000
6	-3.948451000	0.768736000	-2.298895000
1	-4.910417000	0.268346000	-2.158184000
1	-4.024803000	1.790653000	-1.920601000
1	-3.722228000	0.801337000	-3.367964000
1	0.203019000	-3.665199000	0.994737000
1	1.518779000	-2.934184000	-0.893811000
6	1.320646000	2.738965000	2.047864000

1	1.689862000	2.253177000	2.961728000
1	1.687906000	3.773648000	2.087354000
6	3.547357000	-0.528101000	-0.795824000
6	3.925203000	-1.392940000	0.408260000
1	3.279888000	-2.268252000	0.510744000
1	4.957797000	-1.749455000	0.303583000
1	3.863081000	-0.810786000	1.331467000
6	3.789406000	-1.276761000	-2.111484000
1	3.544918000	-0.634515000	-2.962717000
1	4.844327000	-1.564823000	-2.196369000
1	3.193436000	-2.191158000	-2.183530000
8	4.363825000	0.655145000	-0.785137000
1	5.283978000	0.365800000	-0.752810000
1	2.098076000	0.813939000	-1.522638000
6	-0.928220000	3.359933000	0.886911000
1	-0.569715000	4.389203000	0.751095000
1	-1.987446000	3.457958000	1.158169000
6	-0.205450000	2.738905000	2.091252000
1	-0.547716000	1.708822000	2.248282000
1	-0.525698000	3.288282000	2.986361000

X = 8 (r,s)

t8

C₂₂H₃₂O₄

C1

6	1.851062000	0.779789000	-0.372951000
6	1.695425000	2.076566000	-1.162149000
6	0.886289000	0.443649000	0.769290000
6	0.299748000	2.727965000	-1.214017000
6	0.381874000	1.190960000	1.758329000
6	0.080562000	3.887224000	-0.224461000
6	0.716667000	2.636408000	1.978504000
1	2.049241000	1.865603000	-2.179293000
1	2.417036000	2.790795000	-0.747171000
1	-0.494272000	1.978667000	-1.111246000
1	0.174844000	3.148869000	-2.218953000
1	-0.730847000	4.517190000	-0.612669000
1	0.977805000	4.523173000	-0.240898000
1	0.669139000	2.852648000	3.052527000
1	1.744397000	2.847841000	1.662366000
1	-0.375296000	0.754081000	2.407066000
6	1.486260000	-0.594627000	-1.006403000
6	0.648143000	-0.905324000	0.236368000
8	3.237761000	0.628993000	-0.063866000
8	2.700732000	-1.277862000	-1.209615000
6	3.685936000	-0.692610000	-0.356067000
1	0.926577000	-0.583903000	-1.947175000
6	0.005962000	-2.026340000	0.613205000
6	-0.763156000	-2.166665000	1.867448000
6	-1.952759000	-1.613717000	2.178385000

6	-2.792505000	-0.727244000	1.366826000
6	-2.910705000	-0.760237000	0.032819000
1	-3.393578000	-0.019091000	1.936832000
1	-2.353385000	-1.500560000	-0.539139000
6	0.088148000	-3.286280000	-0.217651000
1	0.675153000	-3.114645000	-1.121842000
1	0.605368000	-4.071397000	0.361917000
8	-1.191008000	-3.743246000	-0.639571000
1	-1.735061000	-3.822878000	0.154839000
6	3.845585000	-1.497641000	0.931983000
1	4.167345000	-2.517417000	0.701435000
1	4.597701000	-1.028403000	1.572651000
1	2.902047000	-1.541191000	1.478264000
6	4.985004000	-0.599440000	-1.140360000
1	5.336351000	-1.598416000	-1.412163000
1	4.818772000	-0.019937000	-2.050764000
1	5.754504000	-0.107774000	-0.539599000
6	-3.788918000	0.125679000	-0.816694000
6	-4.428200000	1.285730000	-0.054769000
1	-3.660083000	1.907968000	0.411225000
1	-5.003438000	1.912340000	-0.745832000
1	-5.118937000	0.935155000	0.718502000
6	-4.863827000	-0.740142000	-1.492040000
1	-4.396249000	-1.545823000	-2.064764000
1	-5.539565000	-1.183081000	-0.754187000
1	-5.467650000	-0.134426000	-2.179810000
8	-2.896735000	0.637730000	-1.817815000
1	-3.432187000	1.129136000	-2.453094000
1	-0.330444000	-2.850260000	2.602914000
1	-2.342796000	-1.827970000	3.174316000
6	-0.265625000	3.569817000	1.235780000
1	-0.322904000	4.524936000	1.773978000
1	-1.271415000	3.132739000	1.288455000

TS¹

C22H32O4

C1

6	1.328248000	-0.764137000	0.554862000
6	0.943643000	-1.754493000	1.646318000
6	0.251482000	-0.081023000	-0.310314000
6	0.945064000	-3.226085000	1.226715000
6	-0.803339000	-0.513179000	-1.134549000
6	-0.102241000	-3.670981000	0.203400000
6	-1.040013000	-1.955713000	-1.554215000
1	-0.034291000	-1.468603000	2.053159000
1	1.670063000	-1.638147000	2.460832000
1	0.812299000	-3.830261000	2.133439000
1	1.942500000	-3.465020000	0.840938000
1	-1.109573000	-3.519417000	0.613900000
1	0.001138000	-4.758684000	0.103595000
1	-2.022182000	-2.293806000	-1.201731000

1	-1.138985000	-1.933962000	-2.647267000
1	-1.032731000	0.188595000	-1.924231000
6	1.782770000	0.663910000	0.954809000
6	0.679470000	1.203503000	0.051020000
8	2.445082000	-1.277080000	-0.169786000
8	3.128795000	0.783928000	0.542174000
6	3.408338000	-0.246712000	-0.401497000
1	1.721614000	0.959900000	2.005877000
6	0.353307000	2.550785000	-0.193776000
6	-0.714250000	3.109173000	-0.905676000
6	-1.961988000	2.650582000	-1.370117000
6	-2.736028000	1.545735000	-1.042904000
6	-2.459765000	0.553659000	-0.087841000
1	-3.655778000	1.440745000	-1.614681000
1	-1.760535000	0.830140000	0.693834000
6	1.328248000	3.550544000	0.417514000
1	2.355919000	3.186481000	0.350816000
1	1.270664000	4.505134000	-0.128115000
8	1.083042000	3.736765000	1.806410000
1	0.151837000	3.973624000	1.896194000
6	3.311028000	0.273774000	-1.834296000
1	4.046027000	1.068346000	-1.992196000
1	3.515807000	-0.536198000	-2.540527000
1	2.315963000	0.672105000	-2.036617000
6	4.786822000	-0.806932000	-0.090175000
1	5.545576000	-0.029482000	-0.212132000
1	4.809758000	-1.166733000	0.940483000
1	5.021318000	-1.634928000	-0.764336000
6	-3.624510000	-0.286228000	0.440458000
6	-3.141423000	-1.323626000	1.452257000
1	-2.498919000	-2.076729000	0.992327000
1	-2.584094000	-0.832077000	2.255124000
1	-3.995171000	-1.846453000	1.900575000
6	-4.479528000	-0.937618000	-0.650265000
1	-3.910295000	-1.636293000	-1.268811000
1	-5.300170000	-1.498283000	-0.187797000
1	-4.925869000	-0.182571000	-1.301433000
8	-4.429514000	0.685641000	1.135392000
1	-5.115633000	0.195937000	1.607973000
1	-0.549577000	4.161438000	-1.146852000
1	-2.439838000	3.339137000	-2.066606000
6	-0.012812000	-3.047754000	-1.205634000
1	-0.183180000	-3.849344000	-1.934264000
1	1.001970000	-2.681719000	-1.391562000

c8

C₂₂H₃₂O₄

C1

6	-1.640024000	0.756602000	0.484553000
6	-1.823341000	1.886298000	1.488147000
6	-0.240073000	0.175616000	0.181830000
6	-1.717007000	3.297353000	0.890663000
6	1.067677000	0.848448000	-0.146059000
6	-0.612197000	3.508908000	-0.146265000

6	1.337123000	2.022344000	0.831643000
1	-1.103517000	1.743641000	2.301330000
1	-2.818419000	1.771723000	1.936456000
1	-1.604000000	4.020771000	1.709405000
1	-2.671177000	3.527542000	0.404305000
1	-0.735419000	4.516877000	-0.563942000
1	-0.785491000	2.824138000	-0.984689000
1	0.944017000	1.782130000	1.825886000
1	2.412782000	2.144346000	0.940043000
1	0.988700000	1.302807000	-1.143160000
6	-2.030954000	-0.681923000	0.894056000
6	-0.629022000	-1.097941000	0.472220000
8	-2.450878000	1.012228000	-0.659442000
8	-3.117763000	-1.053699000	0.074469000
6	-3.155194000	-0.171395000	-1.046500000
1	-2.296386000	-0.871487000	1.937958000
6	-0.135888000	-2.469855000	0.421246000
6	0.681785000	-2.974115000	-0.536067000
6	1.279356000	-2.229527000	-1.631831000
6	1.864052000	-1.023735000	-1.538349000
6	2.156718000	-0.271687000	-0.270772000
1	2.199650000	-0.541053000	-2.455880000
1	2.026731000	-0.961318000	0.571654000
6	-0.771167000	-3.404367000	1.427299000
1	-1.854335000	-3.439308000	1.263420000
1	-0.383735000	-4.424689000	1.284028000
8	-0.610254000	-2.967907000	2.768605000
1	0.335990000	-2.861196000	2.920559000
6	-2.504704000	-0.807716000	-2.272727000
1	-3.037913000	-1.723595000	-2.543976000
1	-2.549133000	-0.114389000	-3.117958000
1	-1.459771000	-1.052044000	-2.076687000
6	-4.606958000	0.202822000	-1.300377000
1	-5.185922000	-0.686325000	-1.564257000
1	-5.031312000	0.648744000	-0.398421000
1	-4.674482000	0.922229000	-2.120727000
6	3.652665000	0.178960000	-0.224435000
6	4.574251000	-0.826223000	-0.933301000
1	4.386766000	-0.854466000	-2.008375000
1	5.621801000	-0.537938000	-0.778125000
1	4.447323000	-1.838332000	-0.537834000
6	4.154161000	0.297589000	1.226110000
1	3.505509000	0.901817000	1.860395000
1	4.234432000	-0.695970000	1.679507000
1	5.155295000	0.745117000	1.240002000
8	3.719235000	1.432798000	-0.907943000
1	4.649605000	1.679351000	-0.973657000
1	0.830403000	-4.055287000	-0.544159000
1	1.241042000	-2.709134000	-2.610738000
6	0.831615000	3.389388000	0.342454000
1	1.489145000	3.691559000	-0.483812000
1	1.001858000	4.121319000	1.144699000

TS²
C22H32O4
C1

6	-1.256595000	1.045129000	-0.534114000
6	-1.330254000	2.569433000	-0.739626000
6	0.020887000	0.256522000	-0.127654000
6	-0.152707000	3.483095000	-0.375923000
6	1.433206000	0.794112000	0.073519000
6	0.184143000	3.677962000	1.105139000
6	1.674202000	1.554357000	1.393939000
1	-2.238020000	2.929397000	-0.234712000
1	-1.516975000	2.699509000	-1.810695000
1	-0.398034000	4.473118000	-0.782454000
1	0.739566000	3.168328000	-0.925811000
1	-0.662612000	4.177644000	1.596370000
1	1.022971000	4.385339000	1.165337000
1	1.893529000	0.806848000	2.168741000
1	2.579278000	2.167607000	1.298603000
1	1.682838000	1.421396000	-0.786885000
6	-1.965929000	0.341785000	0.662803000
6	-0.731756000	-0.540573000	0.776354000
8	-1.914680000	0.431672000	-1.646106000
8	-3.163917000	-0.210366000	0.177276000
6	-3.077904000	-0.295741000	-1.247223000
1	-2.196673000	0.965498000	1.530236000
6	-0.614640000	-1.859549000	1.207751000
6	0.083163000	-2.806299000	0.427799000
6	0.688485000	-2.488977000	-0.785152000
6	1.201443000	-1.213541000	-1.071534000
6	2.176528000	-0.527979000	-0.119785000
1	1.378025000	-0.964741000	-2.117901000
1	2.193372000	-1.083584000	0.826529000
6	-1.567505000	-2.344220000	2.279839000
1	-2.599740000	-2.235445000	1.929081000
1	-1.393486000	-3.414811000	2.473166000
8	-1.497134000	-1.582699000	3.474886000
1	-0.573108000	-1.575386000	3.750557000
6	-2.931456000	-1.743674000	-1.693196000
1	-3.801138000	-2.326052000	-1.375347000
1	-2.856295000	-1.793510000	-2.783294000
1	-2.029013000	-2.178777000	-1.260069000
6	-4.320280000	0.366593000	-1.829814000
1	-5.220608000	-0.163773000	-1.507128000
1	-4.381187000	1.402336000	-1.487815000
1	-4.277915000	0.355392000	-2.922261000
6	3.619916000	-0.479844000	-0.667970000
6	4.136784000	-1.894117000	-0.951247000
1	3.502383000	-2.404735000	-1.679242000
1	5.156801000	-1.851529000	-1.352999000
1	4.165681000	-2.498066000	-0.038543000
6	4.571639000	0.232829000	0.298335000

1	4.299477000	1.284338000	0.408188000
1	4.568550000	-0.234979000	1.288114000
1	5.599233000	0.190472000	-0.083265000
8	3.541630000	0.259379000	-1.891188000
1	4.424008000	0.273079000	-2.279731000
1	-0.122124000	-3.854123000	0.648773000
1	0.629902000	-3.230593000	-1.582550000
6	0.534034000	2.431657000	1.920686000
1	0.807867000	2.761636000	2.931389000
1	-0.356183000	1.810508000	2.059136000

f8

C22H32O4

C1

6	-0.875967000	1.136458000	-0.480084000
6	-0.577588000	2.637039000	-0.595620000
6	0.189741000	0.063448000	-0.053601000
6	0.421552000	3.372451000	0.320881000
6	1.556991000	0.557269000	0.498046000
6	0.357975000	3.227095000	1.850335000
6	1.735264000	0.975650000	1.954681000
1	-1.555652000	3.129825000	-0.508087000
1	-0.255840000	2.808444000	-1.629920000
1	0.272237000	4.439887000	0.109272000
1	1.444478000	3.173093000	-0.009934000
1	-0.613962000	3.595590000	2.208186000
1	1.097752000	3.936055000	2.246322000
1	1.784152000	0.075224000	2.581704000
1	2.703718000	1.481581000	2.070579000
1	1.868565000	1.363830000	-0.167821000
6	-1.829742000	0.638082000	0.644525000
6	-0.898187000	-0.556280000	0.787192000
8	-1.573476000	0.726943000	-1.653004000
8	-3.087648000	0.419564000	0.050581000
6	-2.934865000	0.402850000	-1.372520000
1	-1.969997000	1.299607000	1.502744000
6	-1.171307000	-1.869853000	0.893801000
6	-0.355158000	-2.815112000	0.125894000
6	0.505853000	-2.399318000	-0.823330000
6	0.969178000	-0.984479000	-0.935229000
6	2.236153000	-0.711505000	-0.059084000
1	1.129064000	-0.665078000	-1.969459000
1	2.323597000	-1.486005000	0.712370000
6	-2.407622000	-2.396441000	1.580273000
1	-3.066843000	-1.572842000	1.859739000
1	-2.970519000	-3.048819000	0.891877000
8	-2.100229000	-3.084943000	2.787585000
1	-1.502508000	-3.808175000	2.566311000
6	-3.224704000	-0.984024000	-1.929183000

1	-4.243286000	-1.287785000	-1.672167000
1	-3.125710000	-0.978594000	-3.018436000
1	-2.516660000	-1.705318000	-1.517903000
6	-3.862776000	1.461829000	-1.957729000
1	-4.904576000	1.222241000	-1.726738000
1	-3.628994000	2.441259000	-1.534421000
1	-3.745378000	1.508945000	-3.043733000
6	3.585548000	-0.575707000	-0.772403000
6	3.966549000	-1.890528000	-1.460428000
1	3.221418000	-2.158979000	-2.214204000
1	4.936407000	-1.794715000	-1.964119000
1	4.047056000	-2.711732000	-0.740971000
6	4.680580000	-0.152110000	0.211894000
1	4.445716000	0.819245000	0.654244000
1	4.800261000	-0.882305000	1.018723000
1	5.646224000	-0.065535000	-0.301710000
8	3.408545000	0.444608000	-1.759905000
1	4.247070000	0.548250000	-2.224517000
1	-0.590844000	-3.876427000	0.201865000
1	0.952434000	-3.127776000	-1.497681000
6	0.611876000	1.858695000	2.510640000
1	0.817994000	2.045681000	3.572508000
1	-0.300987000	1.258892000	2.509621000

References of Supporting Information

1. J. Suffert, *J. Org. Chem.* **1989**, *54*, 509-510
2. (a) J. Suffert, B. Salem, P. Klotz, *J. Am. Chem. Soc.* **2001**, *123*, 12107-12108. (b) B. Salem, J. Suffert, *Angew. Chem. Int. Ed.* **2004**, *43*, 2826-2830. (c) C. Hulot, G. Blond, J. Suffert, *J. Am. Chem. Soc.* **2008**, *130*, 5046-5047.
3. H. X. Zhang, F. Guibé, G. Balavoine, *J. Org. Chem.* **1990**, *55*, 1857-1867
4. W. P. Gallagher, I. Terstiege, R. E. Maleczka, *J. Am. Chem. Soc.* **2001**, *123*, 14, 3194-3204
5. C. Morril, R. H. Grubbs, *J. Org. Chem.* **2003**, *68*, 15, 6031-6034
6. B. M. Trost, M. T. Rudd, *Org. Lett.* **2003**, *5*, 24, 4599-4602
7. C. Spino, V. G. Gund, C. Nadeau, *J. Comb. Chem.* **2005**, *7*, 345-352
8. R. N. Hanson, L. Franke, F. Murphy, *Nuclear Medicine and Biology* **1996**, *23*, 5, 585-588.
9. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, revision C.02; Gaussian, Inc.: Wallingford, CT, **2004**.

18a

ppm

139,294

127,339
126,900

81,981

64,810

52,445

40,285

38,351

37,149

35,142

30,557

30,205

29,751

28,667

25,795

24,652

21,459

18c

ppm

160

150

140

130

120

110

100

90

80

70

60

50

40

30

20