

Supporting Information

Site-selectivity Control in the Hetero-Diels-Alder Reactions of Methylidene Derivatives of Lawsone through Modification of the Reactive Carbonyl Group: An Experimental and Theoretical Study

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Detailed experimental procedures

Spectral and analytical data of the prepared new compounds

Preparation of 4,4-dimethoxynaphthalene-1,3-dione (12)

A catalytic amount of conc. H_2SO_4 (two drops) was added to a hot suspension of lawsone (1000 mg, 5.7 mmol) in acetic anhydride (1.4 mL, 14.4 mmol) and the mixture was heated in an oil bath for 15 min. Upon addition of water, acetyl lawsone **11** precipitated²⁶ and was collected by filtration. It was thoroughly washed with water and then dried under vacuum. The crude ester **11** (1186 mg, 5.49 mmol) was dissolved in methanol (30 mL) and K_2CO_3 (2273 mg, 16.47 mmol) was added. After stirring for 30 min at rt, potassium carbonate was removed by filtration and the filtrate was concentrated in a rotary evaporator. The resulting mixture was carefully neutralized with a dilute hydrochloric acid solution and was then extracted with CH_2Cl_2 (3 x 20 mL) and washed with brine. The organic layer was dried (Na_2SO_4) and concentrated to afford the acetal **12** in 78% total yield (983 mg, 4.47 mmol).

4,4-Dimethoxynaphthalene-1,3-(2H,4H)-dione (12). Yellow solid; Yield 84%; mp 110–111 °C; ^1H NMR (CDCl_3 , 500 MHz) δ (mixture of tautomers **A**, **B**) **A**: 8.03 (ddd, $J = 7.8, 1.4, 0.4$ Hz, 1H), 7.86 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.71–7.67 (m, 1H), 7.58–7.54 (m, 1H), 3.84 (s, 2H), 3.32 (s, 6H); **B**: 8.14 (ddd, $J = 7.8, 1.2, 0.6$ Hz, 1H), 7.71–7.67 (m, 2H), 7.58–7.55 (m, 1H), 6.17 (s, 1H), 3.06 (s, 6H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 197.8, 192.6, 138.0, 133.9, 132.8, 130.0, 127.8, 127.5, 126.1, 99.3, 51.6, 50.9; ESI-MS m/z negative 219 (M^-); Anal. Calcd for $\text{C}_{12}\text{H}_{12}\text{O}_4$: C, 65.45; H, 5.49. Found: C, 65.34; H, 5.63.

Prerparation of arylidene-4,4-dimethoxynaphthalene-1,3-diones 14a-d. General procedure.

In a solution of the acetal **12** (40 mg, 0.18 mmol) in CH_2Cl_2 (3 mL) the appropriate aldehyde **13** (0.36 mmol), anhydrous MgSO_4 (65 mg, 0.54 mmol) and a catalytic amount of *S*-proline (4 mg, 0.036 mmol) were added and the mixture was stirred for 2 days at rt. MgSO_4 was removed by filtration and the filtrate was concentrated and subjected to column chromatography (silica gel, PE/ethyl acetate 5:1) to afford the unreacted aldehyde and products **14** in order of elution. The arylidene-1,3-diones **14** were crystallized upon trituration with mixtures of PE/ Et_2O .

(Z)-2-Benzylidene-4,4-dimethoxynaphthalene-1,3(2H,4H)-dione (14a). Yellow oil; Yield 83%; ^1H NMR (CDCl_3 , 300 MHz) δ 8.19 (s, 1H), 8.15 (dd, $J_1 = 7.7$ Hz, $J_2 = 1.1$ Hz, 1H), 7.90–7.80 (m, 3H), 7.65 (ddd appearing as dt, $J = 7.5, 1.2$ Hz, 1H), 7.56 (ddd appearing as dt, $J = 7.5, 1.2$ Hz, 1H), 7.48–7.40 (m, 3H), 3.35 (s, 6H); ^{13}C NMR (CDCl_3 , 75 MHz) δ 193.9, 185.2, 148.1, 137.4, 133.6, 133.5, 133.4, 133.0, 131.8, 131.6, 130.2, 128.6, 128.2, 127.1, 99.4, 51.0; ESI-MS m/z positive 672 ($2\text{M} + \text{Na} + \text{MeOH} + \text{H}$)⁺. Anal. Calcd for $\text{C}_{19}\text{H}_{16}\text{O}_4$: C, 74.01; H, 5.23. Found: C, 74.19; H, 5.54.

(Z)-4,4-Dimethoxy-2-(4-methylbenzylidene)naphthalene-1,3(2H,4H)-dione (14b). Yellow solid; Yield 73%; mp 88–90 °C; IR (KBr) cm^{-1} 1668, 1247, 1049; ^1H NMR (CDCl_3 , 300 MHz) δ 8.17 (s, 1H), 8.14 (dd, $J = 7.5, 1.2$ Hz, 1H), 7.86 (dd, $J = 7.5, 1.2$ Hz, 1H), 7.78 (d, $J = 8.2$ Hz, 2H), 7.65 (ddd appearing as td, $J = 7.5, 1.2$ Hz, 1H), 7.56 (ddd appearing as td, $J = 7.5, 1.2$ Hz, 1H), 7.23 (d, $J = 8.2$ Hz, 2H), 3.35 (s, 6H), 2.40 (s, 3H); ^{13}C NMR (CDCl_3 , 75 MHz) δ 194.0, 185.4, 148.6, 142.8, 137.4, 133.3, 132.5, 132.3, 130.7, 130.2, 129.5, 129.1, 128.6, 127.0, 99.4, 51.1, 21.8; ESI-MS m/z positive 667 ($2\text{M} + \text{Na}$)⁺; Anal. Calcd for $\text{C}_{20}\text{H}_{18}\text{O}_4$: C, 74.52; H, 5.63. Found: C, 74.39; H, 5.92.

(Z)-2-(3,4-Dimethoxybenzylidene)-4,4-dimethoxynaphthalene-1,3(2H,4H)-dione (14c). Yellow solid; Yield 70%; mp 139–141 °C; ^1H NMR (CDCl_3 , 300 MHz) δ 8.16 (s, 1H), 8.14 (d, $J = 7.8$ Hz, 1H), 7.85 (d, $J = 7.2$ Hz, 1H), 7.78 (d, $J = 1.8$ Hz, 1H), 7.64 (ddd appearing as dt, $J = 7.5, 1.2$ Hz, 1H), 7.59–7.50 (m, 2H), 6.92 (d, $J = 8.4$ Hz, 1H), 3.95 (s, 6H), 3.35 (s, 6H); ^{13}C NMR (CDCl_3 , 75 MHz) δ 194.2, 185.4, 153.0, 148.9, 148.7, 137.1, 133.1, 130.5, 130.1, 129.1, 128.5, 126.9, 126.4, 116.1, 114.4, 110.8, 99.3, 56.0, 55.9, 51.1; ESI-MS m/z positive 391 ($\text{M} + \text{Na}$)⁺, 423 ($\text{M} + \text{Na} + \text{MeOH}$)⁺; Anal. Calcd for $\text{C}_{21}\text{H}_{20}\text{O}_6$: C, 68.47; H, 5.47. Found: C, 68.19; H, 5.74.

(Z)-2-(4-Chlorobenzylidene)-4,4-dimethoxynaphthalene-1,3(2H,4H)-dione (14d). Yellow solid; Yield 67%; mp 89–92 °C; IR (KBr) cm^{-1} 1675, 1648; ^1H NMR (CDCl_3 , 300 MHz) δ 8.14 (dd, $J_1 = 7.5$ Hz, $J_2 = 1.5$ Hz, 1H), 8.12 (s, 1H), 7.87 (dd, $J = 7.5, 1.2$ Hz, 1H), 7.79 (d, $J = 8.5$ Hz, 2H), 7.67 (ddd appearing as dt, $J = 7.5, 1.5$ Hz, 1H), 7.57 (ddd appearing as dt, $J = 7.5, 1.2$ Hz, 1H), 7.40 (d, $J = 8.5$ Hz, 2H), 3.34 (s, 6H); ^{13}C NMR (CDCl_3 , 75 MHz) δ

193.9, 185.2, 148.1, 137.4, 133.6, 134.4, 133.5, 133.4, 133.0, 131.8, 131.6, 130.2, 128.7, 128.2, 127.1, 99.4, 51.0; ESI-MS m/z positive 365 / 367 ($M+Na$)⁺; Anal. Calcd for C₁₉H₁₅ClO₄: C, 66.58; H, 4.41. Found: C, 66.89; H, 4.20.

General procedure for the reactions of acetal **12** with formaldehyde and vinyl ethers **17**. Synthesis of the dihydrobenzochromenones **18**, **19**, **22** and **23**.

A solution of the acetal **12** (60 mg, 0.27 mmol) in CH₃CN (6 mL) was placed in an ice bath. Aqueous formaldehyde 37% (0.05 mL), anhydrous MgSO₄ (97.5 mg, 0.814 mmol) and a catalytic amount of *S*-proline (6 mg, 0.054 mmol) were added and the mixture was stirred for 30 min. An excess of the appropriate vinyl ether **17** was added and the mixture was kept at rt overnight. MgSO₄ was removed by filtration and the filtrate was subjected to column chromatography (silica gel, PE/ethyl acetate 7:1) to afford the dihydrobenzochromenones **18**, **19**, **22** and **23**.

Reaction with ethoxyethene (**17a**)

2-Ethoxy-10,10-dimethoxy-3,4-dihydro-2H-benzo[*g*]chromen-5(10*H*)-one (18a). Oil; Yield 16%; ¹H NMR (CDCl₃, 500 MHz) δ 8.12 (d, *J* = 7.5 Hz, 1H), 7.72 (d, *J* = 7.5 Hz, 1H), 7.64 (dd appearing as t, *J* = 7.5 Hz, 1H), 7.51 (dd appearing as t, *J* = 7.5 Hz, 1H), 5.45 (brs, 1H), 4.03 (dq, *J* = 9.6, 7.1 Hz, 1H), 3.75 (dq, *J* = 9.6, 7.1 Hz, 1H), 3.09 (s, 3H), 3.03 (s, 3H), 2.65 (ddd, *J* = 17.0, 6.0, 2.5 Hz, 1H), 2.52 (ddd, *J* = 17.0, 12.0, 6.0 Hz, 1H), 2.15–2.08 (m, 1H), 1.88–1.80 (m, 1H), 1.23 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 183.4, 159.6, 137.7, 132.9, 132.4, 129.4, 126.1, 125.9, 117.9, 98.1, 96.4, 64.6, 51.9, 51.5, 25.6, 14.9, 13.7; ESI-MS m/z positive 327 ($M+Na$)⁺, 359 ($M+Na+MeOH$); Anal. Calcd for C₁₇H₂₀O₅: C, 67.09; H, 6.62. Found: C, 67.35; H, 6.80.

2-Ethoxy-6,6-dimethoxy-3,4-dihydro-2H-benzo[*h*]chromen-5(6*H*)-one (19a). Oil; Yield 75%; ¹H NMR (CDCl₃, 500 MHz) δ 7.80 (d, *J* = 7.5 Hz, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.48 (dd appearing as t, *J* = 7.5 Hz, 1H), 7.43 (dd appearing as t, *J* = 7.5 Hz, 1H), 5.41 (dd, *J* = 4.2, 2.6 Hz, 1H), 3.99 (dq, *J* = 9.6, 7.1 Hz, 1H), 3.74 (dq, *J* = 9.6, 7.1 Hz, 1H), 3.26 (s, 3H), 3.25 (s, 3H), 2.55–2.51 (m, 2H), 2.07–2.00 (m, 1H), 1.98–1.90 (m, 1H), 1.26 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 192.3, 159.0, 137.0, 130.0, 129.1, 129.0, 127.2, 123.4, 110.4, 99.3, 94.5, 64.8, 51.9, 51.6, 25.7, 15.1, 14.4; ESI-MS m/z positive 327 ($M+Na$)⁺; Anal. Calcd for C₁₇H₂₀O₅: C, 67.09; H, 6.62. Found: C, 67.32; H, 6.72.

Reaction with 1-ethoxybut-1-ene (**17b**)

2-Ethoxy-3-ethyl-10,10-dimethoxy-3,4-dihydro-2H-benzo[*g*]chromen-5(10*H*)-one (18b). Mixture of diastereoisomers (~2:1). Oil; Total yield 20%. Spectra of the major isomer: ¹H NMR (CDCl₃, 500 MHz) δ 8.12 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.63 (dd appearing as t, *J* = 7.8 Hz, 1H), 7.50 (dd appearing as t, *J* = 7.8, 1H), 5.16 (d, *J* = 2.6 Hz, 1H), 4.09–3.97 (overlapped m, 1H), 3.76–3.69 (overlapped m, 1H), 3.09 (s, 3H), 3.03 (s, 3H), 2.64 (dd, *J* = 17.2, 6.3 Hz, 1H), 2.47 (dd, *J* = 17.2, 2.8 Hz, 1H), 1.99–1.92 (m, 1H), 1.55–1.44 (m, 2H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.00 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 183.7, 159.3, 137.8, 132.9, 132.4, 129.4, 126.1, 125.9, 116.6, 101.7, 96.4, 64.8, 52.0, 51.5, 36.5, 23.5, 19.1, 14.9, 11.6; Spectra of the minor isomer: ¹H NMR (CDCl₃, 500 MHz) δ 8.12 (d, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.63 (dd appearing as t, *J* = 7.5, 1H), 7.50 (dd appearing as t, *J* = 7.6, 1H), 5.31 (d, *J* = 2.2 Hz, 1H), 4.05–3.97 (overlapped m, 1H), 3.76–3.69 (overlapped m, 1H), 3.08 (s, 3H), 3.01 (s, 3H), 2.72 (dd, *J* = 16.8, 5.5 Hz, 1H), 2.16 (dd, *J* = 16.8, 12.6 Hz, 1H), 1.79–1.71 (m, 1H), 1.64–1.52 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.02 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz) (distinguishable peaks only) δ 183.4, 132.5, 125.9, 100.3, 64.9, 51.8, 51.9, 37.2, 24.1, 19.8, 14.9, 11.4; ESI-MS (mixture of diastereoisomers) m/z positive 355 ($M+Na$)⁺; Anal. Calcd for C₁₉H₂₄O₅ (mixture of diastereoisomers): C, 68.66; H, 7.28. Found: C, 68.79; H, 7.03.

2-Ethoxy-3-ethyl-6,6-dimethoxy-3,4-dihydro-2H-benzo[*h*]chromen-5(6*H*)-one (19b). Oil; Mixture of diastereoisomers (~2:1). Total yield 79%. Spectra of the major isomer: ¹H NMR (CDCl₃, 300 MHz) δ 7.79 (d, *J* = 7.7 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.48 (dd appearing as t, *J* = 7.5, 1H), 7.43 (dd appearing as t, *J* = 7.6, 1H), 5.08 (d, *J* = 5.1 Hz, 1H), 4.02 (dq, *J* = 9.7, 7.1 Hz, 1H), 3.74 (dq, *J* = 9.7, 7.1 Hz, 1H), 3.263 (s, 3H), 3.259 (s, 3H), 2.70 (dd, *J* = 17.2, 6.0 Hz, 1H), 2.25 (dd, *J* = 17.2, 6.3 Hz, 1H), 1.92–1.84 (m, 1H), 1.65–1.52 (overlapped m, 1H), 1.52–1.42 (m, 1H), 1.27 (t, *J* = 7.1 Hz, 3H), 0.99 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 192.7, 158.8, 137.1, 130.0, 129.2, 129.1, 127.3, 123.5, 109.5, 103.4, 94.7, 65.2, 51.9, 51.7, 36.7, 23.3, 20.4, 15.2, 11.2. Spectra of the minor isomer: ¹H NMR (CDCl₃, 300 MHz) δ 7.79 (d, *J* = 7.7 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.48 (dd appearing as t, *J* = 7.5, 1H), 7.43 (dd appearing as t, *J* = 7.6, 1H), 5.32 (d, *J* = 2.3 Hz, 1H), 3.88 (dq, *J* = 9.7, 7.1 Hz, 1H), 3.70 (dq, *J* = 9.7, 7.1 Hz, 1H), 3.27 (s, 3H), 3.25 (s, 3H), 2.62 (dd, *J* = 16.8, 5.6 Hz, 1H), 2.13 (dd, *J* = 16.8, 12.3 Hz, 1H), 1.82–1.74 (m, 1H), 1.65–1.52 (overlapped m, 2H), 1.19 (t, *J* = 7.1 Hz, 3H), 1.01 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 192.5, 158.5, 137.2, 129.9, 129.2, 128.9, 127.2, 123.4, 110.9, 100.7, 94.6, 64.9, 51.9, 51.7, 37.1, 23.8,

19.6, 15.0, 11.4; ESI-MS (mixture of diastereoisomers) m/z positive 371 (M+K)⁺; Anal. Calcd for C₁₉H₂₄O₅ (mixture of diastereoisomers): C, 68.66; H, 7.28. Found: C, 68.43; H, 7.10.

Reaction with 2-methoxyprop-1-ene (17c)

2,10,10-Trimethoxy-2-methyl-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (18c). Oil; Yield 12%; ¹H NMR (CDCl₃, 500 MHz) δ 8.12 (d, J = 7.8 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.63 (dd appearing as t, J = 7.5 Hz, 1H), 7.50 (dd appearing as t, J = 7.5 Hz, 1H), 3.45 (s, 3H), 3.09 (s, 3H), 3.04 (s, 3H), 2.64 (ddd, J = 17.5, 6.1, 2.9 Hz, 1H), 2.54 (ddd, J = 17.5, 11.9, 6.1 Hz, 1H), 2.15 (ddd, J = 13.6, 6.1, 2.9 Hz, 1H), 1.71 (ddd, J = 13.6, 11.9, 6.1 Hz, 1H), 1.65 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 183.5, 160.0, 137.9, 132.9, 132.4, 129.4, 126.1, 125.8, 117.4, 100.9, 96.4, 51.9, 51.7, 49.8, 31.4, 22.9, 15.4; ESI-MS m/z positive 327 (M+Na)⁺, 359 (M+Na+MeOH)⁺; Anal. Calcd for C₁₇H₂₀O₅: C, 67.09; H, 6.62. Found: C, 66.85; H, 6.41.

2,6,6-Trimethoxy-2-methyl-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (19c). Oil; Yield 18%; ¹H NMR (CDCl₃, 500 MHz) δ 7.82 (dd, J = 7.5, 1.0 Hz, 1H), 7.69 (dd, J = 7.5, 1.0 Hz, 1H), 7.47 (ddd appearing as dt, J = 7.5, 1.5 Hz, 1H), 7.42 (ddd appearing as dt, J = 7.5, 1.5 Hz, 1H), 3.36 (s, 3H), 3.28 (s, 3H), 3.25 (s, 3H), 2.53 (ddd, J = 17.0, 6.5, 3.5 Hz, 1H), 2.51 (ddd, J = 17.0, 11.0, 6.0 Hz, 1H), 2.13 (ddd, J = 13.5, 6.0, 3.5 Hz, 1H), 1.77 (ddd, J = 13.5, 11.0, 6.5 Hz, 1H), 1.65 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 192.6, 158.8, 137.2, 130.0, 129.2, 129.1, 127.3, 123.3, 110.7, 101.1, 94.6, 51.9, 51.8, 49.7, 31.0, 22.6, 15.2; ESI-MS m/z positive 327 (M+Na)⁺, 343 (M+K)⁺. Anal. Calcd for C₁₇H₂₀O₅: C, 67.09; H, 6.62. Found: C, 67.19; H, 6.78.

2,10,10-Trimethoxy-2,4,4-trimethyl-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (22). Oil; Yield 11%; ¹H NMR (CDCl₃, 500 MHz) δ 8.09 (d, J = 7.0 Hz, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.60 (dd appearing as t, J = 7.5 Hz, 1H), 7.50 (dd appearing as t, J = 7.0 Hz, 1H), 3.42 (s, 3H), 3.10 (s, 3H), 2.99 (s, 3H), 2.02 (d, J = 14.0 Hz, 1H), 1.80 (d, J = 14.0 Hz, 1H), 1.63 (s, 3H), 1.56 (s, 3H), 1.39 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 183.2, 158.7, 136.9, 133.4, 132.6, 129.4, 125.9, 125.8, 124.8, 101.1, 96.7, 51.9, 51.4, 49.7, 48.9, 30.9, 30.1, 27.6, 23.5; ESI-MS m/z positive 333 (M+H)⁺; Anal. Calcd for C₁₉H₂₄O₅: C, 68.66; H, 7.28. Found: C, 68.47; H, 7.00.

2,6,6-Trimethoxy-2,4,4-trimethyl-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (23). Oil; Yield 27%; ¹H NMR (CDCl₃, 500 MHz) δ 7.86 (dd, J = 7.0, 1.0 Hz, 1H), 7.67 (dd, J = 7.0, 1.0 Hz, 1H), 7.45 (ddd appearing as dt, J = 7.5, 1.0 Hz, 1H), 7.42 (ddd appearing as dt, J = 7.5, 1.0 Hz, 1H), 3.31 (s, 3H), 3.28 (s, 3H), 3.27 (s, 3H), 1.99 (d, J = 14.0 Hz, 1H), 1.84 (d, J = 14.0 Hz, 1H), 1.63 (s, 3H), 1.51 (s, 3H), 1.35 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 193.1, 156.8, 136.8, 129.8, 129.6, 129.3, 127.0, 124.1, 118.1, 101.1, 95.1, 52.3, 51.6, 49.5, 48.2, 30.7, 29.4, 27.8, 23.3; ESI-MS m/z positive 333 (M+H)⁺; Anal. Calcd for C₁₉H₂₄O₅: C, 68.66; H, 7.28. Found: C, 68.50; H, 7.06.

Reaction with 2,3-dihydrofuran (17d).

10,10-Dimethoxy-3a,4,10,11a-tetrahydro-2H-benzo[g]furo[2,3-b]chromen-5(3H)-one (18d). Oil; Yield 45%; ¹H NMR (CDCl₃, 300 MHz) δ 8.11 (d, J = 7.5 Hz, 1H), 7.72 (d, J = 7.5 Hz, 1H), 7.64 (dd appearing as t, J = 7.5 Hz, 1H), 7.51 (dd appearing as t, J = 7.5 Hz, 1H), 5.67 (d, J = 3.0 Hz, 1H), 4.25 (ddd appearing as dt, J = 9.0, 3.3 Hz, 1H), 4.09 (ddd appearing as q, J = 8.7 Hz, 1H), 3.18 (s, 3H), 3.15 (s, 3H), 2.95–2.67 (m, 3H), 2.28–2.10 (m, 1H), 1.84–1.65 (m, 1H); ¹³C NMR (CDCl₃, 75 MHz) δ 183.8, 161.0, 138.2, 132.9, 131.8, 129.4, 126.2, 125.8, 112.1, 101.6, 95.7, 68.7, 51.9, 36.4, 27.6, 19.1; ESI-MS m/z positive 325 (M+Na)⁺, 341 (M+K)⁺, 357 (M+Na+MeOH)⁺; Anal. Calcd for C₁₇H₁₈O₅: C, 67.54; H, 6.00. Found: C, 67.26; H, 5.84.

5,5-Dimethoxy-7,7a,8,9-tetrahydro-5H-benzo[h]furo[2,3-b]chromen-6(10aH)-one (19d). Oil; Yield 37%; ¹H NMR (CDCl₃, 300 MHz) δ 7.87 (d, J = 7.5 Hz, 1H), 7.69 (d, J = 7.5 Hz, 1H), 7.49 (ddd appearing as dt, J = 7.4, 1.0 Hz, 1H), 7.46 (dt, J = 7.5, 1.2 Hz, 1H), 5.68 (d, J = 3.9 Hz, 1H), 4.21 (ddd appearing as dt, J = 8.6, 2.4 Hz, 1H), 4.07 (ddd appearing as q, J = 8.6 Hz, 1H), 3.28 (s, 3H), 3.25 (s, 3H), 2.89–2.61 (m, 3H), 2.20–2.05 (m, 1H), 1.84–1.67 (m, 1H); ¹³C NMR (CDCl₃, 125 MHz) δ 192.9, 159.5, 137.0, 130.2, 129.3, 128.7, 127.2, 124.1, 106.1, 102.0, 94.7, 69.0, 51.9, 51.8, 36.4, 27.4, 18.8; ESI-MS m/z positive 341 (M+K)⁺, 357 (M+Na+MeOH)⁺, 373 (M+K+MeOH)⁺; Anal. Calcd for C₁₇H₁₈O₅: C, 67.54; H, 6.00. Found: C, 67.29; H, 5.77.

Reaction with 3,4-dihydro-2H-pyran (17e)

11,11-Dimethoxy-3,4,4a,5,11,12a-hexahydrobenzo[g]pyrano[2,3-b]chromen-6(2H)-one (18e). Oil; Yield 34%; ¹H NMR (CDCl₃, 500 MHz) δ 8.10 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.63 (dd appearing as t, J = 8.0 Hz, 1H), 7.50 (dd appearing as t, J = 8.0 Hz, 1H), 5.44 (d, J = 2.0 Hz, 1H), 4.01 (ddd appearing as td, J = 12.0, 4.5 Hz, 1H), 3.79 (ddd appearing as broad d, J = 12.0 Hz, 1H), 3.21 (s, 3H), 3.14 (s, 3H), 2.64 (dd, J = 17.5, 6.5 Hz, 1H), 2.55 (dd, J = 17.5, 4.0 Hz, 1H), 2.26–2.20 (m, 1H), 1.78–1.58 (m, 4H); ¹³C NMR (CDCl₃, 125 MHz) δ 183.6, 160.9, 138.2, 132.9, 132.0, 129.4, 126.2, 125.8, 114.3, 98.1, 95.9, 62.9, 52.1, 51.9, 30.8, 24.3, 23.6, 23.0; ESI-MS

m/z positive 339 (M+Na)⁺, 355 (M+K)⁺, 371 (M+Na+MeOH)⁺. Anal. Calcd for C₁₈H₂₀O₅: C, 68.34; H, 6.37. Found: C, 68.70; H, 6.59.

5,5-Dimethoxy-7,7a,8,9,10,11a-hexahydrobenzo[h]pyrano[2,3-b]chromen-6(5H)-one (19e). Oil; Yield 28%; ¹H NMR (CDCl₃, 500 MHz) δ 7.88 (d, J = 7.5 Hz, 1H), 7.70 (d, J = 7.5 Hz, 1H), 7.49 (dd appearing as t, J = 7.5 Hz, 1H), 7.45 (dd appearing as t, J = 7.5 Hz, 1H), 5.51 (s broad, 1H), 3.98 (dt, J = 11.5, 2.5 Hz, 1H), 3.81 (ddd appearing as broad d, J = 11.5 Hz, 1H), 3.27 (s, 3H), 3.26 (s, 3H), 2.58 (dd, J = 17.5, 6.0 Hz, 1H), 2.52 (dd, J = 17.5, 3.0 Hz, 1H), 2.27–2.20 (m, 1H), 1.85–1.72 (m, 1H), 1.72–1.63 (m, 2H), 1.60–1.50 (m, 1H); ¹³C NMR (CDCl₃, 125 MHz) δ 192.8, 159.6, 137.1, 130.2, 129.3, 128.5, 127.3, 123.8, 107.6, 98.3, 94.7, 62.2, 52.0, 51.7, 30.8, 24.0, 23.5, 23.2; ESI-MS m/z positive 339 (M+Na)⁺, 355 (M+K)⁺, 371 (M+Na+MeOH)⁺. Anal. Calcd for C₁₈H₂₀O₅: C, 68.34; H, 6.37. Found: C, 68.64; H, 6.56.

Reaction of acetal **12** with acetaldehyde. Synthesis of the 4-methyl-dihydrobenzochromenones **25** and **26**

In a solution of the acetal **12** (120 mg, 0.54 mmol) in CH₂Cl₂ (6 mL) with a threefold excess of acetaldehyde, anhydrous MgSO₄ (195 mg, 1.625 mmol) and a catalytic amount of *S*-proline (12 mg, 0.1 mmol) were added and the mixture was stirred overnight at rt. MgSO₄ was removed by filtration and the filtrate was concentrated to afford a mixture of compounds **25** and **26**, in 9% and 86% yields, respectively estimated by ¹H NMR. The attempt to separate compounds **25** and **26** by column chromatography (silica gel, PE/ethyl acetate 4:1) resulted to their hydrolysis.

Mixture of **2-hydroxy-10,10-dimethoxy-4-methyl-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (25)** and **2-hydroxy-6,6-dimethoxy-4-methyl-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (26)**. Yield 9% and 86%, respectively, as estimated by ¹H NMR; ¹H NMR (CDCl₃, 300 MHz) δ 8.11 (d), 7.89–7.30 (m), 5.97–5.37 (overlapping broad multiplets), 3.28 (s), 3.23 (s), 3.12 (s), 3.10 (s), 3.09 (s), 3.04 (s), 2.15–1.93 (m), 1.45 (d), 1.31 (d), 1.27 (d), 1.22 (d); ¹³C NMR (CDCl₃, 75 MHz) δ 192.4, 183.0, 182.9, 159.9, 158.5, 137.2, 137.0, 132.8, 132.5, 130.0, 129.5, 129.0, 128.9, 127.1, 125.9, 125.8, 123.9, 122.1, 121.4, 114.4, 96.3, 94.1, 93.8, 93.6, 52.1, 51.7, 51.6, 51.4, 35.3, 25.1, 23.6, 23.5, 23.4, 21.2, 20.7; ESI-MS m/z positive (mixture of isomers) 313 (M+Na)⁺, 345 (M+Na+MeOH)⁺.

Reaction of acetal **12a** with acetaldehyde and ethoxyethene (**17a**). Synthesis of 2-hydroxy-4-methyl-dihydrobenzochromenones **27** and **28**

A solution of the acetal **12** (80 mg, 0.36 mmol) in CH₃CN (6 mL) was placed in an ice bath. An excess of acetaldehyde, anhydrous MgSO₄ (130 mg, 1.08 mmol) and a catalytic amount of *S*-proline (8 mg, 0.072 mmol) were added and the mixture was stirred for 30 min. An excess of ethoxyethene (**17a**) was added and the mixture was kept at rt overnight. MgSO₄ was removed by filtration and the filtrate after concentration was subjected to column chromatography (silica gel, PE/ethyl acetate 5:1) to afford the dihydrobenzochromenones **27** and **28**.

2-Ethoxy-10,10-dimethoxy-4-methyl-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (27) as mixture of diastereoisomers (ratio ~ 5:1). Oil; Total yield 9%; Spectra of the major isomer: ¹H NMR (CDCl₃, 500 MHz) δ 8.12 (d, J = 8.0 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.63 (dd appearing as t, J = 8.0 Hz, 1H), 7.50 (dd appearing as t, J = 8.0 Hz, 1H), 5.46 (dd appearing as t, J = 5.0 Hz, 1H), 4.05 (dq, J = 9.5, 7.1 Hz, 1H), 3.68 (dq, J = 9.5, 7.1 Hz, 1H), 3.10–2.98 (m overlapped, 1H), 3.06 (s, 3H), 3.04 (s, 3H), 2.08–1.98 (m, 2H), 1.38 (d, J = 7.1 Hz, 3H), 1.22 (t, J = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 183.1, 158.7, 137.5, 132.9, 132.7, 129.5, 126.1, 125.9, 122.3, 98.9, 96.5, 65.0, 51.8, 51.5, 32.5, 21.9, 20.8, 15.1; ESI-MS m/z positive 319 (M+H)⁺, 341 (M+Na)⁺. Anal. Calcd for C₁₈H₂₂O₅: C, 67.91; H, 6.97. Found: C, 68.33; H, 7.25.

2-Ethoxy-6,6-dimethoxy-4-methyl-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (28) as mixture of diastereoisomers (ratio ~ 1:1.9). Oil; Total yield 78%; Spectra of the major isomer: ¹H NMR (CDCl₃, 500 MHz) δ 7.81 (d, J = 7.5 Hz, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.48 (dd appearing as t, J = 7.5 Hz, 1H), 7.43 (dd appearing as t, J = 7.5 Hz, 1H), 5.38 (brs, 1H), 3.98 (dq, J = 9.4, 7.2 Hz, 1H), 3.68 (dq, J = 9.4, 7.2 Hz, 1H), 3.31 (s, 3H), 3.22 (s, 3H), 3.01–2.93 (m, 1H), 2.10 (ddd, J = 14.0, 7.2, 3.1 Hz, 1H), 1.94–1.87 (m, 1H), 1.32 (d, J = 7.0 Hz, 3H), 1.25 (t, J = 7.2 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 192.5, 157.9, 137.1, 130.1, 129.2, 127.1, 123.8, 115.3, 99.8, 94.8, 65.1, 52.2, 51.6, 33.5, 22.5, 20.2, 15.2; ESI-MS m/z positive 357 (M+K)⁺. Anal. Calcd for C₁₈H₂₂O₅: C, 67.91; H, 6.97. Found: C, 68.30; H, 7.28.

Reactions of arylidene-1,3-diones **14b**, **c** with ethoxyethene (**17a**).

A solution of the appropriate arylidene-1,3-dione **14** (0.3 mmol) in CH₂Cl₂ (5 mL) was stirred with an excess of ethoxyethene (0.3 mL) for 4 h, at rt. The reaction mixture was concentrated and subjected to column chromatography (silica gel, PE/ethyl acetate 7:1) to afford product **30** and subsequently, by successive increasing the polarity of the elution solvent (PE/ethyl acetate 5:1), the product **29** and finally (PE/ethyl acetate 3:1) products **31** and **33**.

Reaction of **14b**

(2S*,4R*)-2-Ethoxy-6,6-dimethoxy-4-(p-tolyl)-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (29a). Light yellow oil; Yield 76%; ¹H NMR (CDCl₃, 300 MHz) δ 7.86 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.70 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.49 (ddd appearing as td, *J* = 7.4, 1.7 Hz, 1H), 7.45 (ddd appearing as td, *J* = 7.4, 1.7 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 5.31 (dd, *J* = 6.3, 2.4 Hz, 1H), 4.10 (dd appearing as t, *J* = 7.4 Hz, 1H), 3.99 (dq, *J* = 9.5, 7.1 Hz, 1H), 3.66 (dq, *J* = 9.5, 7.1 Hz, 1H), 3.16 (s, 3H), 3.08 (s, 3H), 2.38 (ddd, *J* = 14.0, 7.4, 2.4 Hz, 1H), 2.27 (s, 3H), 2.16 (ddd, *J* = 14.0, 7.4, 6.3 Hz, 1H), 1.19 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz) δ 191.5, 159.3, 140.8, 137.7, 135.4, 130.3, 129.2, 129.0, 128.7, 127.3, 127.1, 123.8, 113.3, 100.5, 95.0, 65.0, 52.3, 51.0, 36.4, 34.6, 20.9, 15.0; ESI-MS *m/z* positive 417 (M+Na)⁺, 433 (M+K)⁺. Anal. Calcd for C₂₄H₂₆O₅: C, 73.08; H, 6.64. Found: C, 72.81; H, 6.37.

(2S*,4S*)-2-Ethoxy-6,6-dimethoxy-4-(p-tolyl)-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (30a). Light yellow oil; Yield 5%; ¹H NMR (CDCl₃, 300 MHz) δ 7.86 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.72 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.51 (ddd appearing as td, *J* = 7.2, 1.6 Hz, 1H), 7.46 (ddd appearing as td, *J* = 7.2, 1.6 Hz, 1H), 7.13 (d, *J* = 8.2 Hz, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 5.17 (dd, *J* = 7.0, 3.9 Hz, 1H), 4.26 (dd appearing as t, *J* = 5.0 Hz, 1H), 4.07 (dq, *J* = 9.5, 7.1 Hz, 1H), 3.67 (dq, *J* = 9.5, 7.1 Hz, 1H), 3.22 (s, 3H), 3.16 (s, 3H), 2.30 (s, 3H), 2.22–2.15 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz) δ 191.6, 160.0, 141.0, 137.8, 136.1, 130.4, 129.3, 129.1, 127.5, 127.3, 124.0, 111.7, 99.4, 95.2, 65.5, 52.5, 51.3, 35.8, 33.7, 21.0, 15.3; ESI-MS *m/z* positive 417 (M+Na)⁺, 433 (M+K)⁺. Anal. Calcd for C₂₄H₂₆O₅: C, 73.08; H, 6.64. Found: C, 72.90; H, 6.55.

(2R*,4R*)-2-Ethoxy-10,10-dimethoxy-4-(p-tolyl)-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (31a). Compound **31a** was obtained as inseparable mixture with **32a** in a ratio **31a**:**32a** ~ 3:1 as estimated by ¹H NMR. The absorptions of **31a** in the NMR spectra are estimated from the spectra of the mixture. Light yellow oil; Yield 14%; ¹H NMR (CDCl₃, 300 MHz) δ 8.00 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.75 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.63 (ddd appearing as td, *J* = 7.5, 1.3 Hz, 1H), 7.46 (ddd appearing as td, *J* = 7.8, 1.3 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 2H), 7.02 (d, *J* = 8.1 Hz, 2H), 5.36 (dd, *J* = 4.1, 2.8 Hz, 1H), 4.18 (dd, *J* = 7.5, 4.8 Hz, 1H), 4.14–3.95 (m, 2H), 3.64–3.54 (m, 1H), 3.29 (s, 3H), 3.12 (s, 3H), 2.36 (ddd, *J* = 14.1, 7.5, 2.8 Hz, 1H), 2.27 (s, 3H), 1.11 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz) δ 182.6, 161.3, 140.6, 137.7, 135.3, 132.8, 132.5, 129.4, 128.8, 127.4, 127.1, 126.1, 119.3, 99.5, 96.6, 64.9, 52.1, 51.8, 35.4, 33.7, 21.0, 14.7; ESI-MS *m/z* positive 417 (M+Na)⁺, 433 (M+K)⁺. Anal. Calcd for C₂₄H₂₆O₅: C, 73.08; H, 6.64. Found: C, 72.75; H, 6.37.

(2R*,4S*)-2-Ethoxy-10,10-dimethoxy-4-(p-tolyl)-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (32a). Light yellow oil, mixture with **33a**; Yield 4%; Prominent peaks in the ¹H NMR spectrum (CDCl₃, 300 MHz) δ 5.23 (dd, *J* = 6.8, 2.8 Hz), 4.26 (dd appearing as t, *J* = 6.0 Hz).

Reaction of **14c**

(2S*,4R*)-4-(3,4-Dimethoxyphenyl)-2-ethoxy-6,6-dimethoxy-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (29b). Light yellow oil; Yield 73%; ¹H NMR (CDCl₃, 300 MHz) δ 7.87 (dd, *J* = 7.0, 1.6 Hz, 1H), 7.71 (dd, *J* = 7.0, 1.6 Hz, 1H), 7.54–7.42 (m, 2H), 6.89–6.72 (m, 3H), 5.34 (dd, *J* = 6.4, 2.2 Hz, 1H), 4.10 (dd appearing as t, *J* = 7.2 Hz, 1H), 4.10–3.96 (m, 1H), 3.83 (s, 3H), 3.80 (s, 3H), 3.68 (dq, *J* = 9.4, 7.0 Hz, 1H), 3.20 (s, 3H), 3.09 (s, 3H), 2.40 (ddd, *J* = 13.9, 7.2, 2.2 Hz, 1H), 2.18 (ddd, *J* = 13.9, 7.2, 6.4 Hz, 1H), 1.21 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz) δ 191.8, 159.1, 148.5, 147.2, 137.3, 136.4, 130.4, 129.3, 128.9, 127.1, 124.0, 119.8, 113.1, 110.8, 110.3, 100.4, 95.1, 65.1, 55.8, 55.6, 52.5, 51.0, 36.3, 34.5, 15.1; ESI-MS *m/z* positive 463 (M+Na)⁺, 479 (M+K)⁺, 495 (M+Na+MeOH)⁺; Anal. Calcd for C₂₅H₂₈O₇: C, 68.17; H, 6.41. Found: C, 68.34; H, 6.27.

(2S*,4S*)-4-(3,4-Dimethoxyphenyl)-2-ethoxy-6,6-dimethoxy-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (30b). Light yellow oil; Yield 6%; ¹H NMR (CDCl₃, 300 MHz) δ 7.86 (d, *J* = 7.5 Hz, 1H), 7.72 (d, *J* = 7.4 Hz, 1H), 7.53–7.45 (m, 2H), 6.82–6.76 (m, 3H), 5.18 (dd, *J* = 6.6, 4.0 Hz, 1H), 4.24 (dd appearing as t, *J* = 5.0 Hz, 1H), 4.12–4.05 (m, 1H), 3.84 (s, 6H), 3.69 (m, 1H), 3.24 (s, 3H), 3.16 (s, 3H), 2.21–2.16 (m, 2H), 1.28 (t, *J* = 7.0, 3H); ¹³C NMR (CDCl₃, 75 MHz) δ 191.9, 159.9, 149.0, 147.6, 137.3, 136.5, 130.3, 129.3, 128.9, 127.2, 124.0, 119.5,

111.5, 111.1, 110.9, 99.4, 95.2, 65.5, 55.9, 55.8, 52.7, 51.2, 35.8, 33.5, 15.3; ESI-MS m/z positive 463 (M+Na)⁺, 479 (M+K)⁺, 495 (M+Na+MeOH)⁺; Anal. Calcd for C₂₅H₂₈O₇: C, 68.17; H, 6.41. Found: C, 68.44; H, 6.57.

(2R*,4R*)-4-(3,4-dimethoxyphenyl)-2-ethoxy-10,10-dimethoxy-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (31b). Light yellow oil; Yield 20%; ¹H NMR (CDCl₃, 300 MHz) δ 8.01 (d, J = 7.6 Hz, 1H), 7.74 (d, J = 7.5 Hz, 1H), 7.64 (dd appearing as t, J = 7.0 Hz, 1H), 7.48 (dd appearing as t, J = 7.1 Hz, 1H), 6.82–6.71 (m, 3H), 5.38 (t, J = 3.0 Hz, 1H), 4.18 (dd, J = 7.1, 4.2 Hz, 1H), 4.07–3.93 (m, 1H), 3.81 (s, 3H), 3.76 (s, 3H), 3.68–3.54 (m, 1H), 3.29 (s, 3H), 3.12 (s, 3H), 2.41–2.23 (m, 2H), 1.11 (t, J = 7.0 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz) δ 182.6, 161.4, 148.8, 147.5, 137.7, 136.5, 132.9, 132.5, 129.5, 126.2, 126.1, 119.9, 119.2, 111.6, 111.4, 99.5, 96.6, 65.0, 56.0, 55.8, 51.8, 35.4, 33.5, 14.8. ESI-MS m/z positive 463 (M+Na)⁺, 479 (M+K)⁺, 495 (M+Na+MeOH)⁺; Anal. Calcd for C₂₅H₂₈O₇: C, 68.17; H, 6.41. Found: C, 68.69; H, 6.65.

Reactions of acetal 12 with formaldehyde and alkenes 33 performed at rt

The same procedure as that previously described for the reactions of acetal 12 with enol ethers 17 was followed. After removal of MgSO₄ by filtration, the mixture was concentrated and subjected to column chromatography (silica gel, PE/ethyl acetate 5:1) to afford mixtures of products 34 and 35 whose composition was estimated from their ¹H NMR spectra. After repeated chromatography columns, small amounts of pure compounds 34 and 35 were isolated, sufficient for obtaining their analytical and spectroscopic data.

Reaction with styrene (33a)

10,10-Dimethoxy-2-phenyl-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (34a). Oil; Yield 9%; ¹H NMR (CDCl₃, 500 MHz) δ 8.13 (d, J = 7.8 Hz, 1H), 7.74 (d, J = 7.75 Hz, 1H), 7.64 (dd appearing as t, J = 7.5 Hz, 1H), 7.52 (dd appearing as t, J = 7.5 Hz, 1H), 7.46–7.37 (m, 5H), 5.16 (dd, J = 10.3, 2.5 Hz, 1H), 3.23 (s, 3H), 3.13 (s, 3H), 2.78 (ddd, J = 17.3, 5.2, 3.0 Hz, 1H), 2.59 (ddd, J = 17.3, 11.0, 6.1 Hz, 1H), 2.36–2.30 (m, 1H), 2.05–1.95 (m, 1H); ¹³C NMR (CDCl₃, 125 MHz) δ 183.6, 163.0, 140.0, 138.2, 132.9, 132.0, 129.4, 128.7, 128.3, 126.2, 125.9, 116.3, 96.2, 79.2, 52.2, 52.0, 29.0, 18.7; ESI-MS m/z positive 359 (M+Na)⁺, 391 (M+Na+MeOH)⁺; Anal. Calcd for C₂₁H₂₀O₄: C, 74.98; H, 5.99. Found: C, 74.80; H, 6.06.

6,6-Dimethoxy-2-phenyl-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (35a). Oil; Yield 13%; ¹H NMR (CDCl₃, 500 MHz) δ 7.84 (d, J = 7.8 Hz, 1H), 7.71 (d, J = 7.6 Hz, 1H), 7.49 (ddd appearing as dt, J = 7.6, 1.1 Hz, 1H), 7.45–7.38 (m, 6H), 5.19 (dd, J = 10.5, 2.4 Hz, 1H), 3.30 (s, 3H), 3.29 (s, 3H), 2.74 (ddd, J = 17.3, 5.3, 2.7 Hz, 1H), 2.53 (ddd, J = 17.3, 11.2, 6.1 Hz, 1H), 2.33–2.27 (m, 1H), 2.05–1.96 (m, 1H); ¹³C NMR (CDCl₃, 125 MHz) δ 192.5, 161.7, 140.1, 136.8, 130.2, 129.3, 129.1, 128.7, 128.4, 127.2, 125.9, 123.8, 109.9, 94.8, 79.5, 52.1, 51.8, 28.9, 18.4; ESI-MS m/z positive 359 (M+Na)⁺, 391 (M+Na+MeOH)⁺; Anal. Calcd for C₂₁H₂₀O₄: C, 74.98; H, 5.99. Found: C, 75.10; H, 6.10.

Reaction with prop-1-en-2-ylbenzene (33b)

Mixture of 10,10-Dimethoxy-2-methyl-2-phenyl-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (34b) and 6,6-dimethoxy-2-methyl-2-phenyl-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (35b). Oil; Yield 23% and 25%, respectively; ¹H NMR (CDCl₃, 500 MHz) δ 8.10 (d, J = 7.7 Hz), 8.01 (d, J = 6.9 Hz), 7.75–7.61 (m), 7.54–7.47 (m), 7.39–7.25 (m), 3.27 (s), 3.20 (s), 3.16 (s), 3.10 (s), 2.62–2.50 (m), 2.48–2.40 (m), 2.38–2.27 (m), 2.18–2.04 (m), 1.74 (s), 1.71 (s); ¹³C NMR (CDCl₃, 125 MHz) δ 192.4, 183.4, 161.8, 160.4, 144.7, 144.2, 130.2, 129.3, 128.7, 128.6, 127.4, 127.3, 124.5, 124.2, 123.6, 115.7, 110.0, 96.4, 94.6, 81.7, 80.9, 52.2, 51.9, 51.8, 32.4, 32.1, 29.0, 28.5, 16.5, 16.1; ESI-MS m/z positive 373 (M+Na)⁺, 405 (M+Na+MeOH)⁺; Anal. Calcd for C₂₂H₂₂O₄: C, 75.41; H, 6.33. Found: C, 75.08; H, 6.07.

Reaction with 2-methylbut-2-ene (33c)

10,10-Dimethoxy-2,2,3-trimethyl-3,4-dihydro-2H-benzo[g]chromen-5(10H)-one (34c). Oil; Yield 7%; ¹H NMR (CDCl₃, 500 MHz) δ 8.10 (dd, J = 7.8, 0.9 Hz, 1H), 7.71 (dd, J = 7.65, 0.7 Hz, 1H), 7.61 (ddd appearing as dt, J = 7.45, 1.3 Hz, 1H), 7.49 (ddd appearing as dt, J = 7.8, 1.2 Hz, 1H), 3.11 (s, 3H), 3.06 (s, 3H), 2.69 (dd, J = 17.4, 5.4 Hz, 1H), 2.14 (dd, J = 17.4, 9.9 Hz, 1H), 1.91–1.83 (m, 1H), 1.50 (s, 3H), 1.27 (s, 3H), 1.07 (d, J = 6.85, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 183.5, 161.7, 138.2, 132.7, 132.3, 129.3, 126.2, 125.7, 115.1, 96.1, 81.7, 51.8, 51.7, 35.0, 29.7, 27.1, 24.7, 16.4; ESI-MS m/z positive 303 (M+H)⁺; Anal. Calcd for C₁₈H₂₂O₄: C, 71.50; H, 7.33. Found: C, 71.17; H, 7.45.

6,6-Dimethoxy-2,2,3-trimethyl-3,4-dihydro-2H-benzo[h]chromen-5(6H)-one (35c). Oil; Yield 6%; ¹H NMR (CDCl₃, 500 MHz) δ 7.80 (d, J = 7.6 Hz, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.47 (dd appearing as t, J = 7.5 Hz, 1H),

7.42 (dd appearing as t, $J = 7.5$ Hz, 1H), 3.27 (s, 3H), 3.24 (s, 3H), 2.64 (dd, $J = 17.4, 5.25$ Hz, 1H), 2.06 (dd, $J = 17.4, 10.4$ Hz, 1H), 1.92–1.84 (m, 1H), 1.50 (s, 3H), 1.24 (s, 3H), 1.05 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 192.3, 160.4, 137.1, 130.0, 129.5, 129.1, 127.1, 123.7, 109.1, 94.6, 81.8, 51.9, 51.8, 35.0, 29.7, 27.2, 24.3, 16.4; ESI-MS m/z positive 303 ($\text{M}+\text{H}$) $^+$; Anal. Calcd for $\text{C}_{18}\text{H}_{22}\text{O}_4$: C, 71.50; H, 7.33. Found: C, 71.25; H, 7.60.

Reactions of acetal **12** with formaldehyde and alkenes **33** under MW irradiation

A mixture of acetal **12** (40 mg, 0.18 mmol), aqueous formaldehyde 37% (0.04 mL), anhydrous MgSO_4 (65 mg, 0.54 mmol), a catalytic amount of *S*-proline (4 mg, 0.036 mmol), and the appropriate alkene **33** (0.36 mmol) in CH_2Cl_2 (2 mL) was irradiated in a closed vessel in a microwave oven at 75 °C for 35 min. After filtration of MgSO_4 and evaporation, the crude mixture was analyzed by ^1H NMR and the two desired products **34**, **35** were identified in the mixture by relative integrations of the peaks of the methoxy groups. The $\alpha:\beta$ ratios for the products **34a:35a**, **34b:35b**, and **34c:35c** were found to be 1:1.75, 1:1.29, and 1:1.19 respectively. The crude mixtures of the products **34** and **35** also contained the corresponding hydrolyzed compounds **36** and **37** and thus purification by silica column chromatography was inefficient. The reaction was then repeated and after removal of MgSO_4 by filtration, TFA (2 drops) was added into the crude mixture. After 1 h at rt, the mixture was evaporated and the hydrolyzed products **36** and **37** were purified by column chromatography in order to verify the structures and obtain the yield of the reactions.

Reaction with styrene (**33a**)

2-Phenyl-3,4-dihydro-2*H*-benzo[*g*]chromene-5,10-dione (**36a**)

Yellow solid; mp 167–169 °C (lit.¹ mp 168–170 °C); Yield 30%.

2-Phenyl-3,4-dihydro-2*H*-benzo[*h*]chromene-5,6-dione (**37a**)

Yellow solid; mp 161–162 °C (lit.¹ mp 161–163 °C); Yield 28%.

Reaction with prop-1-en-2-ylbenzene (**33b**)

2-Methyl-2-phenyl-3,4-dihydro-2*H*-benzo[*g*]chromene-5,10-dione (**36b**)

Yellow solid; mp 138–140 °C (lit.² mp 138–140 °C); Yield 38%.

2-Methyl-2-phenyl-3,4-dihydro-2*H*-benzo[*h*]chromene-5,6-dione (**37b**)

Yellow solid; mp 114–116 °C (lit.² mp 115–117 °C); Yield 33%.

Reaction with 2-methylbut-2-ene (**33c**)

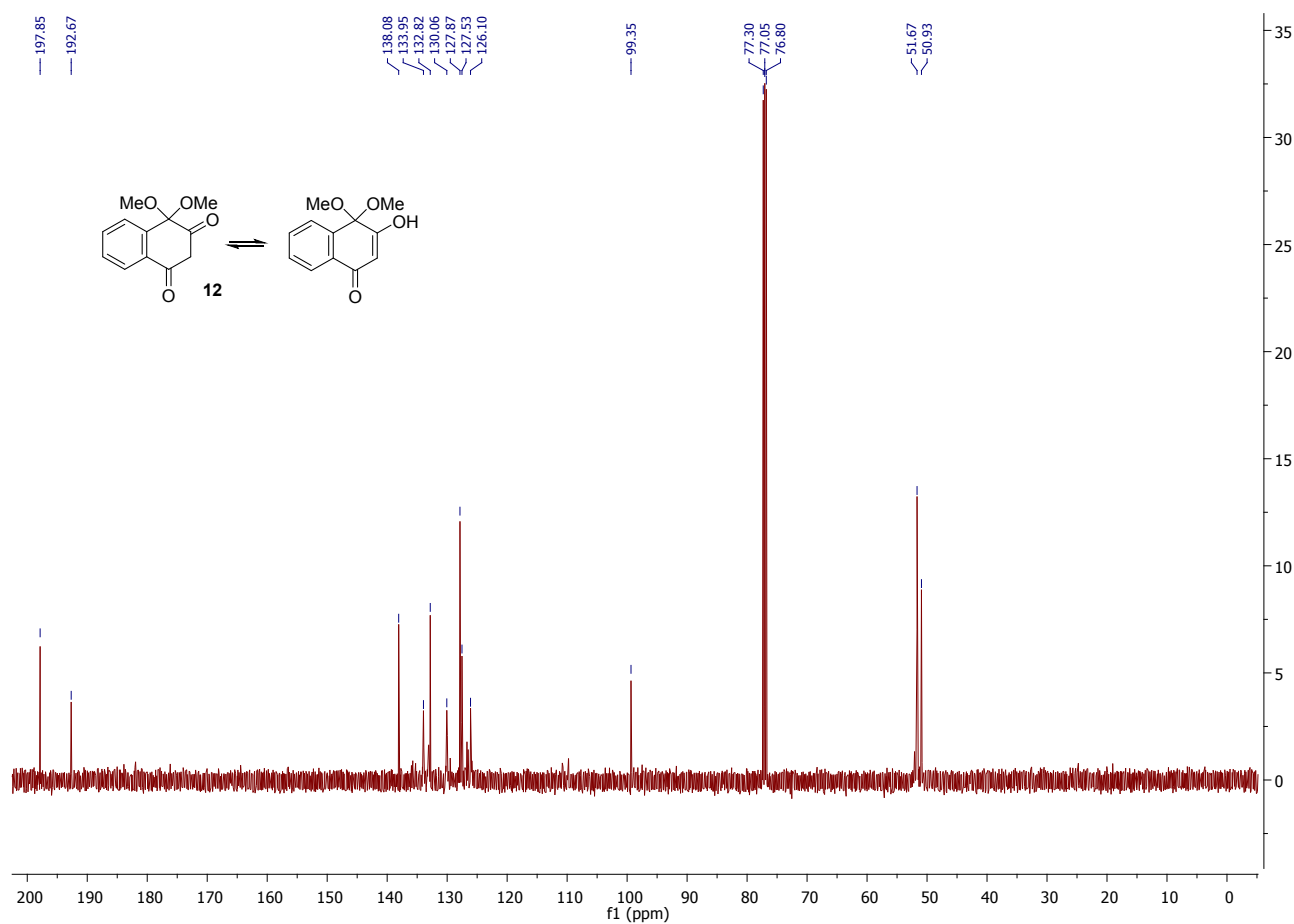
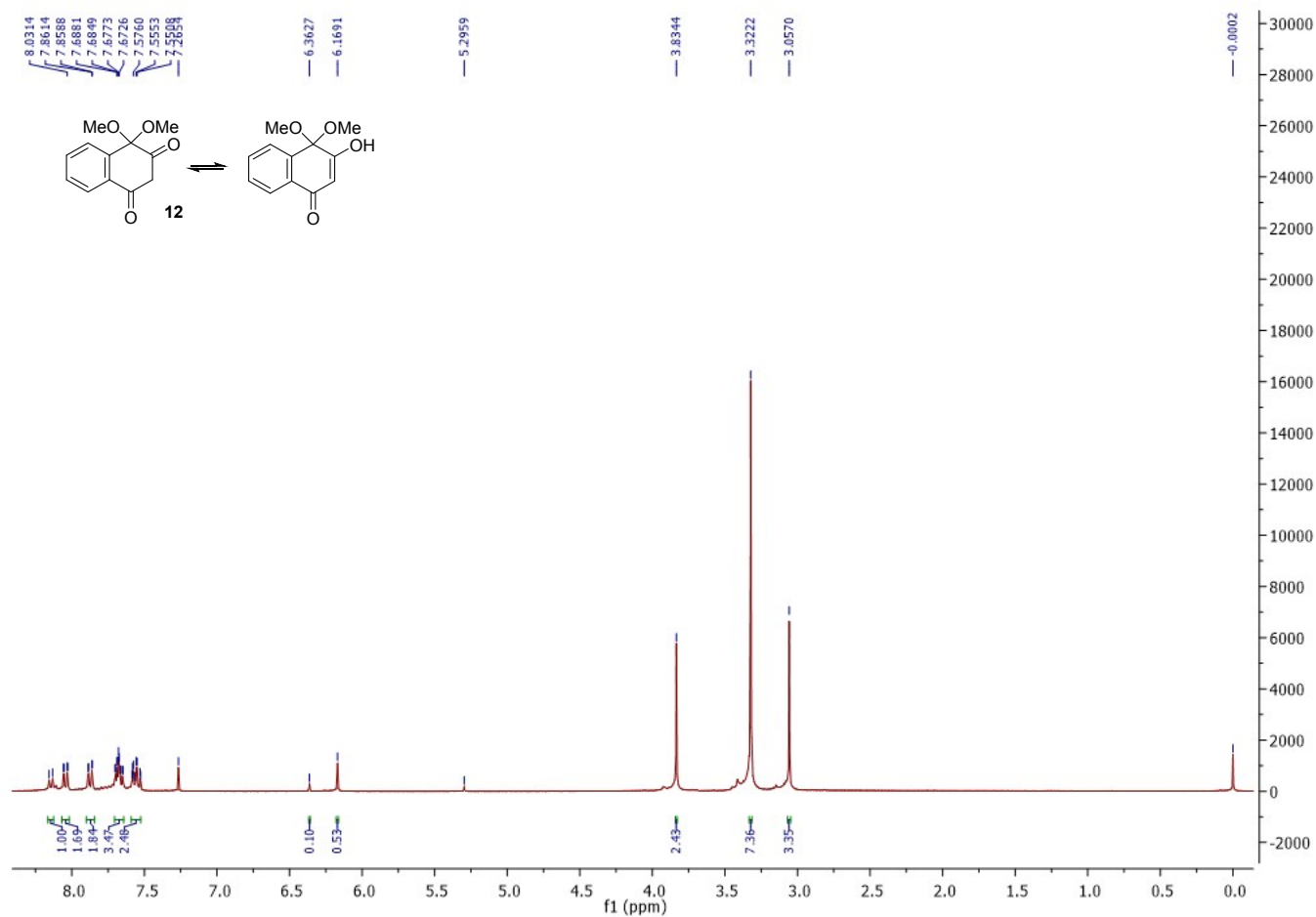
2,2,3-Trimethyl-3,4-dihydro-2*H*-benzo[*g*]chromene-5,10-dione (36c**)**³ Oil; Yield 16%; ^1H NMR (CDCl_3 , 500 MHz) δ 8.08 (dd, $J = 7.5, 1.1$ Hz, 1H), 8.07 (d, $J = 7.5$ Hz, 1H), 7.69 (ddd appearing as dt, $J = 7.5, 1.4$ Hz, 1H), 7.65 (ddd appearing as dt, $J = 7.5, 1.4$ Hz, 1H), 2.73 (dd, $J = 18.8, 4.3$ Hz, 1H), 2.19 (dd, $J = 18.8, 9.9$ Hz, 1H), 1.92–1.84 (m, 1H), 1.50 (s, 3H), 1.24 (s, 3H), 1.07 (d, $J = 6.9, 3\text{H}$); ^{13}C NMR (CDCl_3 , 125 MHz) δ 184.4, 180.0, 154.3, 133.9, 132.9, 132.2, 131.2, 126.3, 126.0, 120.4, 81.9, 34.6, 26.9, 25.1, 20.2, 16.4. ESI-MS m/z positive 257 ($\text{M}+\text{H}$) $^+$, 279 ($\text{M}+\text{Na}$) $^+$; Anal. Calcd for $\text{C}_{16}\text{H}_{16}\text{O}_3$: C, 74.98; H, 6.29. Found: C, 74.60; H, 6.01.

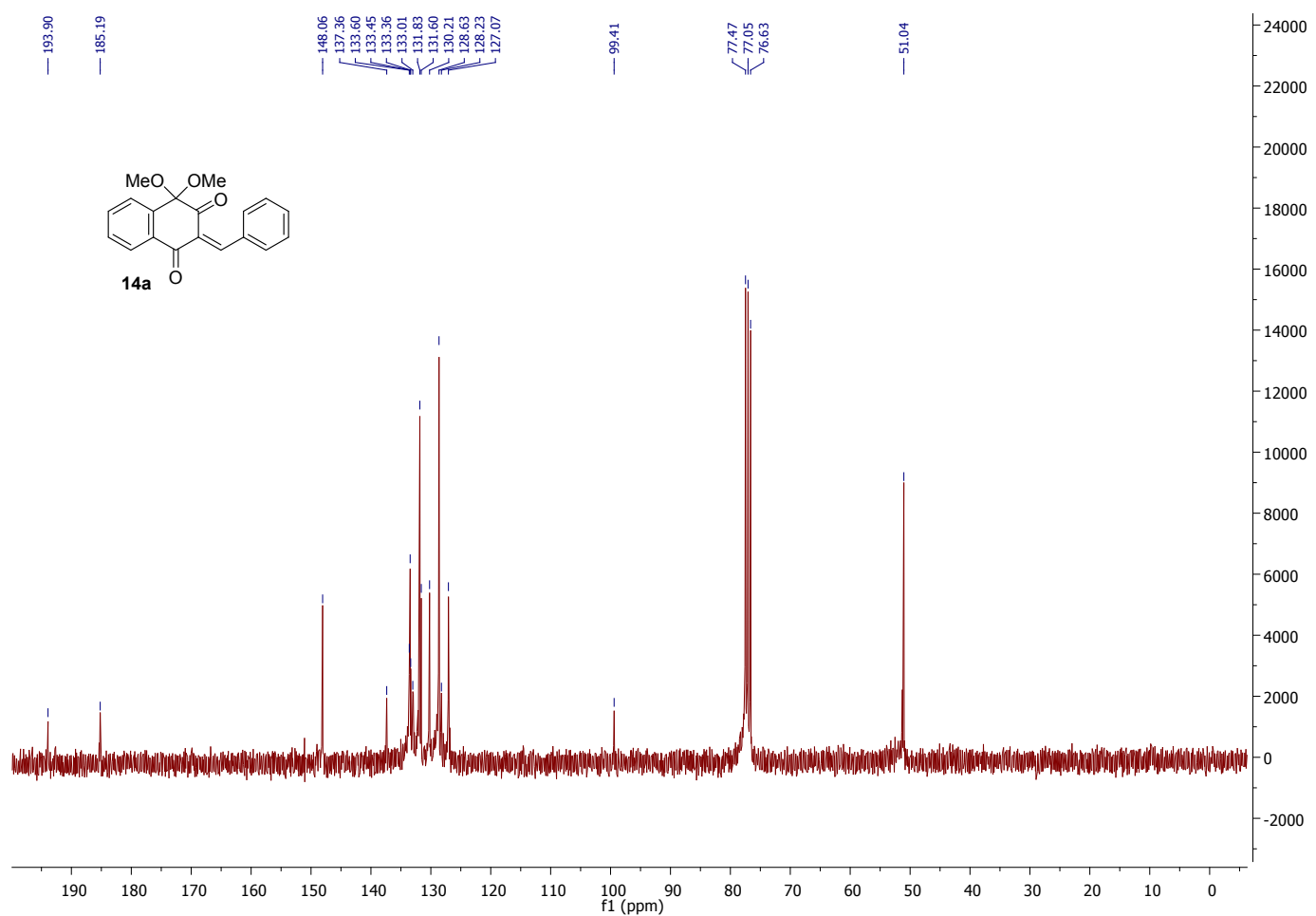
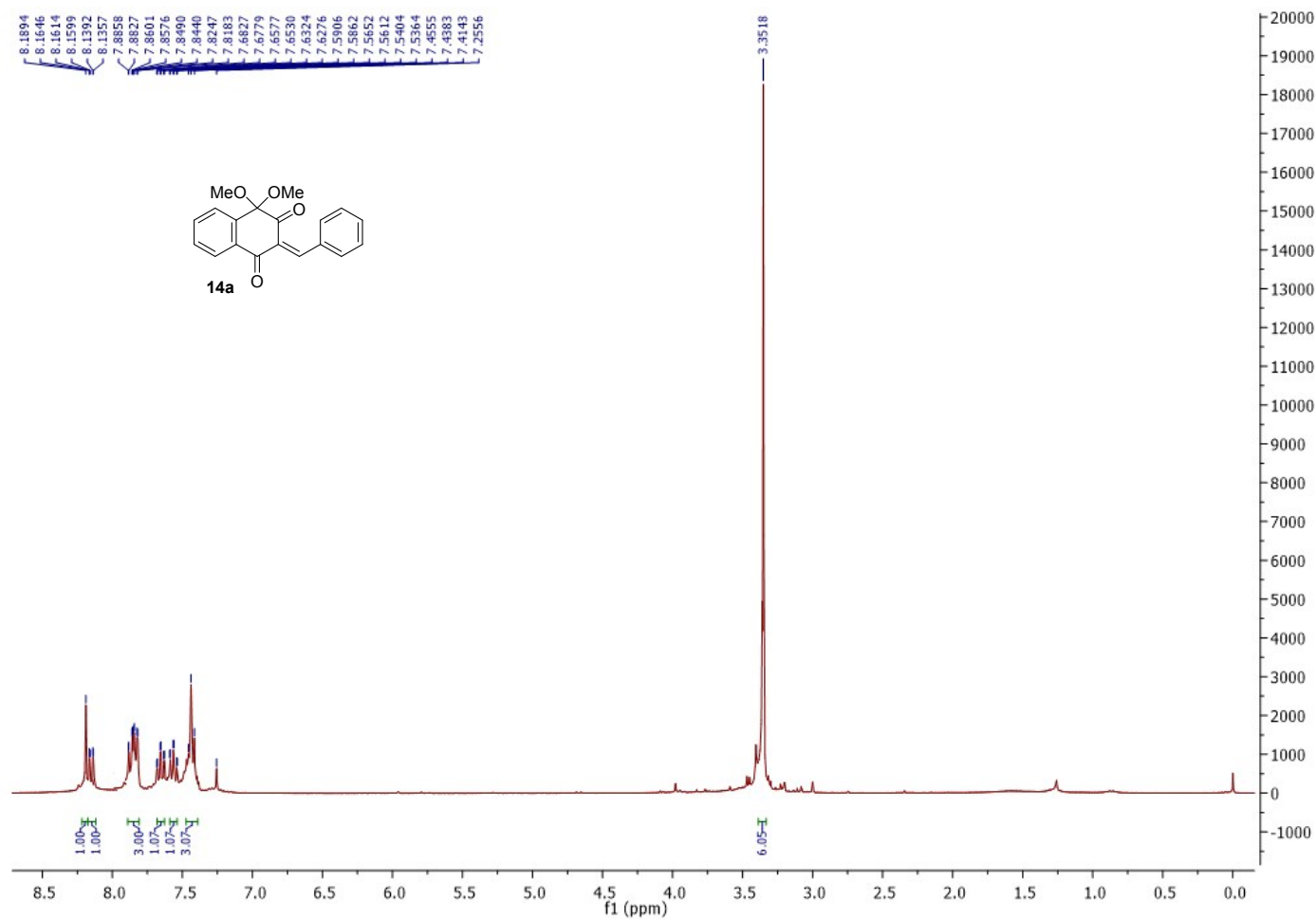
2,2,3-Trimethyl-3,4-dihydro-2*H*-benzo[*h*]chromene-5,6-dione (37c**)**³ Oil; Yield 12%; ^1H NMR (CDCl_3 , 500 MHz) δ 8.06 (d, $J = 7.6, 1.1$ Hz, 1H), 7.81 (d, $J = 7.6$ Hz, 1H), 7.69 (dd appearing as t, $J = 7.6$ Hz, 1H), 7.51 (dd appearing as t, $J = 7.6$ Hz, 1H), 2.70 (dd, $J = 17.6, 5.3$ Hz, 1H), 2.15 (dd, $J = 18.8, 10.1$ Hz, 1H), 1.97–1.90 (m, 1H), 1.54 (s, 3H), 1.29 (s, 3H), 1.08 (d, $J = 6.9, 3\text{H}$); ^{13}C NMR (CDCl_3 , 125 MHz) δ 179.9, 178.6, 161.8, 134.8, 132.5, 130.7, 130.2, 128.6, 124.1, 113.1, 83.1, 34.9, 27.1, 24.6, 20.5, 16.4. ESI-MS m/z positive 257 ($\text{M}+\text{H}$) $^+$, 279 ($\text{M}+\text{Na}$) $^+$; Anal. Calcd for $\text{C}_{16}\text{H}_{16}\text{O}_3$: C, 74.98; H, 6.29. Found: C, 75.30; H, 6.00.

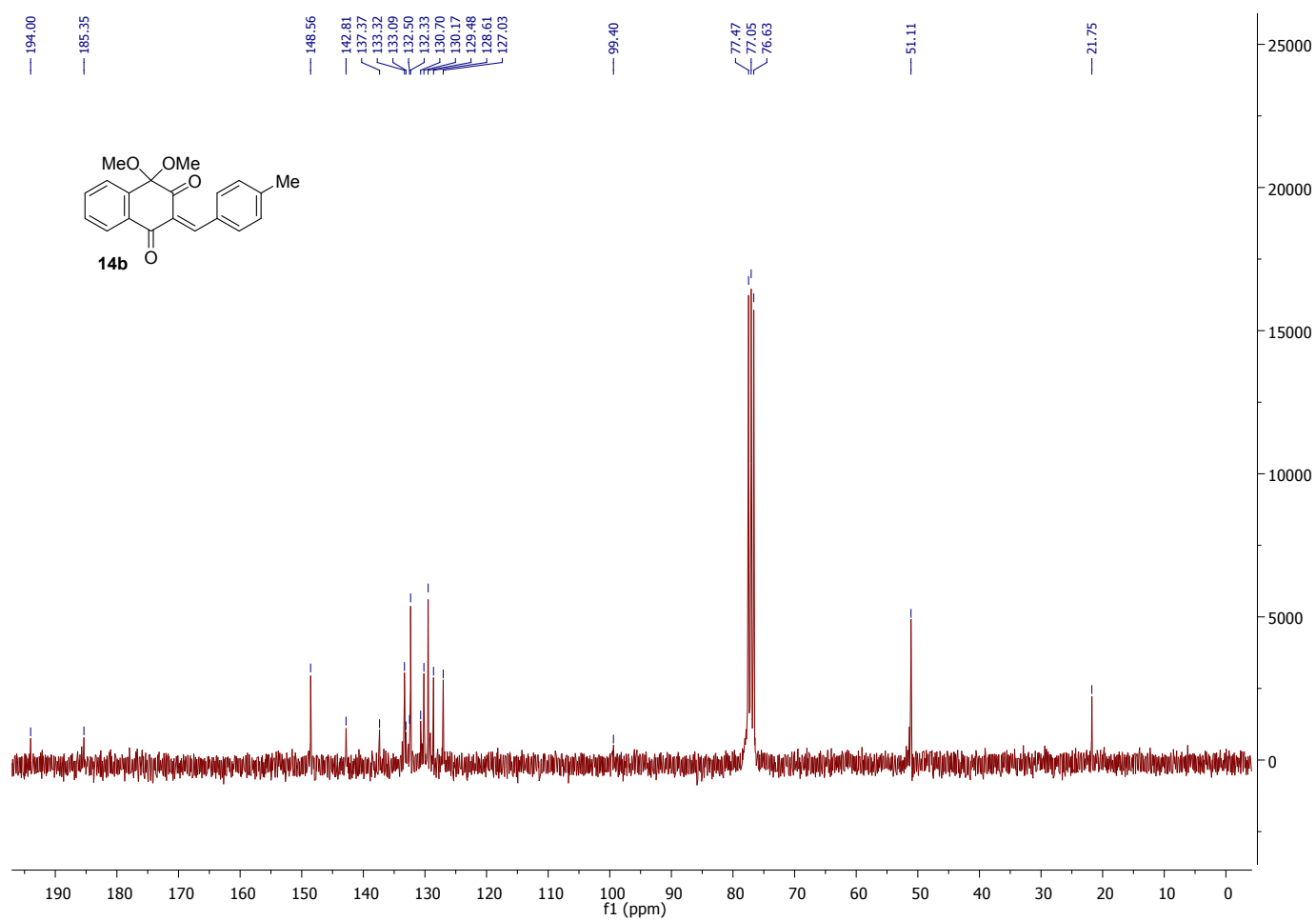
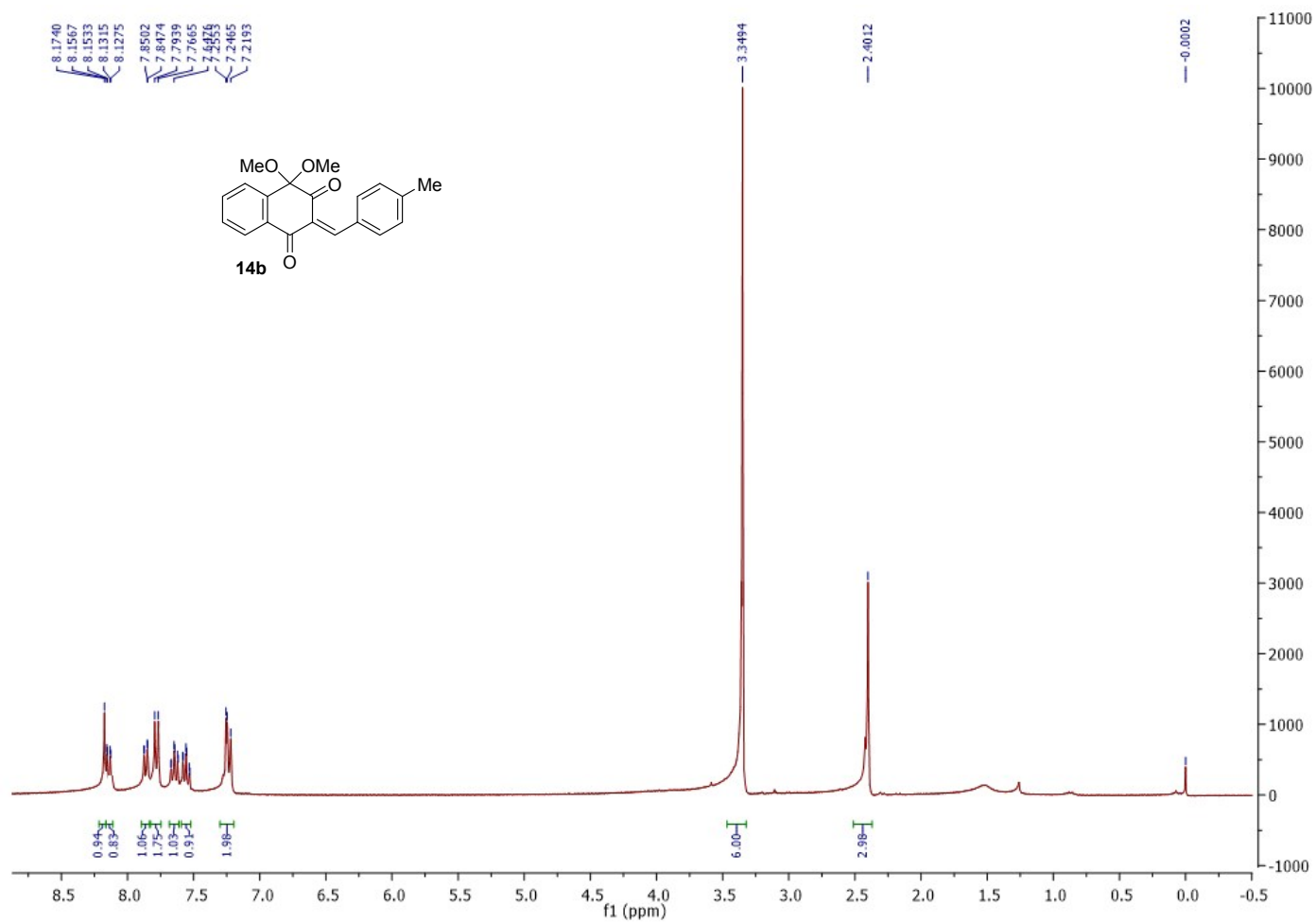
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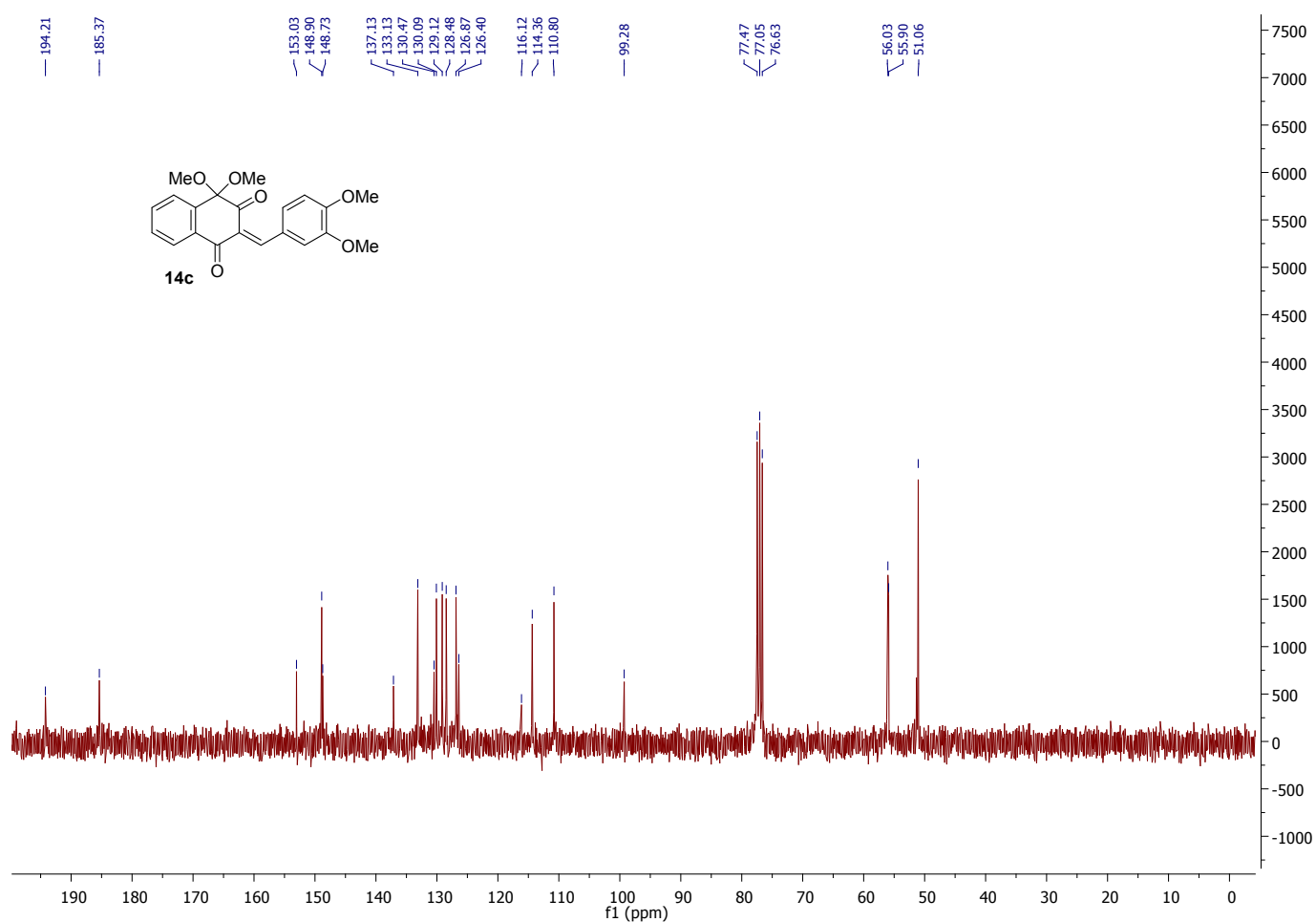
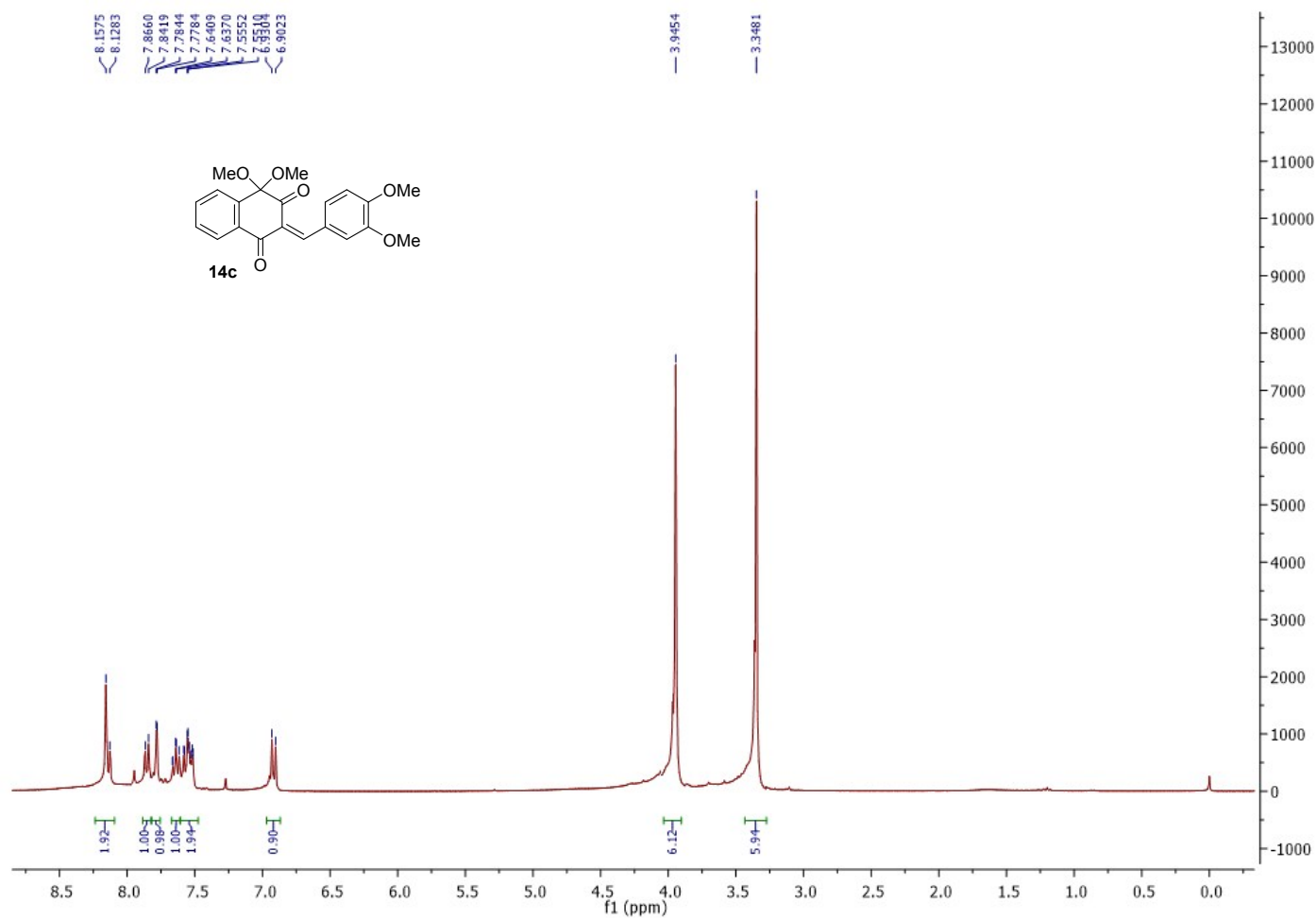
1. S. B. Ferreira, F. de C. da Silva, F. A. F. M. Bezerra, M. C. S. Lourenco, C. R. Kaiser, A. C. Pinto, V. F. Ferreira, Arch. Pharm. Chem. Life Sci., 2010, 343, 81–90.
2. Y. Gu, J. Barrault, F. Jérôme, Adv. Synth. Catal., 2009, 351, 3269–3278.
3. (a) R. G. Cooke, Austral. J. Sci. Res., 1950, 3A, 480; (b) R. G. Cooke, T. C. Sommers, Austral. J. Sci. Res., 1950, 3A, 466.

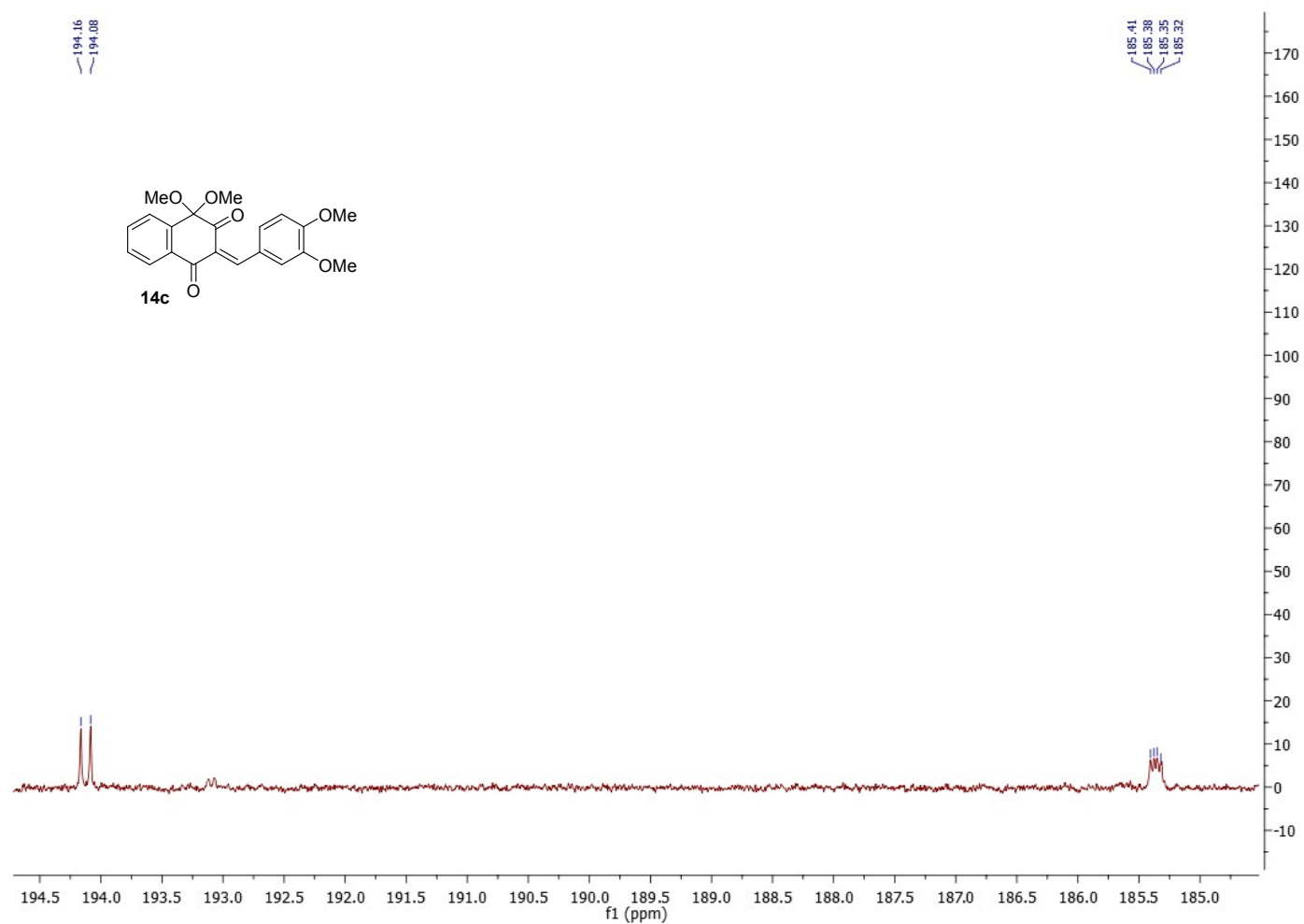
Copies of ^1H NMR and ^{13}C NMR spectra



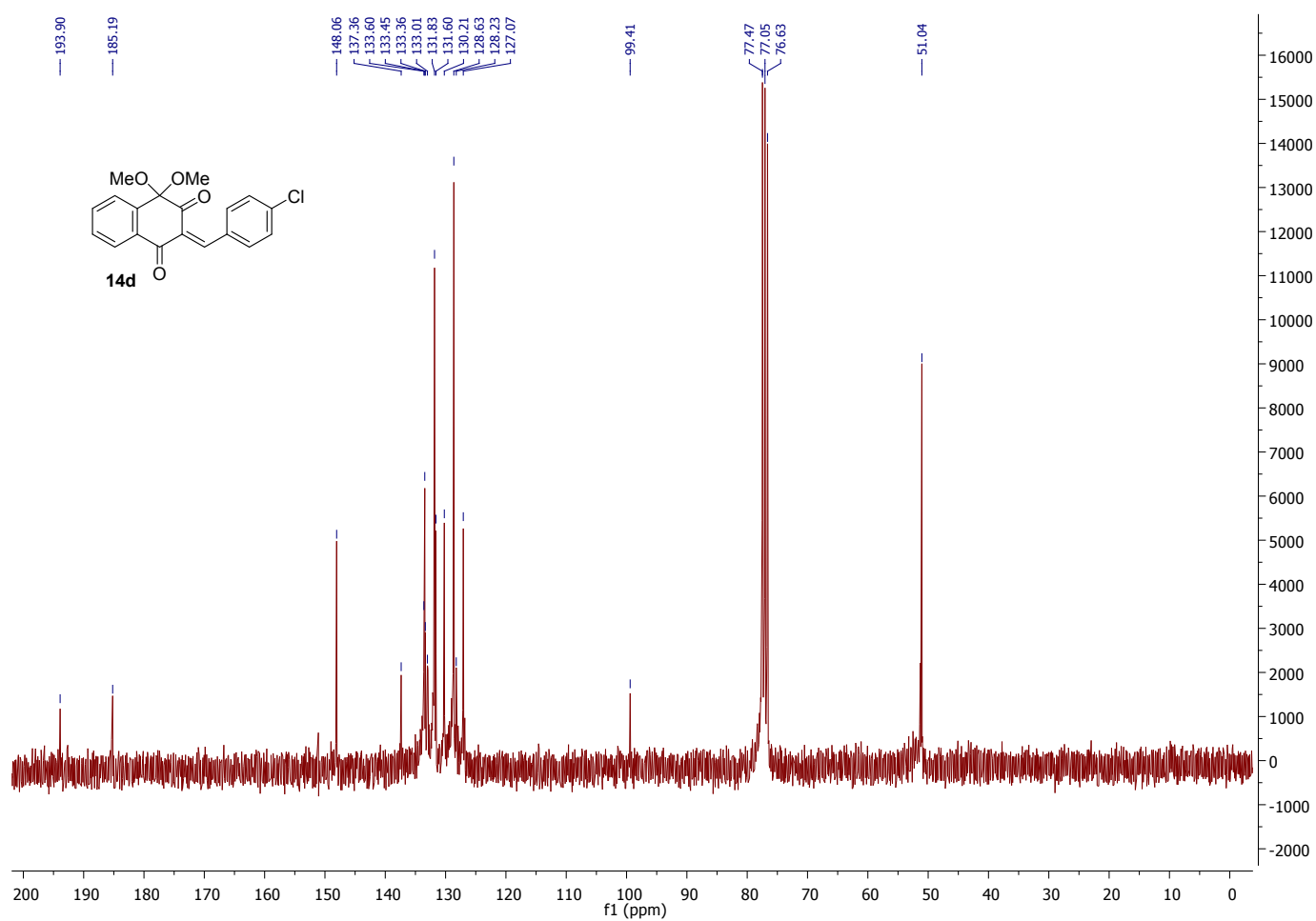
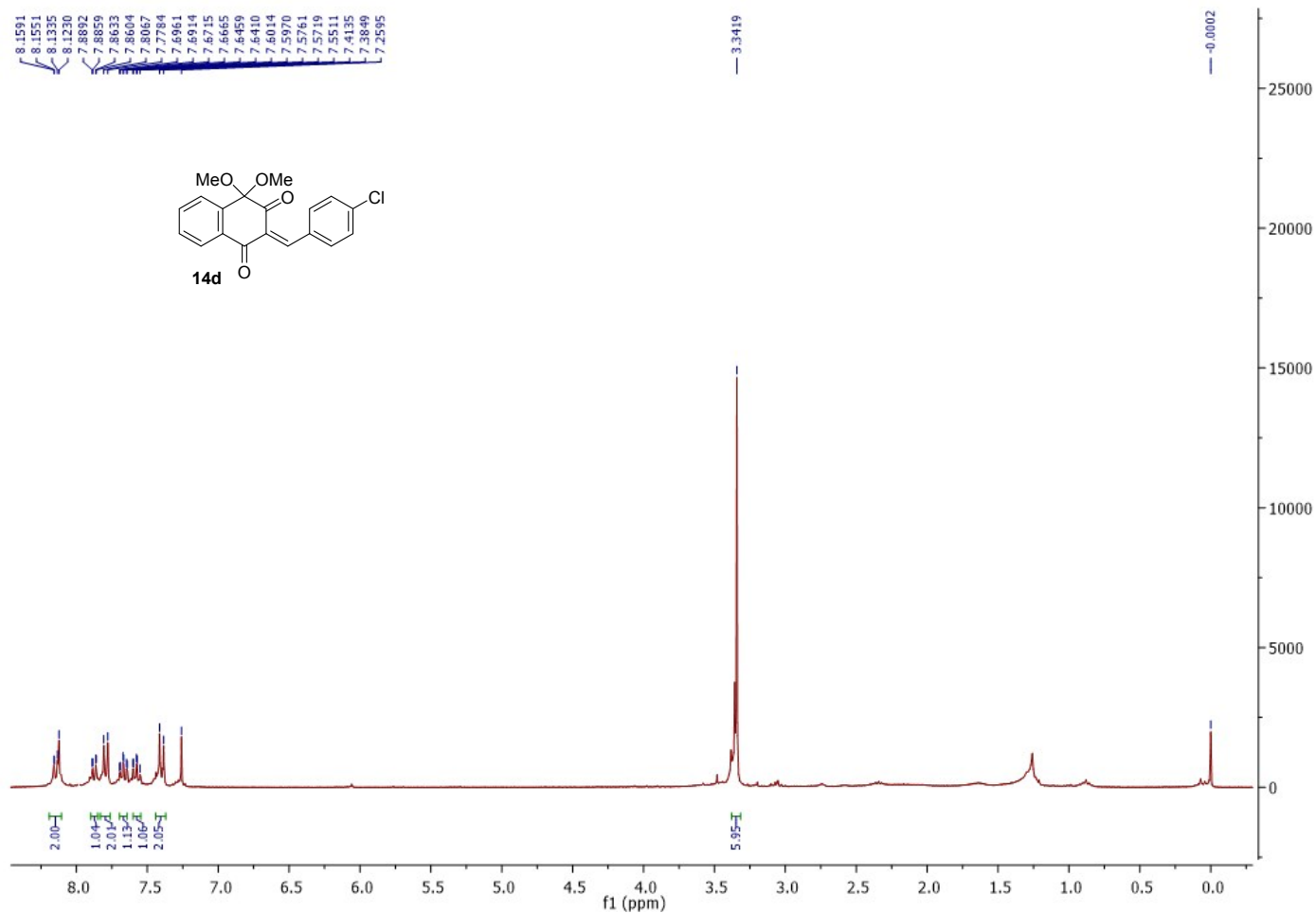


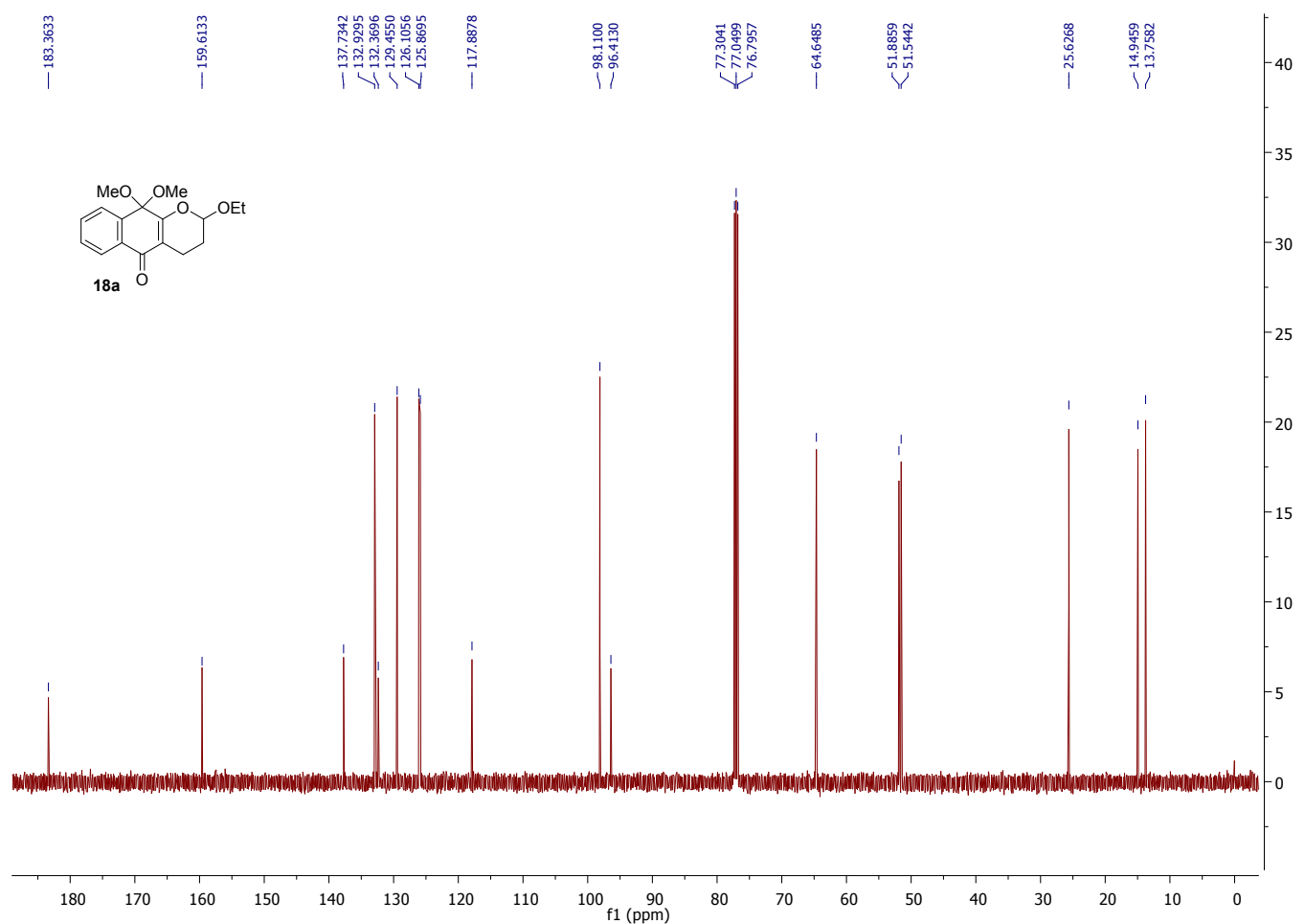
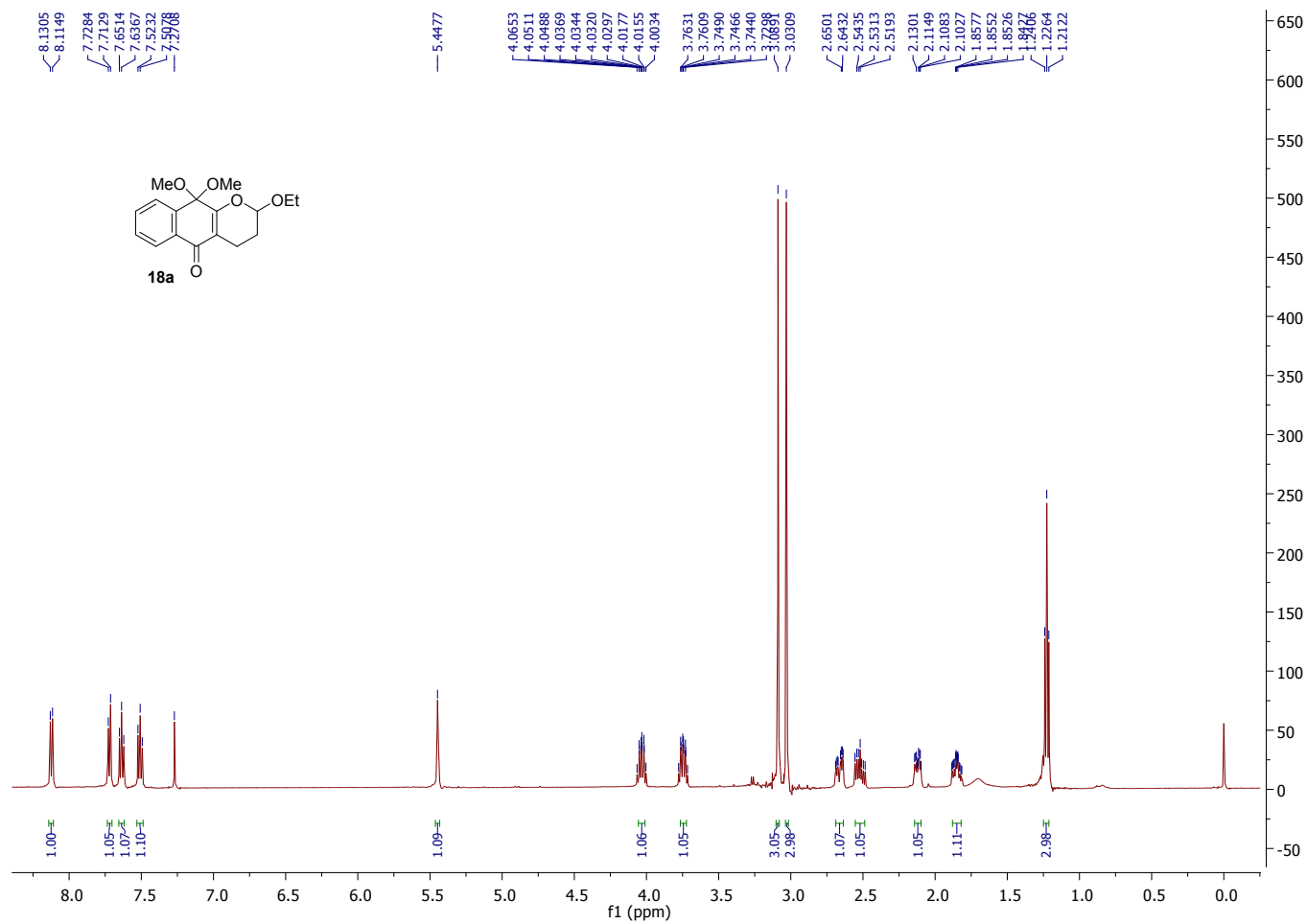


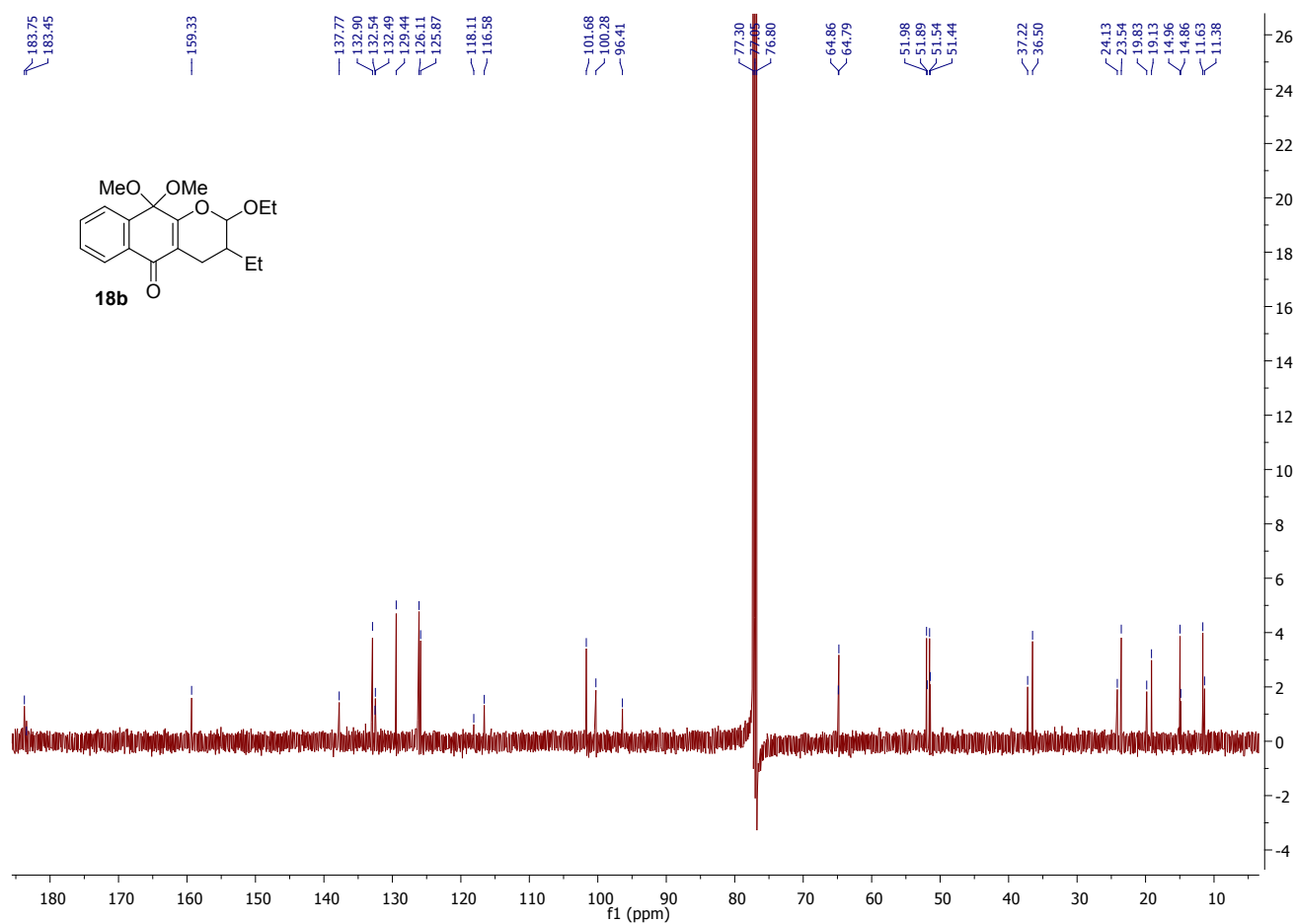
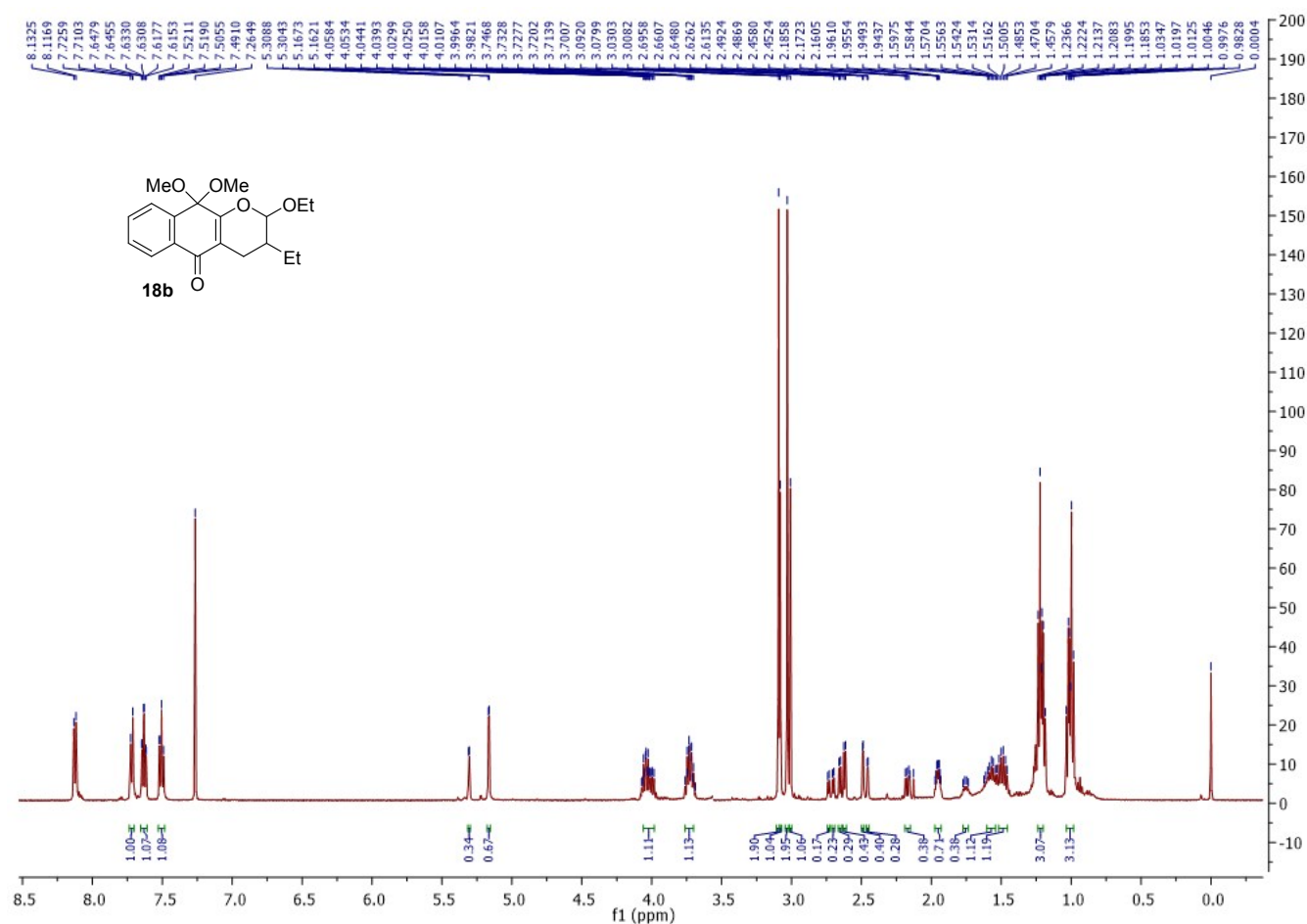




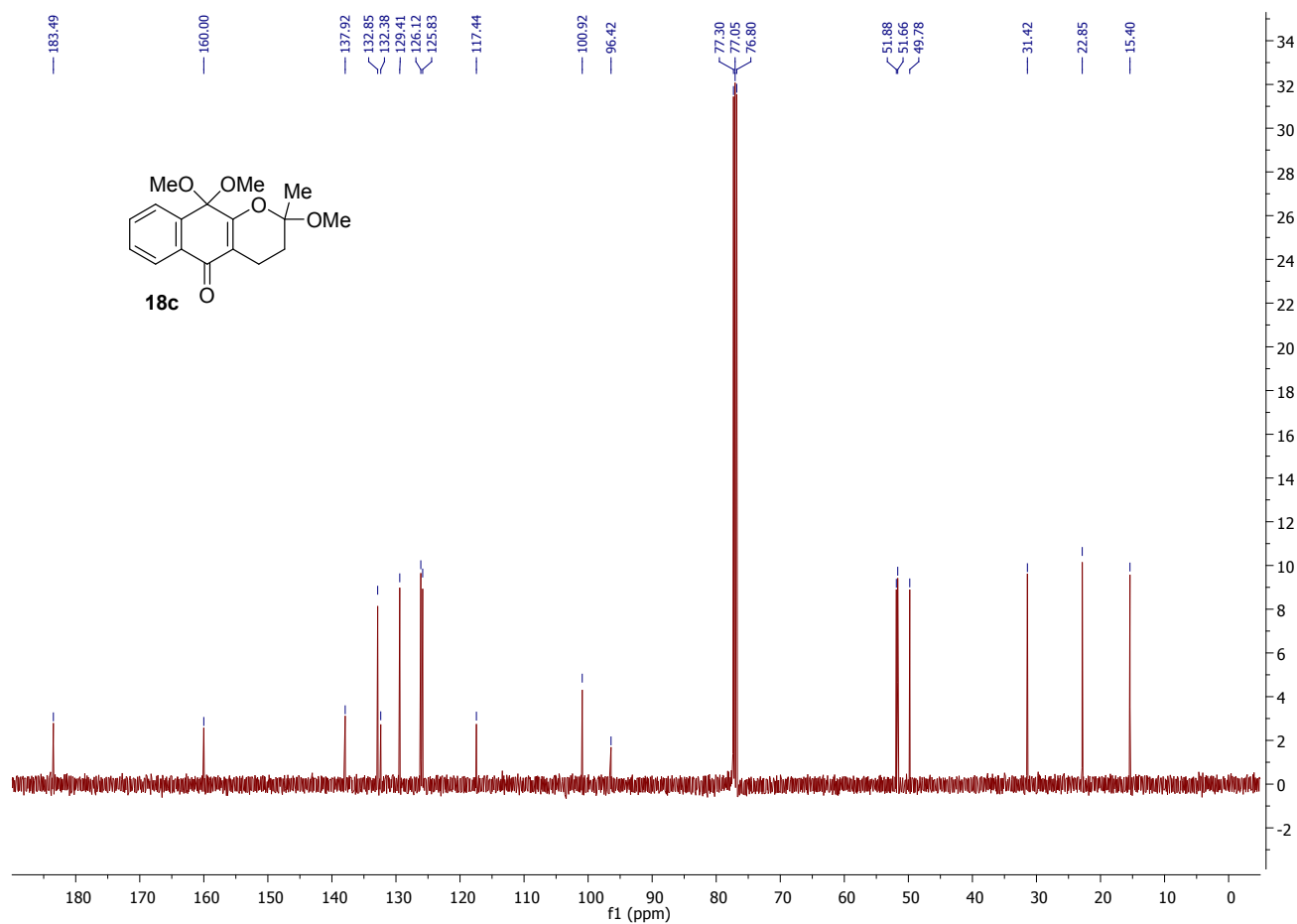
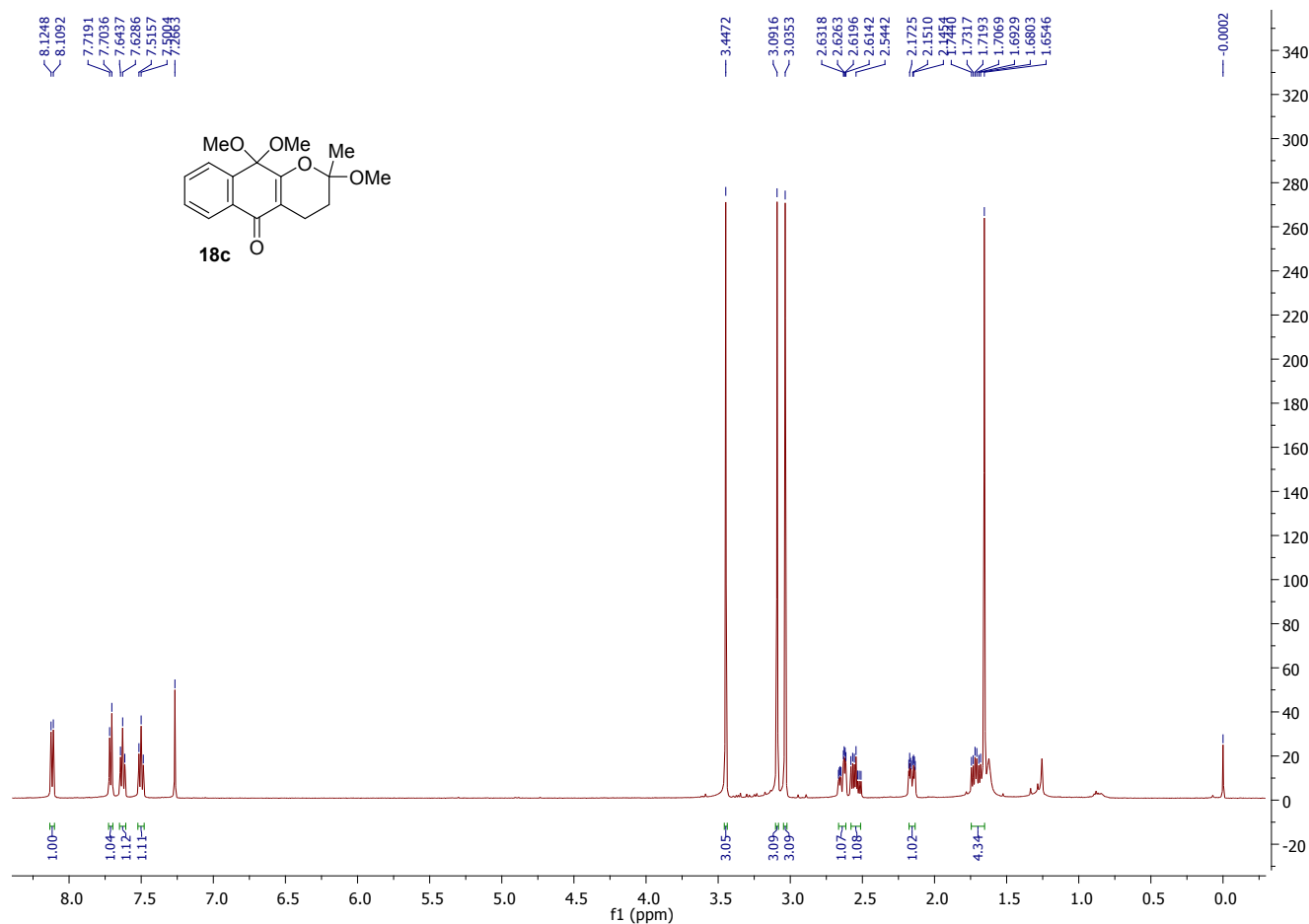
³J_{CH} coupling constants between C1 and C3 carbonyl carbons with the alkenyl hydrogen of compound 14c

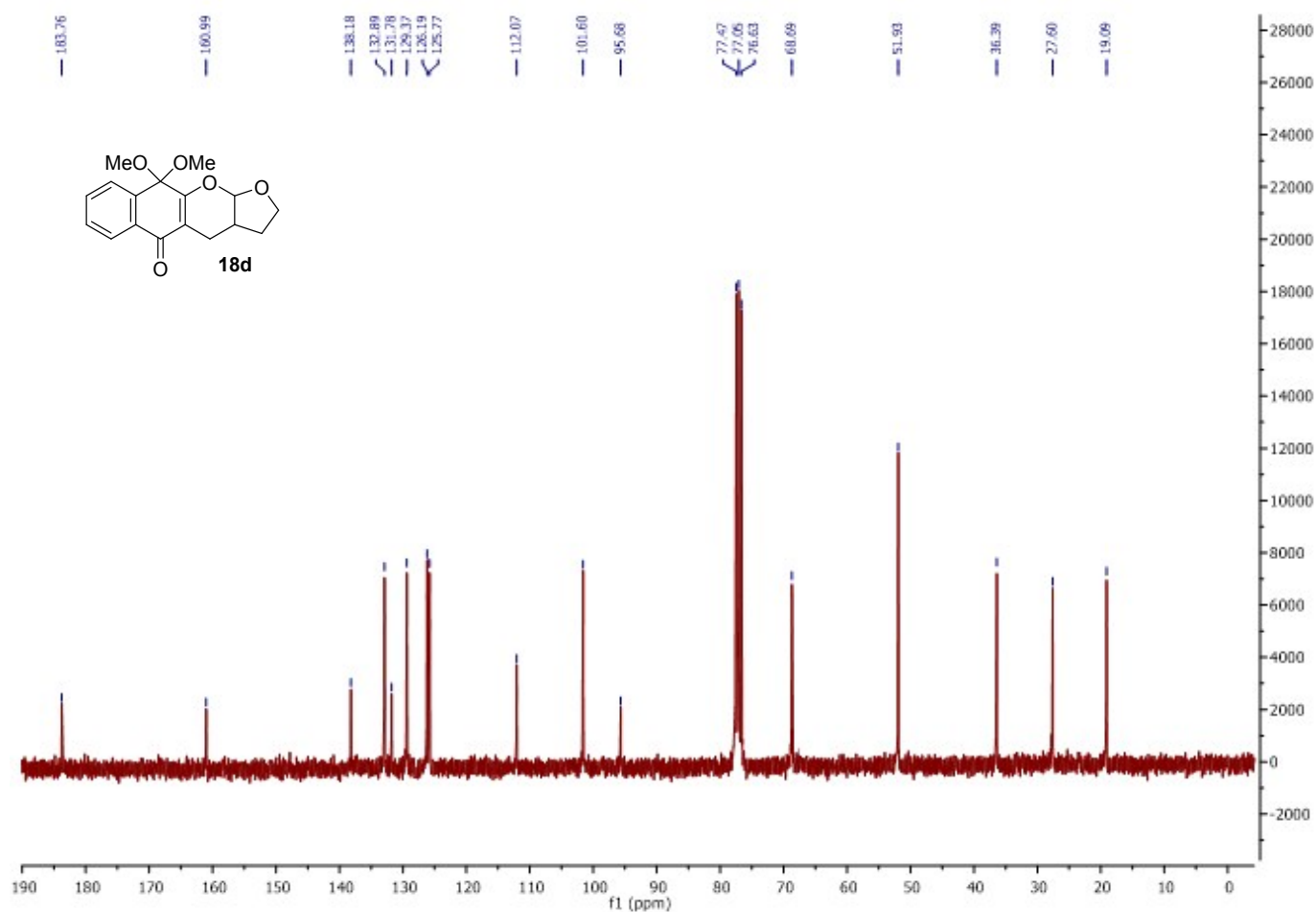
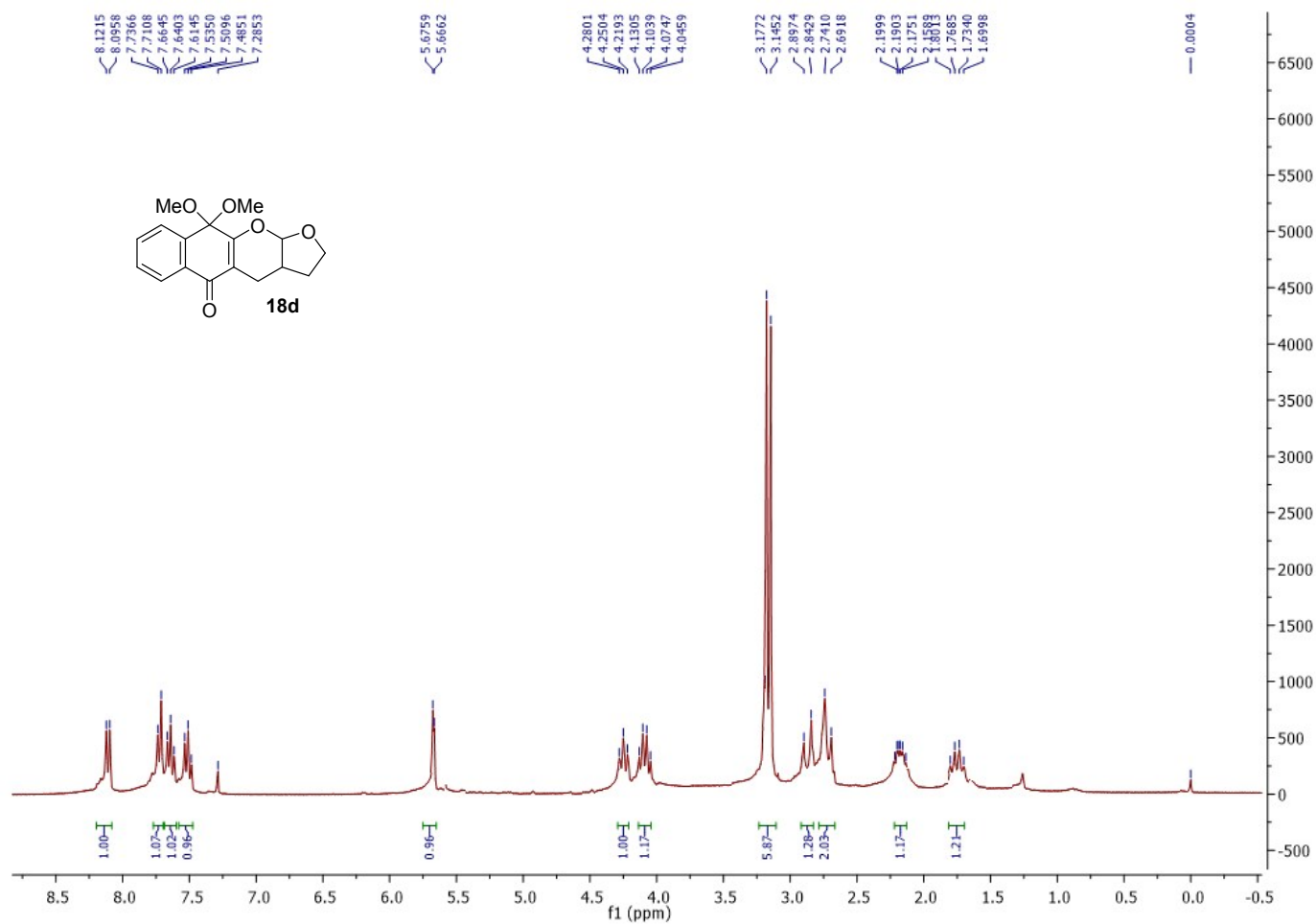


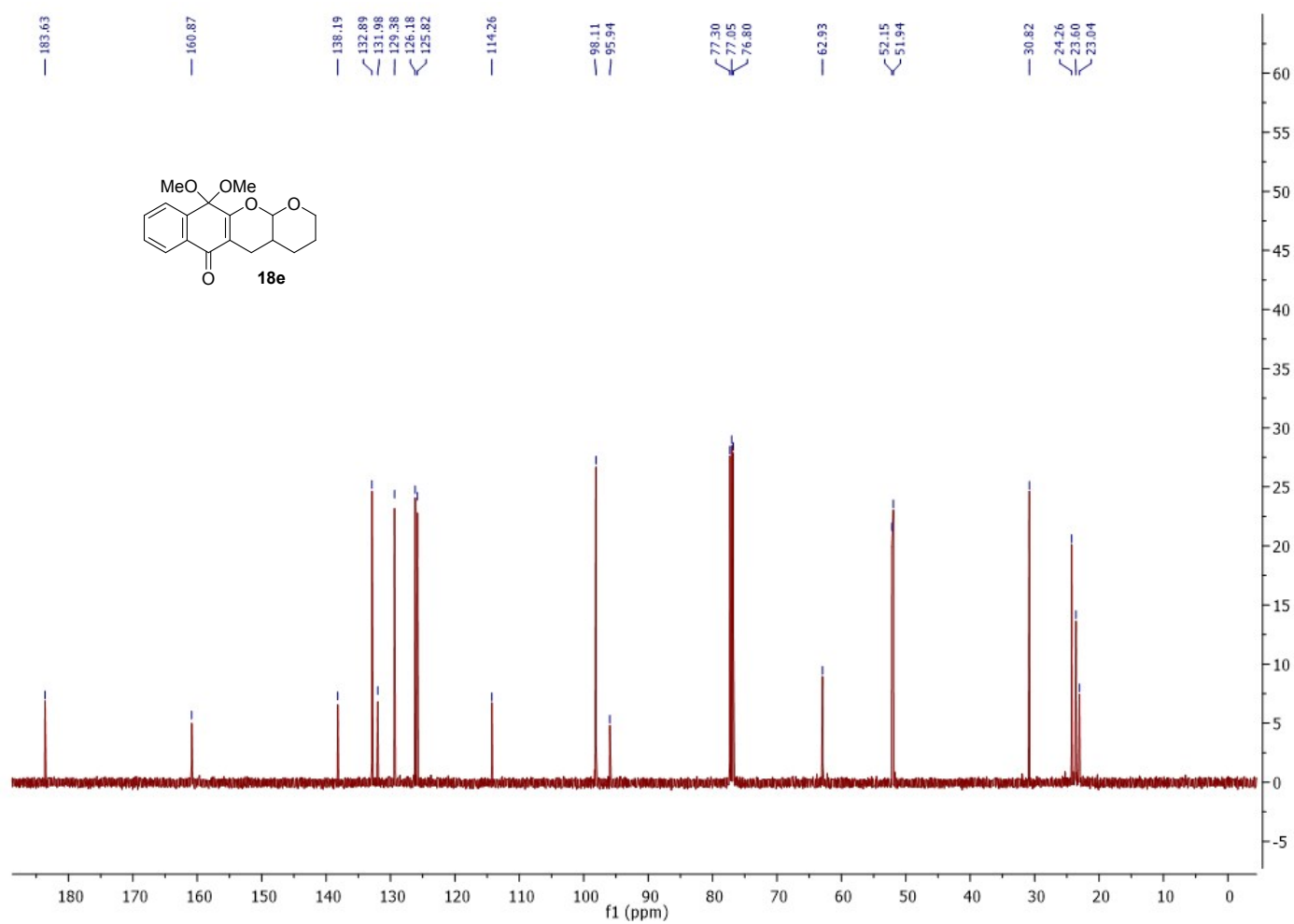
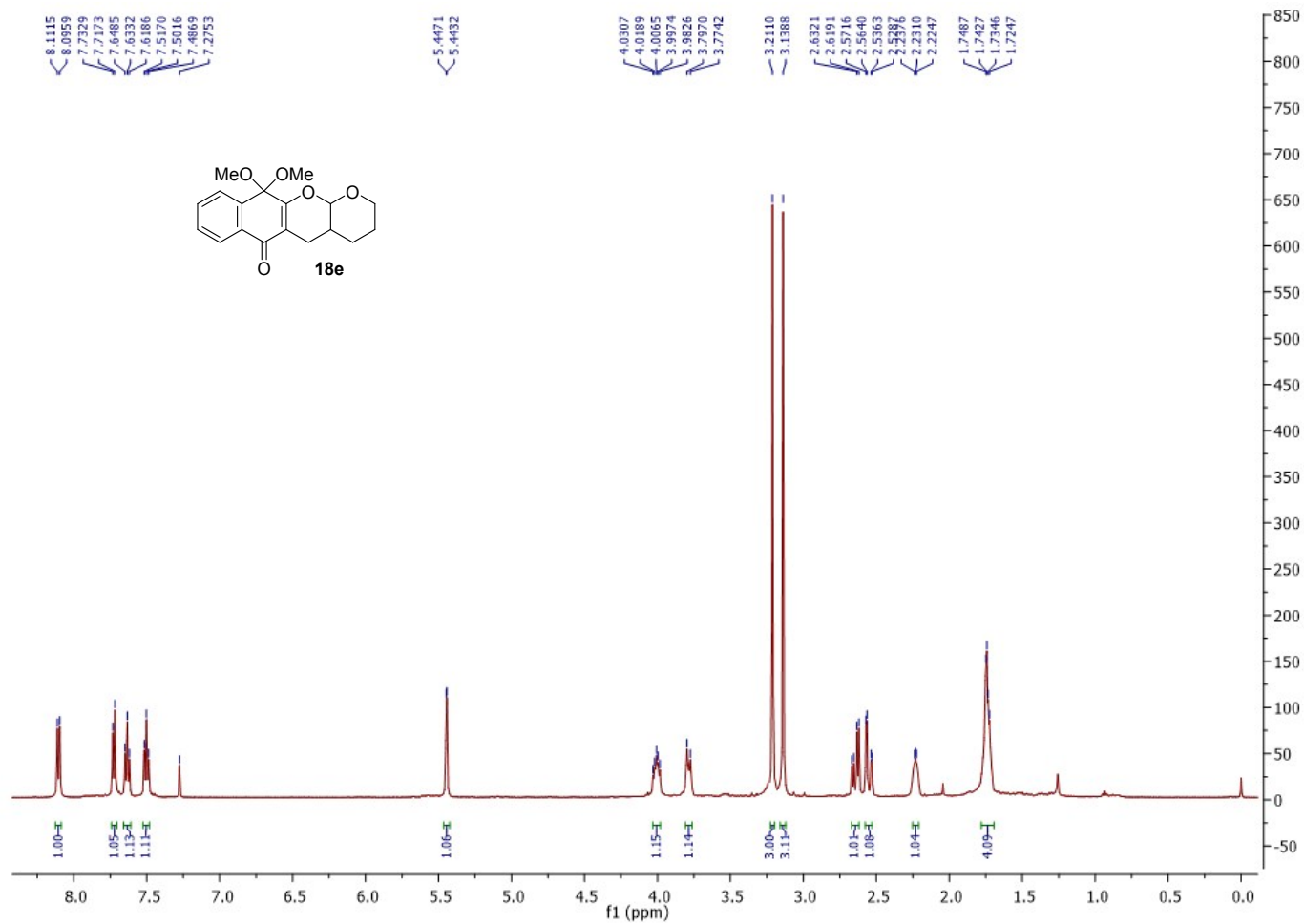


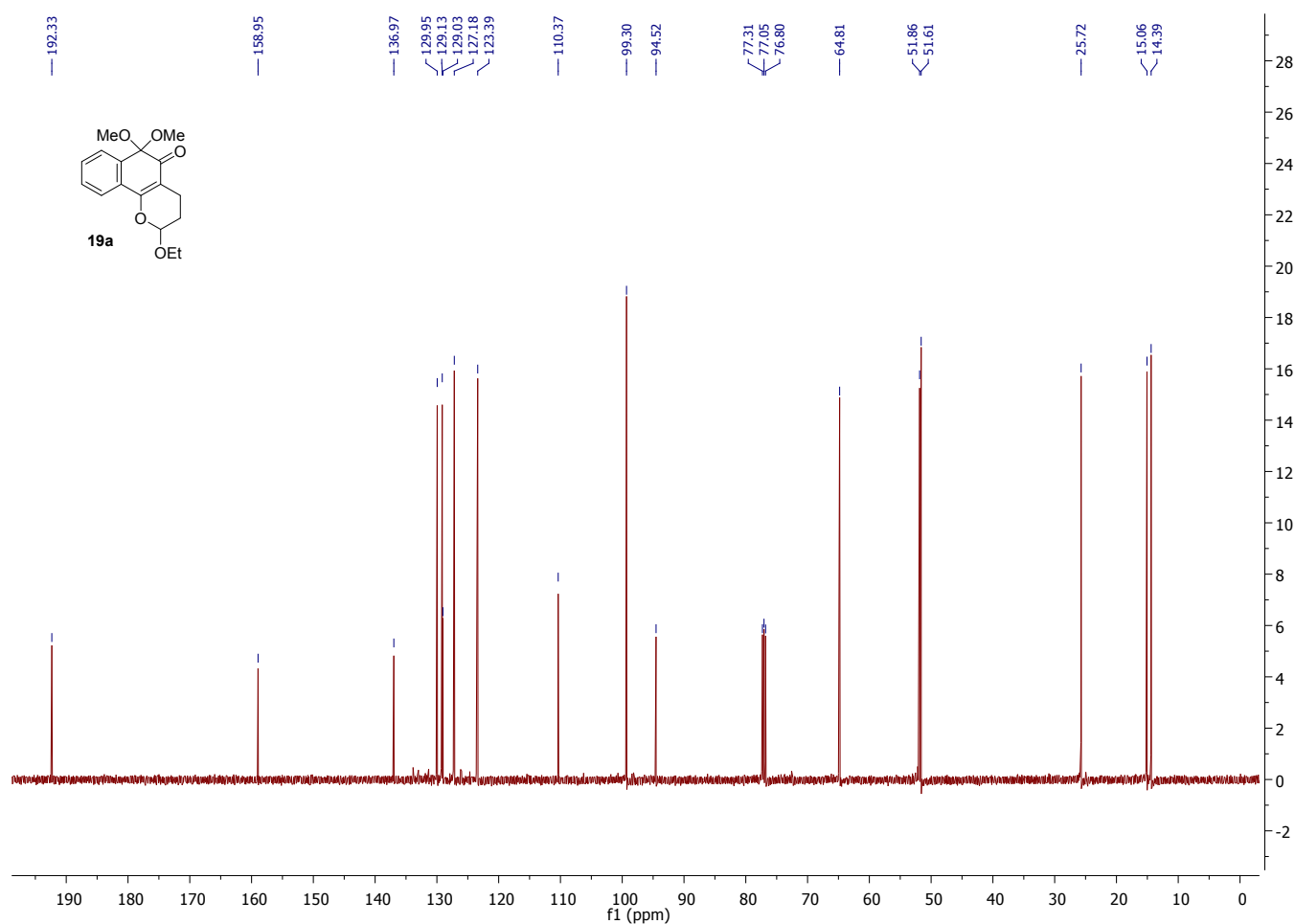
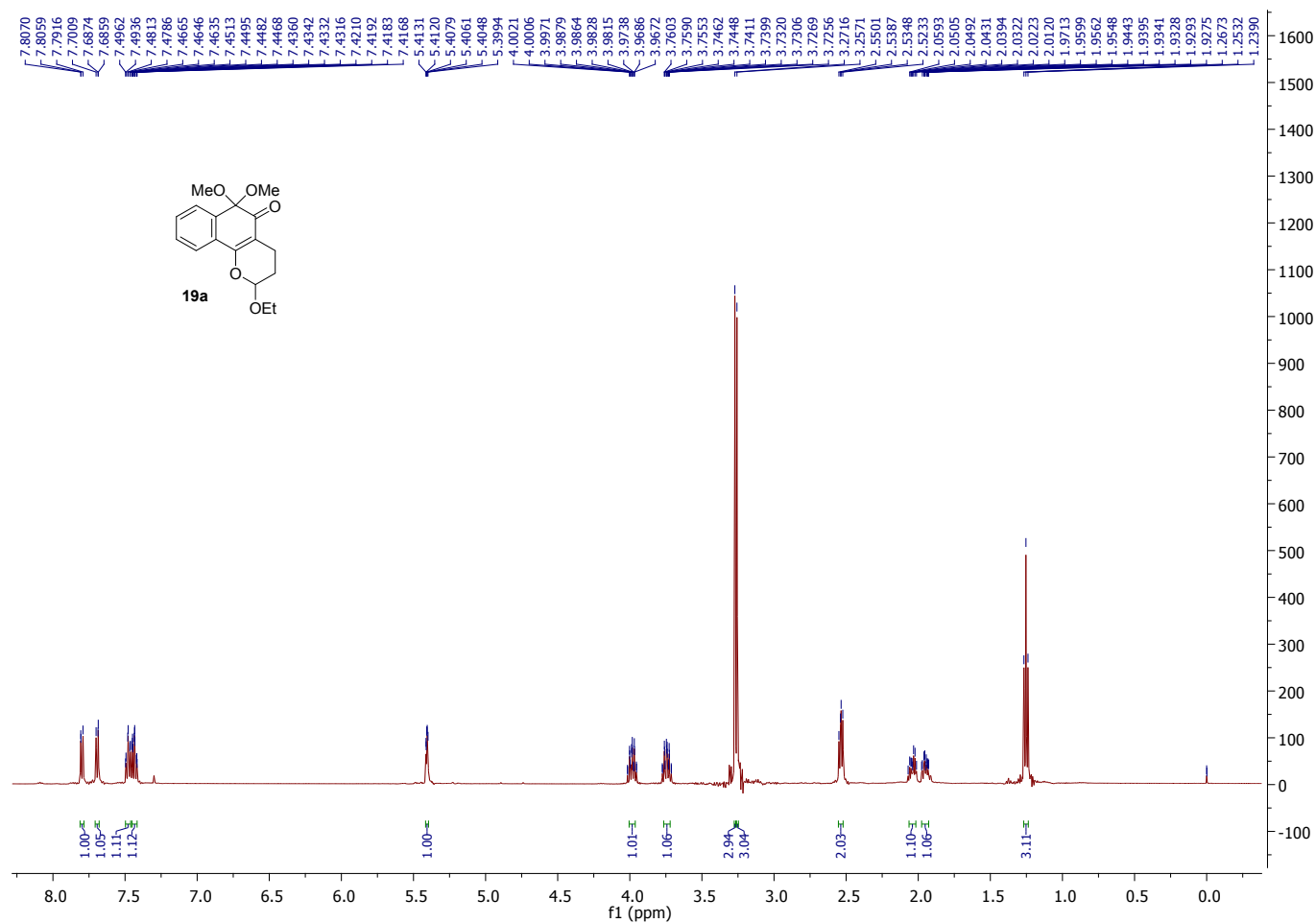


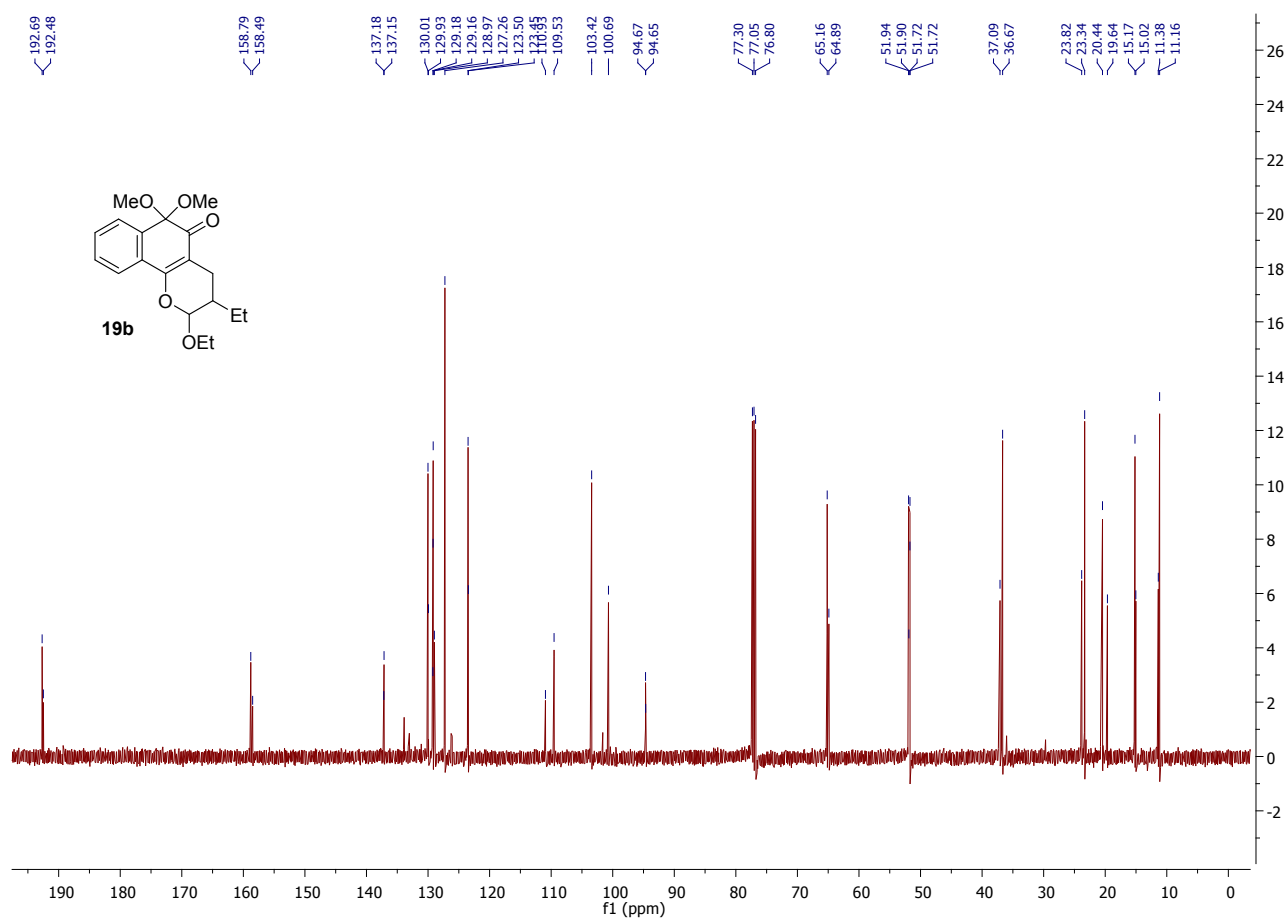
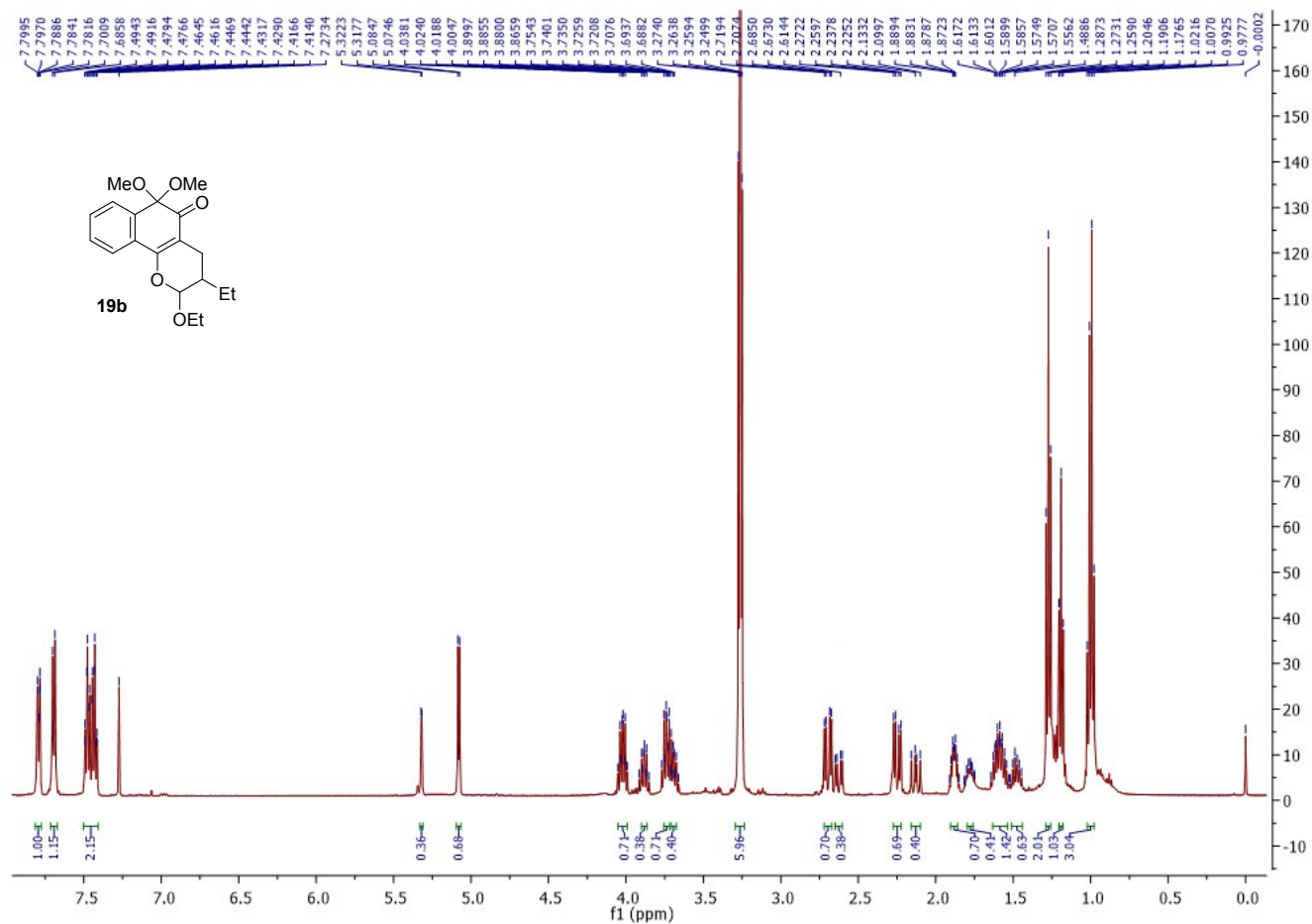
Mixture of diastereoisomers 18b



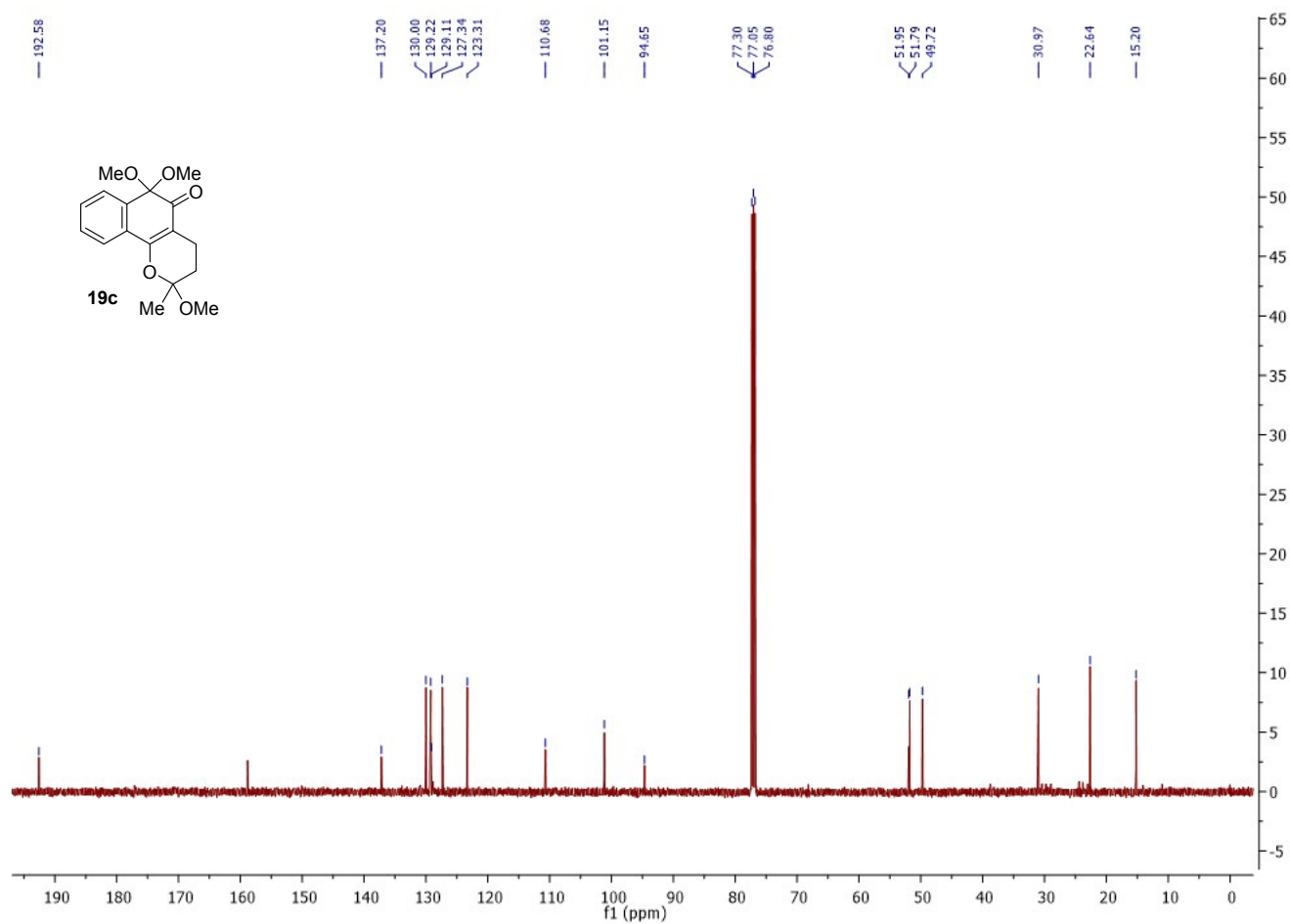
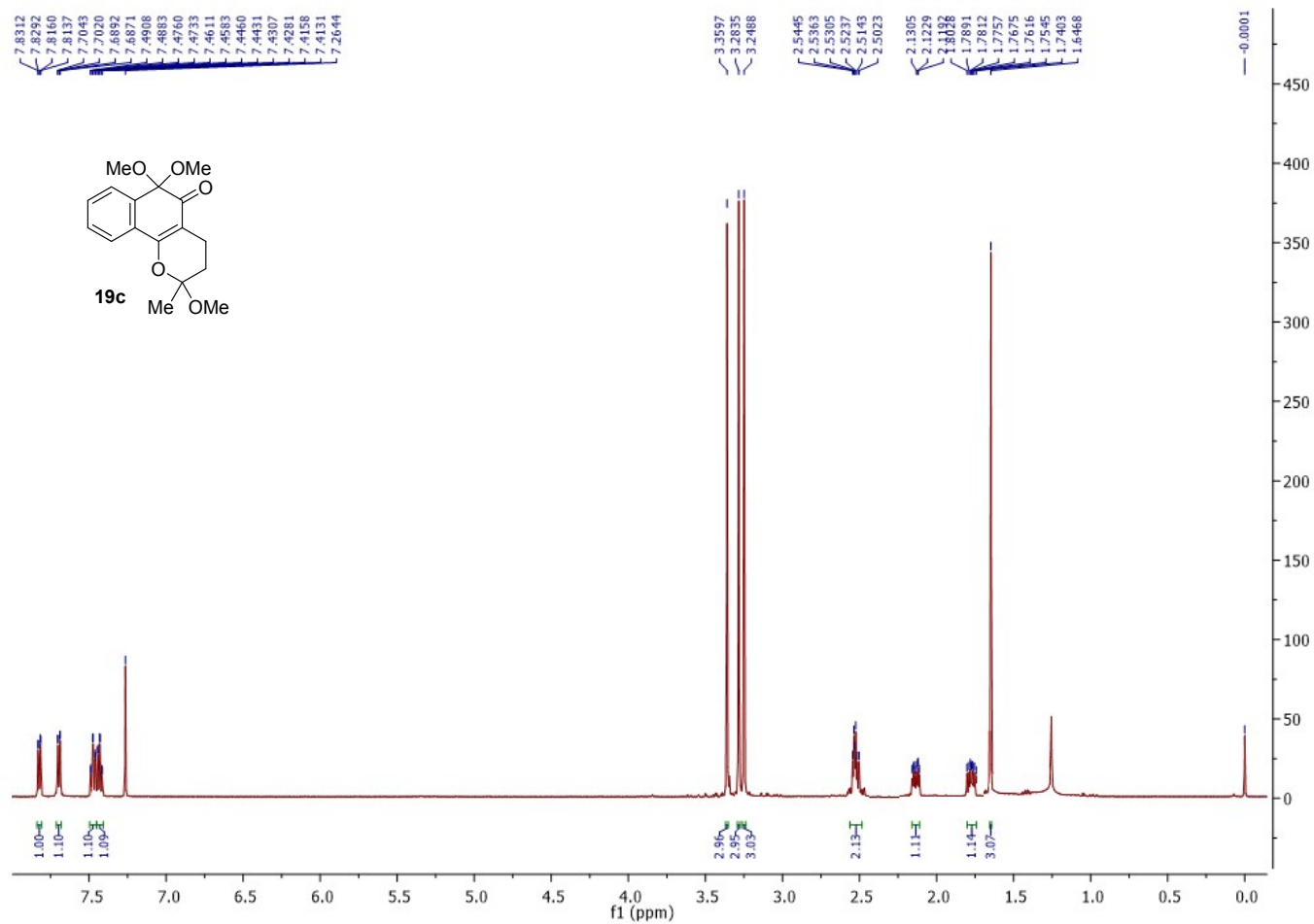


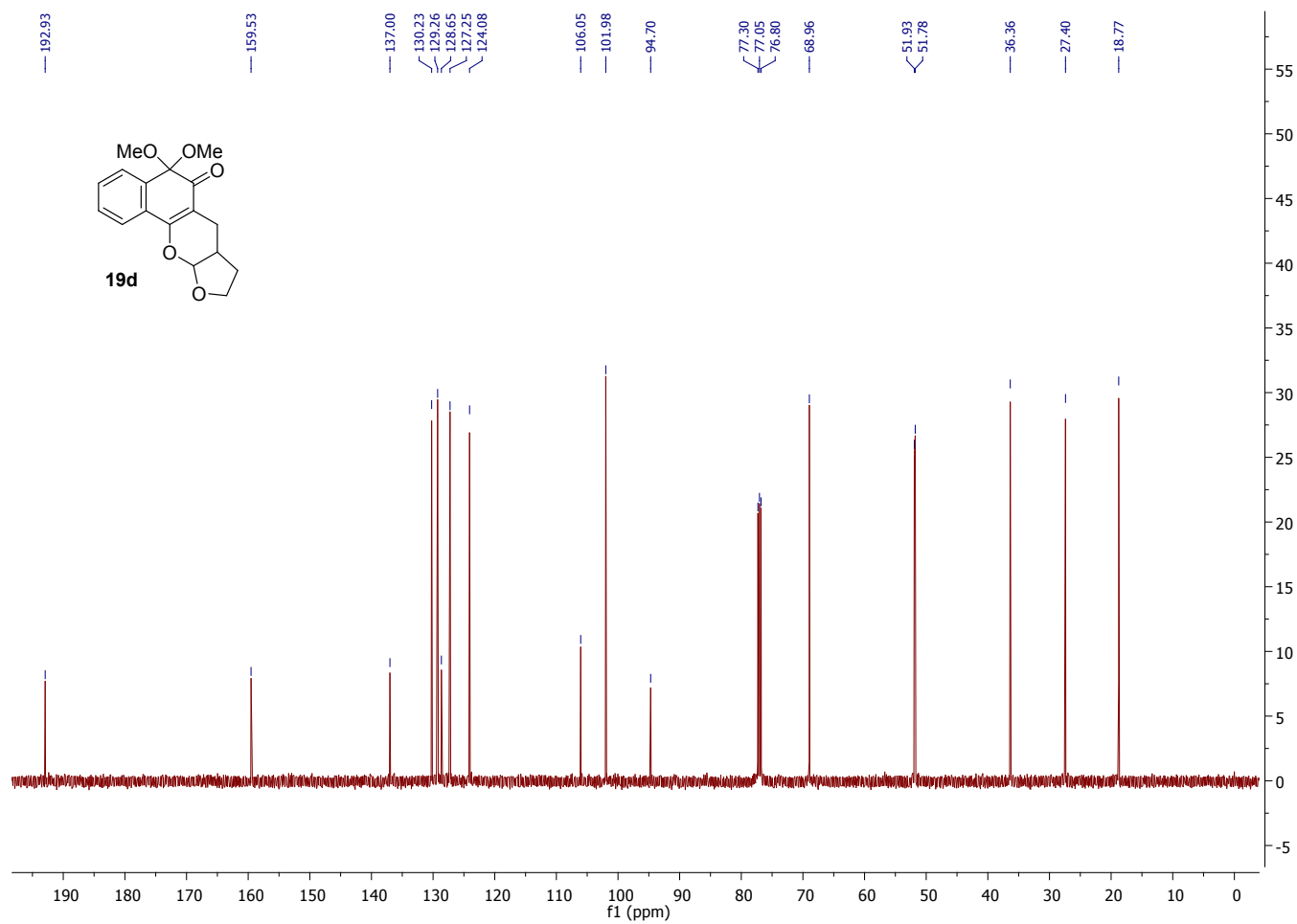
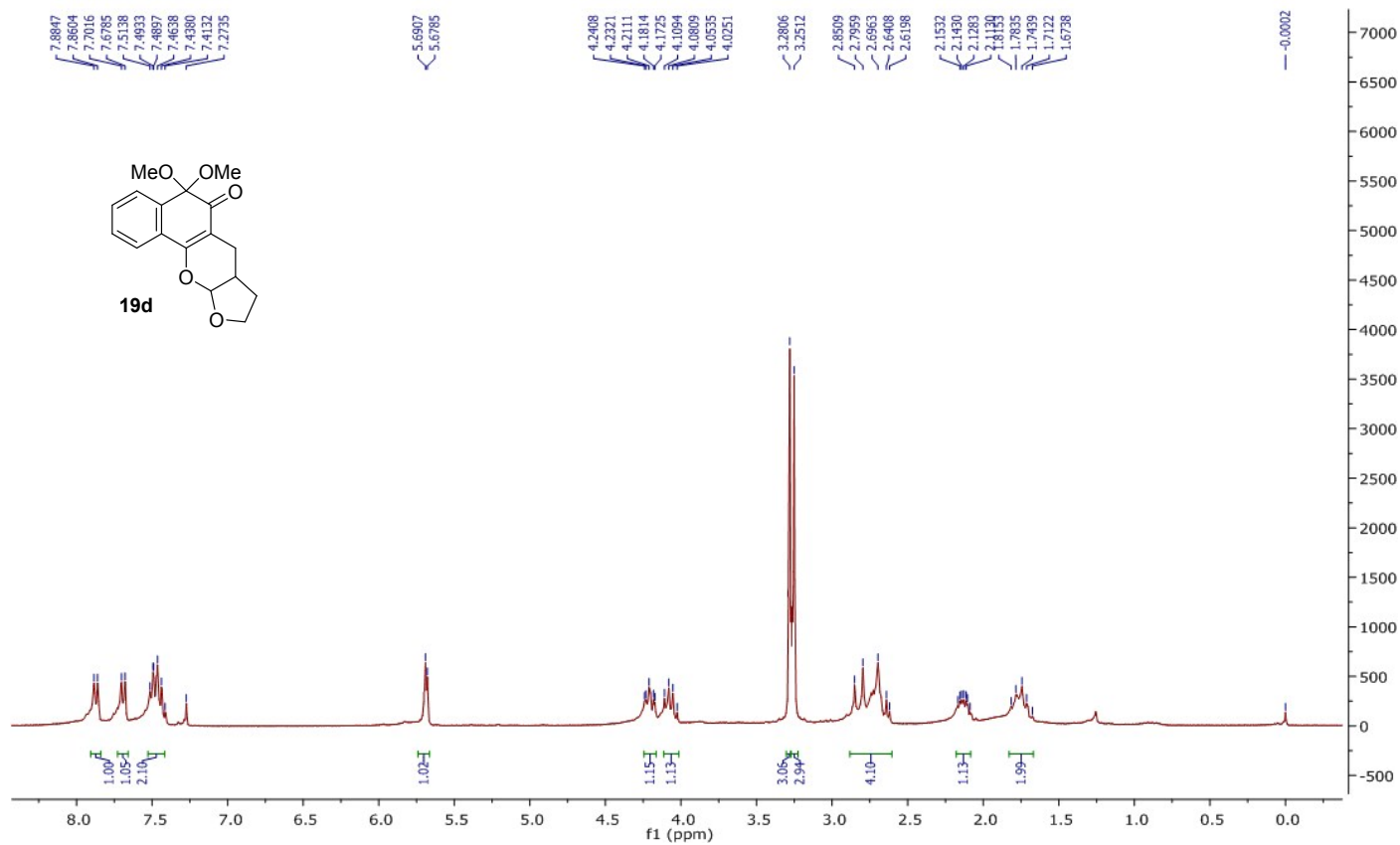


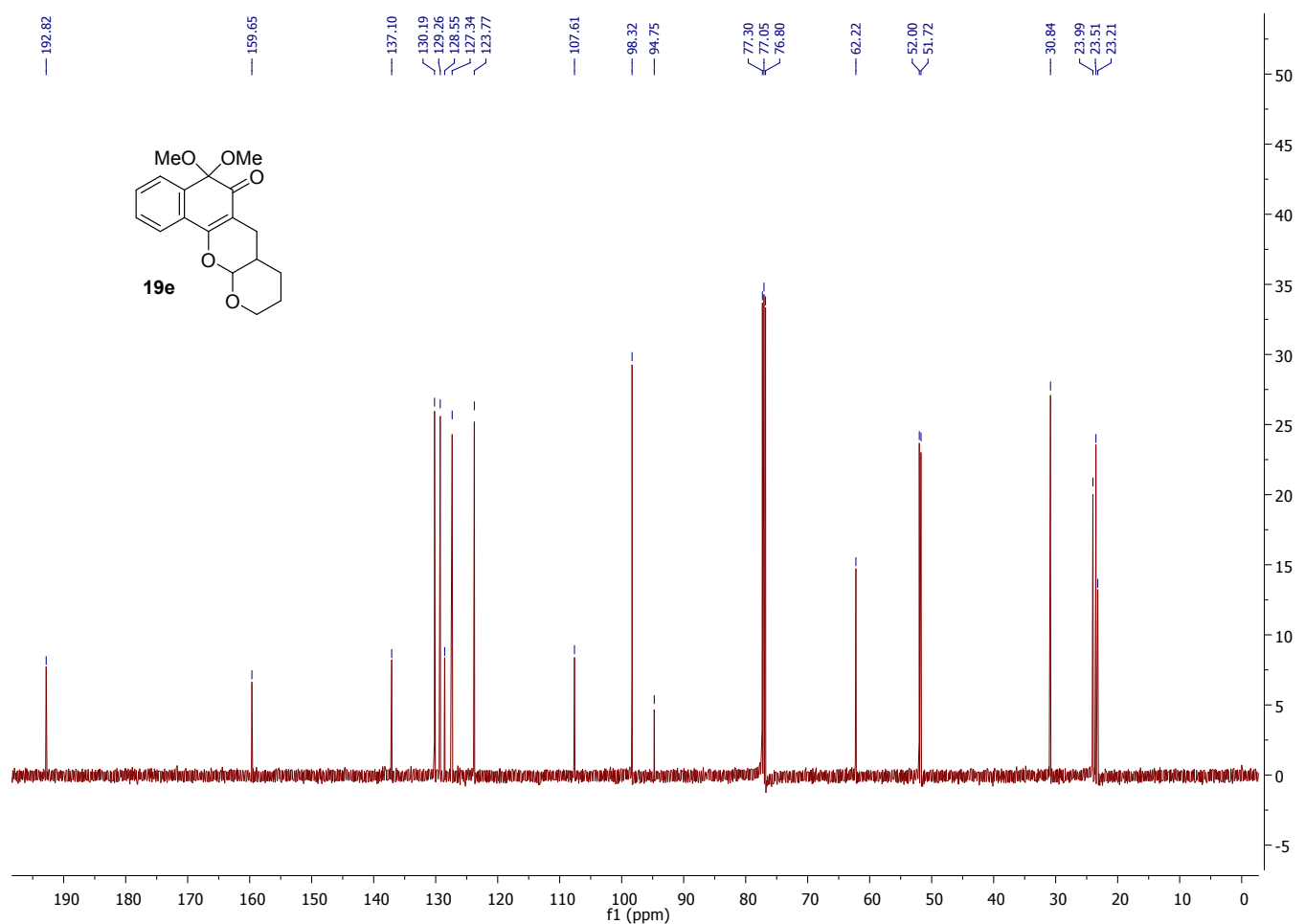
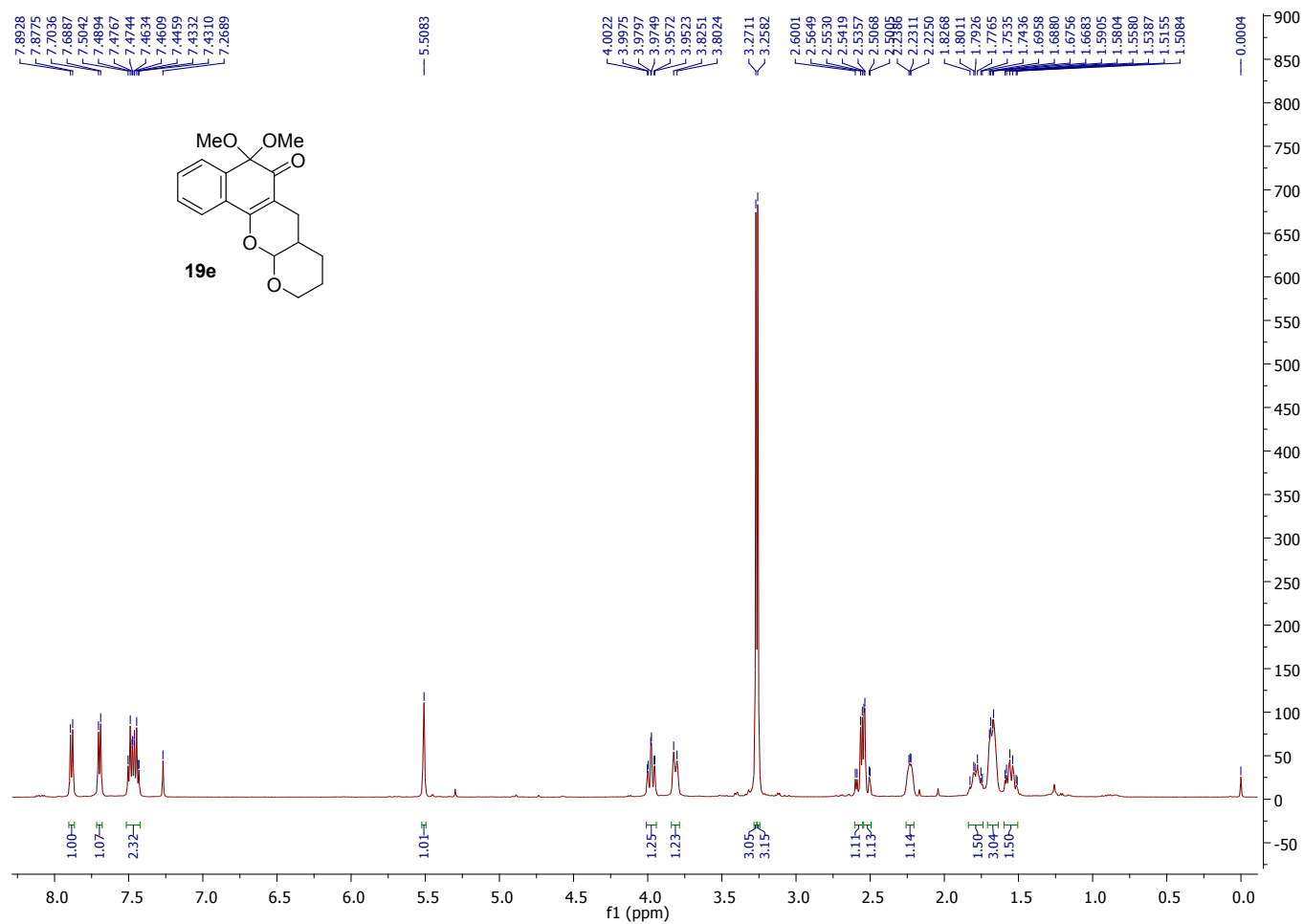


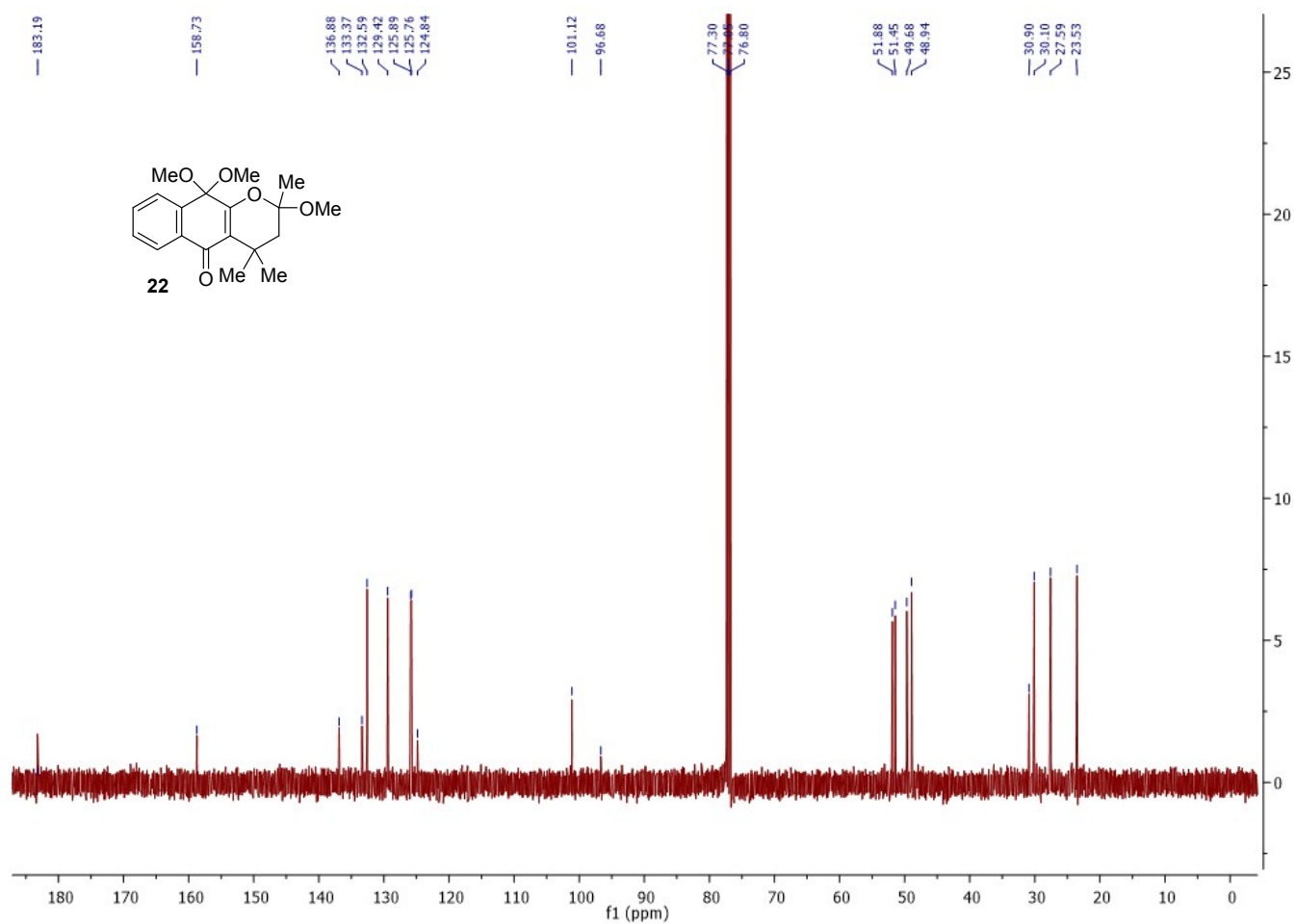
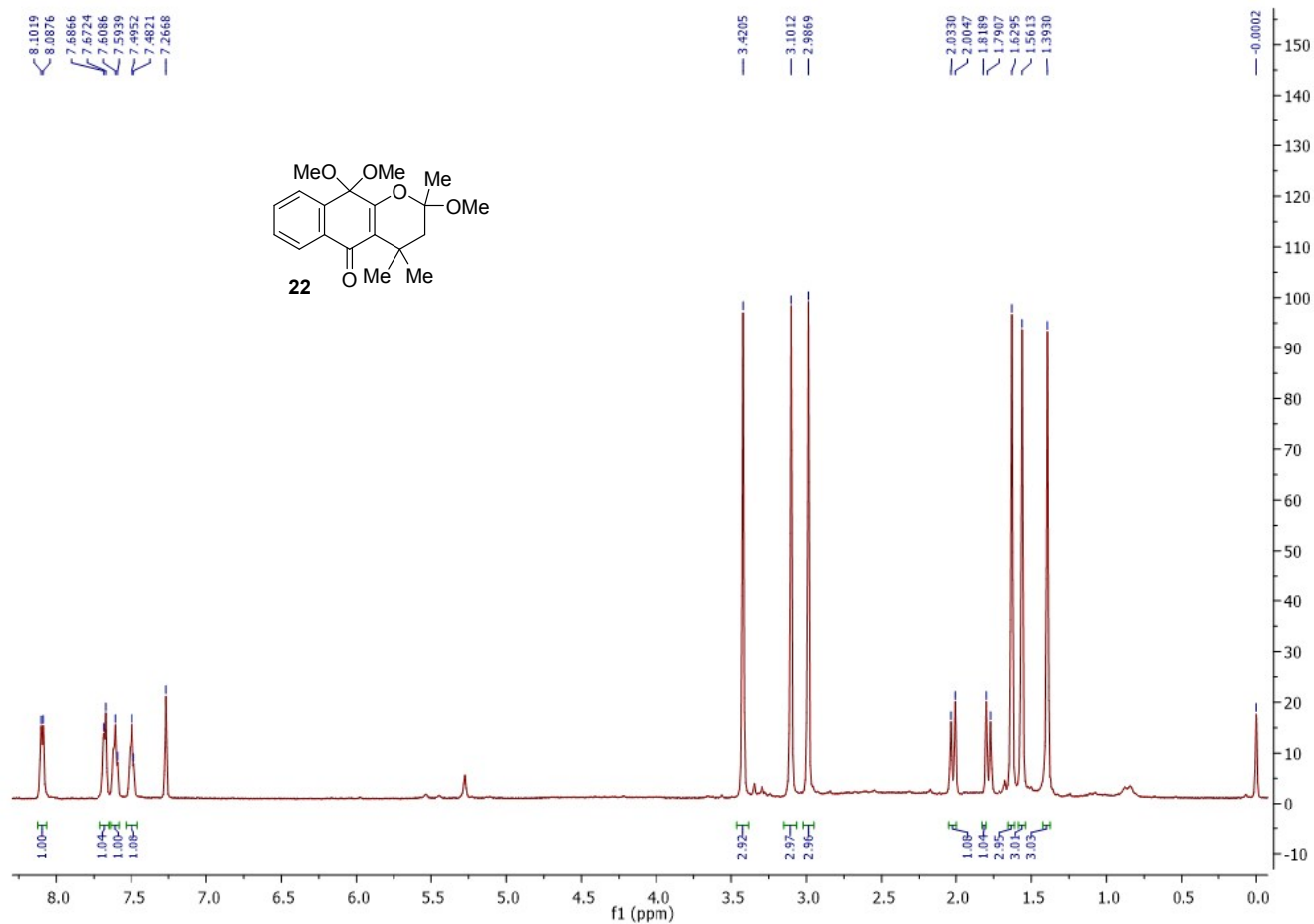


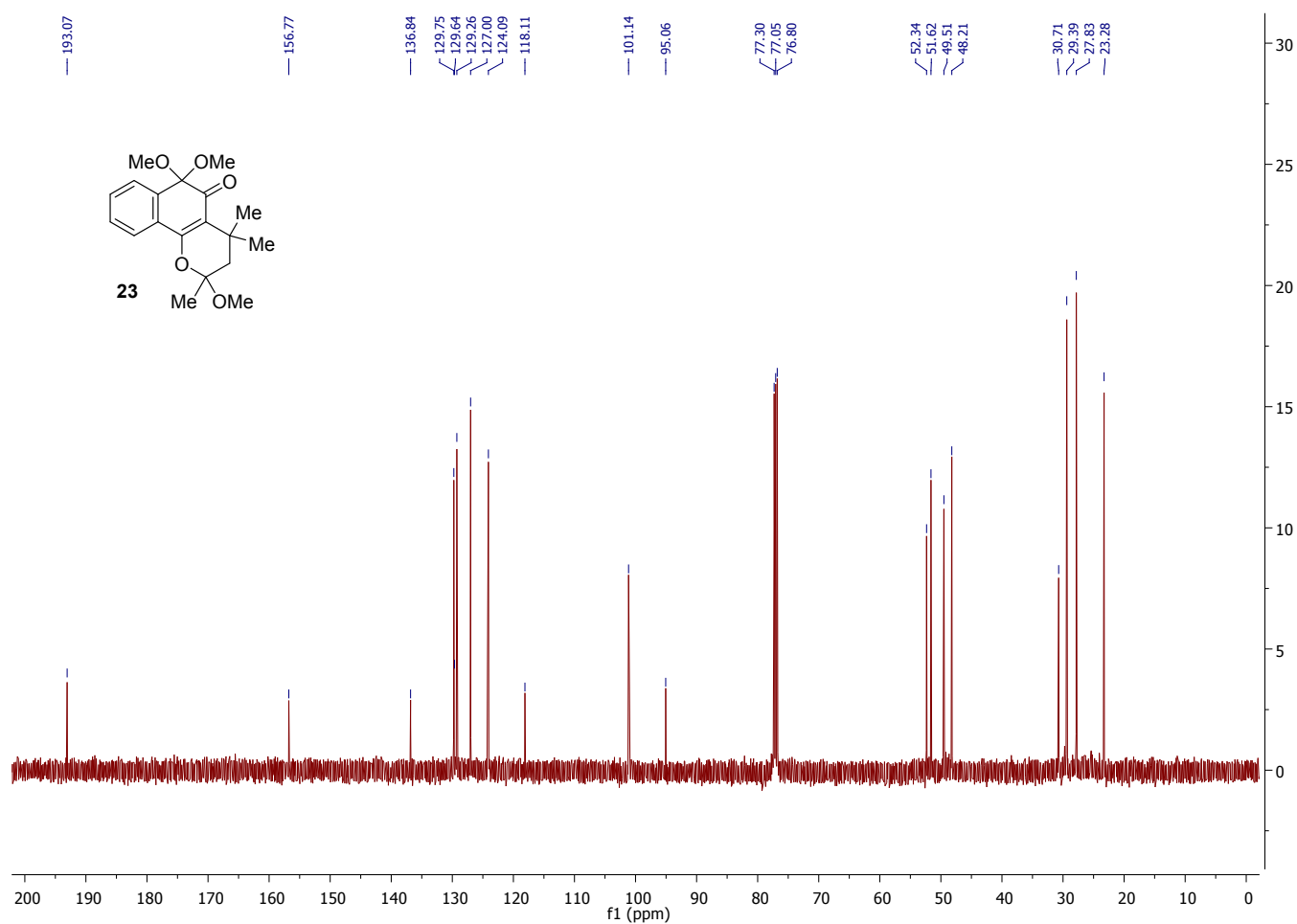
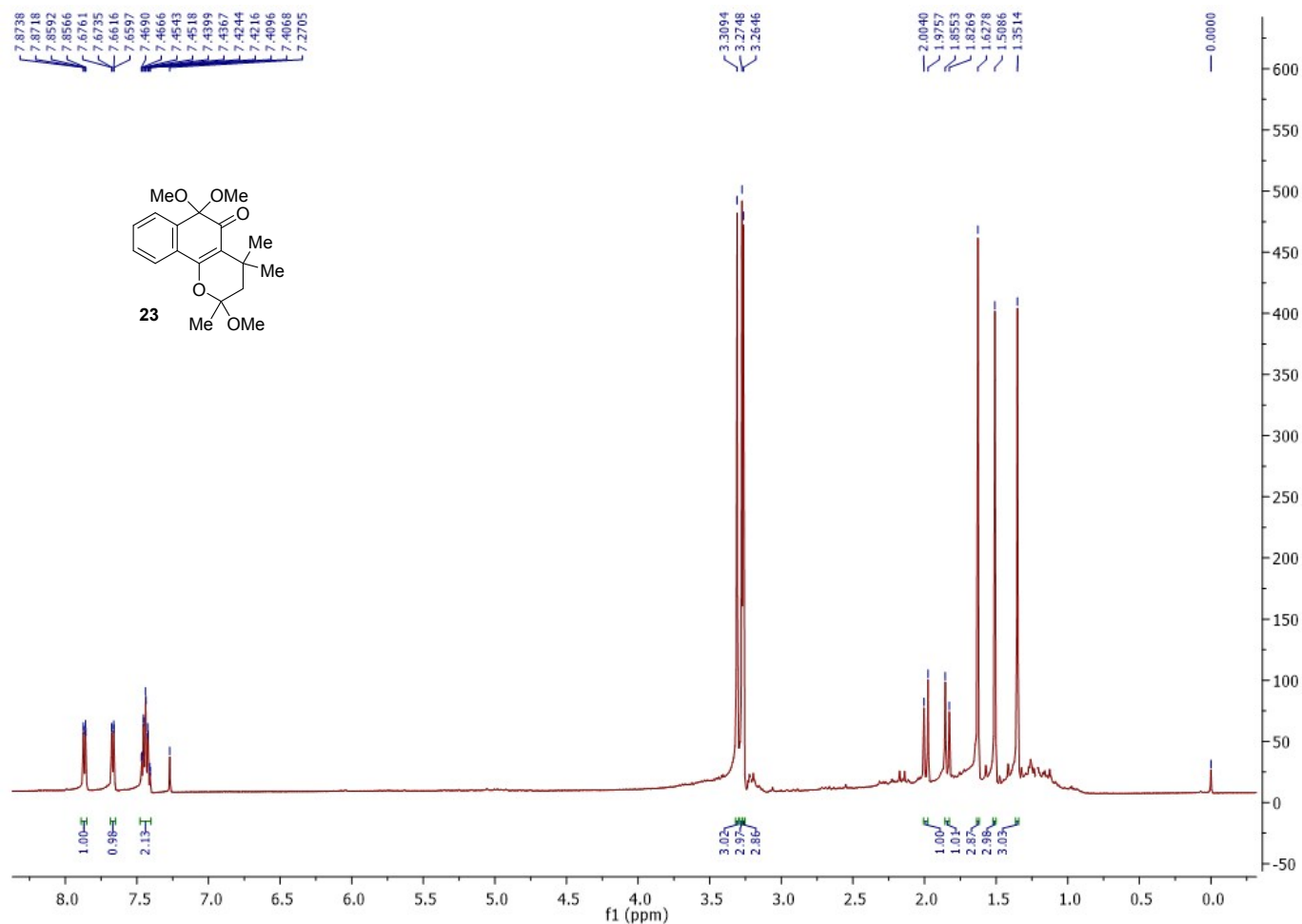
Mixture of diastereoisomers 19b

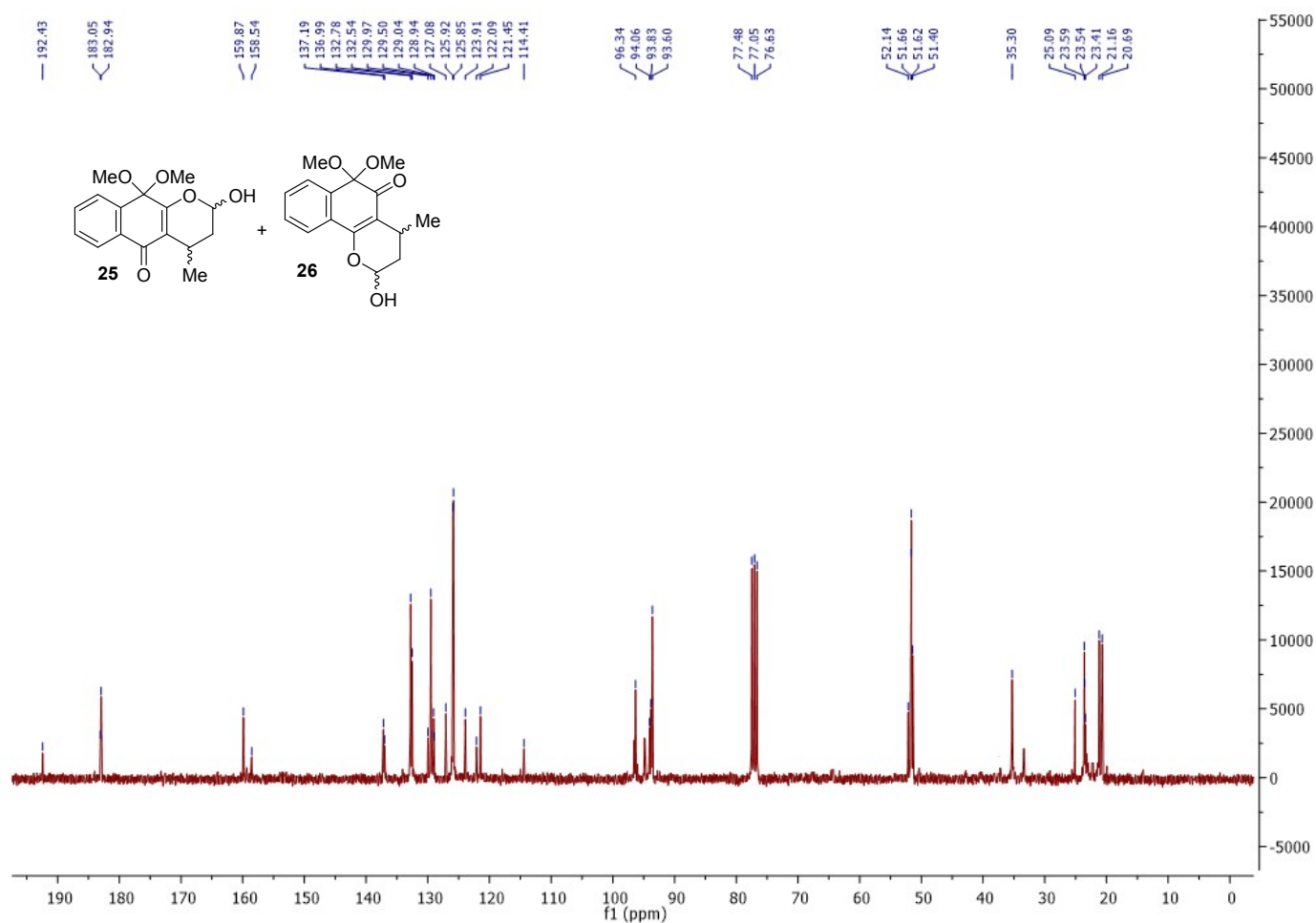
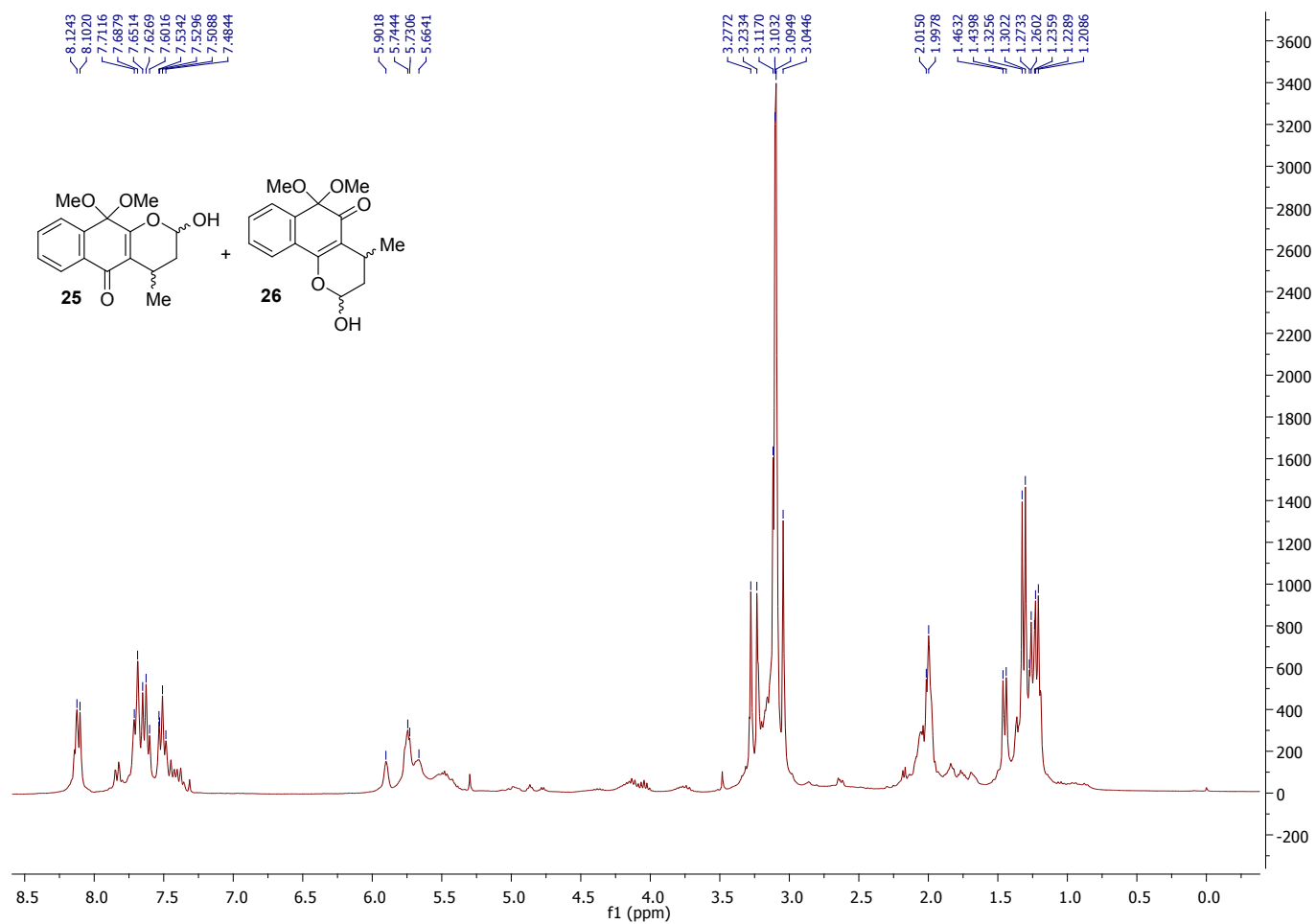


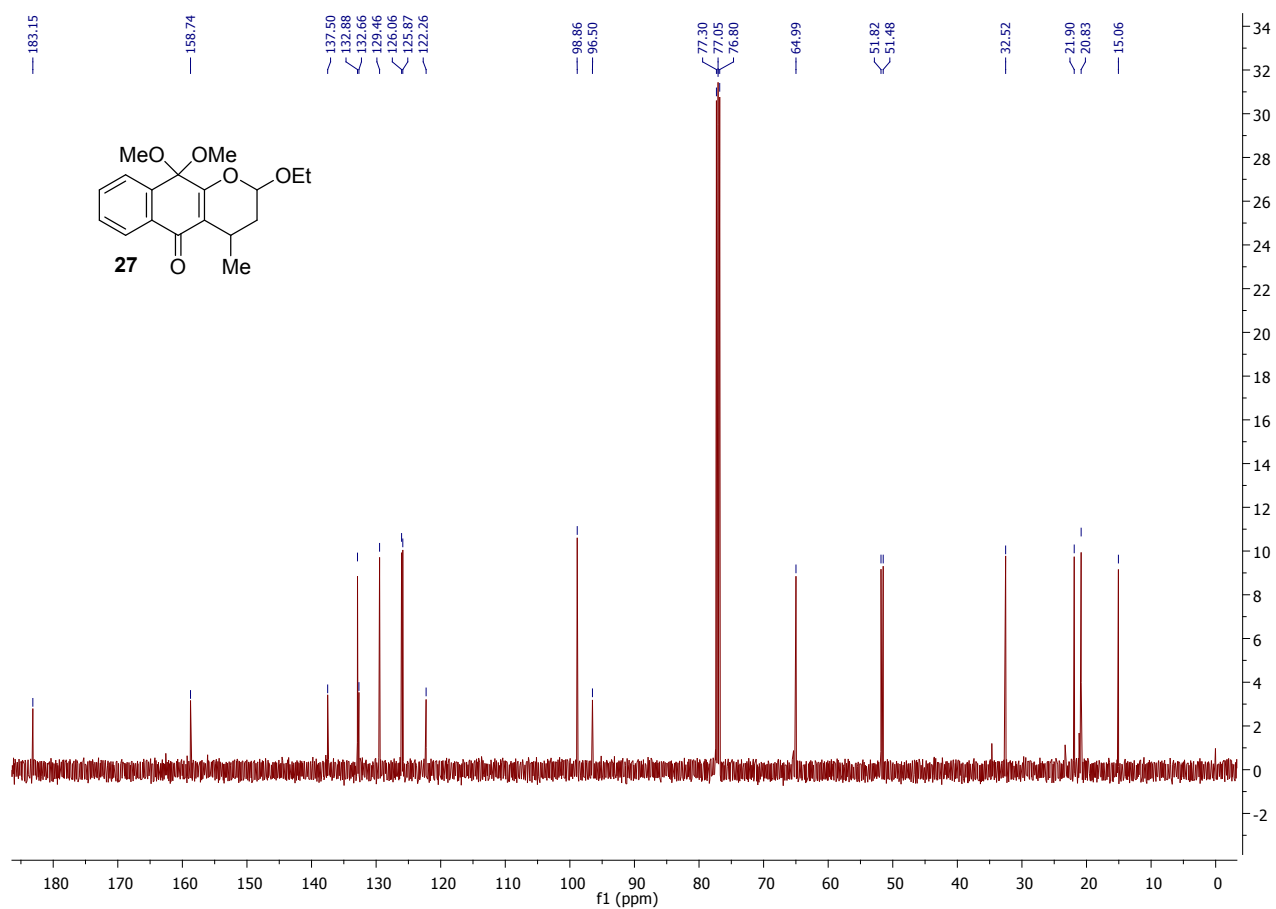
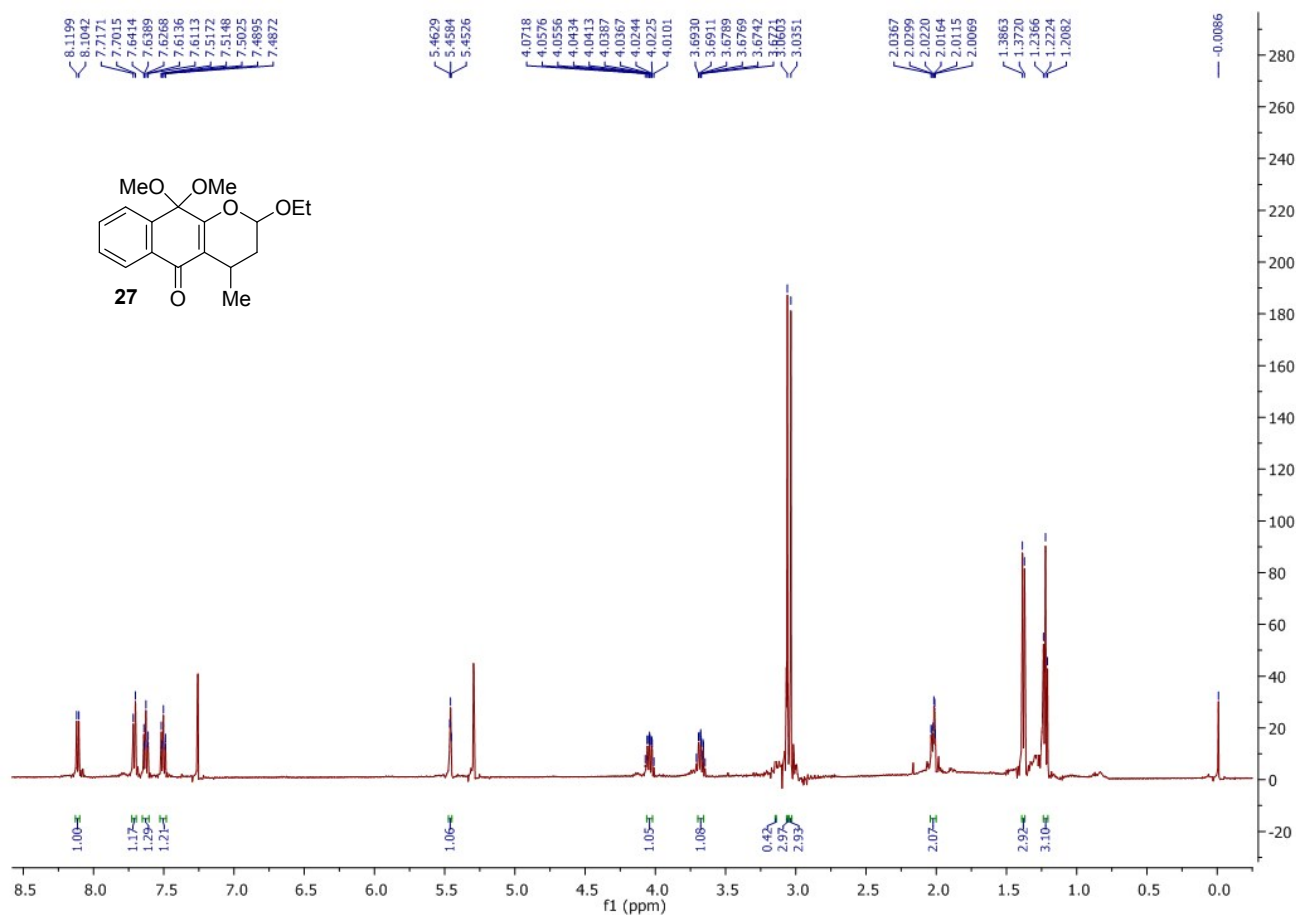




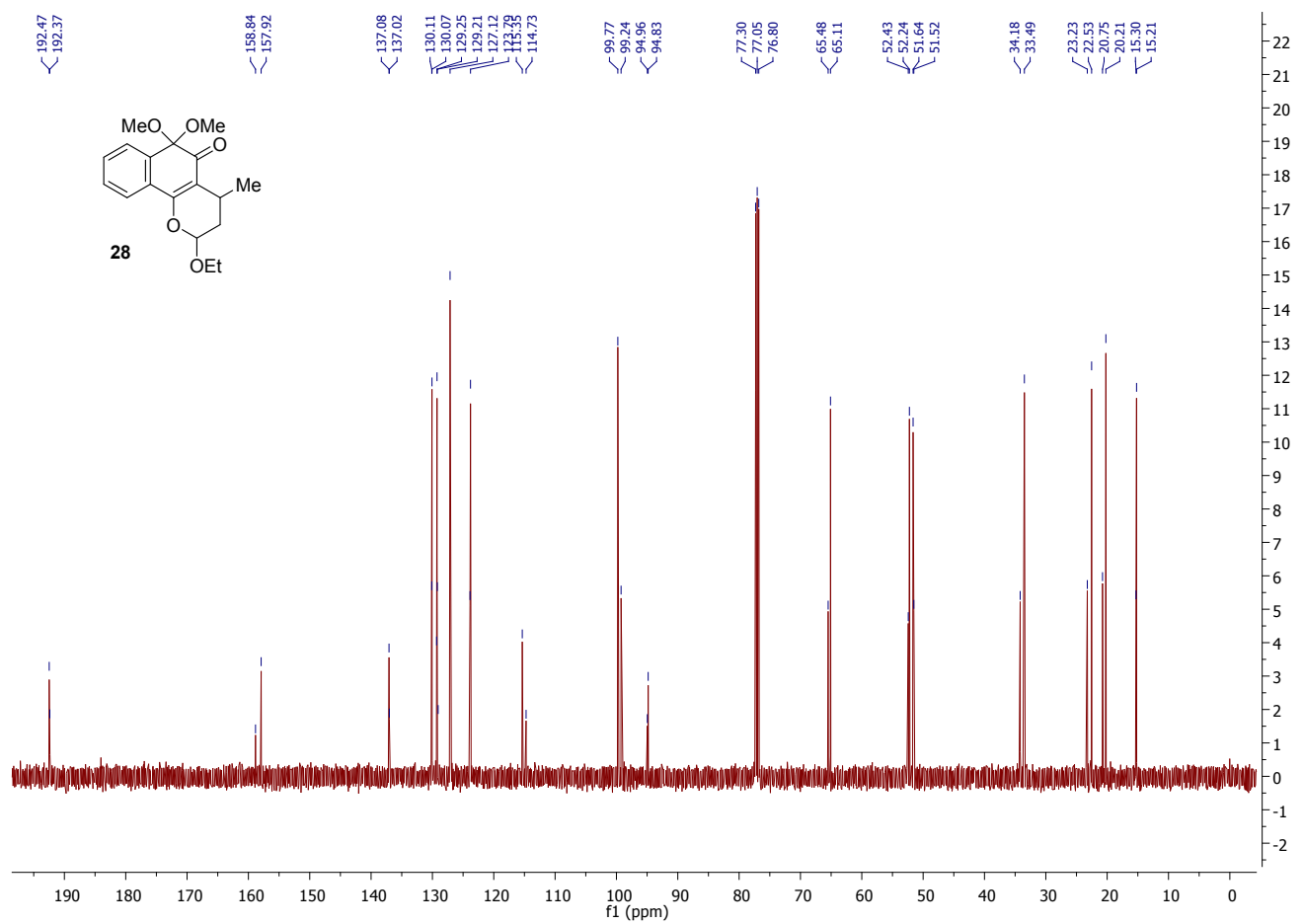
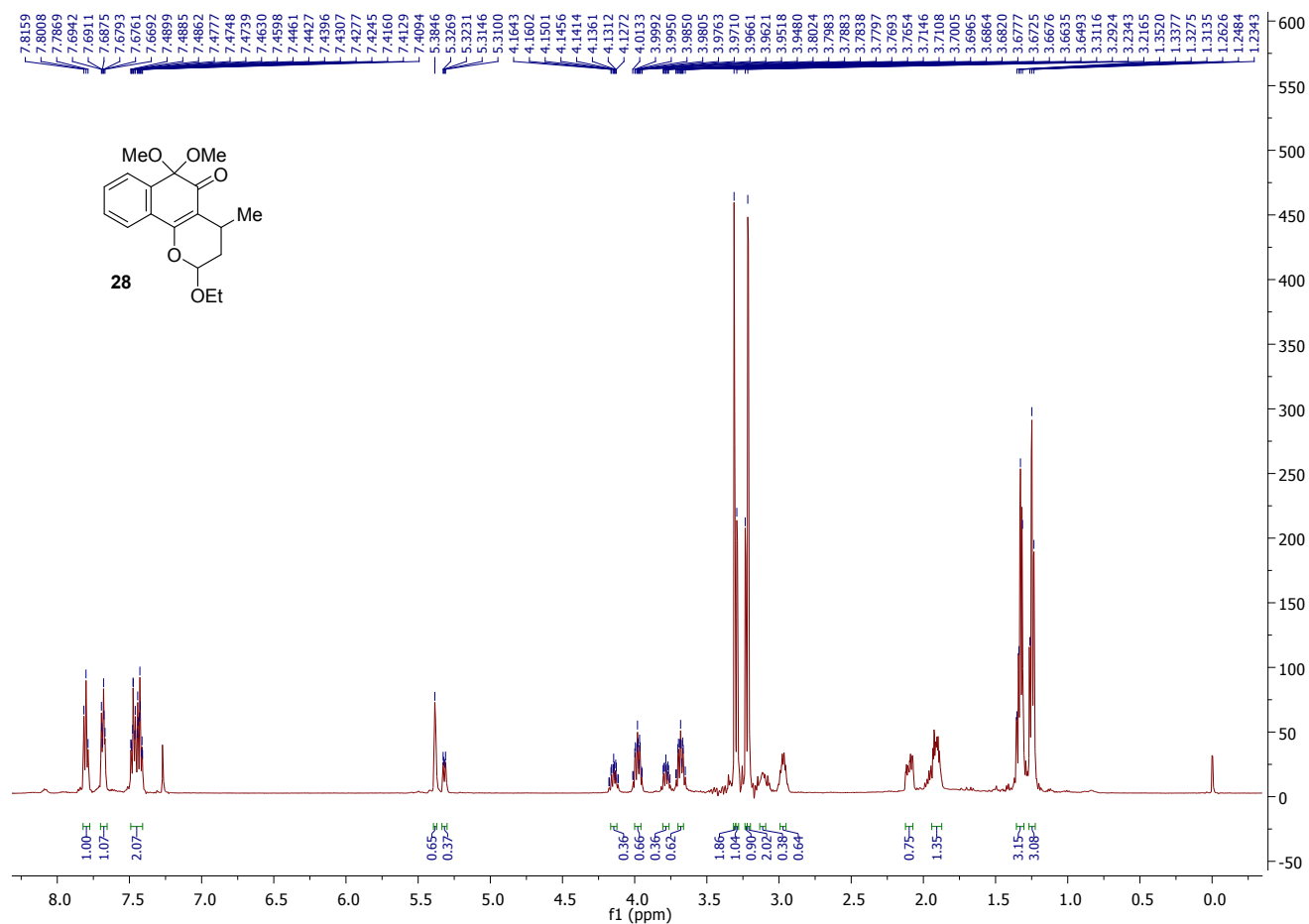




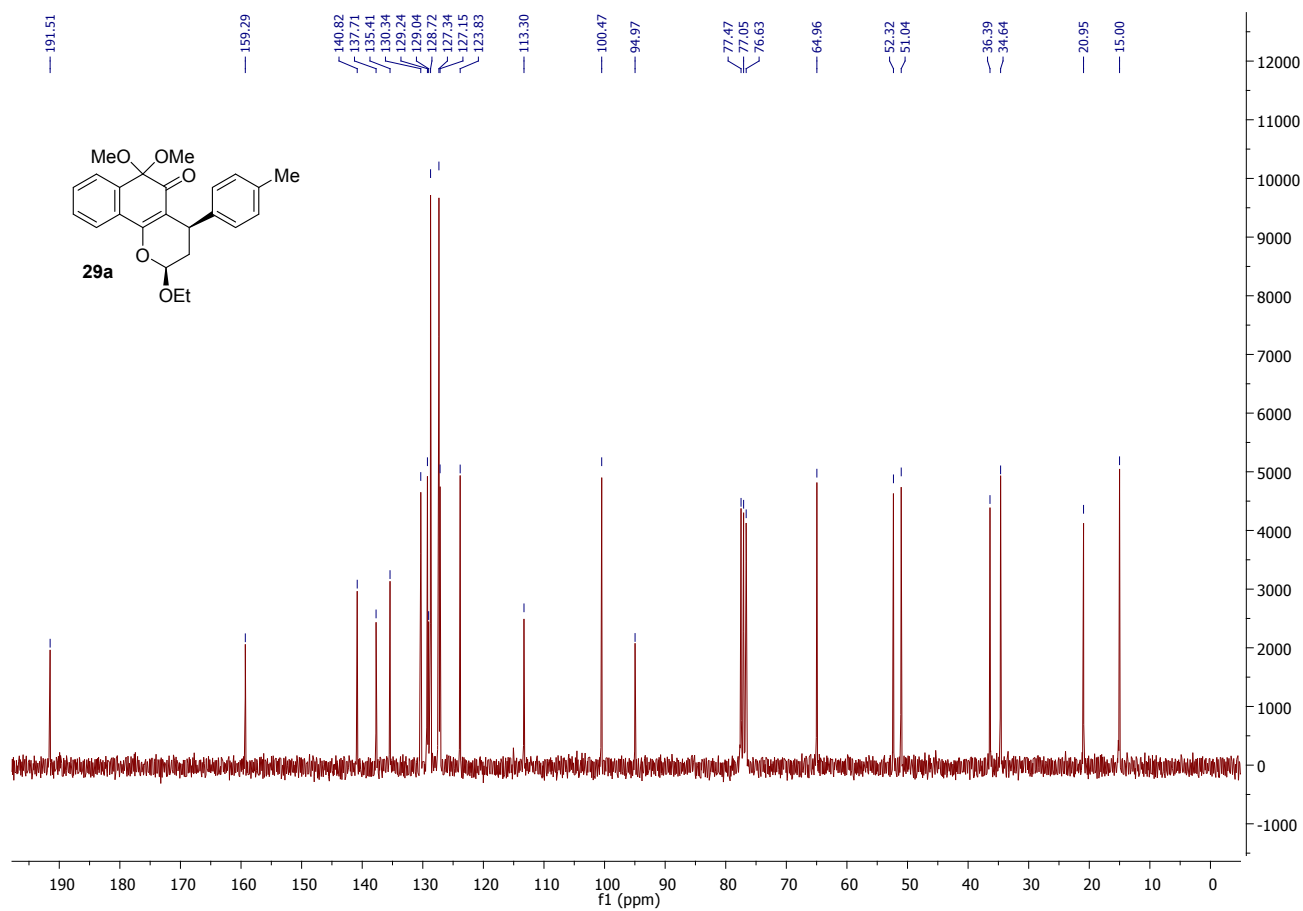
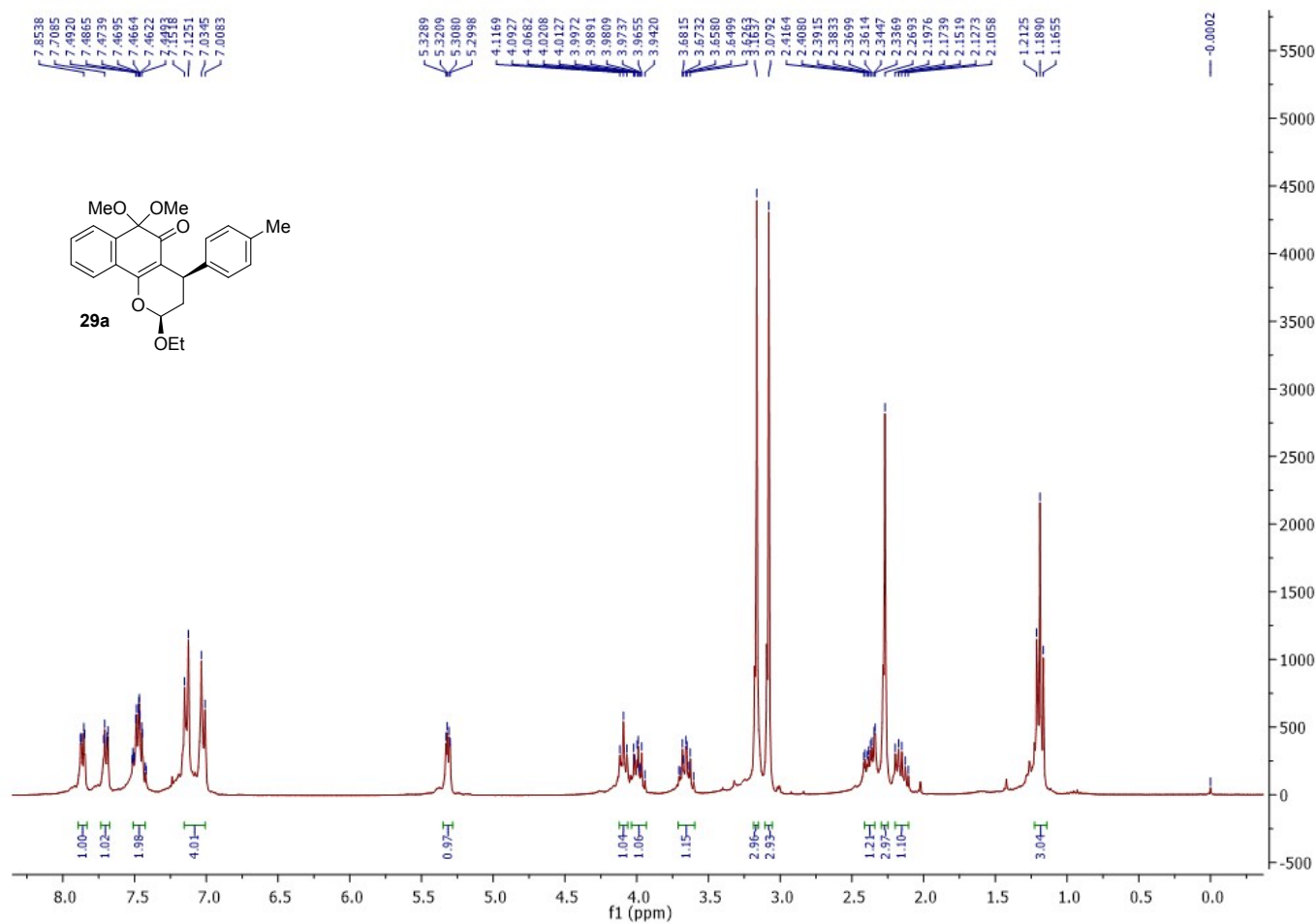


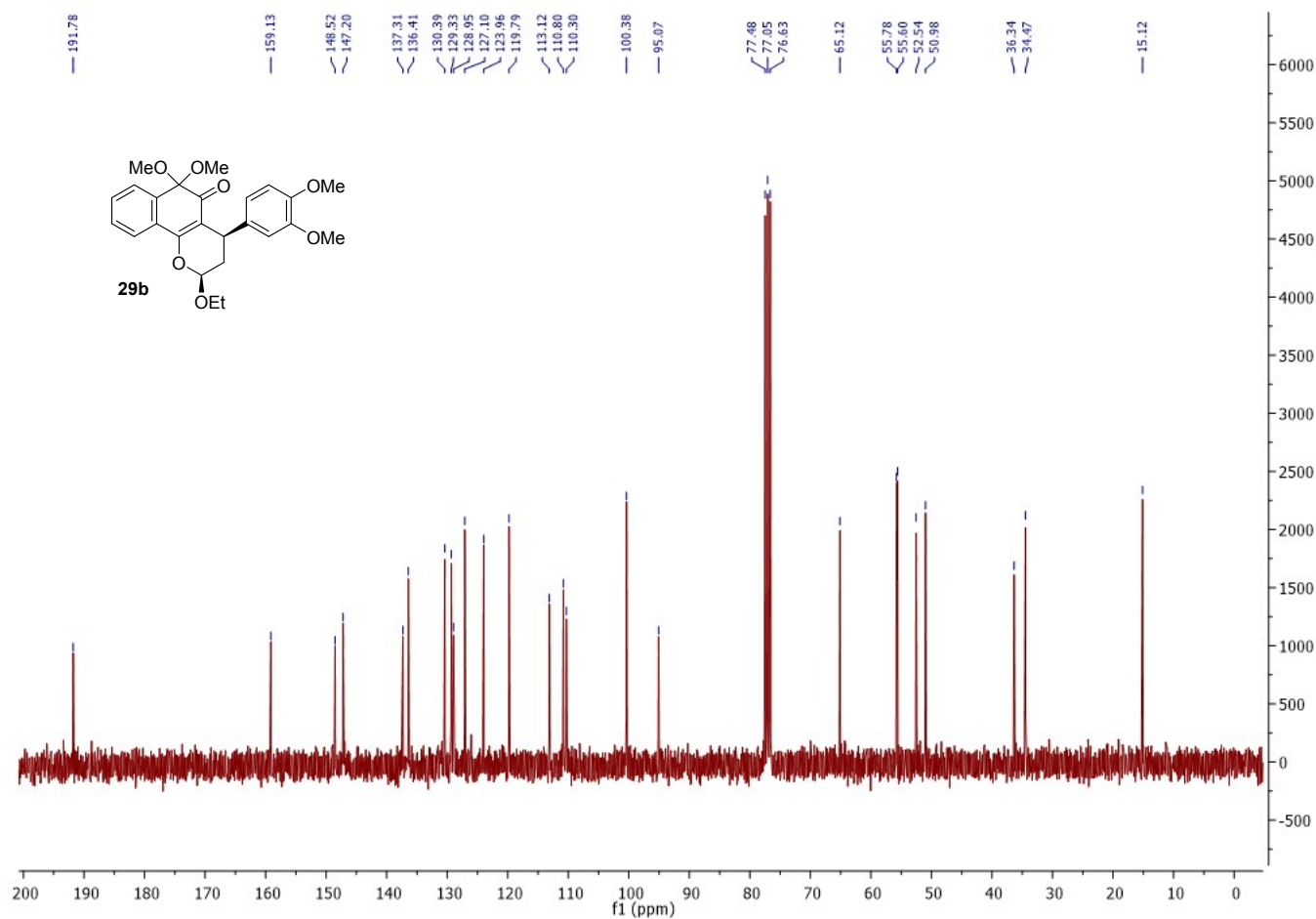
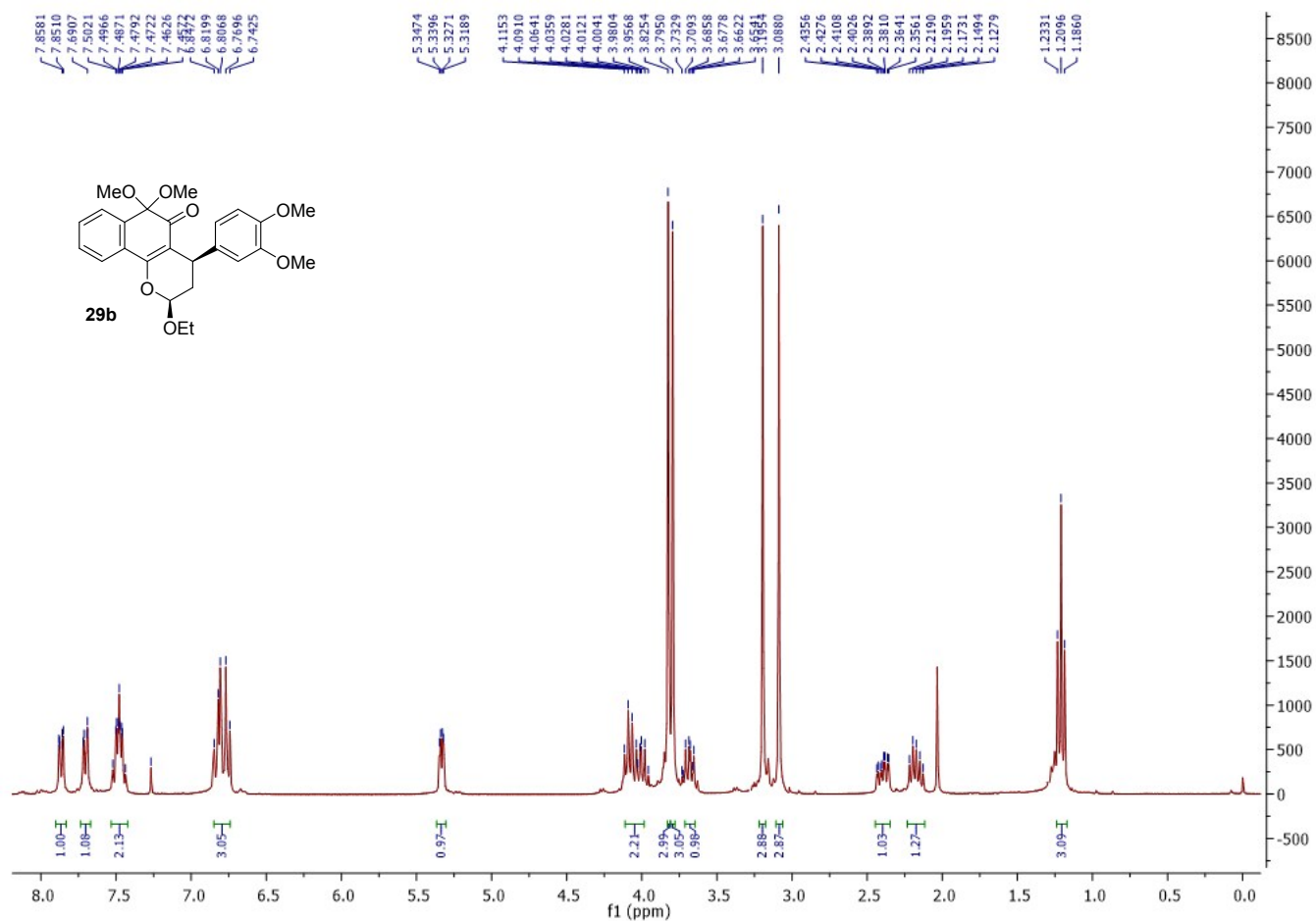


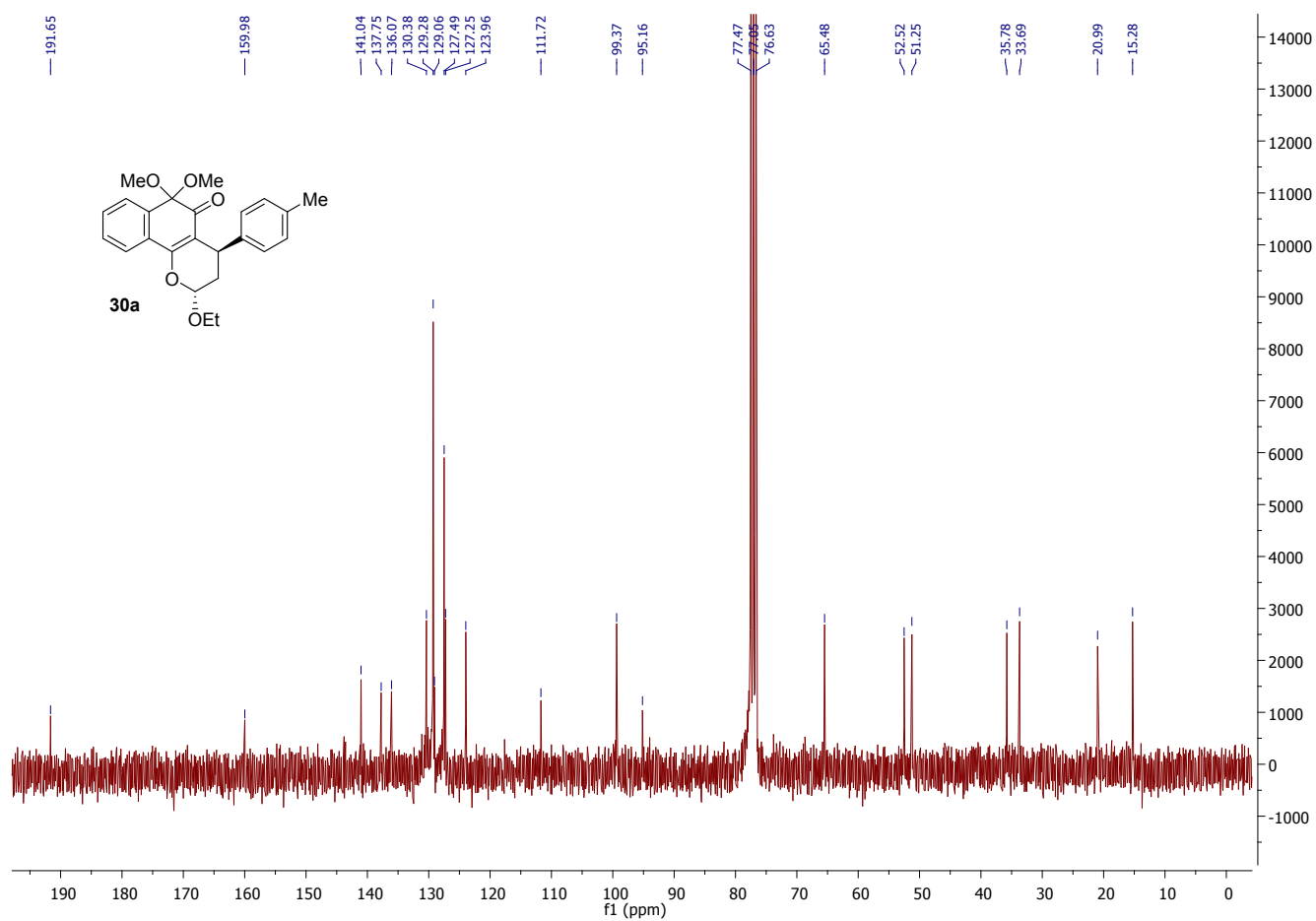
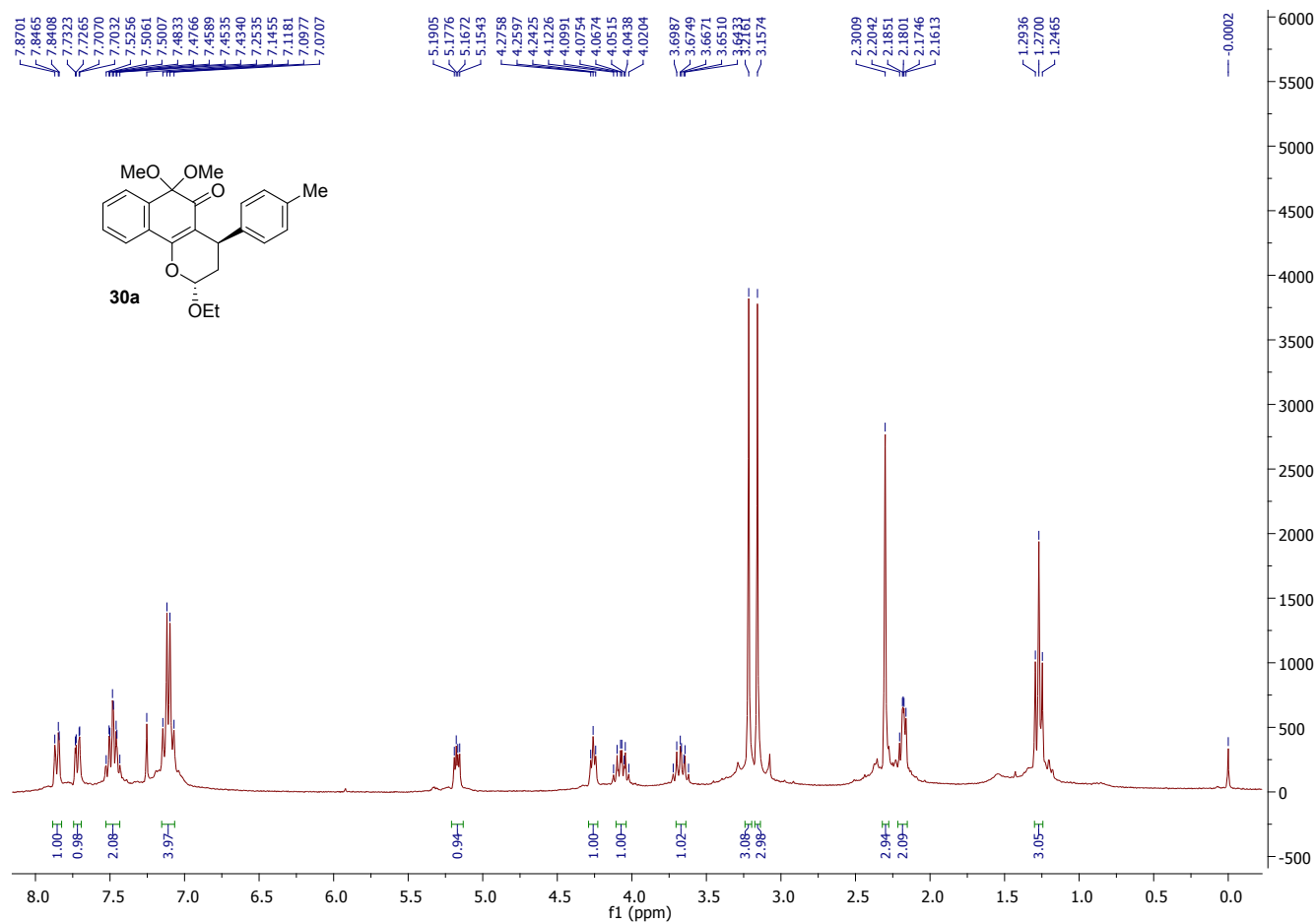
Mixture of diastereoisomers

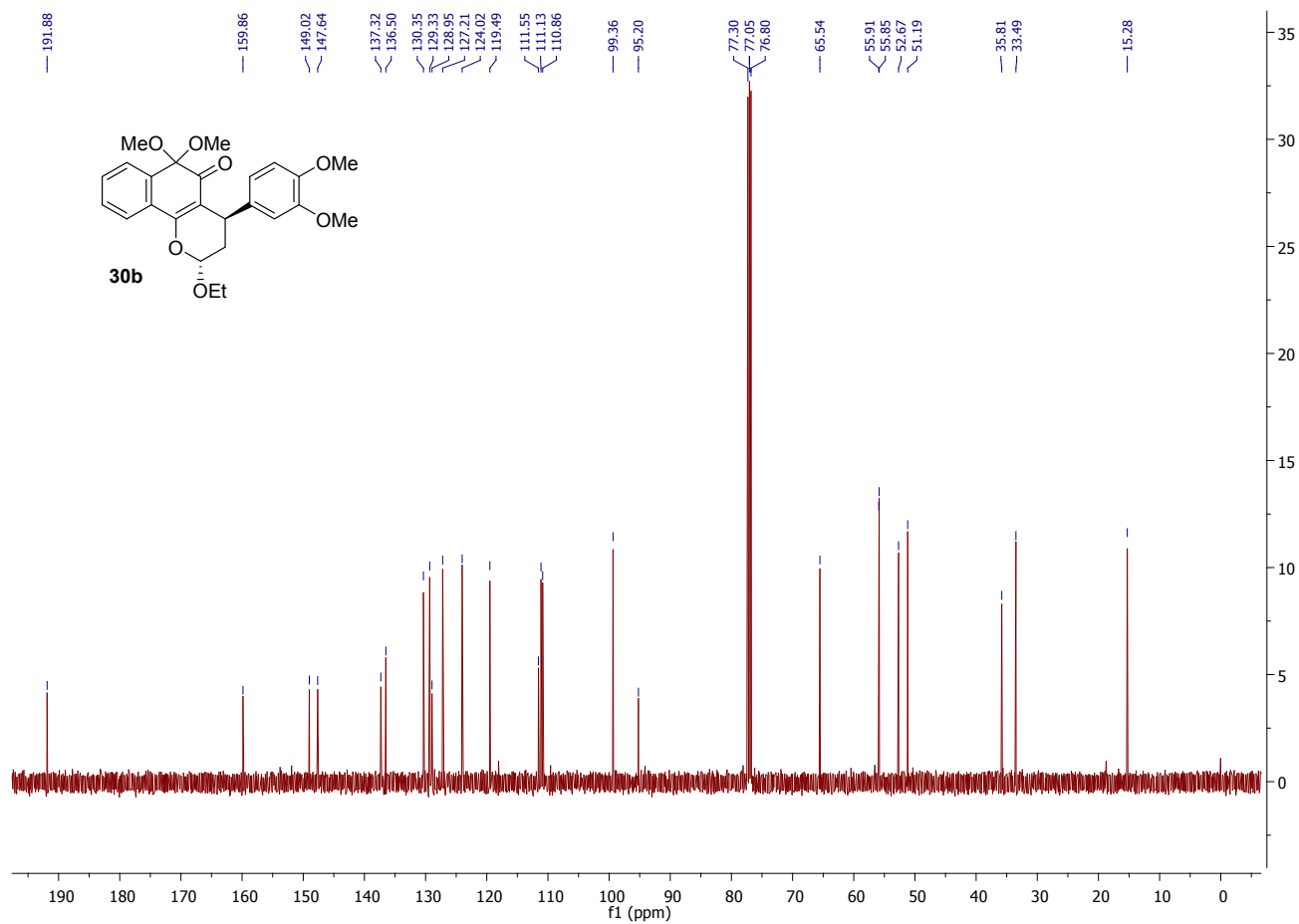
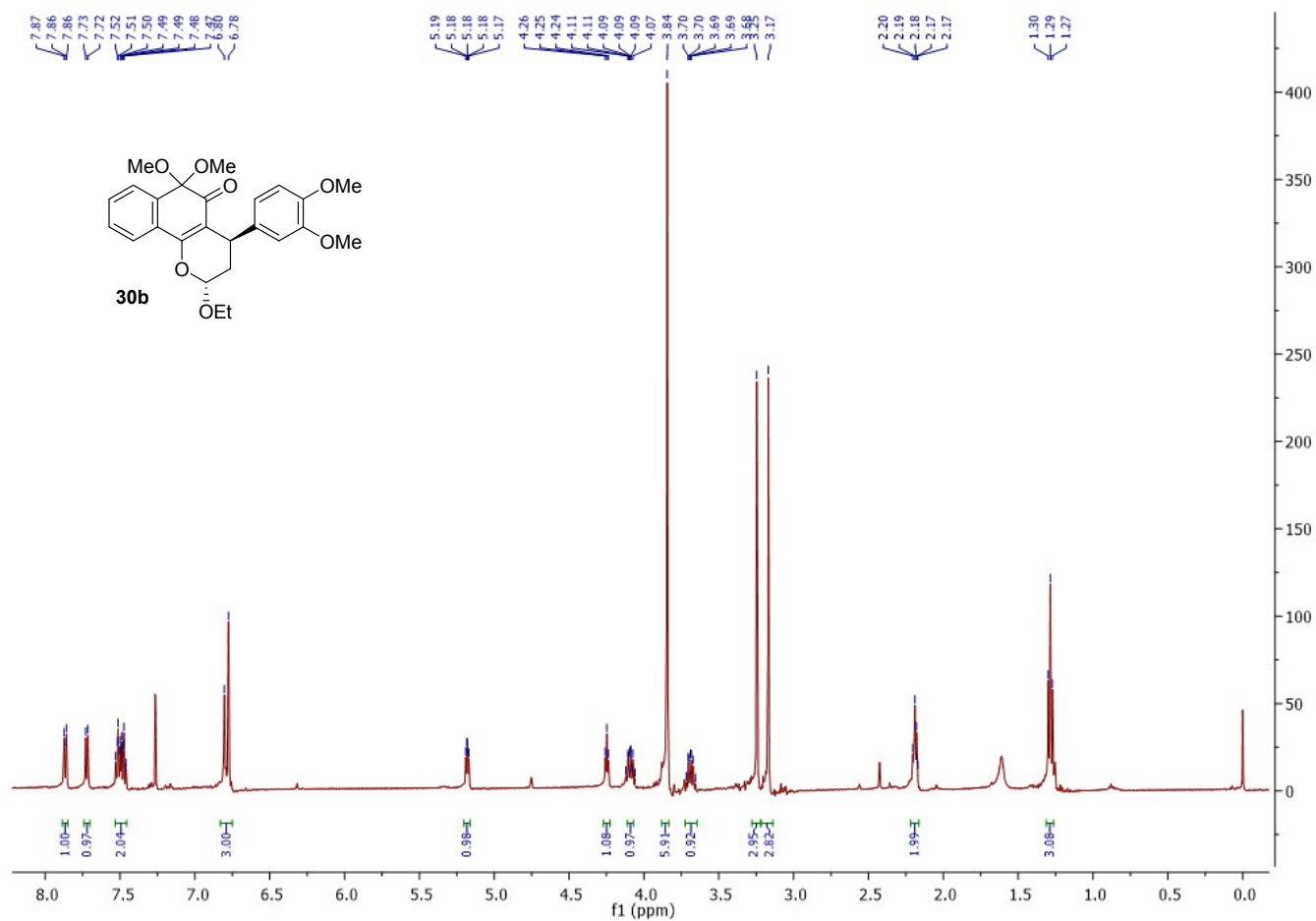


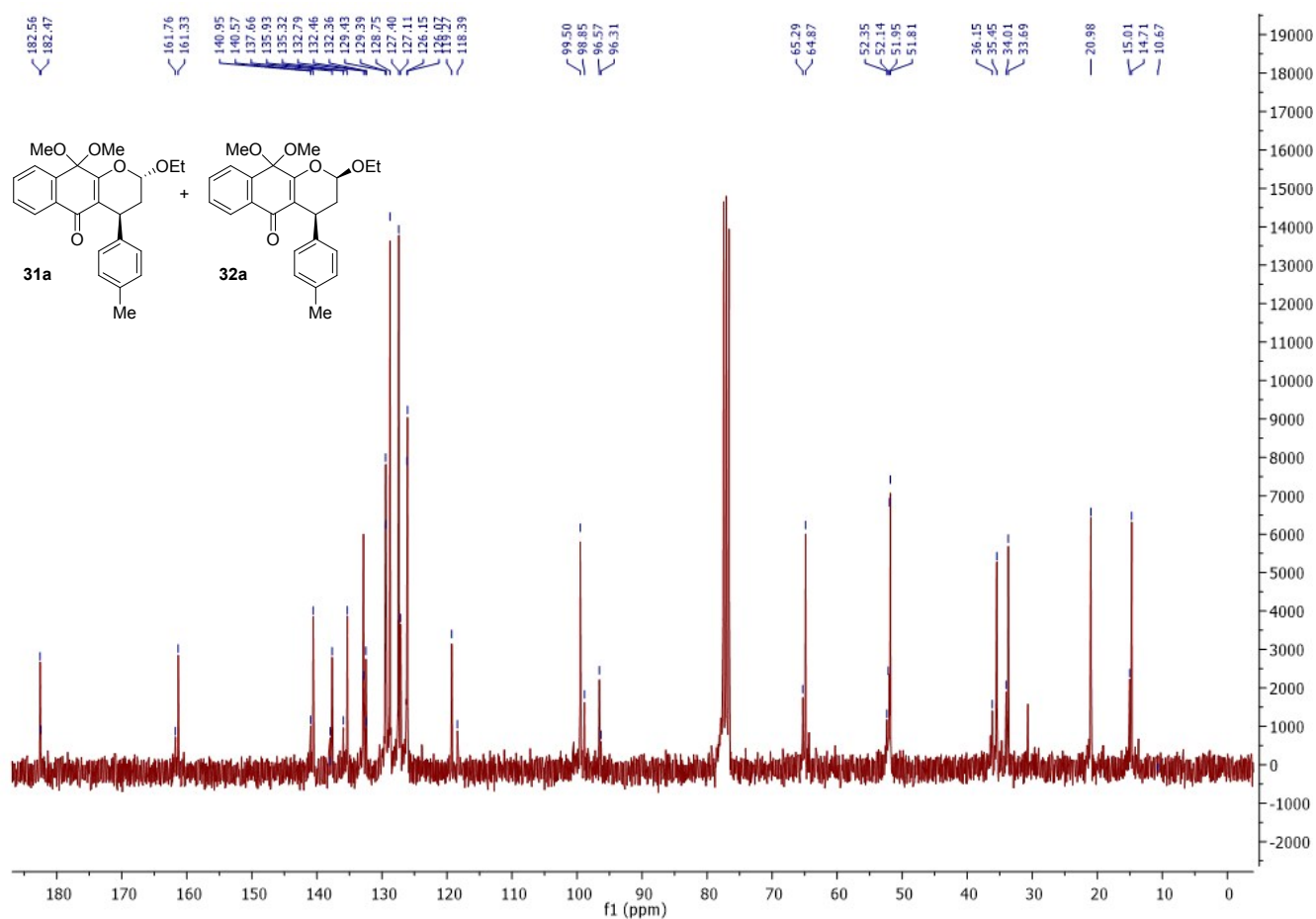
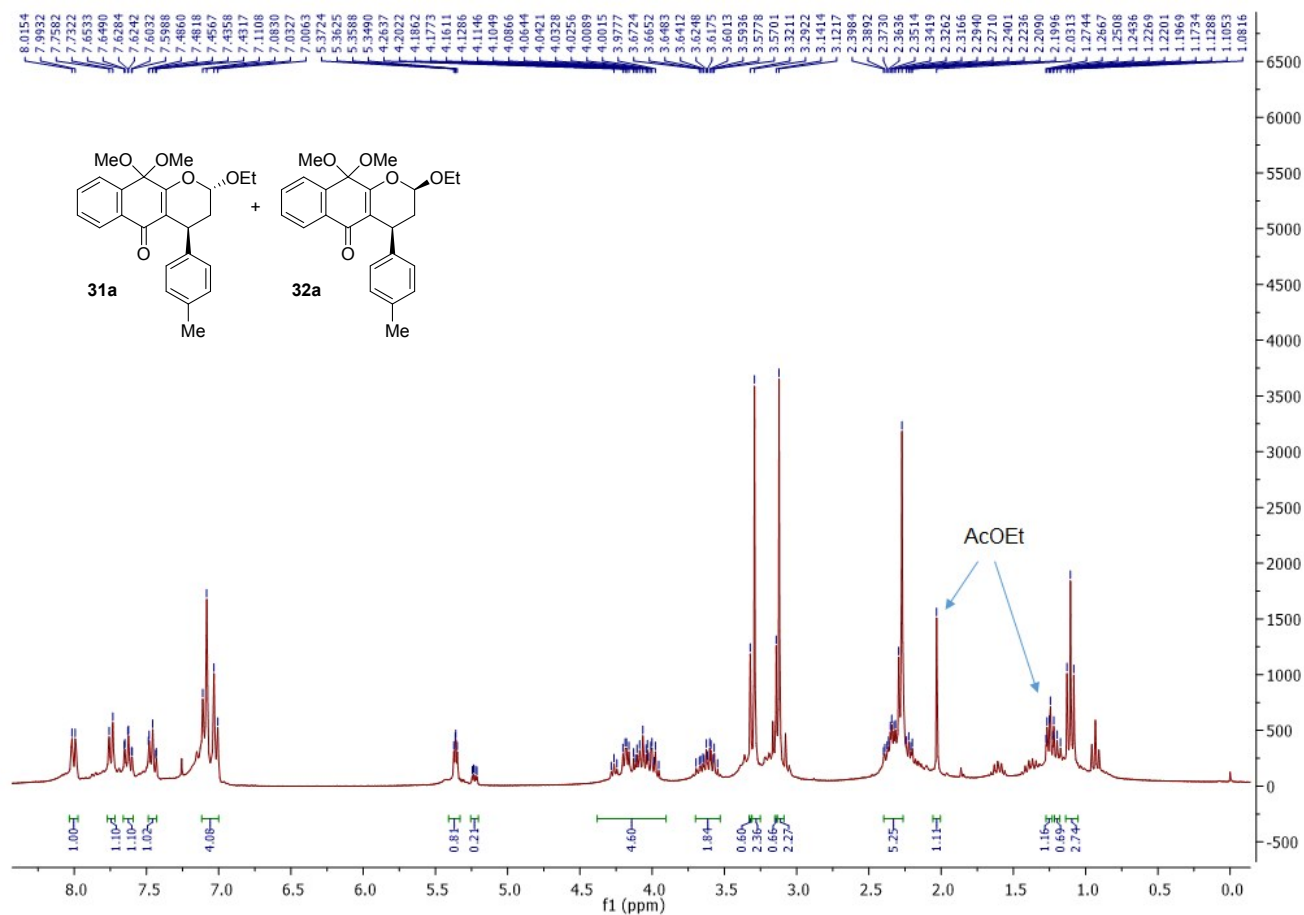
Mixture of diastereoisomers



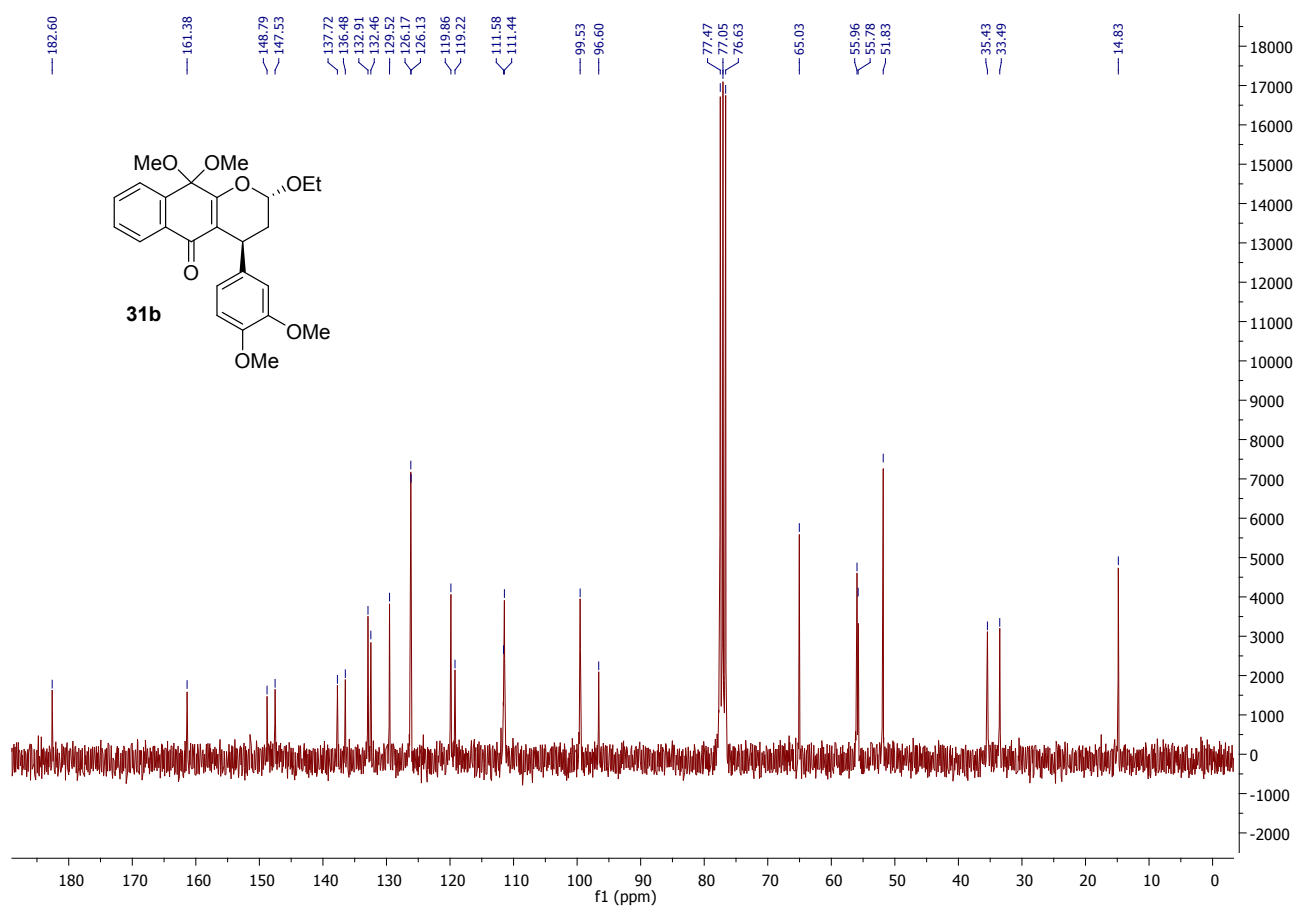
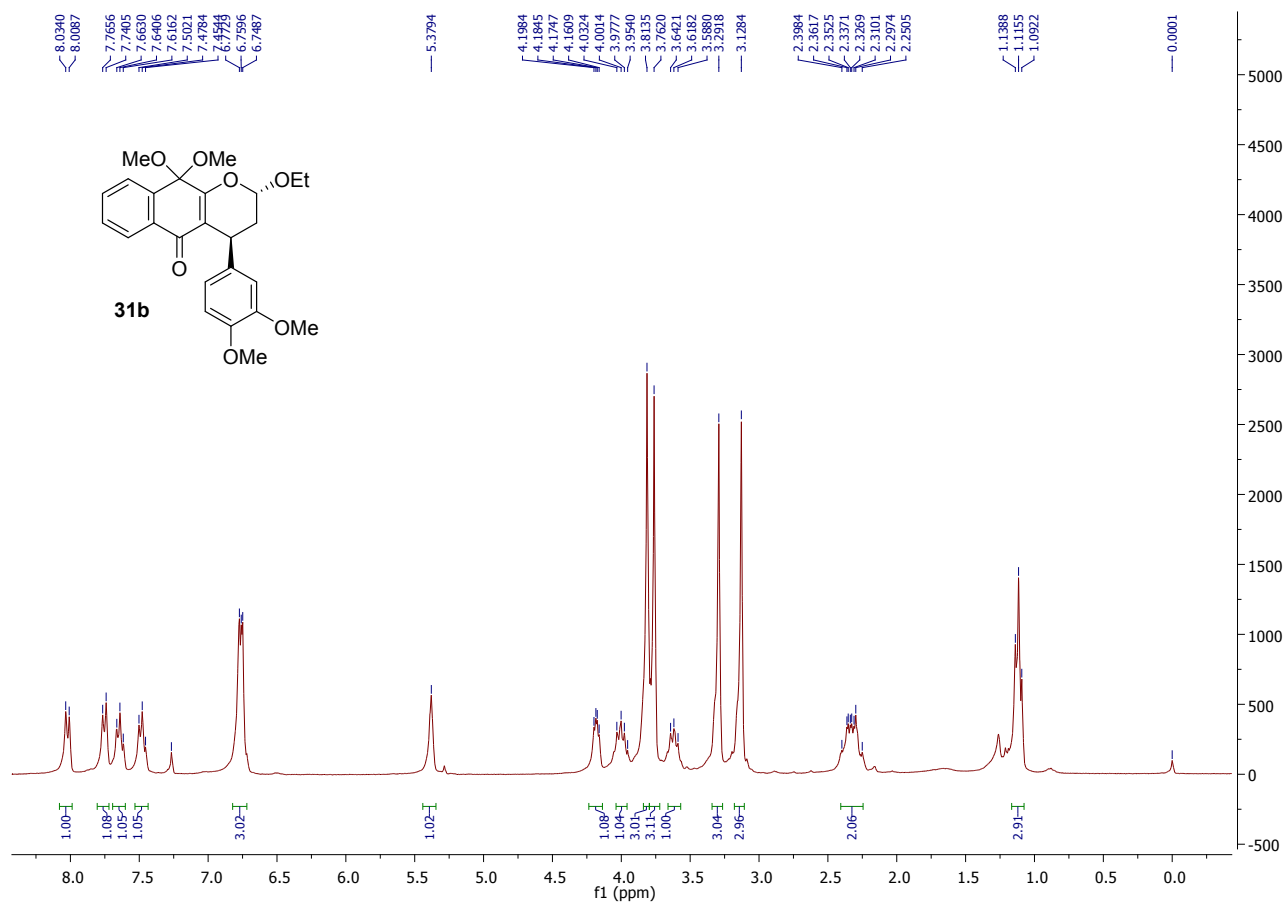


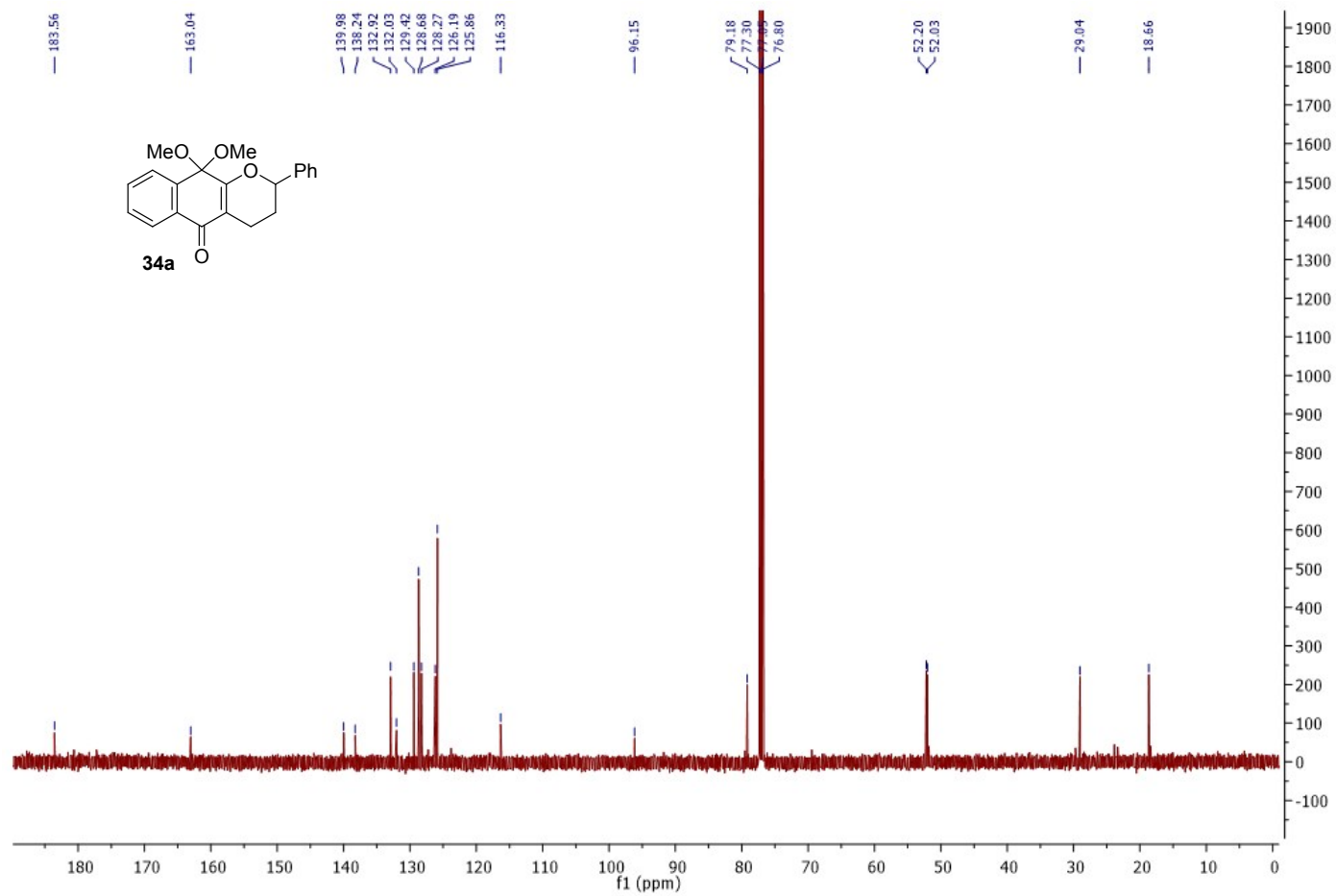
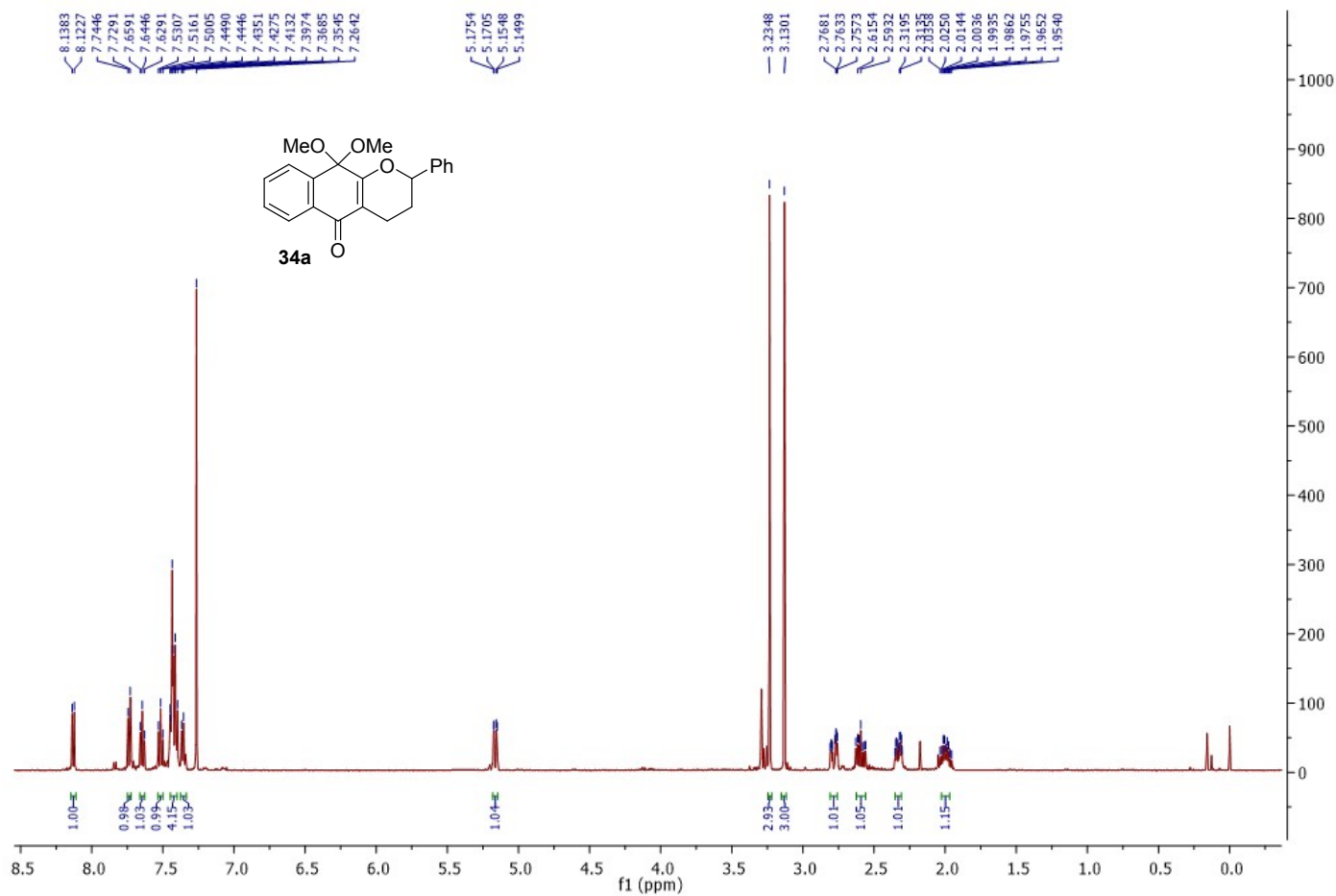


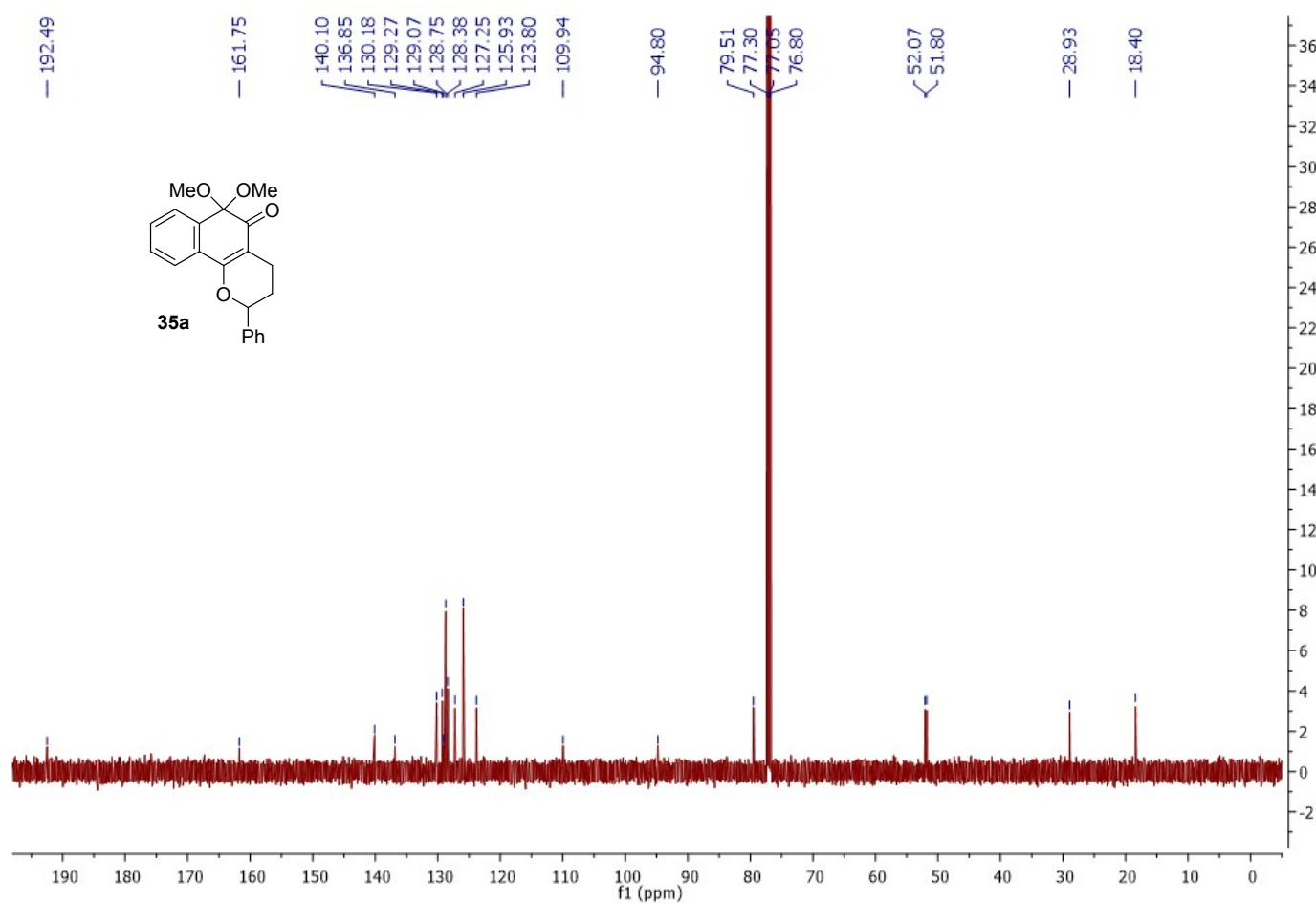
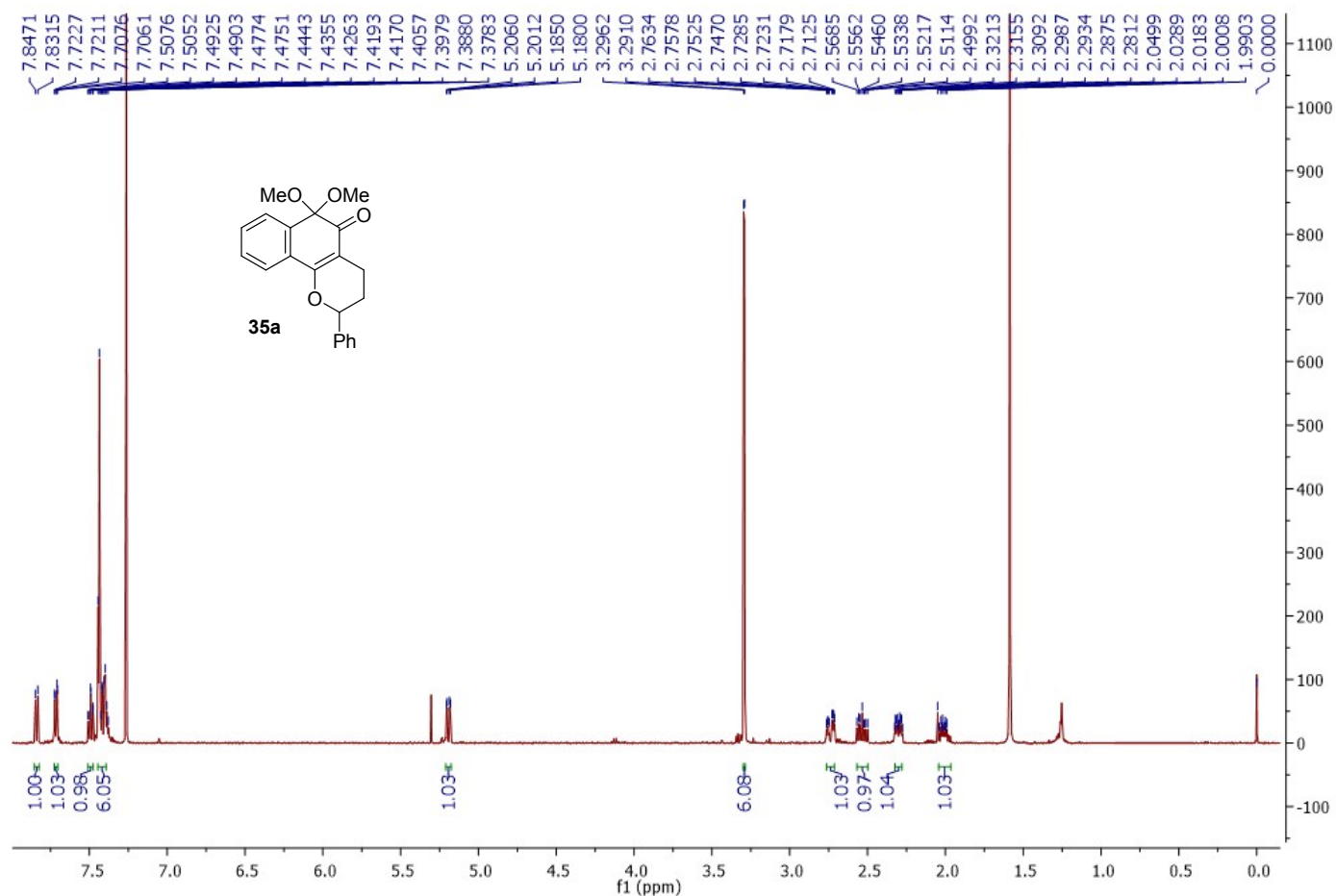


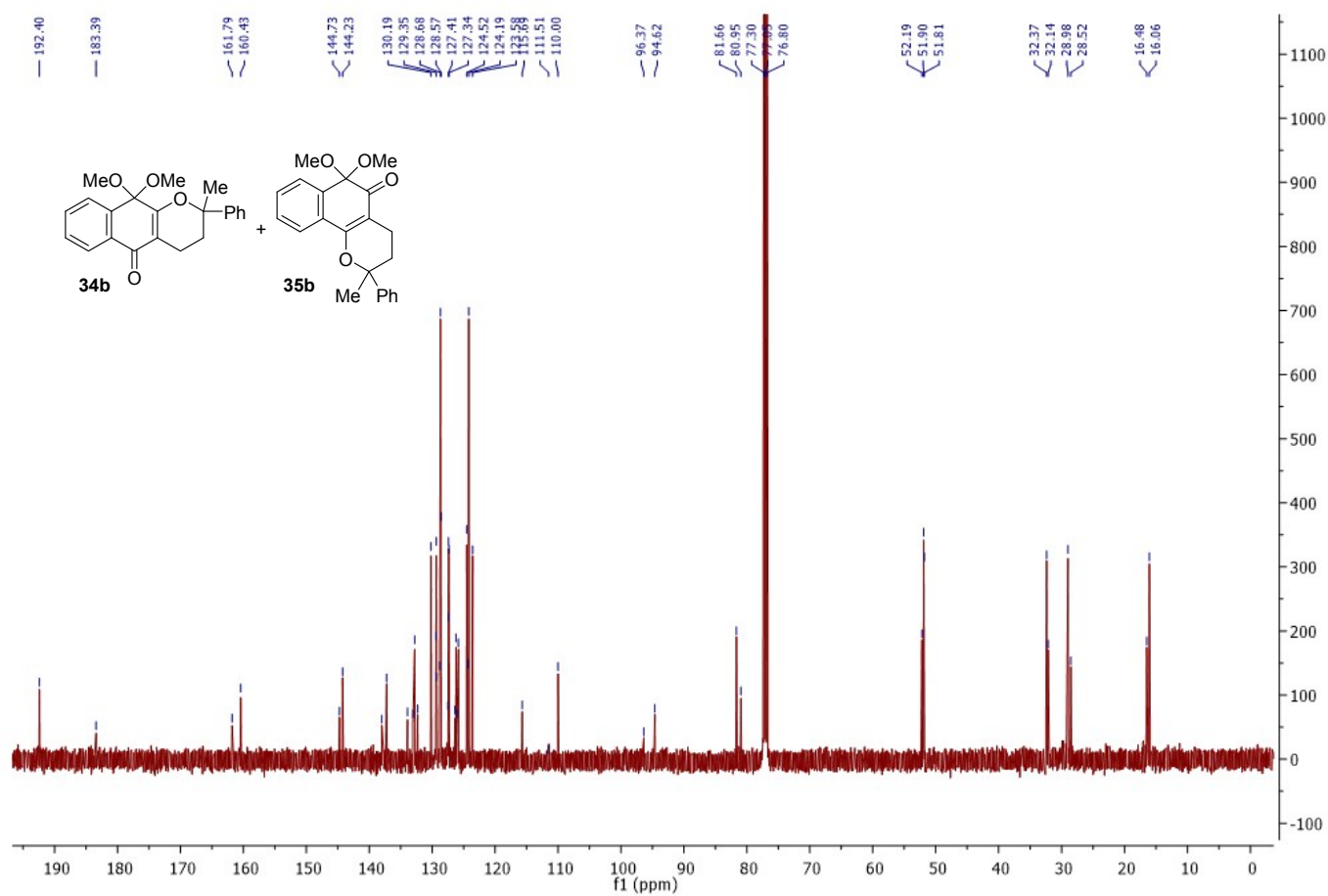
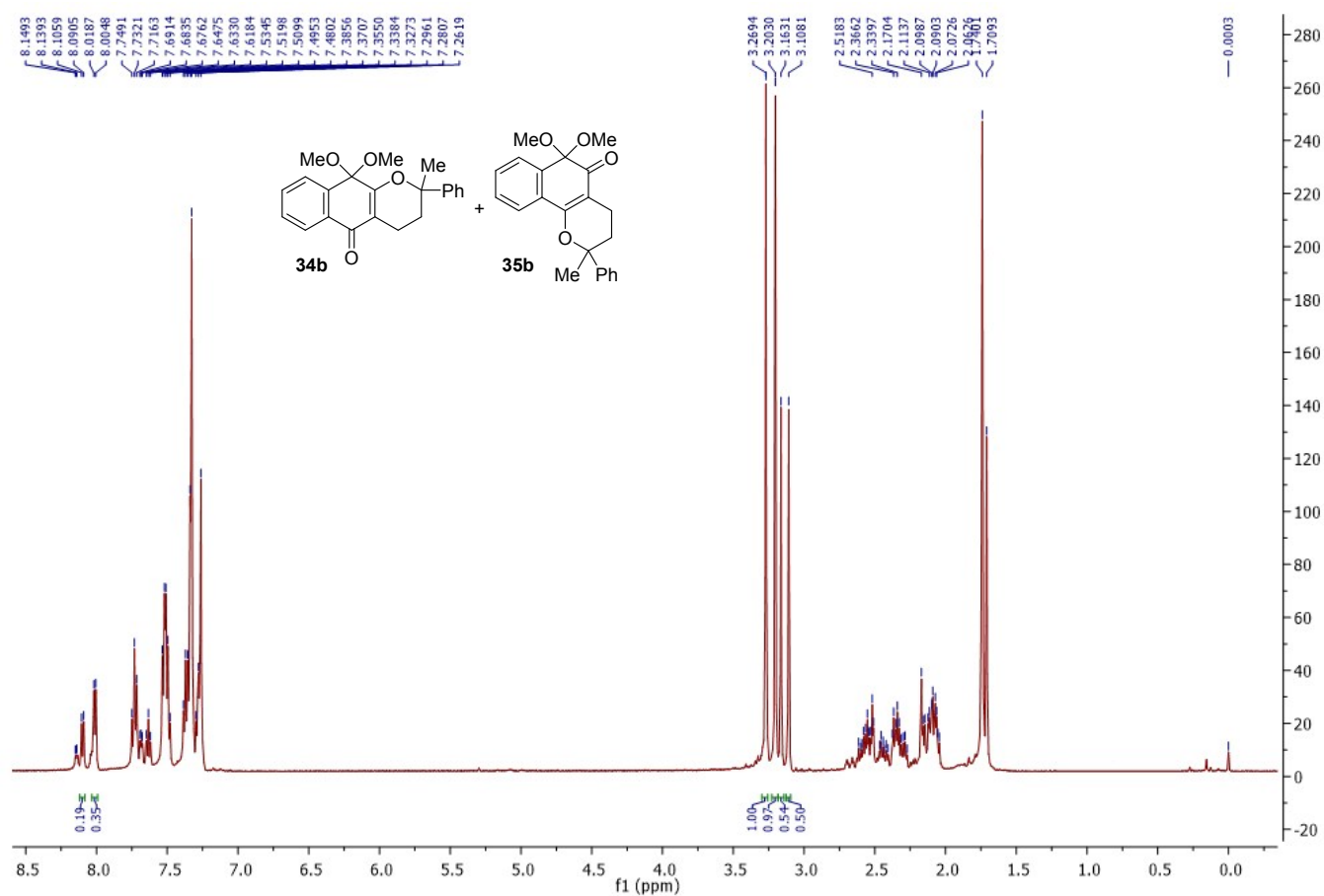


Mixture of 31a and 32a (ratio 4 : 1)

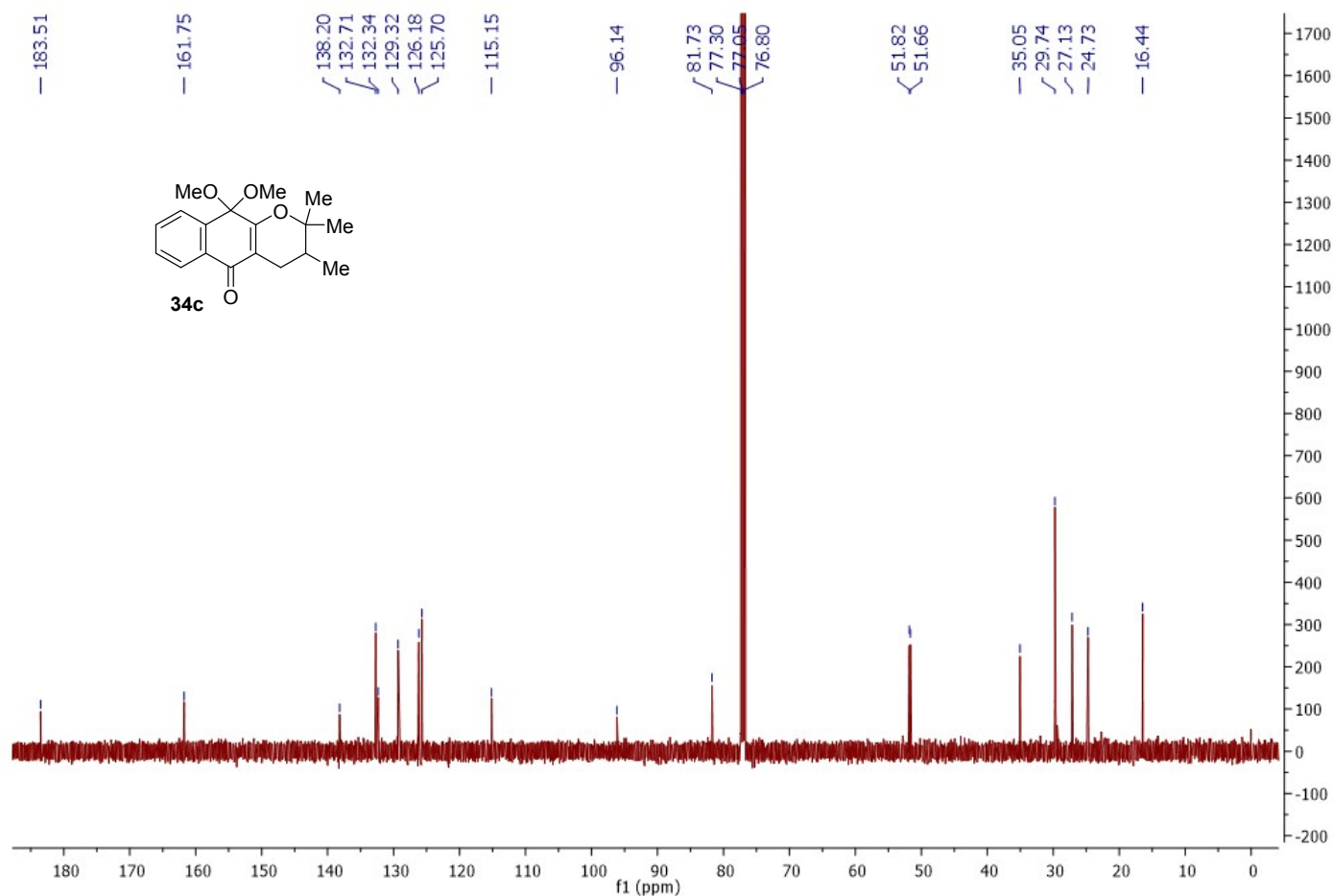
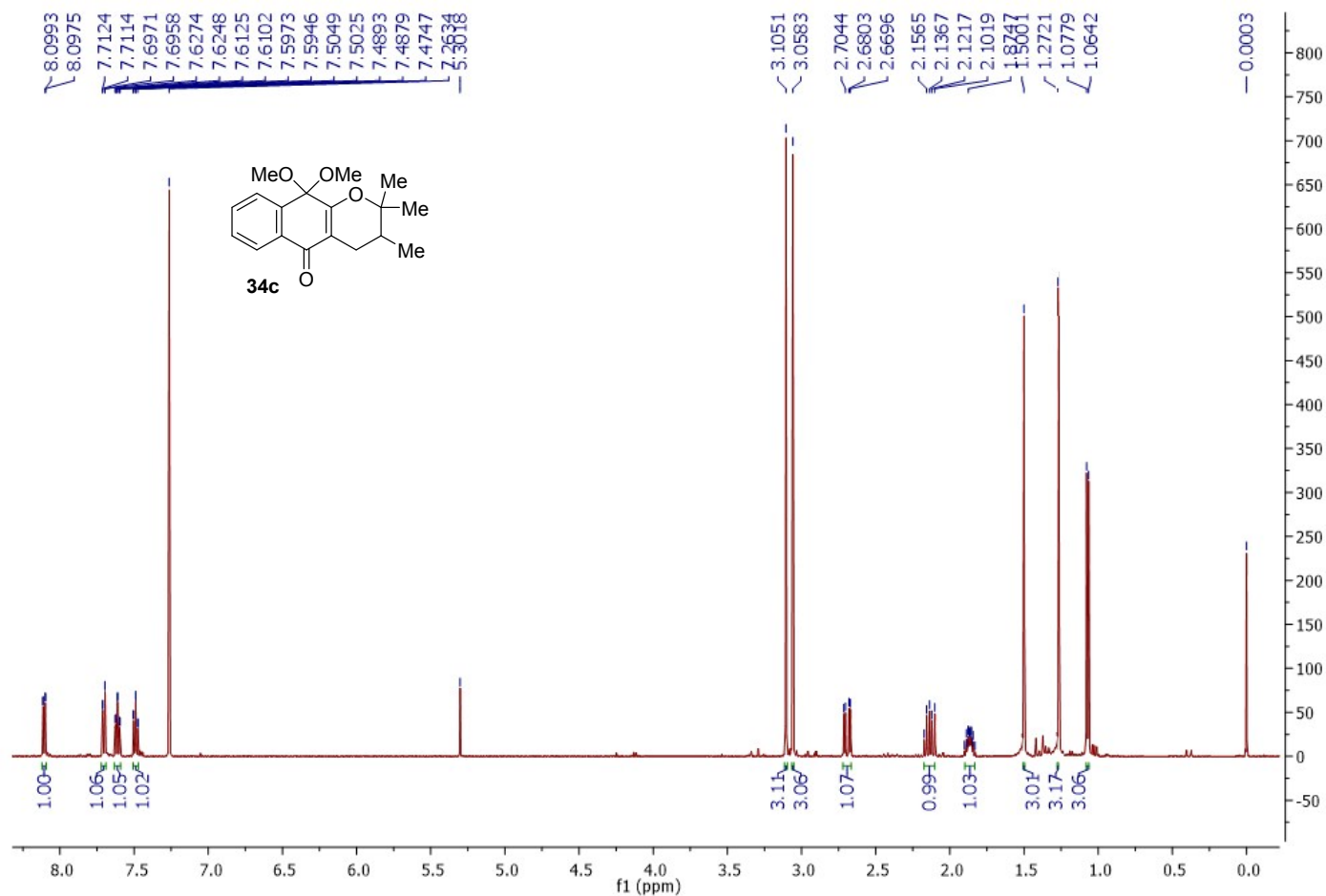


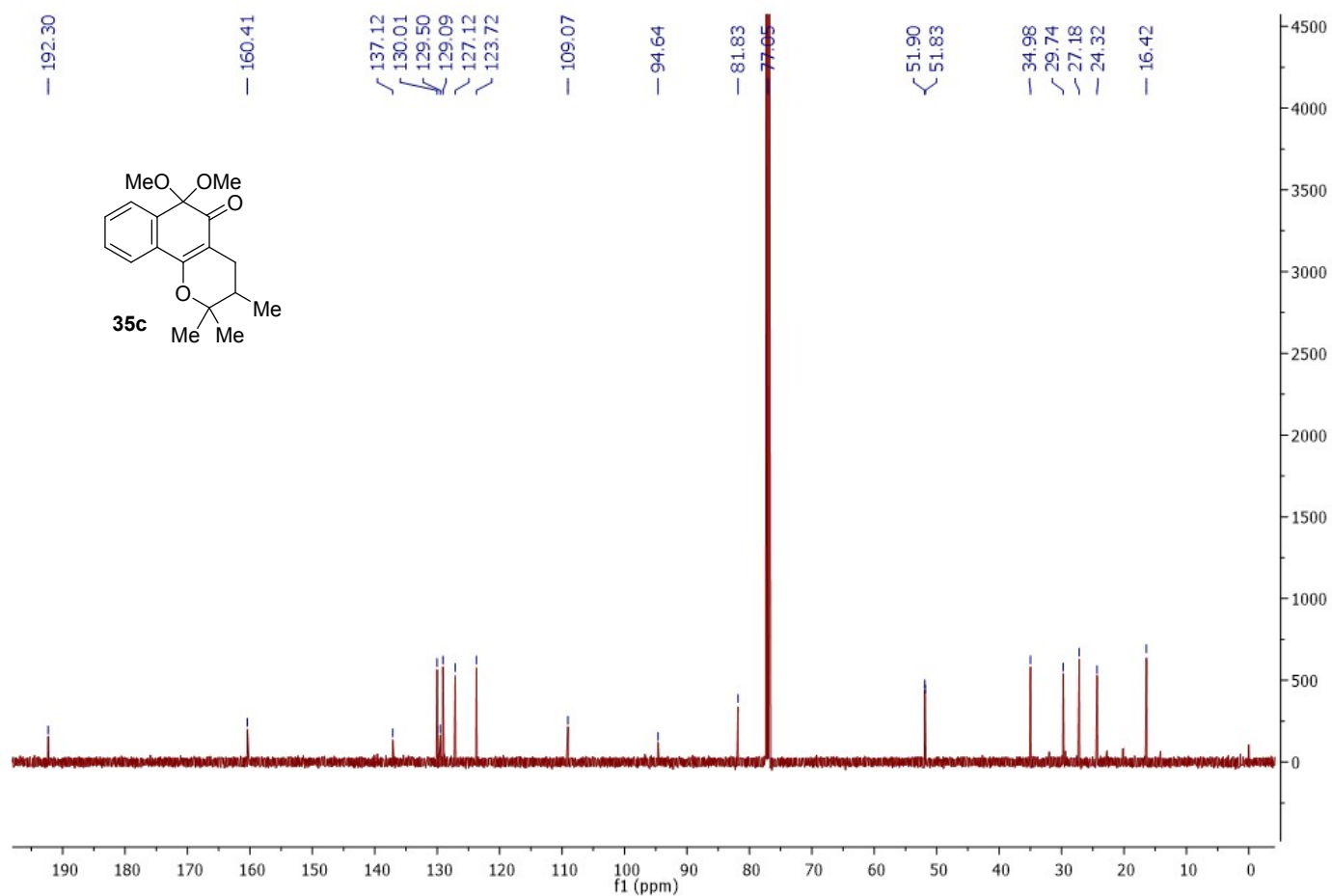
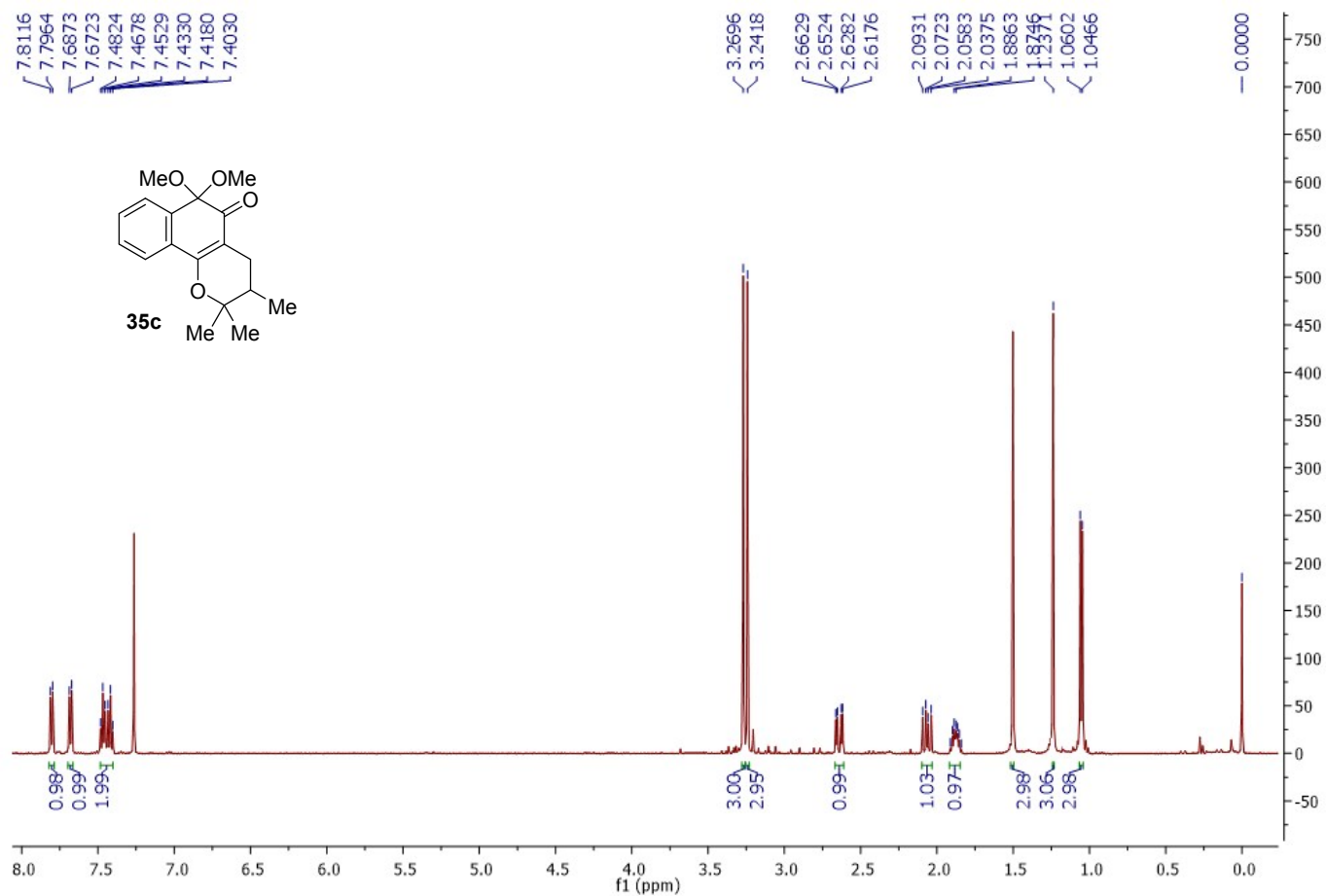


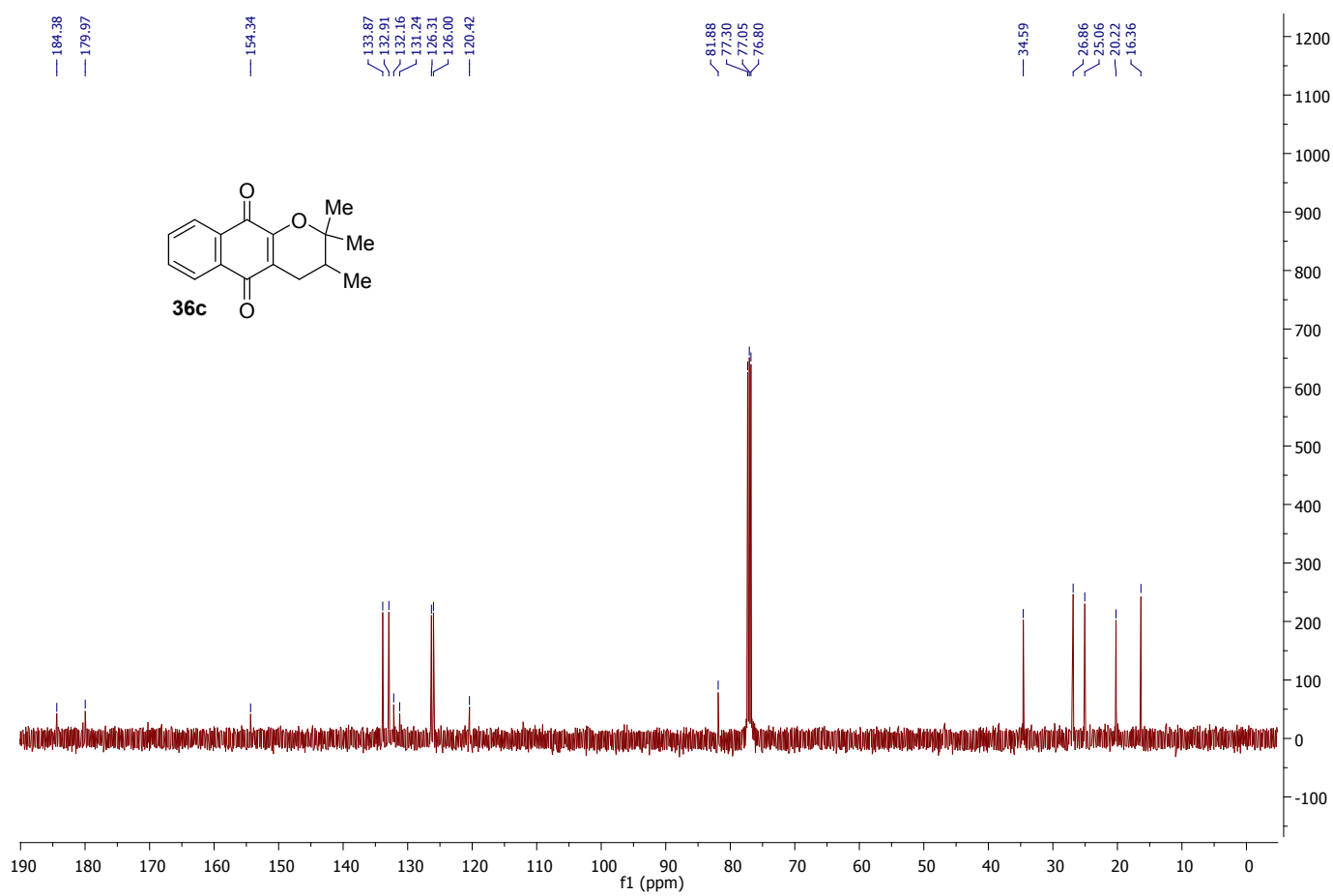
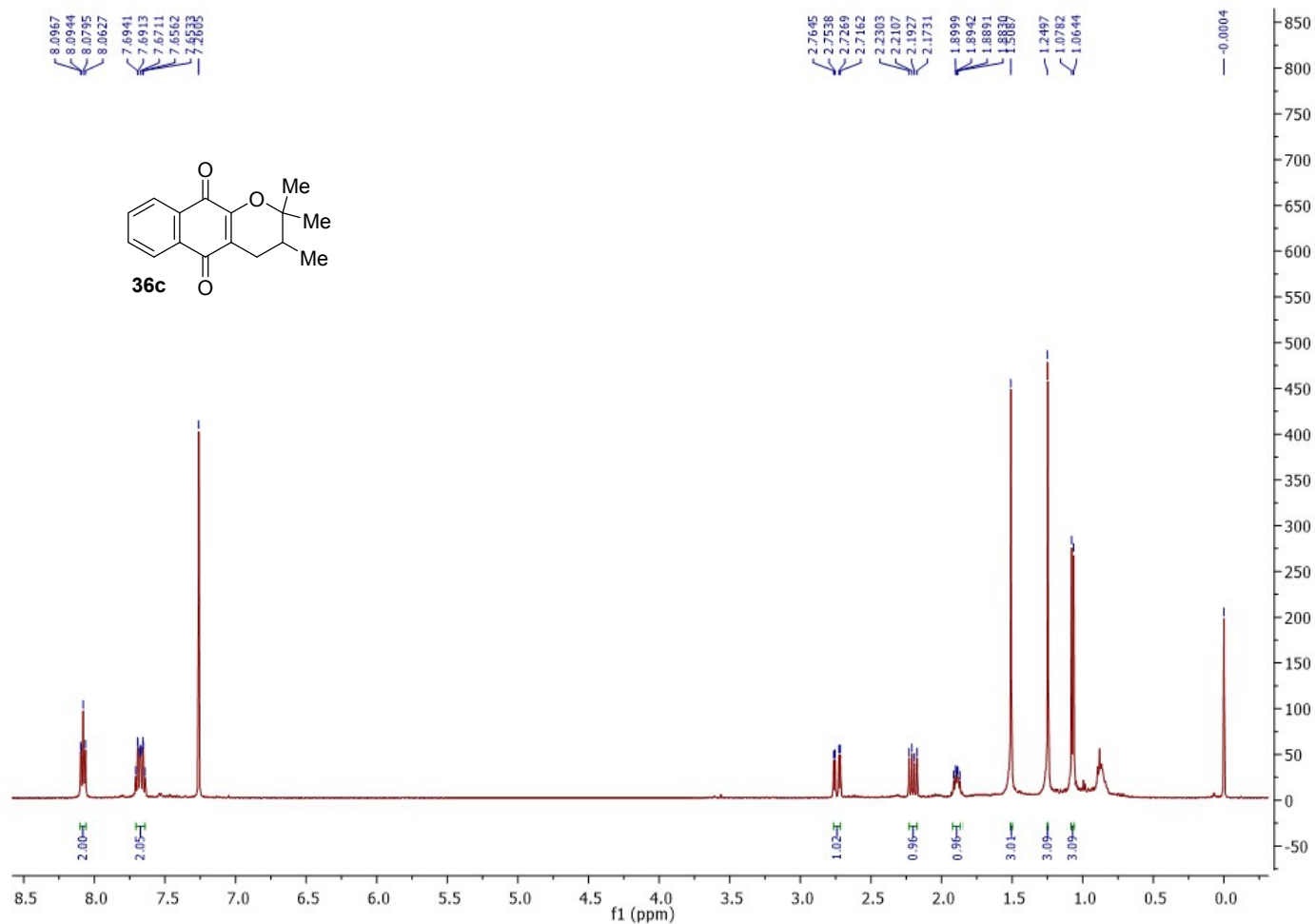


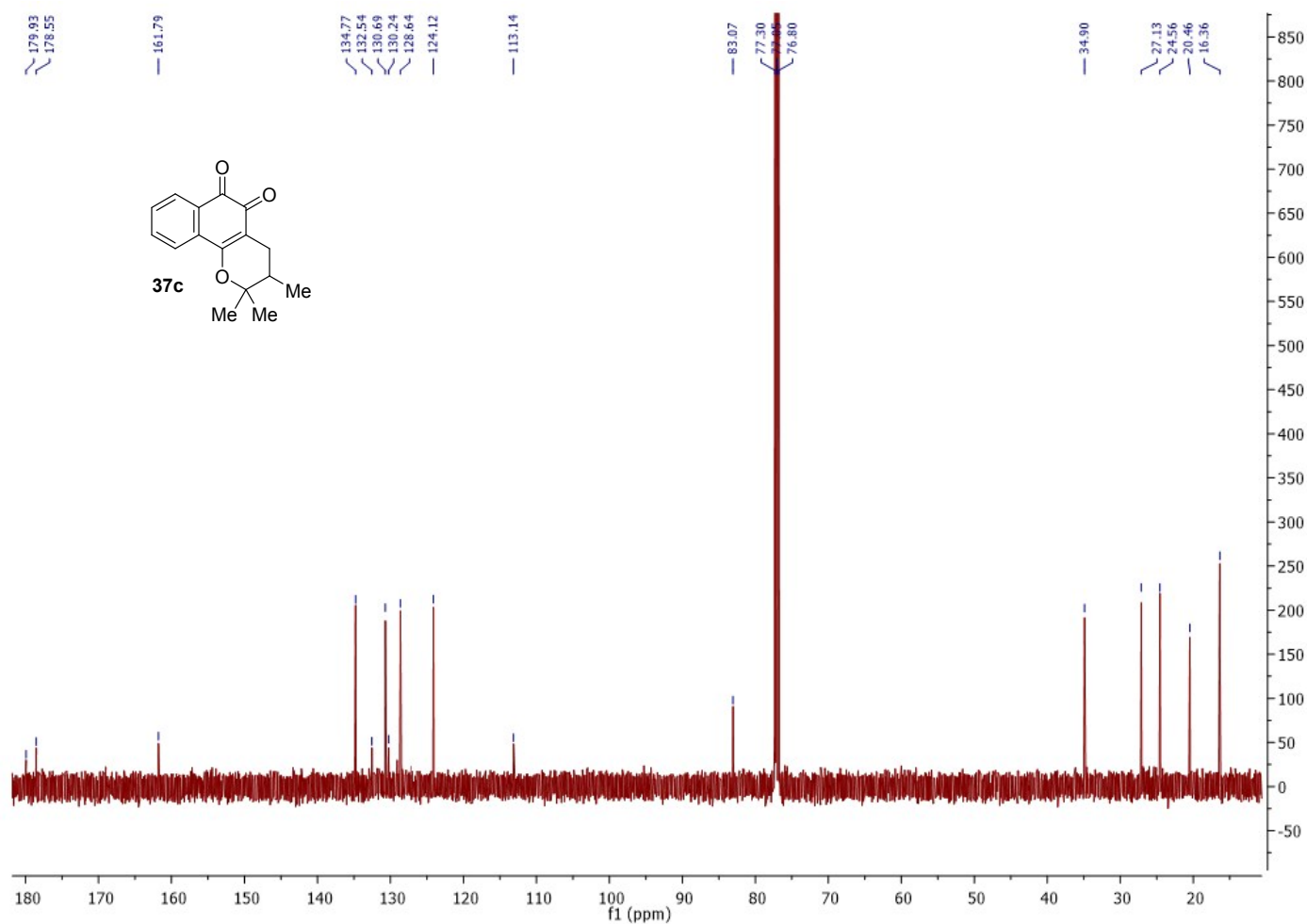
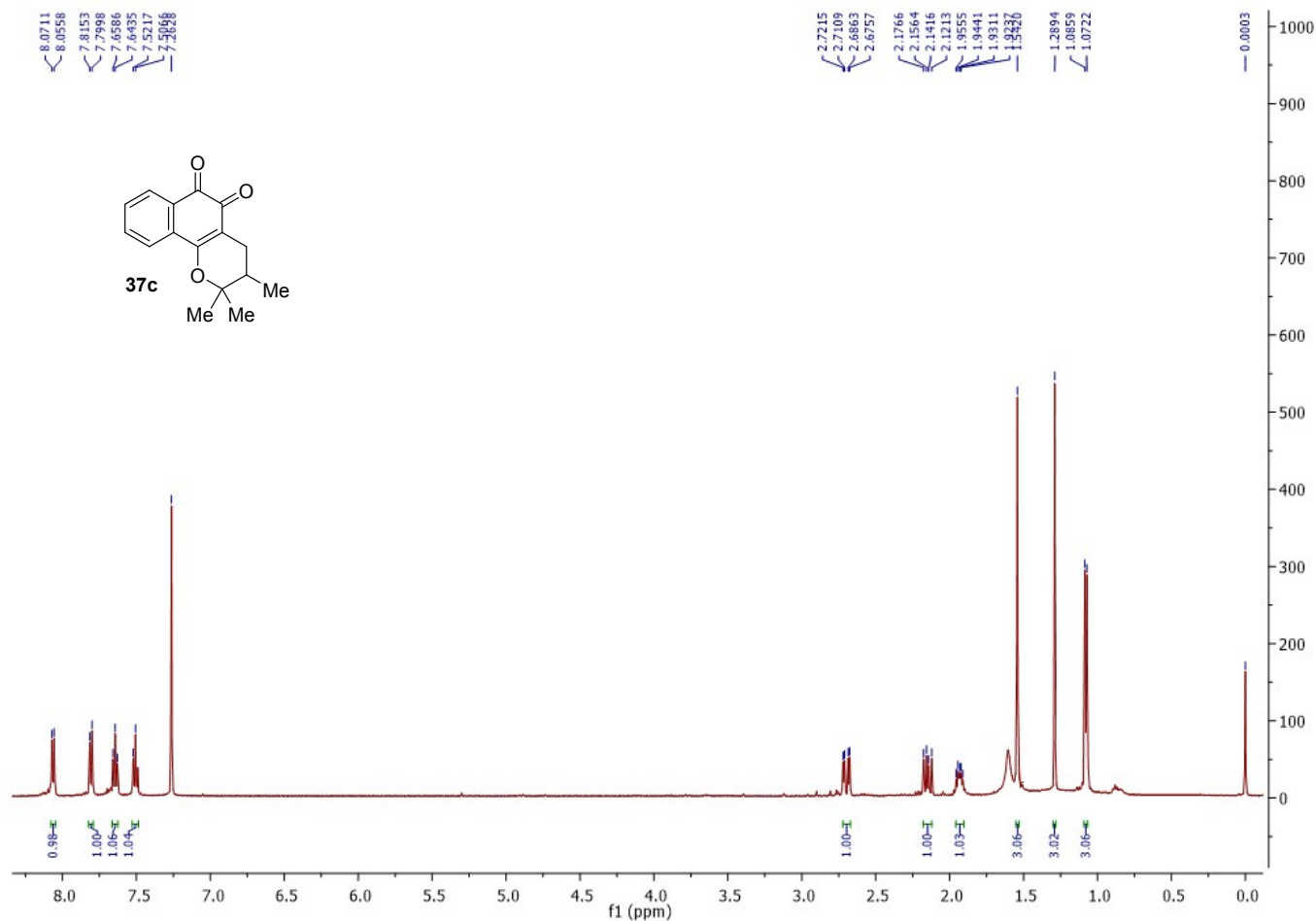


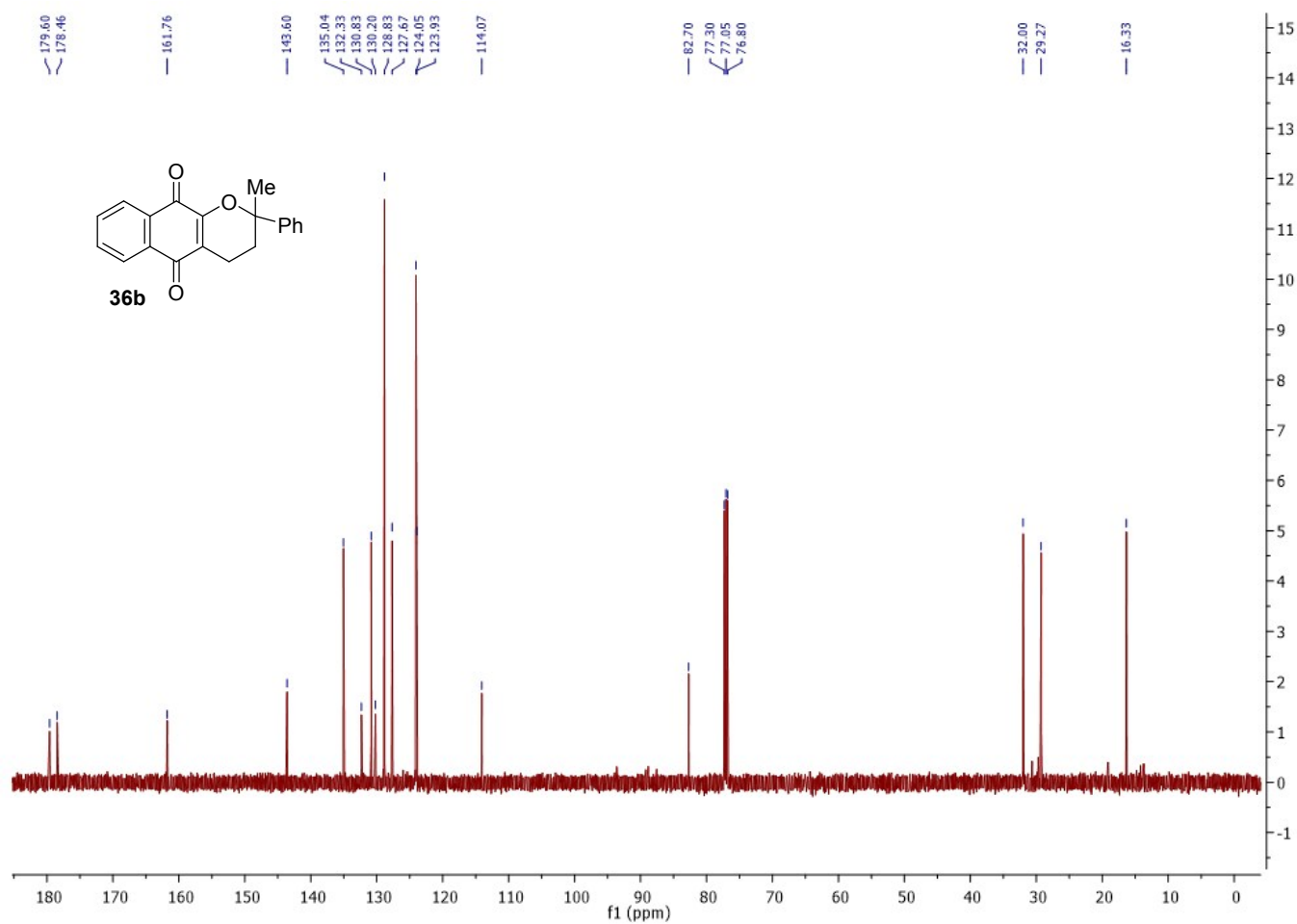
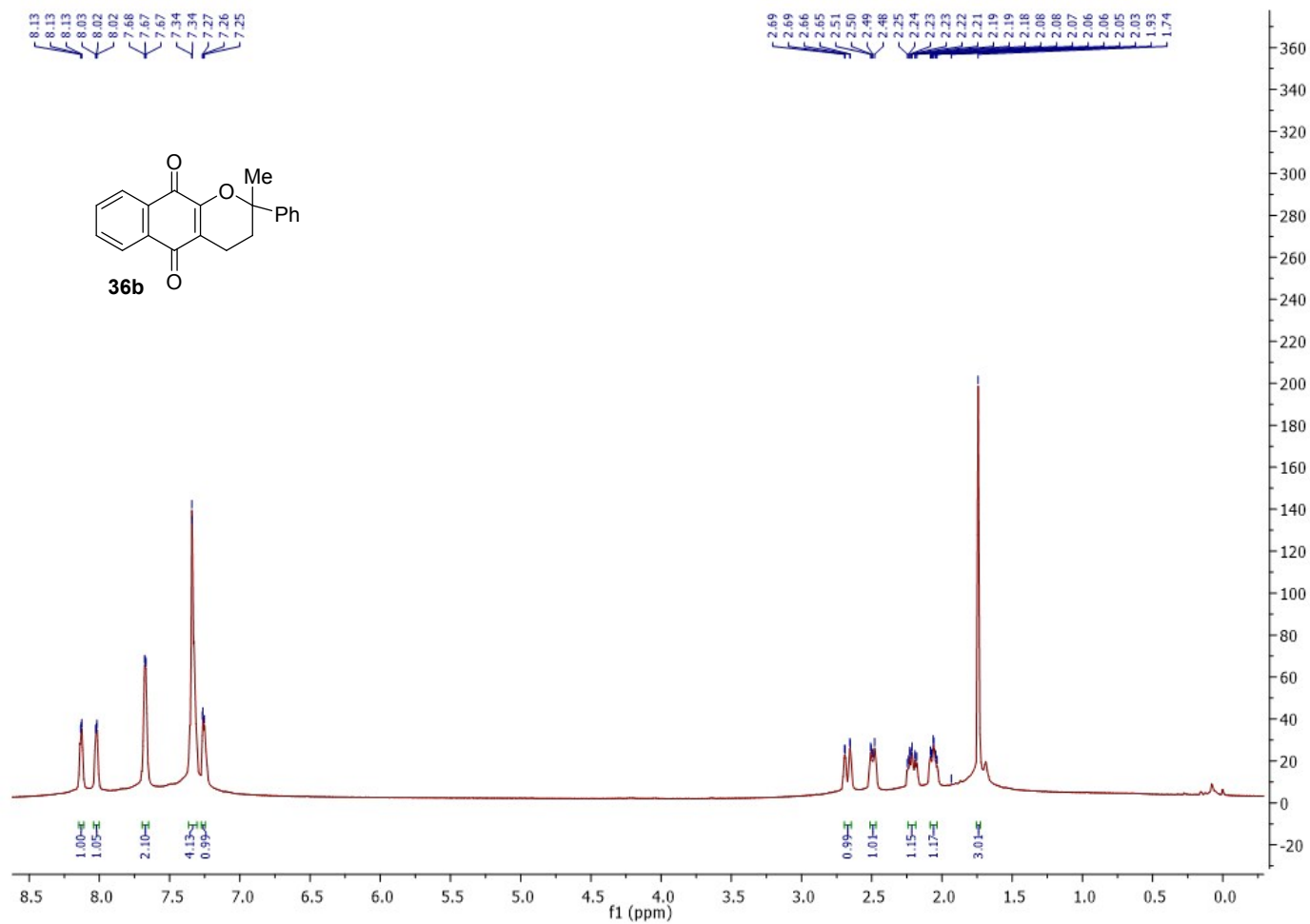
Mixture of compounds 34b and 35b

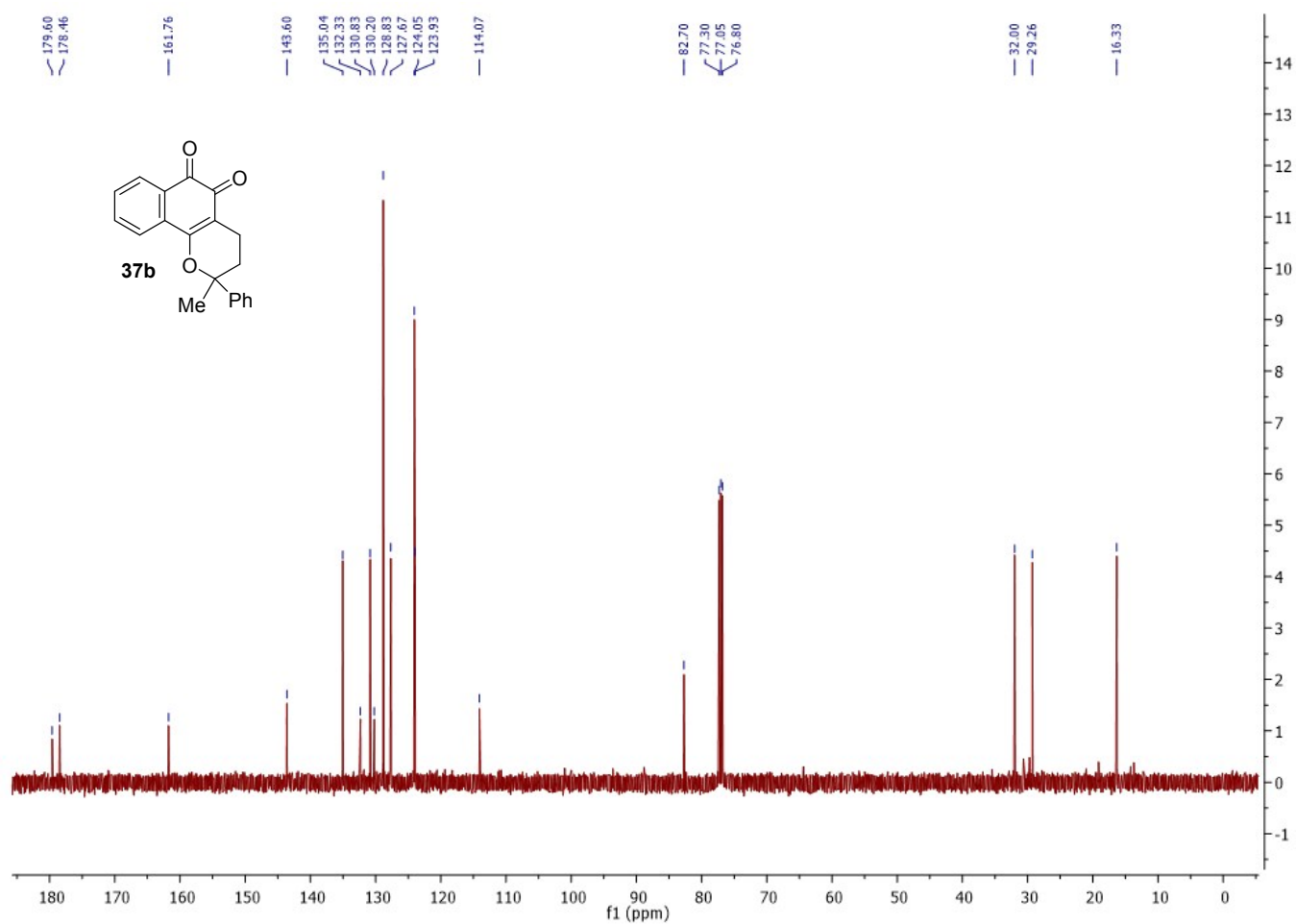
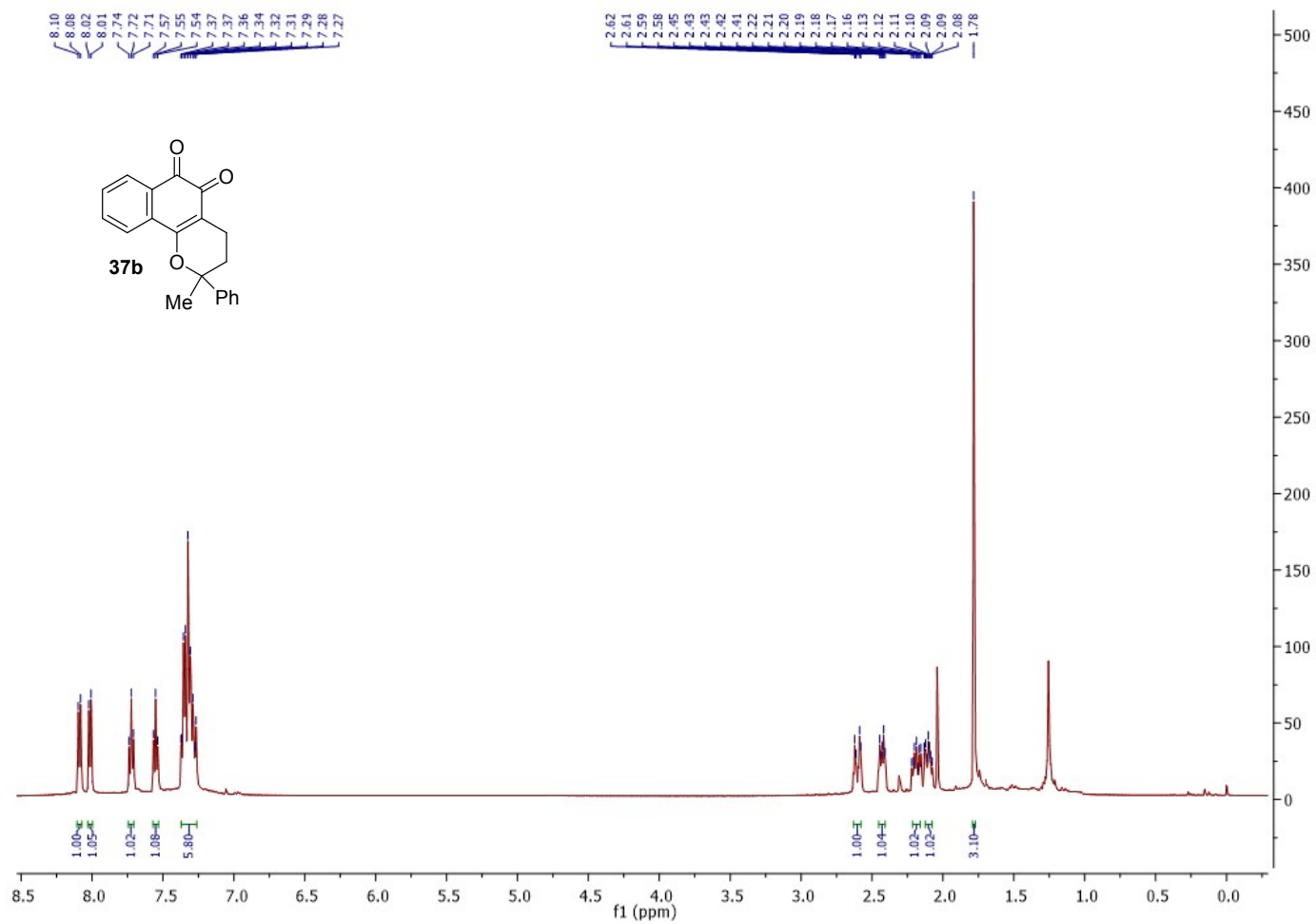








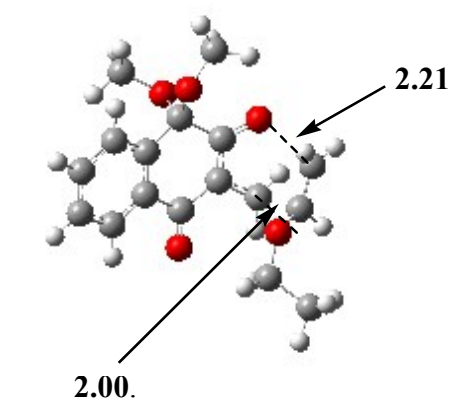




Computational data

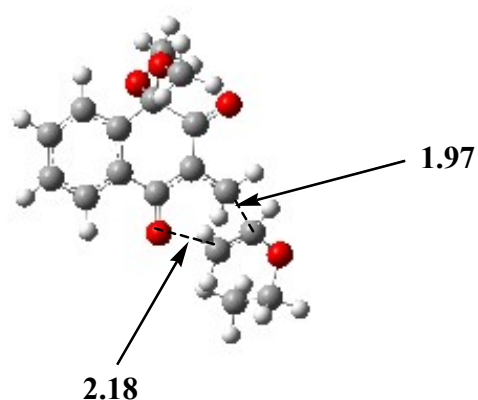
Complete Reference 46

GAUSSIAN09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2010**.



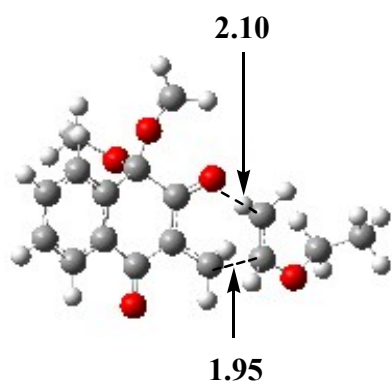
TS α -endo

$$\Delta E^\ddagger = 18.2 \text{ kcal/mol}$$



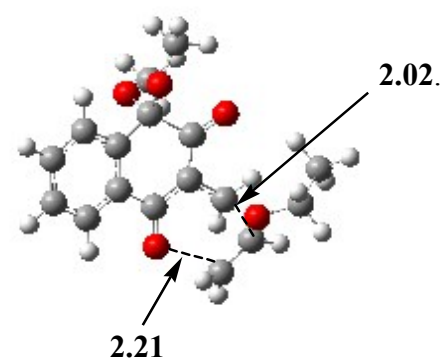
TS β -exo

$$\Delta E^\ddagger = 20.4 \text{ kcal/mol}$$



TS α -exo

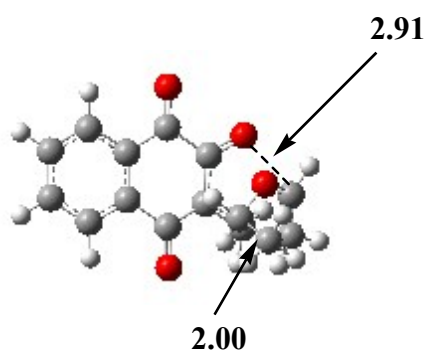
$$\Delta E^\ddagger = 21.8 \text{ kcal/mol}$$



TS β -endo

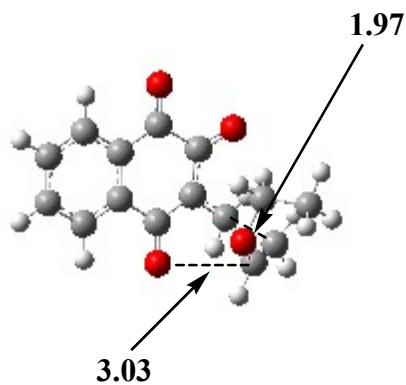
$$\Delta E^\ddagger = 22.0 \text{ kcal/mol}$$

FIGURE S1. The four possible TSs involved in the polar Diels-Alder reaction of **10** with **17a**, presenting the *meta* mode. (Distances are given in angstroms, energies in kcal/mol).



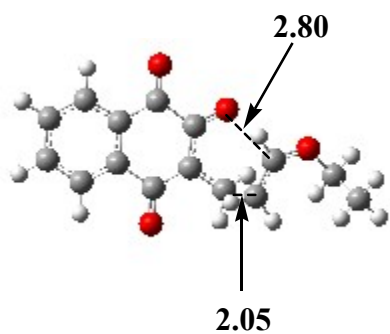
TS α -endo

$$\Delta E^\ddagger = 5.3$$



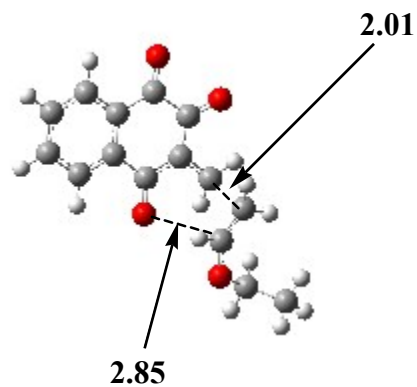
TS β -endo

$$\Delta E^\ddagger = 5.5$$



TS α -exo

$$\Delta E^\ddagger = 7.2$$



TS β -exo

$$\Delta E^\ddagger = 7.9$$

FIGURE S2. The four possible TSs involved in the polar Diels-Alder reaction of **5** with **17a**. (Distances are given in angstroms, energies in kcal/mol).

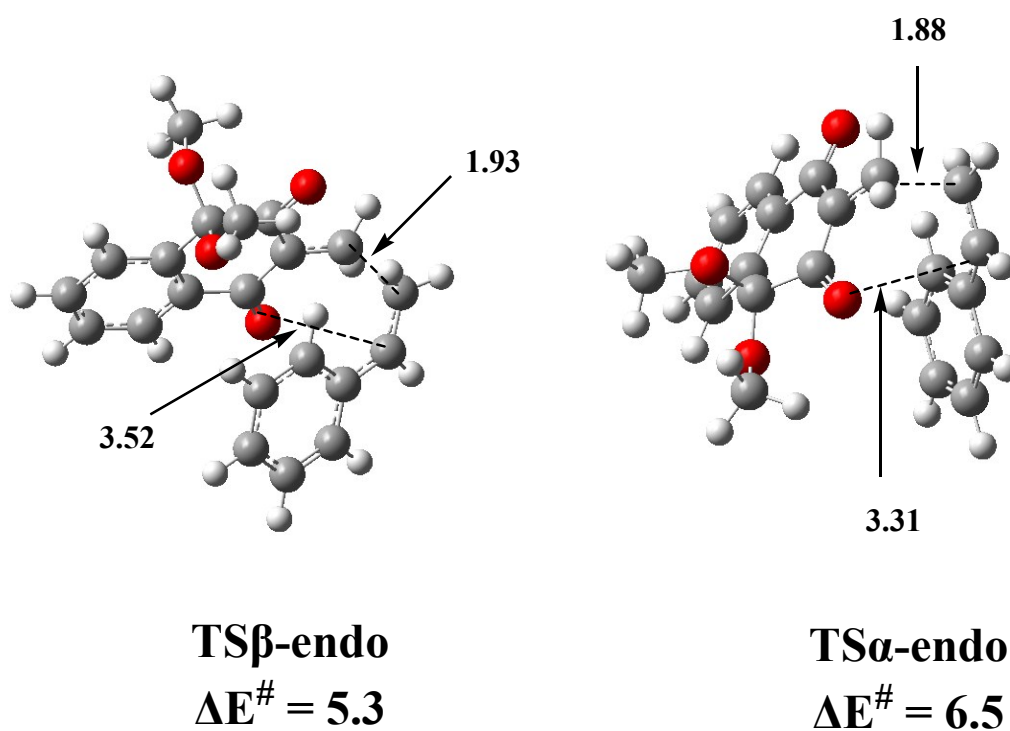


FIGURE S3. The two most probable TSs involved in the polar Diels-Alder reaction of **10** with **33a**. (Distances are given in angstroms, energies in kcal/mol).

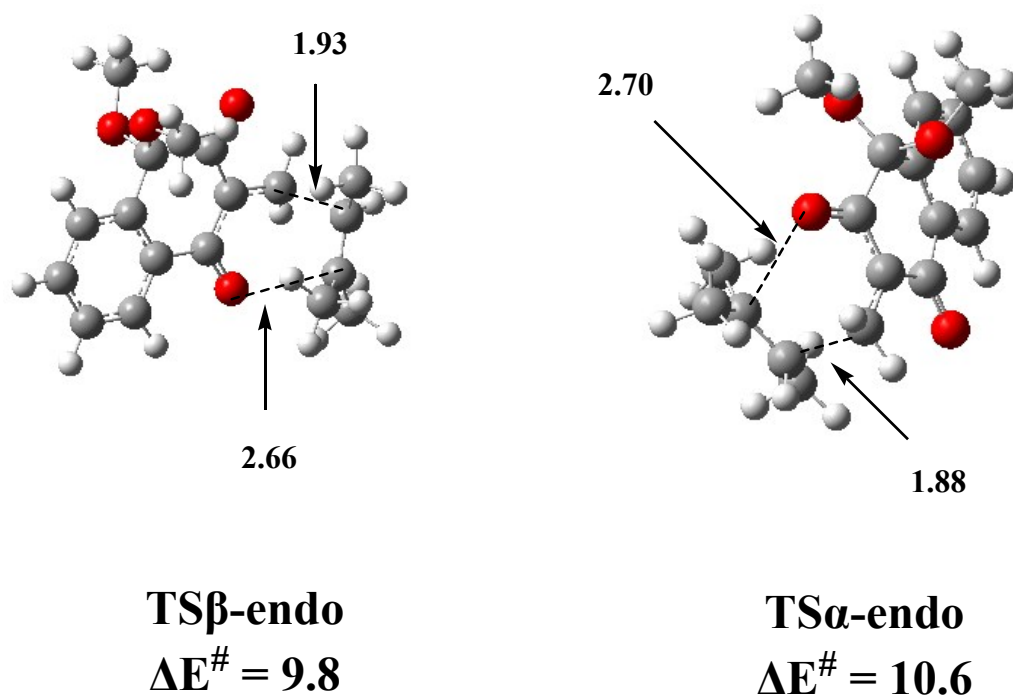


FIGURE S4. The two most probable TSs involved in the polar Diels-Alder reaction of **10** with **33c**. (Distances are given in angstroms, energies in kcal/mol).

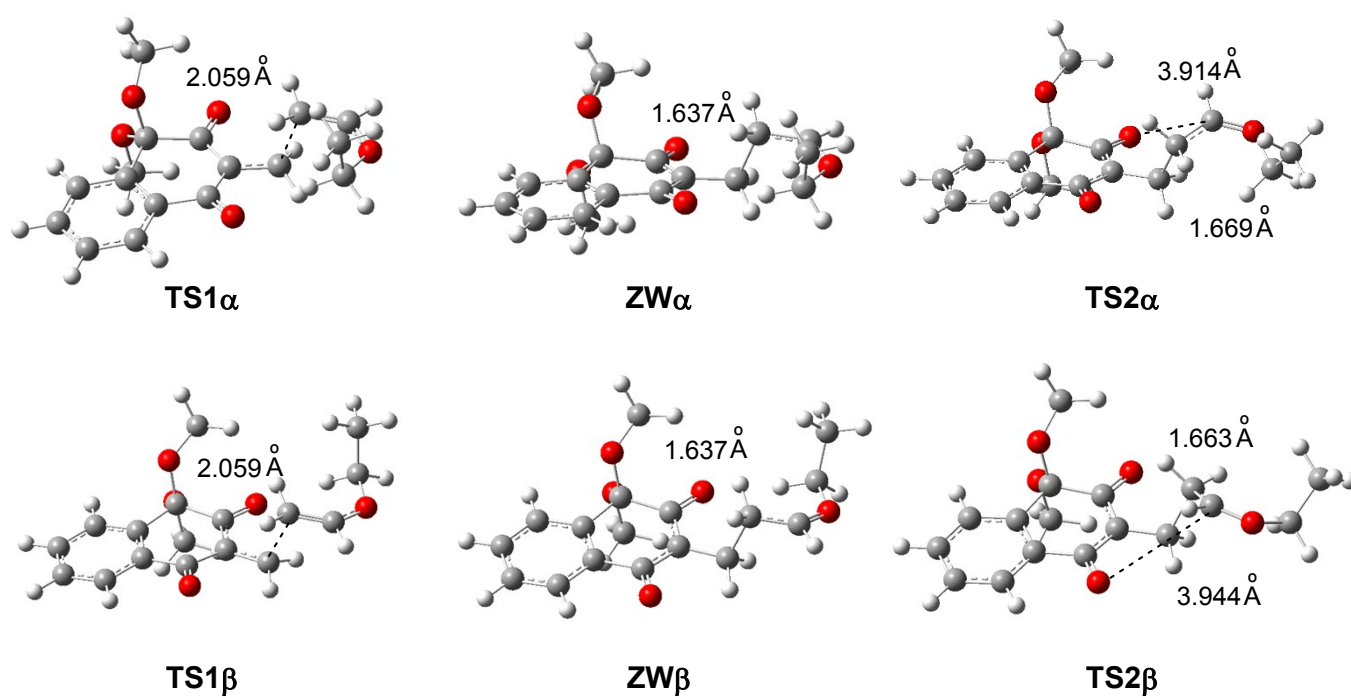
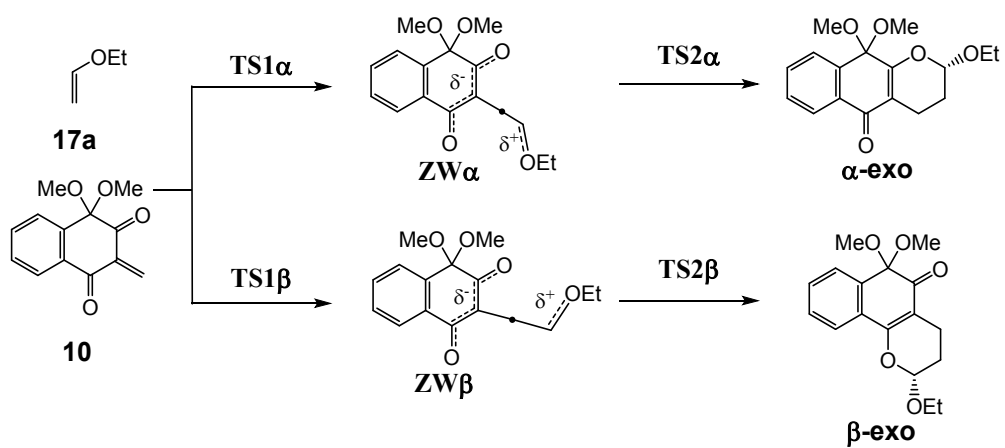


Figure S5. Geometries of the stationary points involved in the *anti* reaction paths associated with the hetero-Diels-Alder reaction of **10** with **17a**.



Scheme S1. *anti* stereoisomeric reaction paths associated with the polar hetero-Diels-Alder reaction of **10** with **17a**.

Table S1. Liquid-phase thermodynamic data, computed at 298.15 K in dichloromethane, of the Diels-Alder reaction of **10** with **17a**.

	H (a.u.)	ΔH (kcal/mol)	S (cal/mol·K)	ΔS (cal/mol·K)	G (a.u.)	ΔG (kcal/mol)
10	-803.213155		125.0		-803.272544	
17a	-232.312214		75.4		-232.348048	
TSα-endo	-1035.518996	4.0	156.9	-43.5	-1035.593559	17.0
TSα-exo	-1035.517621	4.9	158.3	-42.0	-1035.592870	17.4
TSβ-endo	-1035.520393	3.1	156.8	-43.5	-1035.594926	16.1
TSβ-exo	-1035.518577	4.3	158.4	-42.0	-1035.593855	16.8
α-endo	-1035.573828	-30.4	149.4	-50.9	-1035.644843	-15.2
α-exo	-1035.571533	-29.0	149.4	-50.9	-1035.642554	-13.8
β-endo	-1035.577409	-32.7	149.9	-50.4	-1035.648653	-17.6
β-exo	-1035.574716	-31.0	150.8	-49.6	-1035.646373	-16.2
TS1α	-1035.52034	3.2	157.7	-42.7	-1035.595303	15.9
TS1β	-1035.52009	3.3	157.9	-42.5	-1035.595142	16.0
ZWα	-1035.52454	0.5	156.6	-43.8	-1035.598974	13.6
ZWβ	-1035.52435	0.6	157.9	-42.5	-1035.599394	13.3
TS2α	-1035.51838	4.4	156.0	-44.4	-1035.592522	17.6
TS2β	-1035.51847	4.3	155.5	-44.9	-1035.592364	17.7

Table S2. Energetic data of the Diels-Alder reaction of **14b** with **17a**.

Compound	E (a.u.)
14b (Z-)	-1073.8316491
14b (E-)	-1073.8310400
17a	-232.4307407
TSβ-endo	-1306.2375029
TSβ-exo	-1306.2337462
β-endo	-1306.3007597
β-exo	-1306.2959684

TABLE S3. HOMO (au) and LUMO (au) Energies of Tetracyanoethylene (TCE), and all Reactants Studied

No.	HOMO	LUMO
TCE	-0.33520	-0.18226
5	-0.25573	-0.11477
6	-0.24101	-0.09992
7	-0.23204	-0.06542
8	-0.25314	-0.08630
9	-0.24557	-0.06932
10	-0.24397	-0.08928
14b	-0.23356	-0.09278
17a	-0.22121	+0.04416
17b	-0.20896	+0.04906
17c	-0.21858	+0.04816
17d	-0.20426	+0.04251
17e	-0.21016	+0.04465
35a	-0.22166	-0.03053
35b	-0.22132	-0.02197
35c	-0.22564	+0.03801

Table S4. Cartesian Coordinates of all Stationary Points Found in the Potential Energy Surface (B3LYP/6-31G*) of the Reactions Studied in the Gas-phase.

5/17a reaction

5

C	-1.26575900	-0.04244200	-0.19923400
C	0.06510700	0.50418000	-0.77245200
C	1.31812400	0.26171600	0.00443200
C	1.29336600	-0.48698100	1.30330800
C	-0.02251700	-0.98624700	1.80087700
C	-0.04853800	-1.68626700	3.01454100
C	-1.24972600	-2.17192000	3.52046900
C	-2.44438100	-1.96418900	2.81841000
C	-2.43125700	-1.27146300	1.61302500
C	-1.22605300	-0.77699100	1.09343100
O	0.04948600	1.10803500	-1.82689000
C	2.48821000	0.72350300	-0.46901900
O	2.32257000	-0.68283000	1.93674900
O	-2.29612400	0.14415100	-0.81871200
H	0.88879200	-1.83538500	3.53988800
H	-1.26045600	-2.71374400	4.46203000
H	-3.38145400	-2.34436600	3.21528500
H	-3.34225400	-1.09740000	1.04987500
H	2.52215800	1.26760300	-1.40754200
H	3.40647300	0.55529300	0.08432800

17a

C	-0.62711000	2.31555300	2.18847600
C	-1.38013300	1.27266500	1.82308400
O	0.17069800	3.11367500	1.43264000
C	0.25781400	2.85767100	0.02686800
C	-0.90736300	3.46451300	-0.74809700
H	-0.57527100	2.64021900	3.22487900
H	-1.93696500	0.73982700	2.58521100
H	-1.47311200	0.91727500	0.80340200
H	0.34125800	1.77711100	-0.14738800

H	1.20125100	3.31957700	-0.27909400
H	-0.77807700	3.28470200	-1.82178700
H	-0.95062500	4.54586900	-0.58280400
H	-1.86336500	3.03234300	-0.43938900

TS α -endo

C	0.91449600	-0.58291800	-0.53008200
C	0.14156300	-0.26454000	0.76402600
C	-1.29837100	-0.18898200	0.69715400
C	-2.01677500	-0.11567700	-0.56468300
C	-1.25865900	-0.44590400	-1.81643900
C	-1.95275500	-0.51866300	-3.02865800
C	-1.27753000	-0.82603900	-4.20802100
C	0.10294000	-1.05717200	-4.18894400
C	0.80369200	-0.97907700	-2.98857400
C	0.13198400	-0.67669900	-1.79739100
O	0.76803900	-0.05726800	1.80959600
C	-1.99011300	-0.02044300	1.91646600
O	-3.20746300	0.22525800	-0.62921200
O	2.12131700	-0.74922500	-0.49725400
H	-3.02168500	-0.33191800	-3.01810100
H	-1.82493900	-0.88612200	-5.14502100
H	0.62792400	-1.29500100	-5.11017500
H	1.87525100	-1.14656400	-2.94527800
H	-1.49457700	-0.41968300	2.79497200
H	-3.07011700	-0.13112800	1.87927600
C	-0.80109900	2.35417000	2.27431400
C	-2.05256000	1.85454400	2.60631200
O	-0.45184200	2.85251000	1.10983400
C	-1.45012200	3.24831200	0.12011800
C	-1.99044500	4.63550900	0.43023300
H	0.06064400	2.21933100	2.91987200
H	-2.21578500	1.65301000	3.66023500
H	-2.92640800	2.20268000	2.06648300
H	-2.23438400	2.49204300	0.05401100
H	-0.88942000	3.24146900	-0.81605500

H	-2.53758600	4.65447500	1.37818200
H	-2.67863600	4.94039900	-0.36556600
H	-1.17771900	5.36627700	0.48320800

TS β -endo

C	-1.25473800	-0.01576900	-0.19019000
C	0.06085100	0.64271900	-0.66682800
C	1.27422200	0.28288500	0.02978900
C	1.25825300	-0.35541900	1.33178200
C	-0.03554600	-0.92529800	1.82695800
C	-0.05367700	-1.62416100	3.03769600
C	-1.24122700	-2.17901000	3.51057900
C	-2.42560000	-2.03814500	2.77775700
C	-2.41804900	-1.33930900	1.57378200
C	-1.22825000	-0.77998100	1.09030700
O	0.01867900	1.45459200	-1.59617900
C	2.52756700	0.69719400	-0.47982800
O	2.28174600	-0.41211600	2.03373400
O	-2.27188800	0.11734800	-0.84849300
H	0.87721700	-1.72049300	3.58693500
H	-1.24676800	-2.72393500	4.45095500
H	-3.35028100	-2.47206900	3.14856200
H	-3.32232500	-1.20972500	0.98751000
H	2.54911100	0.95587600	-1.53518500
H	3.38646900	0.14907400	-0.10684500
C	2.79936200	2.51258500	1.44044800
C	3.14070900	2.47948200	0.09429500
O	1.62974800	2.83664300	1.93689900
C	0.63230400	3.55121100	1.13952400
C	0.92953700	5.04204700	1.12510600
H	3.44727600	2.08978400	2.20253800
H	4.20100700	2.38322400	-0.11839300
H	2.58740200	3.09154100	-0.60975400
H	-0.30118100	3.33773200	1.66262600
H	0.57212000	3.11973900	0.13886000
H	0.97901700	5.43997300	2.14330900

H	0.12825600	5.56165600	0.58883300
H	1.87470500	5.26187500	0.61849700

Cycloadduct α -endo

C	0.41764500	0.52846900	-0.63435400
C	-0.43879200	0.43656900	0.59676000
C	-1.67493800	-0.13227900	0.59367300
C	-2.21815400	-0.74638000	-0.62919000
C	-1.38176000	-0.72153800	-1.86927400
C	-1.86660500	-1.30945200	-3.03985400
C	-1.09991000	-1.28060600	-4.20448500
C	0.15465500	-0.66198600	-4.20623000
C	0.64402900	-0.07204700	-3.04225800
C	-0.11995300	-0.10072200	-1.87125400
O	0.14923100	0.98242300	1.67534100
C	-2.53278500	-0.11822400	1.83278800
O	-3.33482600	-1.26245900	-0.62948800
O	1.49877900	1.09545400	-0.60002100
H	-2.84405200	-1.78001800	-3.01456300
H	-1.47972300	-1.73986900	-5.11303100
H	0.74937600	-0.64100800	-5.11520500
H	1.61389100	0.41425800	-3.01736800
H	-2.54034200	-1.11372700	2.29847900
H	-3.57139200	0.07986200	1.54952100
C	-0.50127300	0.80014300	2.96780600
C	-2.01494200	0.93890000	2.81620600
O	0.11322100	1.65012100	3.86608400
C	-0.04345700	3.06255200	3.65222700
C	0.97282400	3.76726900	4.53391700
H	-0.24516900	-0.21143300	3.30532800
H	-2.47667500	0.82876800	3.80288500
H	-2.25464300	1.94152900	2.44451100
H	-1.06431400	3.37160200	3.91685400
H	0.12724900	3.29678500	2.59531100
H	0.81373800	3.51199400	5.58664700

H	0.88068800	4.85320300	4.42231200
H	1.98940600	3.47217800	4.25694900

Cycloadduct β -endo

C	0.19979300	-1.64254400	-1.66487500
C	0.27880200	-0.75062900	-0.39987800
C	-0.90880200	-0.00038900	-0.00663400
C	-2.05817400	-0.09153800	-0.73836500
C	-2.21041600	-0.96820800	-1.91508400
C	-3.43052900	-1.06944300	-2.59390400
C	-3.54900800	-1.90381300	-3.70669400
C	-2.45379500	-2.64229300	-4.16002600
C	-1.23528100	-2.54785000	-3.48995400
C	-1.10711000	-1.72178500	-2.37089400
O	1.32844000	-0.70368100	0.22865500
C	-0.83580600	0.84358400	1.24057600
O	-3.17783000	0.61010300	-0.44985200
O	1.18514200	-2.25259700	-2.03729200
H	-4.28357300	-0.50101100	-2.24305400
H	-4.50324200	-1.97505000	-4.22150600
H	-2.55048600	-3.28758800	-5.02842400
H	-0.36415000	-3.10847900	-3.81392900
H	-0.24656000	1.75169300	1.04931900
H	-0.28232500	0.29532900	2.00989900
C	-3.09715400	1.66319600	0.56472700
C	-2.24099900	1.20331600	1.73133400
O	-4.37418900	1.94260100	0.99620200
C	-5.16938600	2.81886100	0.18415600
C	-5.93154800	2.10107600	-0.92359100
H	-2.64838000	2.53048900	0.05401100
H	-2.73361500	0.33666200	2.18699300
H	-2.21500100	2.00111900	2.47984400
H	-4.52917700	3.61220800	-0.22934200
H	-5.86840500	3.28622300	0.88463700
H	-5.25309100	1.69974800	-1.68114000
H	-6.62083300	2.80014300	-1.41215200

H	-6.51613300	1.27426900	-0.50764700
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10/17a reaction

10

C	0.49069700	-0.42633000	-0.61760900
C	-0.20756300	-0.96019600	0.66207800
C	-1.56616100	-0.39505100	0.92269100
C	-2.38767800	0.12706800	-0.22085600
C	-1.83760800	-0.08842900	-1.58615900
C	-2.70715100	0.02427500	-2.68000300
C	-2.24870900	-0.22229500	-3.96876700
C	-0.91224800	-0.58138000	-4.16962800
C	-0.03676900	-0.68437100	-3.08867600
C	-0.48937500	-0.43741900	-1.79138000
O	0.33977900	-1.73319700	1.42712100
C	-2.06457500	-0.39241100	2.16805100
O	-3.48847000	0.62776300	-0.03188900
O	1.57760500	-1.21887600	-0.99250400
C	2.79103300	-1.15943900	-0.24559000
O	0.78200400	0.96061700	-0.42858200
C	1.35923500	1.43608000	0.79112600
H	-3.73919300	0.29815000	-2.48652800
H	-2.92629500	-0.14042700	-4.81399900
H	-0.54787600	-0.77802100	-5.17444100
H	1.00151600	-0.95264600	-3.23959400
H	-1.49362200	-0.80423700	2.99444900
H	-3.04874200	0.02382700	2.35961500
H	2.61939300	-1.24921600	0.82902100
H	3.38108400	-2.01564100	-0.58149400
H	3.34473000	-0.24015200	-0.47128400
H	2.45318700	1.40142200	0.75686900
H	1.04069300	2.47745300	0.88674400
H	1.01707700	0.88207900	1.67221800

TS β -endo

C	-1.12049300	0.06183000	-0.23937200
C	0.28929400	0.44987100	-0.78149300
C	1.44690900	0.22220800	0.05290100
C	1.35859100	-0.29677000	1.40349400
C	0.04385900	-0.82603600	1.87010400
C	-0.02209500	-1.47948200	3.10894200
C	-1.22622700	-2.00384900	3.56452500
C	-2.37989700	-1.87439600	2.78293000
C	-2.32181600	-1.21942900	1.55476800
C	-1.11227600	-0.69461200	1.08699100
O	0.35338300	0.99596800	-1.89096600
C	2.73035100	0.59475300	-0.40844800
O	2.35071700	-0.29715400	2.15357100
O	-1.86579800	-0.64169300	-1.21569400
C	-1.24874000	-1.80216900	-1.75581000
O	-1.83625800	1.25745000	0.03770700
C	-2.27122300	2.04617300	-1.07772500
H	0.89118800	-1.56105600	3.68942500
H	-1.27102500	-2.51321600	4.52362700
H	-3.32462700	-2.28157000	3.13407700
H	-3.21125300	-1.10774300	0.94342100
H	2.81657300	0.79356000	-1.47323200
H	3.56485500	0.07824900	0.05337300
H	-0.99253700	-2.52803300	-0.97170100
H	-1.98549600	-2.25030700	-2.42674700
H	-0.34887500	-1.55011700	-2.32937400
H	-2.80508500	1.43326100	-1.80662900
H	-2.95006300	2.78853600	-0.64841400
H	-1.43462200	2.54342900	-1.57766900
C	2.86676100	2.49652000	1.45423100
C	3.31942300	2.40720300	0.14370300
O	1.65192500	2.80753600	1.83893400
C	0.68631900	3.42645600	0.93362600
C	0.78815800	4.93932600	1.03358100
H	3.46208400	2.13701500	2.28752200
H	4.39410300	2.30676500	0.02717700

H	2.83352900	2.98953400	-0.63172700
H	-0.27574800	3.04993600	1.28149600
H	0.83695100	3.06059300	-0.08218000
H	0.64174500	5.27187900	2.06579000
H	0.01239200	5.39733000	0.41025700
H	1.76229400	5.30021800	0.68637200

TS α -endo

C	1.06319100	-0.49632600	-0.43644300
C	0.30376000	0.02538800	0.81470800
C	-1.12418200	-0.15641500	0.85307900
C	-1.91252700	-0.29575600	-0.35254500
C	-1.17327400	-0.37512400	-1.65520400
C	-1.92169100	-0.35821200	-2.83936800
C	-1.28949100	-0.32650200	-4.07845400
C	0.10578700	-0.29098900	-4.13850900
C	0.85948600	-0.31028800	-2.96435600
C	0.23335900	-0.36638300	-1.71440500
O	0.92326600	0.52503800	1.76293800
C	-1.77006800	0.03214100	2.10141900
O	-3.15423100	-0.23846900	-0.34099600
O	1.25678600	-1.86870100	-0.07813700
C	1.87896100	-2.70946500	-1.04392100
O	2.27609900	0.16418700	-0.68302900
C	3.30828500	0.08773000	0.30711100
H	-3.00342500	-0.35864800	-2.75156000
H	-1.87796200	-0.31652700	-4.99223600
H	0.61017700	-0.24666900	-5.10052000
H	1.94177600	-0.26987600	-3.00771300
H	-1.15859200	-0.17175400	2.97499400
H	-2.79504600	-0.32692500	2.15169800
H	2.06525300	-3.65741200	-0.53284600
H	1.23013300	-2.88825500	-1.90988700
H	2.83256000	-2.29392800	-1.39180800
H	4.25616400	0.09225200	-0.24187600
H	3.26187200	0.94567300	0.98064800

H	3.22925100	-0.83025700	0.89428400
C	-1.10856900	2.60229400	2.13647700
C	-2.21757700	1.85769800	2.53500900
O	-0.86925300	3.04417600	0.92549900
C	-1.91541200	3.11111600	-0.09260100
C	-2.70761100	4.40055400	0.05216300
H	-0.24598000	2.73376500	2.78188400
H	-2.35336000	1.77664400	3.60972200
H	-3.14136100	1.95945800	1.97418900
H	-2.54493900	2.22145000	-0.04866300
H	-1.35495400	3.08703900	-1.02823900
H	-3.25865800	4.43074500	0.99788600
H	-3.43249800	4.47210600	-0.76592800
H	-2.04686100	5.27167600	0.00607100

Cycloadduct β -endo

C	-1.11163500	0.11911000	-0.39350700
C	0.30651000	0.47984400	-0.92849800
C	1.38360500	0.71728000	0.02113800
C	1.23377900	0.37120700	1.33289100
C	-0.00165500	-0.20308100	1.88619500
C	-0.06844600	-0.61610900	3.22597100
C	-1.24181100	-1.17011300	3.73135700
C	-2.35630900	-1.32164600	2.90378900
C	-2.29280500	-0.91615400	1.57020000
C	-1.12277700	-0.36149500	1.05356200
O	0.46355300	0.64340900	-2.13719800
C	2.67155100	1.31289100	-0.48957800
O	2.21948500	0.50425400	2.25026300
O	-1.77411600	-0.79294700	-1.24545400
C	-1.09595600	-2.01363100	-1.51314000
O	-1.88022000	1.30452000	-0.37972800
C	-2.15375100	1.92681900	-1.64168200
H	0.80426200	-0.50159600	3.85839000
H	-1.28476700	-1.48596900	4.77009400
H	-3.27303300	-1.75422300	3.29535600

H	-3.14896400	-1.02780500	0.91322600
H	2.44347100	2.09053100	-1.22587200
H	3.25537900	0.55715400	-1.03415400
H	-0.86440600	-2.56006500	-0.58801400
H	-1.78323200	-2.61341100	-2.11446600
H	-0.17461800	-1.84641200	-2.08224000
H	-2.54947100	1.20460700	-2.35918400
H	-2.90704300	2.68706200	-1.42051500
H	-1.26271100	2.40198500	-2.06515300
C	3.56093500	0.85537300	1.80034500
C	3.48832800	1.88349300	0.67568100
O	4.29210200	1.20369700	2.92137700
C	3.88805900	2.37554800	3.65342000
C	4.90815400	3.49568100	3.49825500
H	4.02167400	-0.07045400	1.43595400
H	4.50938200	2.12951400	0.36626200
H	3.01998100	2.80231800	1.04751700
H	3.81955000	2.06519300	4.70175000
H	2.88695500	2.69435600	3.34494500
H	5.90520500	3.14478900	3.78360200
H	4.64321800	4.34136900	4.14397500
H	4.95583200	3.85554600	2.46526500

Cycloadduct α -endo

C	0.44692400	-0.18564800	-0.99239900
C	-0.58628800	0.40918100	-0.02765200
C	-1.86912400	-0.01186200	0.06798200
C	-2.38512800	-1.05612300	-0.82139300
C	-1.51580000	-1.49705400	-1.95293300
C	-2.06891500	-2.33510000	-2.92857900
C	-1.33645900	-2.67844300	-4.06020400
C	-0.04944300	-2.16213100	-4.22966000
C	0.50865200	-1.33027500	-3.25832300
C	-0.20945900	-1.00602600	-2.10242500
O	-0.03479800	1.33107300	0.79085300

C	-2.81312800	0.57686200	1.08701200
O	-3.52033000	-1.50977100	-0.67402600
O	1.22634500	-0.99255600	-0.11043900
C	2.25849100	-1.79527300	-0.67537000
O	1.22805500	0.78409500	-1.65744500
C	2.16494300	1.56604000	-0.90987500
H	-3.08429500	-2.68702400	-2.77773500
H	-1.76976400	-3.32863000	-4.81535100
H	0.52184100	-2.40235300	-5.12254300
H	1.49902400	-0.91430700	-3.40281700
H	-2.97345600	-0.13730300	1.90638600
H	-3.79718000	0.72129700	0.62954300
H	2.80982600	-2.20040500	0.17664100
H	1.85423500	-2.62208800	-1.27048300
H	2.94200900	-1.20542400	-1.29775900
H	3.01431900	1.74163100	-1.57766400
H	1.72650700	2.52555600	-0.62056100
H	2.50015100	1.04271700	-0.01229500
C	-0.78484600	1.73578100	1.97520400
C	-2.26095200	1.90135800	1.62658100
O	-0.14320900	2.83365500	2.51881600
C	-0.12586300	4.05448500	1.75899300
C	-0.98513600	5.12246100	2.42316100
H	-0.65564600	0.93430100	2.71159100
H	-2.79710200	2.22049000	2.52632700
H	-2.37303600	2.68936400	0.87260900
H	-0.44031500	3.87041600	0.72621900
H	0.92146800	4.37532100	1.72670400
H	-2.04435900	4.84512900	2.41894600
H	-0.87846000	6.07765800	1.89537200
H	-0.67456500	5.26778100	3.46290100

10/33c reaction

33c

C	-0.59918600	0.71841300	-0.44497600
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C	0.18880400	-0.30277600	-0.07548700
C	-0.52083100	2.16185600	-0.03314600
C	-0.05528900	-1.69641100	-0.60562400
C	1.35989300	-0.19228800	0.87033100
H	-1.41210300	0.49184100	-1.13713500
H	0.30084800	2.37004700	0.65737600
H	-1.45297700	2.48065700	0.45366300
H	-0.39080200	2.81161800	-0.90972100
H	0.82331900	-2.07478100	-1.14750900
H	-0.91263800	-1.73074000	-1.28543200
H	-0.24228600	-2.40566600	0.21332900
H	2.28753400	-0.51852800	0.37927200
H	1.22115500	-0.85291800	1.73768500
H	1.52017300	0.82103600	1.24560300

TS β -endo

C	-0.71169200	-2.28984700	0.85354200
C	-1.13038300	-1.36729700	-0.33245300
C	-0.12173500	-1.06567500	-1.33339200
C	1.28494800	-1.19171700	-1.06717000
C	1.72462700	-1.80279000	0.21891600
C	3.09438900	-1.87626200	0.50749500
C	3.53319100	-2.44055800	1.70044400
C	2.60062200	-2.93646400	2.61761200
C	1.23718000	-2.86538100	2.33656100
C	0.78829100	-2.29640600	1.14122000
O	-2.31083700	-1.02404300	-0.43143100
C	-0.48921000	-0.48209800	-2.57254900
O	2.11646400	-0.71845500	-1.87449900
O	-1.01255400	-3.62215600	0.48910800
C	-2.39152300	-3.94571100	0.27805100
O	-1.45667300	-2.00917400	2.02285700
C	-1.40787600	-0.67357000	2.50293100
H	3.79176000	-1.48504400	-0.22625600
H	4.59657000	-2.49785200	1.91775000
H	2.93728800	-3.38142800	3.55044500

H	0.50455600	-3.24709700	3.03994600
H	-1.55489600	-0.49434900	-2.78972500
H	0.15548300	-0.72361700	-3.41244800
H	-2.79187800	-3.46684400	-0.62217400
H	-2.40979000	-5.03152300	0.15567900
H	-3.00095800	-3.65581600	1.13746900
H	-1.95987700	-0.67235800	3.44620400
H	-0.37560400	-0.34921900	2.69796800
H	-1.88863800	0.02162300	1.80577400
C	-0.27876400	1.43278700	-2.64341300
C	1.10818900	1.64597500	-2.55713200
C	-1.22744400	1.98794200	-1.59361500
C	1.97003100	1.55990000	-3.77551700
C	1.73242600	2.10317000	-1.27790000
H	-0.66150900	1.49849500	-3.66371100
H	-1.24395200	3.08500800	-1.62955000
H	-0.94057300	1.68769800	-0.58253400
H	-2.24441800	1.62402800	-1.75791200
H	2.86234000	0.96024000	-3.57639900
H	2.30262200	2.57046300	-4.05986500
H	1.43477500	1.13380900	-4.62943200
H	2.81915800	2.00109600	-1.29121600
H	1.33650900	1.54310000	-0.42262000
H	1.47861900	3.16030900	-1.09961700

TS α -endo

C	-0.11936700	-0.94874500	-1.09748300
C	-0.55960100	-1.70439400	0.18298900
C	-1.91785200	-1.59037500	0.61133200
C	-2.79320500	-0.52022400	0.15065600
C	-2.19153300	0.49603500	-0.77600200
C	-2.93184900	1.65204700	-1.05202100
C	-2.38685000	2.67687700	-1.81973100
C	-1.08384100	2.55385300	-2.30765800
C	-0.34214300	1.40111500	-2.04539400
C	-0.88808400	0.35889300	-1.28892300

O	0.24622600	-2.42699200	0.79927200
C	-2.34241200	-2.48032800	1.63801600
O	-3.95812800	-0.39575200	0.54627500
O	-0.45718000	-1.90571600	-2.10571700
C	-0.26786500	-1.51416700	-3.46180500
O	1.24553800	-0.61617800	-1.11635000
C	2.20351200	-1.67998600	-1.11479300
H	-3.93161300	1.72186800	-0.63573700
H	-2.96747000	3.57194300	-2.02704400
H	-0.64170600	3.35606300	-2.89307700
H	0.67220900	1.30626000	-2.41558200
H	-1.89159300	-3.46897900	1.60983600
H	-3.41670900	-2.47596500	1.81299000
H	-0.45011600	-2.41347600	-4.05540200
H	-0.97448900	-0.73226500	-3.76448900
H	0.75468900	-1.16216000	-3.64501400
H	3.04971700	-1.33010700	-1.71585600
H	2.53531600	-1.90075200	-0.09789000
H	1.78937900	-2.58855300	-1.55804200
C	-0.42587400	-2.01476800	3.37742300
C	-1.83645100	-1.97998200	3.38227600
C	0.34862000	-0.75234000	3.20718000
C	0.30658300	-3.28896300	3.64265200
C	-2.57636400	-0.68148500	3.67251500
H	-2.28194400	-2.85176200	3.86658400
H	0.22396700	-0.11014200	4.09265400
H	1.41270700	-0.93359800	3.04489500
H	-0.04607500	-0.17601500	2.35821800
H	1.14043100	-3.41468100	2.94753800
H	-0.35122100	-4.16080300	3.57567200
H	0.72101100	-3.26311700	4.66319900
H	-2.38957800	-0.35422900	4.70337500
H	-2.27126900	0.12412600	3.00041500
H	-3.65350500	-0.81417400	3.54577800

Cycloadduct β -endo

C	-2.26605400	-0.33424800	-0.69820800
C	-1.32372400	0.31287600	-1.75702700
C	0.09833800	0.42461200	-1.46467100
C	0.55935400	0.20389700	-0.19878500
C	-0.31398600	-0.13864100	0.93540800
C	0.19868000	-0.23552500	2.23810900
C	-0.64308400	-0.54838400	3.30254500
C	-2.00261400	-0.77205900	3.07595600
C	-2.51556000	-0.68262200	1.78133000
C	-1.68317600	-0.36021700	0.71043300
O	-1.79133100	0.63945100	-2.84705200
C	1.02079800	0.87335300	-2.56979600
O	1.85968700	0.31893000	0.14470600
O	-2.43121800	-1.69608700	-1.03891600
C	-3.08271500	-1.98633600	-2.28191100
O	-3.55049100	0.25359000	-0.71584100
C	-3.60628300	1.66151500	-0.52547100
C	2.35271800	1.40805500	-2.00784400
C	2.86847400	0.43877300	-0.91309200
C	2.20065700	2.85777100	-1.51631400
C	3.12879500	-0.97083800	-1.46442200
C	4.11045100	0.95004800	-0.18242900
H	1.25583000	-0.06374400	2.40354300
H	-0.23717100	-0.61904600	4.30801900
H	-2.66141300	-1.01949600	3.90399000
H	-3.56818200	-0.85913100	1.58643500
H	0.51505400	1.64559800	-3.15903800
H	1.19774400	0.04659800	-3.27143600
H	-2.46172500	-1.71820000	-3.14307500
H	-3.24477000	-3.06698700	-2.26665500
H	-4.04017500	-1.46536500	-2.35568200
H	-3.13306500	2.19911500	-1.35446000
H	-4.66793500	1.91780300	-0.49263000
H	-3.13957900	1.96127000	0.42351900
H	3.09960800	1.39884900	-2.81271200

H	1.53124100	2.92323700	-0.65168000
H	1.77546400	3.47695800	-2.31345000
H	3.16067900	3.30047000	-1.23436500
H	3.49560600	-1.62278200	-0.66549300
H	3.88729600	-0.93386800	-2.25436300
H	2.22325800	-1.42110500	-1.87825300
H	4.44055900	0.21443100	0.55799400
H	3.91051200	1.88891900	0.33904600
H	4.92780900	1.11188600	-0.89365000

Cycloadduct α -endo

C	0.27476500	-0.41049100	-1.33575100
C	1.44290100	-0.83335700	-0.43687200
C	1.31937300	-1.62815600	0.65191100
C	0.00542800	-2.10654700	1.08744600
C	-1.20068300	-1.54862000	0.40497500
C	-2.46167500	-1.84578100	0.93605000
C	-3.60650500	-1.26267500	0.40329100
C	-3.48903300	-0.35704900	-0.65404900
C	-2.23545700	-0.05958700	-1.18917400
C	-1.08211500	-0.66721300	-0.68071300
O	2.62327900	-0.39637200	-0.91770000
C	2.52631100	-2.06981700	1.44100800
O	-0.10271000	-2.90422300	2.01976200
O	0.49224900	-1.23282200	-2.48328500
C	-0.46667800	-1.18308400	-3.53477200
O	0.26970600	0.96393500	-1.66090100
C	1.31117600	1.50044100	-2.48095100
C	3.85632100	-1.02386400	-0.42607600
C	3.76024900	-1.20810100	1.11030400
C	4.96319100	-0.06088900	-0.85495200
C	4.00842800	-2.36280700	-1.16219700
C	3.72607600	0.12164000	1.88334200
H	-2.50779100	-2.52689200	1.77958200
H	-4.58304400	-1.49595000	0.81895500

H	-4.37411700	0.12498600	-1.06100500
H	-2.14547700	0.66176500	-1.99299200
H	2.72490200	-3.13235800	1.24889300
H	2.29544400	-2.01242500	2.51024200
H	-0.03319800	-1.76618500	-4.35115300
H	-1.42235800	-1.63112000	-3.23937300
H	-0.64287600	-0.15733600	-3.88061000
H	0.85770100	2.32557700	-3.03903200
H	2.13339600	1.88289900	-1.86939500
H	1.70117900	0.75362900	-3.17638700
H	4.66088000	-1.75600000	1.41825000
H	5.93457800	-0.41997000	-0.49771700
H	5.00248400	0.00570400	-1.94682200
H	4.79661500	0.94352400	-0.45860700
H	4.07893700	-2.18996600	-2.24036900
H	3.15587800	-3.02231800	-0.98420000
H	4.91861200	-2.87578300	-0.83162500
H	4.64830900	0.69640900	1.75527100
H	2.88720000	0.75107900	1.56707700
H	3.60819200	-0.07482100	2.95444900

10/33a reaction

33a

C	1.32061300	1.35793700	0.03208600
C	2.54805900	1.05380500	0.47212100
C	0.09531600	0.55070500	0.15319000
C	0.06193600	-0.71055100	0.77642900
C	-1.12426300	-1.43251200	0.86495500
C	-2.30956700	-0.91481100	0.33319300
C	-2.29464200	0.33372600	-0.28849900
C	-1.10474200	1.05542800	-0.37600300
H	1.18284000	2.31041300	-0.48018500
H	3.37882900	1.73643500	0.32191400
H	2.77692600	0.12790100	0.99290800
H	0.97197200	-1.13032200	1.19526900

H	-1.12630900	-2.40481700	1.35090200
H	-3.23406400	-1.48144700	0.40395200
H	-3.20887700	0.74734900	-0.70606800
H	-1.09943400	2.02863700	-0.86205300

TS β -endo

C	-1.37935800	-0.38176700	0.09921800
C	-0.60973500	-0.57807400	-1.23978200
C	0.75225400	-1.07306100	-1.21959000
C	1.46090800	-1.39755600	0.01620300
C	0.68820600	-1.33703800	1.29426000
C	1.31835200	-1.75732700	2.47499000
C	0.63638600	-1.73283000	3.68545700
C	-0.68898400	-1.28437800	3.72652700
C	-1.31965300	-0.86257800	2.55873900
C	-0.64008500	-0.88662700	1.33543000
O	-1.17639500	-0.24956800	-2.28978300
C	1.43444400	-1.22657000	-2.44724300
O	2.65052000	-1.73537000	0.00689800
O	-2.67521800	-0.95106200	0.02266800
C	-2.73992600	-2.32275900	-0.34203100
O	-1.56205500	1.00627500	0.32429800
C	-2.45157000	1.71573300	-0.55004100
H	2.34582400	-2.09945900	2.40593700
H	1.12968400	-2.06228800	4.59619600
H	-1.22834200	-1.26319100	4.67006600
H	-2.34621000	-0.51186900	2.57893300
H	0.80205200	-1.37955800	-3.31810500
H	2.34237500	-1.81974700	-2.41048700
H	-2.16122400	-2.95447600	0.34591700
H	-3.79424900	-2.60171000	-0.27705400
H	-2.39064600	-2.48528300	-1.36899500
H	-3.39804400	1.18368200	-0.66235600
H	-2.62035500	2.67761800	-0.05815900
H	-2.00994100	1.87291700	-1.53839500
C	3.11384900	0.89442400	-2.28922000

C	2.09731400	0.44780400	-3.13479800
C	2.93282300	1.56181600	-1.03808600
C	4.06442100	1.84243900	-0.22936800
C	3.91745300	2.42177200	1.01833000
C	2.63456400	2.72045900	1.50543000
C	1.50751300	2.45596000	0.72849000
C	1.64987400	1.89834400	-0.54065400
H	4.13744700	0.61753400	-2.53809800
H	2.40779700	0.12059600	-4.12458000
H	1.13093000	0.94695000	-3.12435100
H	5.05265700	1.57879100	-0.59755400
H	4.79207700	2.62973500	1.62801800
H	2.52124700	3.16017400	2.49260000
H	0.51166200	2.66439600	1.10483100
H	0.76911600	1.74375100	-1.15043100

TS α -endo

C	0.69568800	-1.69117500	-1.06460400
C	0.87852400	-1.38489900	0.44971000
C	-0.31445200	-1.41372100	1.27455300
C	-1.64117400	-1.21565900	0.71315300
C	-1.74512600	-1.03330600	-0.77034600
C	-2.98096200	-0.64289500	-1.30175000
C	-3.11202300	-0.36169500	-2.65840800
C	-1.99482200	-0.45531500	-3.49229900
C	-0.76108900	-0.84878100	-2.97205500
C	-0.62432200	-1.15237600	-1.61354900
O	2.00151700	-1.22096200	0.92744300
C	-0.15575900	-1.51147800	2.67878700
O	-2.64240000	-1.09689800	1.43599500
O	0.69888000	-3.12334900	-1.03962500
C	0.46733600	-3.79061100	-2.27640700
O	1.71139700	-1.17185800	-1.87807800
C	3.05385000	-1.62598600	-1.66802700
H	-3.82031500	-0.55779800	-0.61902100
H	-4.07478800	-0.06119200	-3.06342100

H	-2.08252100	-0.22253300	-4.55056400
H	0.10951500	-0.91461900	-3.61430100
H	0.80378100	-1.89725600	3.01024200
H	-1.02112300	-1.90995200	3.20419800
H	0.67104600	-4.84696300	-2.08423300
H	-0.57022100	-3.67868900	-2.61389800
H	1.14025400	-3.43025500	-3.06361900
H	3.53169000	-1.62498000	-2.65357400
H	3.58718600	-0.95446300	-0.99249400
H	3.07085500	-2.63666900	-1.25350800
C	0.83079400	0.96029100	3.13040900
C	-0.21600800	0.14063200	3.57252000
C	0.81713400	1.75366300	1.94283500
C	-0.31725300	1.82265400	1.09585500
C	-0.27061400	2.56090500	-0.08523800
C	0.88814100	3.25330400	-0.43517500
C	2.01643000	3.21037500	0.39924900
C	1.98422000	2.46774300	1.56601700
H	1.77429400	0.92226900	3.67222900
H	-0.13430200	-0.21217200	4.59881900
H	-1.23367900	0.40080200	3.28769800
H	-1.23847900	1.32585400	1.37547500
H	-1.14301600	2.59468000	-0.73081300
H	0.91854800	3.82961300	-1.35572400
H	2.91722000	3.75067600	0.12263500
H	2.86251000	2.41177600	2.20398500

Cycloadduct β -endo

C	-0.56792900	0.30026300	-0.34526000
C	0.91327800	0.31873100	-0.82664400
C	1.96277300	-0.08554700	0.09952000
C	1.64282700	-0.71562200	1.26646400
C	0.26305400	-1.02886500	1.67102100
C	-0.00074000	-1.78049600	2.82666600
C	-1.31301900	-2.07820800	3.18622500
C	-2.37359400	-1.62606500	2.39892100

C	-2.11620300	-0.87396400	1.25201000
C	-0.80639900	-0.57761600	0.87830600
O	1.16815400	0.75408300	-1.94794200
C	3.39978000	0.12089100	-0.30381000
O	2.56289300	-1.13980400	2.16631100
O	-1.45372800	-0.02558800	-1.39649800
C	-1.21231400	-1.25333200	-2.07191600
O	-0.89984800	1.60482600	0.08420000
C	-0.87289500	2.64532300	-0.90151200
H	0.82751000	-2.12647200	3.43393900
H	-1.50647900	-2.66238900	4.08172900
H	-3.39847900	-1.85483200	2.67833800
H	-2.92793900	-0.50989400	0.63099200
H	3.49026900	-0.01888900	-1.38544600
H	3.70889900	1.15619300	-0.10350400
H	-1.22444300	-2.10647700	-1.37899500
H	-2.03067400	-1.36806300	-2.78670800
H	-0.26148500	-1.23374500	-2.61554700
H	-1.43828500	2.35930800	-1.79122100
H	-1.34556400	3.50285100	-0.41625700
H	0.14983300	2.90527200	-1.19437100
C	3.96182000	-0.83734500	1.95634700
C	4.29600100	-0.85695100	0.45788100
H	4.47235800	-1.67036300	2.45187700
H	4.13959200	-1.87686500	0.08507300
H	5.35529000	-0.61691000	0.32138400
C	4.35532100	0.45646400	2.65836900
C	5.71844500	0.76161600	2.78506800
C	3.41455900	1.34288000	3.19112100
C	6.13149200	1.93353500	3.41599600
H	6.46536200	0.07372600	2.39377800
C	3.82829600	2.51909300	3.82165400
H	2.35678400	1.11444000	3.12484800
C	5.18486600	2.82008400	3.93467900
H	7.19226000	2.15202700	3.50624000
H	3.08319700	3.19808300	4.22750200
H	5.50439100	3.73422400	4.42749100

Cycloadduct α -endo

C	0.76050400	-1.72503500	-1.04741700
C	1.02531000	-1.68078000	0.46055800
C	0.06138800	-1.54824700	1.40045700
C	-1.33626000	-1.33649800	1.01204000
C	-1.61993500	-1.05996400	-0.42916300
C	-2.90114200	-0.62196100	-0.78380700
C	-3.18204600	-0.25392300	-2.09586700
C	-2.16973900	-0.30472400	-3.05709300
C	-0.89217900	-0.74645900	-2.71048100
C	-0.60983500	-1.14465000	-1.39985300
O	2.33504900	-1.87215900	0.73288300
C	0.39036700	-1.64697700	2.86792000
O	-2.23775500	-1.32868100	1.85023800
O	0.85149300	-3.11928600	-1.32899300
C	0.54814200	-3.55503000	-2.65117500
O	1.69111800	-0.96491500	-1.79529000
C	3.03989000	-1.43013900	-1.92376500
H	-3.65215100	-0.56630800	-0.00246700
H	-4.17751000	0.08764500	-2.36634000
H	-2.37129100	0.00514300	-4.07917300
H	-0.10247000	-0.76480400	-3.45265500
H	-0.41776800	-2.18112000	3.37705100
H	0.42456400	-0.64552200	3.31813100
H	0.81795900	-4.61358300	-2.67653700
H	-0.51766200	-3.44774900	-2.88182600
H	1.13452500	-3.01669000	-3.40551400
H	3.35756800	-1.16804000	-2.93811300
H	3.69073300	-0.93431800	-1.19854100
H	3.10609600	-2.51095500	-1.78407800
C	2.78695000	-1.77620200	2.10347300
C	1.73065700	-2.36092500	3.05242800
C	3.20621900	-0.35008100	2.44139900
C	2.95414400	0.73191400	1.59115500

C	3.36098700	2.02028400	1.94777400
C	4.02964600	2.24314100	3.15060100
C	4.29587600	1.16595100	3.99899500
C	3.88795000	-0.11881300	3.64512600
H	3.67793800	-2.41335200	2.11593800
H	2.08584100	-2.28185400	4.08488200
H	1.62154300	-3.42793900	2.82299100
H	2.44685400	0.57277100	0.64590300
H	3.15442300	2.85007600	1.27709100
H	4.34653800	3.24586000	3.42414200
H	4.82464800	1.32498200	4.93508000
H	4.10960100	-0.95145800	4.30956000

14b/17a reaction

14b-Z

C	1.90921200	1.89355100	1.74473400
C	1.54761100	0.42261900	1.37471900
C	0.98944100	0.18214100	0.02887400
C	0.21484100	1.28912600	-0.63114300
C	0.17312000	2.62418100	0.03007400
C	-0.65890400	3.61192500	-0.52075300
C	-0.71156400	4.88039700	0.04267500
C	0.07869600	5.17773400	1.15915500
C	0.90910900	4.20396300	1.70874100
C	0.95375500	2.92007600	1.15608700
O	1.83084200	-0.46152600	2.17404900
C	1.11132600	-0.95286100	-0.73116400
O	-0.38937100	1.10503000	-1.68433200
O	3.16158400	2.15950900	1.13959300
C	4.29256100	1.45046300	1.66058000
O	2.07239800	2.06003800	3.13198100
C	0.95297900	1.76817300	3.96483700
C	3.00577000	-4.80695500	-0.70588600
C	2.49437400	-4.21837700	-1.87206900
C	1.87915400	-2.97561500	-1.82818700

C	1.75974100	-2.24836400	-0.61902200
C	2.25860200	-2.85548000	0.55532000
C	2.86509800	-4.10478400	0.50047500
C	3.69635900	-6.14717300	-0.74992400
H	-1.24863000	3.35334700	-1.39370000
H	-1.35982100	5.64006100	-0.38531800
H	0.04845100	6.17137200	1.59844500
H	1.53206700	4.42526400	2.56878400
H	0.63440200	-0.81446200	-1.70199400
H	4.19182800	0.36578200	1.53840700
H	5.14237500	1.80513700	1.07327100
H	4.44698800	1.67843200	2.71813100
H	1.25466200	2.05491700	4.97497700
H	0.07088300	2.35560300	3.67772400
H	0.70935300	0.70203300	3.94900200
H	2.57409100	-4.74565500	-2.81971600
H	1.48572000	-2.54217800	-2.74421100
H	2.14411300	-2.34389600	1.50019900
H	3.23193700	-4.55304700	1.42108500
H	3.31703300	-6.76879500	-1.56761000
H	3.56624300	-6.69673800	0.18812400
H	4.77669000	-6.02560600	-0.90775400

14b-E

C	1.88869800	1.93306900	1.65078500
C	1.45811200	0.53827900	1.12028100
C	0.76872200	0.45857300	-0.20816300
C	0.12747300	1.67910900	-0.75262400
C	0.16163500	2.92627900	0.07346100
C	-0.63439700	4.00700900	-0.33920900
C	-0.63617200	5.19623000	0.37888700
C	0.17001300	5.32305300	1.51569900
C	0.96742100	4.25847500	1.92834600
C	0.96016000	3.05384200	1.21858800
O	1.80638600	-0.45520900	1.74450600
C	0.77608900	-0.80450700	-0.75166800

O	-0.46583700	1.70090200	-1.83078500
O	3.13028100	2.22138000	1.03245000
C	4.24951700	1.41315800	1.41719900
O	2.10287300	1.92890600	3.04111700
C	1.00999200	1.53492600	3.86639400
C	-0.44933900	-3.08560600	-4.17692400
C	0.20340300	-3.65583700	-3.07389800
C	0.57792100	-2.87406900	-1.99127500
C	0.31672000	-1.48145700	-1.95098400
C	-0.33662400	-0.91324800	-3.06877800
C	-0.70262600	-1.70570100	-4.14949600
C	-0.88628500	-3.93321000	-5.34526900
H	-1.23957900	3.88361000	-1.23071700
H	-1.25876700	6.02595700	0.05557200
H	0.17879300	6.25384000	2.07671500
H	1.60537200	4.34650400	2.80132700
H	1.27770500	-1.49789200	-0.07624900
H	4.11774500	0.36360300	1.12979900
H	5.09945900	1.83590600	0.87688900
H	4.42364200	1.46992700	2.49427800
H	1.34429000	1.69168000	4.89461600
H	0.12129100	2.15393000	3.68378100
H	0.76177000	0.47902700	3.72401600
H	0.42136800	-4.72111600	-3.06943500
H	1.08707800	-3.33879200	-1.15058600
H	-0.54445500	0.14668500	-3.06749600
H	-1.19940000	-1.24101400	-4.99822000
H	-0.25185200	-4.81813600	-5.45973400
H	-0.86074400	-3.36780200	-6.28264400
H	-1.91725600	-4.28677200	-5.20786300

TS β -exo

C	1.89649100	1.79959000	1.80497200
C	1.37920700	0.38937000	1.37258000
C	0.75030200	0.28463900	0.07315100
C	0.02531600	1.40932400	-0.45355900

C	0.19954500	2.75620000	0.16140500
C	-0.51839300	3.84242000	-0.35804400
C	-0.35208800	5.11547400	0.17758100
C	0.53741800	5.31252300	1.23896200
C	1.25139500	4.23506400	1.76130600
C	1.08249300	2.95286600	1.23197400
O	1.59701700	-0.56516700	2.12508500
C	0.53914200	-0.93826000	-0.66322200
O	-0.80026400	1.25185500	-1.38841200
O	3.19760000	1.96589500	1.27773600
C	4.19834700	1.05075400	1.73577400
O	2.01537500	1.90316800	3.21057300
C	0.83453200	1.69974500	3.97423500
C	3.06690700	-4.46330200	-0.82165000
C	2.78768600	-3.68525400	-1.95130800
C	1.96997100	-2.56088400	-1.86106200
C	1.41771100	-2.15223200	-0.63451600
C	1.68790300	-2.93998800	0.49661100
C	2.49408600	-4.07158400	0.39607700
C	3.97151000	-5.66984700	-0.90576000
H	-1.19498400	3.65846100	-1.18615300
H	-0.90935300	5.95475800	-0.23046800
H	0.67441500	6.30606800	1.65817500
H	1.94162500	4.37279400	2.58715400
H	0.30817300	-0.67261600	-1.69298200
H	4.00899500	0.02827600	1.38991000
H	5.13382500	1.41429900	1.30342500
H	4.26600100	1.05245300	2.82678000
H	1.11209700	1.89906100	5.01256500
H	0.03704700	2.39745300	3.68216300
H	0.47384000	0.66962300	3.88970500
H	3.21049000	-3.96370000	-2.91422600
H	1.76959100	-1.97722100	-2.75733900
H	1.28371000	-2.64710000	1.45598500
H	2.68548300	-4.66293500	1.28907900
H	5.00440700	-5.40975700	-0.63775100
H	3.99370100	-6.08638100	-1.91838500

H	3.65062900	-6.46135600	-0.21963500
C	-2.18591800	-0.79075200	-0.84267400
C	-1.22091000	-1.60721600	-0.23018100
O	-2.72025900	-0.96925800	-2.03379100
C	-2.30665500	-2.08419600	-2.85921900
C	-3.01173300	-1.94170600	-4.19377700
H	-2.61210300	0.07600200	-0.35394100
H	-1.18011100	-1.53553300	0.85205800
H	-1.13589500	-2.62407200	-0.60061100
H	-2.58453100	-3.01549600	-2.35032700
H	-1.21869500	-2.05967600	-2.97157900
H	-4.09804900	-1.95201400	-4.06273500
H	-2.73305800	-2.77448500	-4.84792000
H	-2.72799000	-1.00472000	-4.68161600

TS β -endo

C	1.14481000	1.73541800	1.45076600
C	0.64282400	0.32123700	1.01242700
C	0.40959300	0.12365900	-0.39514200
C	-0.10661800	1.21785600	-1.17515300
C	-0.04706500	2.60457200	-0.62578900
C	-0.56374200	3.66280000	-1.38451900
C	-0.48175700	4.97030400	-0.91489300
C	0.12338700	5.22944100	0.31885500
C	0.63811800	4.17946900	1.07897600
C	0.54840200	2.86406400	0.61683500
O	0.51785600	-0.56013800	1.87653900
C	0.40020500	-1.14909100	-1.10026700
O	-0.65351700	1.00307400	-2.28383600
O	2.53745800	1.79787300	1.22139900
C	3.34408700	0.86332300	1.94526200
O	0.96142100	1.95887800	2.83636000
C	-0.36443200	1.91209600	3.33956100
C	3.08079200	-4.49662600	-0.39515500
C	3.01333600	-3.83351500	-1.62628100
C	2.14047500	-2.76476100	-1.81747200

C	1.31221900	-2.30213700	-0.78099100
C	1.36807200	-2.97653800	0.44937900
C	2.23792600	-4.05005800	0.63118600
C	4.04308200	-5.63947200	-0.17362800
H	-1.01680100	3.42974900	-2.34257500
H	-0.88264000	5.78787500	-1.50844200
H	0.19536100	6.24949400	0.68756200
H	1.10939400	4.36635900	2.03850500
H	0.46410700	-0.91721800	-2.16242700
H	3.15445000	-0.17055300	1.63376300
H	4.37572500	1.13021100	1.70381500
H	3.17954600	0.94967300	3.02276400
H	-0.29807800	2.21718000	4.38747400
H	-1.02514500	2.61443900	2.81159200
H	-0.77836500	0.90006000	3.28625400
H	3.64773700	-4.15890900	-2.44792900
H	2.10752900	-2.27258700	-2.78698900
H	0.74700200	-2.63797000	1.26871600
H	2.26135700	-4.55246600	1.59608000
H	4.27726500	-6.15524600	-1.11095700
H	3.63672700	-6.37661300	0.52751900
H	4.99274400	-5.28239400	0.24723500
C	-2.23835400	-0.94236500	-1.48676500
C	-1.27616200	-1.93138300	-1.19434300
O	-2.89284500	-0.24280500	-0.59613500
C	-2.86548300	-0.60620100	0.82019700
C	-3.64003100	0.46570900	1.55926900
H	-2.46602300	-0.62762900	-2.49778700
H	-1.11774900	-2.63379000	-2.00895100
H	-1.36116600	-2.41859700	-0.22690500
H	-3.34260600	-1.58933600	0.90993100
H	-1.83230500	-0.67690500	1.16535900
H	-3.66632700	0.22327100	2.62671100
H	-4.66859200	0.53288000	1.19190600
H	-3.15957100	1.44072200	1.43690400

Cycloadduct β -endo

C	2.53639000	2.14741400	0.82051200
C	2.20569900	0.76119000	0.18510600
C	0.81408500	0.37413700	-0.02778500
C	-0.19055200	1.21909600	0.35720500
C	0.02595100	2.43197900	1.16054600
C	-1.06034700	3.16084100	1.66973200
C	-0.83971000	4.28399300	2.46258600
C	0.46477000	4.69382500	2.74751700
C	1.54668700	3.98061400	2.23055800
C	1.33635300	2.84981900	1.44281300
O	3.14045000	0.06180400	-0.19597500
C	0.53608700	-0.95774400	-0.70915100
O	-1.48840600	1.00885100	0.04423700
O	2.95801400	3.02272300	-0.20256200
C	4.15665900	2.68720000	-0.91395800
O	3.60581600	2.03917600	1.74020800
C	3.44236400	1.09237200	2.78864100
C	2.41340400	-4.43676100	1.14403900
C	2.49459100	-4.21473600	-0.23579600
C	1.91734100	-3.08827500	-0.82076700
C	1.23353000	-2.14574800	-0.04799100
C	1.14174100	-2.36891800	1.33121800
C	1.72357700	-3.49281200	1.91582000
C	3.07285900	-5.63714200	1.78272900
H	-2.06918900	2.83906300	1.43854700
H	-1.68593900	4.84039700	2.85615800
H	0.63907200	5.57179800	3.36364000
H	2.56658700	4.29243100	2.42957900
H	0.91249000	-0.89834500	-1.73929000
H	3.99273400	1.87328900	-1.62735000
H	4.42683900	3.59989500	-1.45146800
H	4.95740000	2.40561200	-0.22694300
H	4.32587000	1.19220800	3.42358800
H	2.54715600	1.30491500	3.39035800
H	3.39149400	0.06682300	2.40528900

H	3.02254300	-4.93036000	-0.86272700
H	2.00715400	-2.93612200	-1.89407900
H	0.61497500	-1.65238400	1.95819400
H	1.63943400	-3.64013800	2.99076000
H	2.55950900	-5.93450000	2.70357700
H	4.11770700	-5.42523900	2.04719100
H	3.07966500	-6.49891000	1.10635800
C	-1.75178600	0.06189900	-1.03322000
C	-0.98847800	-1.22174300	-0.75074300
O	-3.12294300	-0.04355500	-1.16952200
C	-3.84520500	-0.69352300	-0.11196500
C	-5.31949400	-0.39390500	-0.32166100
H	-1.40091100	0.53437100	-1.95850200
H	-1.31381400	-1.62371300	0.21428000
H	-1.22655000	-1.96870500	-1.51550000
H	-3.66349400	-1.77647200	-0.14264700
H	-3.50336200	-0.31537600	0.85915100
H	-5.91936500	-0.88813900	0.45039200
H	-5.65003800	-0.75439400	-1.30108800
H	-5.50388500	0.68369000	-0.27209200

Cycloadduct β -exo

C	1.75003300	1.63483100	0.48767400
C	1.67733000	0.13955500	0.05209300
C	0.38089300	-0.52307800	-0.05754800
C	-0.75911600	0.16093300	0.25864400
C	-0.75964200	1.48594100	0.90186400
C	-1.95277300	2.05565300	1.37413600
C	-1.93379200	3.29172700	2.01500200
C	-0.72681000	3.97326500	2.18523300
C	0.45937600	3.41619700	1.70678700
C	0.45183600	2.17558500	1.07101700
O	2.72100300	-0.41693500	-0.27941100
C	0.34923200	-1.93886800	-0.60385000

O	-2.00981200	-0.30846800	0.04644600
O	1.96881000	2.42330900	-0.66340300
C	3.19928500	2.23530900	-1.37457200
O	2.84148000	1.85862700	1.35797300
C	2.89858900	1.04152600	2.52076400
C	2.88831300	-4.80680900	1.49398800
C	2.88699400	-4.72195100	0.09636600
C	2.09557000	-3.78669200	-0.56900300
C	1.27315500	-2.90537800	0.13858400
C	1.26370700	-2.99394700	1.53562000
C	2.05921200	-3.92617800	2.20034700
C	3.77600100	-5.79442700	2.21525400
H	-2.88540600	1.52164200	1.23632800
H	-2.86172200	3.72282000	2.38055900
H	-0.70987900	4.93900400	2.68311300
H	1.40500000	3.93584100	1.81999500
H	0.69998200	-1.90695800	-1.64281300
H	3.19659600	1.30847300	-1.95713200
H	3.26657600	3.09418400	-2.04746800
H	4.05163200	2.22643300	-0.69205900
H	3.75763300	1.39652400	3.09492700
H	1.99309500	1.14741700	3.13508200
H	3.04874100	-0.01385400	2.26657300
H	3.51873700	-5.39380600	-0.48112300
H	2.12477800	-3.73641900	-1.65530300
H	0.63261200	-2.32138900	2.11298800
H	2.03492900	-3.97094400	3.28733700
H	3.88240900	-6.72687800	1.64980600
H	3.37815100	-6.04347600	3.20487600
H	4.78619600	-5.38931300	2.36309100
C	-2.22326800	-1.49226700	-0.76789600
C	-1.09379800	-2.50008200	-0.56001100
O	-2.56225300	-1.14688100	-2.07237200
C	-1.56788700	-0.59799900	-2.94743000
C	-2.27739200	-0.18647500	-4.22675300
H	-3.15112900	-1.90170400	-0.36317600
H	-1.25866700	-2.93591500	0.43171600

H	-1.21355600	-3.31468800	-1.28180100
H	-0.79580400	-1.34872600	-3.16241300
H	-1.08367900	0.26754400	-2.48006400
H	-2.76688800	-1.04888500	-4.69067300
H	-1.55856000	0.23176900	-4.93966600
H	-3.03982100	0.56974100	-4.01567000

Table S5. Cartesian Coordinates of all Stationary Points Found in the Potential Energy Surface (B3LYP/6-31G*) of the Reactions Studied in the Liquid-phase.

5/17a reaction

5

C	-1.26276700	-0.04389700	-0.19382600
C	0.06765100	0.50552500	-0.76433200
C	1.31897300	0.26283200	0.00457200
C	1.29109600	-0.48432900	1.30267300
C	-0.02220500	-0.98438700	1.80076600
C	-0.04972800	-1.68406100	3.01391600
C	-1.25102600	-2.17185100	3.52025300
C	-2.44578200	-1.96642300	2.81817800
C	-2.43235800	-1.27354700	1.61228700
C	-1.22777000	-0.77710400	1.09259200
O	0.04206600	1.11336400	-1.81974600
C	2.48972300	0.72125300	-0.47310500
O	2.32283200	-0.67811100	1.93692200
O	-2.28901400	0.14728700	-0.82531700
H	0.88370600	-1.83533600	3.54473300
H	-1.26065700	-2.71305600	4.46154600
H	-3.38205700	-2.34759500	3.21439300
H	-3.34655000	-1.10399000	1.05367100
H	2.52845100	1.26439900	-1.41149100
H	3.41118300	0.55328200	0.07411600

17a

C	-0.62655800	2.31439300	2.19264000
C	-1.37991800	1.27126500	1.82599500
O	0.17050800	3.11343300	1.43502800
C	0.25669100	2.85783100	0.02340400
C	-0.90739600	3.46621800	-0.74990800
H	-0.57448300	2.63708300	3.22991600
H	-1.93609800	0.73925100	2.58972300
H	-1.47437300	0.91831700	0.80544900
H	0.33851900	1.77794400	-0.14958500
H	1.20014000	3.31920100	-0.28138700
H	-0.77177100	3.28850900	-1.82269400
H	-0.95215400	4.54756400	-0.58376700
H	-1.86410700	3.02999100	-0.44881300

TS α -endo

C	0.93546000	-0.60022500	-0.56574800
C	0.19071200	-0.31152000	0.75475300
C	-1.25026700	-0.21533600	0.71929200
C	-1.99591200	-0.18631600	-0.53193300
C	-1.25569000	-0.47837600	-1.80319500
C	-1.97069800	-0.54818100	-3.00312200
C	-1.31336100	-0.81955400	-4.20216500
C	0.07192200	-1.02055000	-4.21582500
C	0.79407400	-0.94876200	-3.02760900
C	0.14017100	-0.68059400	-1.81745800
O	0.85944300	-0.17036900	1.78518100
C	-1.93197100	-0.06647400	1.93811300
O	-3.20725900	0.07832700	-0.57043200
O	2.14809600	-0.75546900	-0.54769700
H	-3.04304600	-0.38722000	-2.97510100
H	-1.87878500	-0.87432700	-5.12807800
H	0.58296900	-1.23034000	-5.15089700
H	1.86891200	-1.09697400	-3.01489500
H	-1.41125200	-0.37271400	2.83734200

H	-3.00918900	-0.19342300	1.93199700
C	-0.91060700	2.38944400	2.32611700
C	-2.17675500	1.92054600	2.59599600
O	-0.46708100	2.86540300	1.18097100
C	-1.39440400	3.27673600	0.12790800
C	-1.93508000	4.67017400	0.40194800
H	-0.10036800	2.26467000	3.03860100
H	-2.40407900	1.69473900	3.63181500
H	-3.01961100	2.18924500	1.97053400
H	-2.18487200	2.53159700	0.02196500
H	-0.77841600	3.25688900	-0.77195400
H	-2.53965900	4.69690300	1.31372700
H	-2.56760100	4.97924600	-0.43690200
H	-1.11693700	5.38976900	0.50158900

TS β -endo

C	-1.23217700	-0.05999900	-0.20728300
C	0.09739800	0.55882500	-0.69785800
C	1.30026100	0.24515700	0.03806500
C	1.26397900	-0.41408400	1.33624900
C	-0.04647400	-0.95174500	1.82707900
C	-0.08735200	-1.63543900	3.04613100
C	-1.28901600	-2.15679700	3.52344600
C	-2.46778700	-1.99993600	2.78477000
C	-2.43853800	-1.31965600	1.57040600
C	-1.23430100	-0.79266900	1.08386500
O	0.06353800	1.29372800	-1.69127400
C	2.54747200	0.64605400	-0.46980800
O	2.28283200	-0.53197300	2.03435800
O	-2.23994700	0.07842600	-0.88564300
H	0.83520300	-1.74954200	3.60517700
H	-1.30928200	-2.68701500	4.47133500
H	-3.40313500	-2.40668900	3.15788300
H	-3.34010800	-1.18343400	0.98211700
H	2.59661700	0.91862000	-1.51869700
H	3.42876500	0.17737100	-0.04901500
C	2.84621300	2.57554000	1.37007100

C	3.15188500	2.59761000	0.02779600
O	1.68577800	2.84741500	1.92896400
C	0.64224500	3.55723000	1.18953900
C	0.90379600	5.05399600	1.19351600
H	3.54539800	2.17200000	2.09715400
H	4.19743200	2.48404800	-0.23615800
H	2.53755000	3.14045000	-0.68068700
H	-0.26718900	3.30943300	1.73834900
H	0.56075900	3.14599800	0.18190200
H	0.97891500	5.43088300	2.21792700
H	0.07060800	5.56309000	0.69764800
H	1.82469100	5.30485400	0.65826200

Cycloadduct α -endo

C	0.43466300	0.49242800	-0.63265600
C	-0.42635400	0.42028700	0.59455500
C	-1.67048500	-0.13131100	0.59156400
C	-2.21472100	-0.73887800	-0.63154300
C	-1.38139500	-0.71934000	-1.87298100
C	-1.87406800	-1.29294300	-3.04703400
C	-1.10845500	-1.26837200	-4.21389900
C	0.15469000	-0.66854000	-4.21354200
C	0.65346300	-0.09355600	-3.04499100
C	-0.10938200	-0.11690200	-1.87312500
O	0.16788600	0.96072000	1.67183000
C	-2.52566000	-0.10578500	1.83198400
O	-3.33701100	-1.24985500	-0.63308600
O	1.53280000	1.03273300	-0.58830900
H	-2.85703900	-1.75164700	-3.03024200
H	-1.49665400	-1.71635200	-5.12396500
H	0.74894400	-0.65014400	-5.12225600
H	1.63150200	0.37572100	-3.02405200
H	-2.54112600	-1.09986200	2.29955100
H	-3.56192700	0.10922200	1.55316800
C	-0.48984700	0.79274500	2.97105600
C	-1.99886600	0.94775800	2.81461700
O	0.14112300	1.64493700	3.85707200
C	-0.07596100	3.05938000	3.68364900
C	0.96164300	3.78382500	4.52291600
H	-0.24147700	-0.21904800	3.31021100
H	-2.46534300	0.83944800	3.79872300
H	-2.22995000	1.95105100	2.44126300
H	-1.08997200	3.32242600	4.00999600
H	0.02590500	3.32111000	2.62434700
H	0.86954100	3.50559000	5.57802500
H	0.82103800	4.86659500	4.43819500
H	1.97352100	3.53689300	4.18598300

Cycloadduct β -endo

C	0.19395000	-1.64400300	-1.66637500
C	0.27589000	-0.73996200	-0.40989300
C	-0.90153600	0.00499700	-0.01317900
C	-2.05648200	-0.09594600	-0.74251100

C	-2.20933800	-0.97883400	-1.91589400
C	-3.42927400	-1.08088100	-2.59306600
C	-3.55056600	-1.92247200	-3.70180100
C	-2.45769200	-2.66645000	-4.15166300
C	-1.23732900	-2.56896100	-3.48402400
C	-1.10654100	-1.73552300	-2.36986300
O	1.34139700	-0.69224500	0.20386200
C	-0.83244000	0.86115300	1.22659700
O	-3.17244200	0.59666300	-0.45373700
O	1.18923500	-2.25234400	-2.02812400
H	-4.28133600	-0.50651300	-2.25013800
H	-4.50486600	-1.99366400	-4.21535100
H	-2.55627400	-3.31689500	-5.01535600
H	-0.37145300	-3.13494900	-3.81181900
H	-0.26377800	1.77905900	1.02238300
H	-0.27028500	0.32838500	2.00043800
C	-3.11079500	1.65425000	0.57075200
C	-2.23842400	1.20317500	1.72760800
O	-4.39510300	1.89198000	1.00356700
C	-5.19467600	2.80517400	0.22627000
C	-5.90111200	2.14608600	-0.95127900
H	-2.68770600	2.52966300	0.05811000
H	-2.71306300	0.32991900	2.18984300
H	-2.21094200	2.00284900	2.47347600
H	-4.56338500	3.63937500	-0.10862000
H	-5.92572900	3.20171100	0.93663100
H	-5.18893700	1.80641900	-1.70836600
H	-6.58266800	2.86636100	-1.41857100
H	-6.48912100	1.28614500	-0.61379000

10/17a reaction

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C	0.49107000	-0.43601800	-0.62068600
C	-0.22168300	-0.98876500	0.64342900
C	-1.56072000	-0.38971200	0.91929800
C	-2.37520000	0.14122600	-0.22263000
C	-1.83413900	-0.08589500	-1.58902700
C	-2.70441300	0.02721700	-2.68284000
C	-2.25004100	-0.22717900	-3.97236900
C	-0.91562500	-0.59366500	-4.17468600
C	-0.03860200	-0.69821700	-3.09366700
C	-0.48759700	-0.44527500	-1.79639600
O	0.29477900	-1.81777300	1.37176500
C	-2.04242400	-0.36075500	2.17164100
O	-3.46835300	0.66475000	-0.03333400
O	1.58189200	-1.22758200	-0.98975200
C	2.79890900	-1.13596400	-0.24476900
O	0.77991500	0.94701700	-0.42261900
C	1.34243800	1.41715900	0.81321700
H	-3.73630300	0.30475300	-2.49478200
H	-2.92902900	-0.14566400	-4.81591900
H	-0.55390700	-0.79496100	-5.17903400
H	0.99785500	-0.97127600	-3.24949000
H	-1.47253900	-0.77198100	2.99864400
H	-3.01105000	0.08329500	2.37775600
H	2.63056500	-1.21592100	0.83135000
H	3.40621400	-1.98232000	-0.57325500
H	3.33131100	-0.20753200	-0.47793500
H	2.43501300	1.43724700	0.76497400
H	0.97111300	2.43612600	0.94644700

H	1.03655200	0.81666200	1.67567100
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TS α -endo

C	1.09397800	-0.51457000	-0.44831300
C	0.35030400	0.02779800	0.80633500
C	-1.08377300	-0.13349700	0.85480200
C	-1.87305900	-0.32416300	-0.34663800
C	-1.14363100	-0.38748500	-1.65448000
C	-1.89758000	-0.36867100	-2.83578200
C	-1.27258200	-0.33555800	-4.07897900
C	0.12277400	-0.30782800	-4.14713600
C	0.88265100	-0.33184000	-2.97639500
C	0.26271700	-0.38127800	-1.72299800
O	0.99930400	0.49979100	1.74742900
C	-1.72843600	0.03736300	2.09758400
O	-3.11681200	-0.34571600	-0.32557500
O	1.27251300	-1.88668700	-0.08194300
C	1.88262000	-2.74359600	-1.04890200
O	2.31432400	0.13414000	-0.70038000
C	3.37404500	0.00966100	0.25739000
H	-2.97908500	-0.36736400	-2.74940300
H	-1.86643700	-0.32005800	-4.98865100
H	0.62202900	-0.26784900	-5.11146700
H	1.96484300	-0.30612400	-3.02981400
H	-1.11951000	-0.08968500	2.98545500
H	-2.75103600	-0.32013500	2.16726400
H	2.06452300	-3.68877300	-0.53220200
H	1.22432000	-2.92143800	-1.90689700
H	2.83585000	-2.33800600	-1.40549700
H	4.30565400	0.00770700	-0.31723000
H	3.36808000	0.85148000	0.95283000
H	3.29373600	-0.92224000	0.82129200
C	-1.21115900	2.65578000	2.16904100
C	-2.32660500	1.92928300	2.54205400
O	-0.92633100	3.10540500	0.96756600
C	-1.95094700	3.19125800	-0.07351100
C	-2.77086400	4.46001900	0.08842800
H	-0.37201500	2.78552300	2.84609800
H	-2.47499300	1.79691200	3.60848500
H	-3.23192300	1.97030800	1.94715000
H	-2.56406100	2.28897600	-0.06357400
H	-1.37030100	3.20436700	-0.99656300
H	-3.34339400	4.45443700	1.02112400
H	-3.47640600	4.53771100	-0.74550400
H	-2.12467800	5.34288900	0.07804300

TS β -endo

C	-1.12142100	0.02088700	-0.24072900
C	0.29563300	0.39481100	-0.77168700
C	1.44309400	0.21245300	0.08969400
C	1.33842400	-0.32935900	1.43360900
C	0.01821300	-0.87115600	1.87580400
C	-0.06259800	-1.53438300	3.10962000
C	-1.26865100	-2.07152500	3.54663500
C	-2.41235800	-1.94766900	2.74925000
C	-2.34039600	-1.28522000	1.52507100
C	-1.12854100	-0.74737000	1.07732000
O	0.37054100	0.88822800	-1.90584300
C	2.72184600	0.58224400	-0.36885500
O	2.31896900	-0.36166500	2.19794400
O	-1.86831400	-0.65974000	-1.23254800

C	-1.28985300	-1.85910000	-1.73958200
O	-1.82357500	1.22108400	0.04862400
C	-2.20290500	2.06154700	-1.05092800
H	0.83992300	-1.61695000	3.70622100
H	-1.32194700	-2.58663100	4.50175500
H	-3.35822200	-2.36525900	3.08332800
H	-3.22305500	-1.18267200	0.90227400
H	2.83204400	0.77257700	-1.43151900
H	3.57220500	0.13578300	0.13221400
H	-1.10777200	-2.58975500	-0.94098600
H	-2.01796900	-2.27261500	-2.44079500
H	-0.35226900	-1.66106300	-2.27183500
H	-2.73813800	1.49306400	-1.81462500
H	-2.86708300	2.81235600	-0.61570000
H	-1.33863800	2.55175200	-1.50789500
C	2.88859900	2.58649600	1.39056400
C	3.29929300	2.52262300	0.07500200
O	1.68375300	2.87351400	1.83373900
C	0.68998700	3.51336000	0.97272700
C	0.84499100	5.02317100	1.02914400
H	3.52880100	2.23827100	2.19567100
H	4.36481800	2.40913600	-0.09192300
H	2.75497100	3.04070400	-0.70565800
H	-0.26246500	3.18099700	1.38554200
H	0.77407800	3.12136400	-0.04109800
H	0.76430100	5.38307400	2.05925900
H	0.05006200	5.48854500	0.43676700
H	1.80887100	5.34205900	0.61979300

Cycloadduct α -endo

C	0.43843000	-0.19268700	-0.99431600
C	-0.59498300	0.39434600	-0.02292700
C	-1.89102800	0.00143600	0.04897500
C	-2.41051600	-1.02518000	-0.85116700
C	-1.53202100	-1.49485000	-1.96232100
C	-2.08091600	-2.33876900	-2.93685300
C	-1.33403400	-2.71543200	-4.04863800
C	-0.03351400	-2.22722100	-4.20024900
C	0.52044800	-1.38883200	-3.23143000
C	-0.21321600	-1.03068600	-2.09477600
O	-0.03539500	1.28400900	0.81806700
C	-2.83379300	0.60701300	1.06061500
O	-3.56176400	-1.45754600	-0.72494100
O	1.24161600	-0.97746200	-0.11641500
C	2.30397700	-1.74905700	-0.68049400
O	1.18783400	0.78988100	-1.67798800
C	2.11646900	1.60726200	-0.95176700
H	-3.10497600	-2.67258100	-2.80623000
H	-1.76517200	-3.36983000	-4.80084200
H	0.55173200	-2.49484500	-5.07556600
H	1.52295600	-0.99954200	-3.36495700
H	-3.01803900	-0.10355500	1.87788200
H	-3.80764900	0.78047800	0.59163800
H	2.87528300	-2.12213000	0.17239200
H	1.92626000	-2.59737800	-1.26150900
H	2.95887700	-1.14014800	-1.31284800
H	2.93507100	1.81997600	-1.64511000
H	1.64844800	2.54540100	-0.64092000
H	2.50422200	1.09015900	-0.07229700
C	-0.80188300	1.71690900	1.99183800
C	-2.26318800	1.91904100	1.61108400
O	-0.13353400	2.79549500	2.53927100
C	-0.10150500	4.03040800	1.79148200

C	-0.95232200	5.09838800	2.46415600
H	-0.70729800	0.91208100	2.72891400
H	-2.81179800	2.24566400	2.49975300
H	-2.34349600	2.70901400	0.85630300
H	-0.41427500	3.85946200	0.75682100
H	0.94925100	4.33804300	1.76809100
H	-2.01392300	4.83102600	2.45551100
H	-0.83463000	6.05435300	1.94098100
H	-0.64027100	5.23674400	3.50469600

Cycloadduct β -endo

C	-1.10524900	0.11285100	-0.39582900
C	0.31542400	0.46964900	-0.92739800
C	1.38720400	0.70917400	0.01918500
C	1.23475000	0.35806600	1.33213200
C	-0.00187300	-0.21991700	1.88149800
C	-0.07212500	-0.63447500	3.22085700
C	-1.24518100	-1.19408200	3.72293800
C	-2.35663400	-1.35033100	2.89162700
C	-2.29043000	-0.94160000	1.55825100
C	-1.12071800	-0.38141800	1.04576800
O	0.46931300	0.62707100	-2.14115200
C	2.67944400	1.30388400	-0.48335500
O	2.21528300	0.48828100	2.24822200
O	-1.77345500	-0.77928900	-1.26393200
C	-1.12625000	-2.02701200	-1.50483700
O	-1.86820800	1.30654300	-0.36601600
C	-2.12143800	1.96813300	-1.61375400
H	0.79615300	-0.51752600	3.85871900
H	-1.28961500	-1.51088400	4.76090700
H	-3.27193200	-1.78892600	3.27872000
H	-3.14625100	-1.06014800	0.90178800
H	2.45873900	2.08281200	-1.22045600
H	3.26964000	0.54567200	-1.01683200
H	-0.95679200	-2.58041500	-0.57226000
H	-1.80485000	-2.60056600	-2.13983700
H	-0.17302100	-1.89186800	-2.02759800
H	-2.52625100	1.27451500	-2.35441500
H	-2.86367300	2.73505300	-1.38036100
H	-1.22012500	2.44154000	-2.01599600
C	3.56377000	0.85657000	1.80785400
C	3.48728100	1.88254100	0.68416600
O	4.27378700	1.20921900	2.94065000
C	3.87709700	2.40635100	3.64547500
C	4.90572100	3.51418500	3.46847800
H	4.03144600	-0.06668500	1.44905100
H	4.50683300	2.13143400	0.37417300
H	3.01286800	2.79982700	1.05003100
H	3.80338300	2.11877600	4.69938200
H	2.88048800	2.72474800	3.32451600
H	5.89861800	3.16691300	3.77308500
H	4.63785700	4.37544000	4.09138300
H	4.96221600	3.84833500	2.42757100

TS α -exo

C	-0.42875900	0.49382300	-0.95948400
C	0.80152900	-0.09225800	-0.21080900
C	0.60980000	-1.31318100	0.53131000
C	-0.70531200	-1.71742400	1.00470100
C	-1.86253100	-0.82235700	0.67593300
C	-3.08913000	-1.06537500	1.30829400

C	-4.17365300	-0.21600900	1.10814000
C	-4.03280200	0.89594400	0.27378200
C	-2.81708900	1.14262800	-0.36663000
C	-1.72595500	0.28727600	-0.17973800
O	1.90681500	0.45561300	-0.31505800
C	1.74701300	-2.01833600	0.96406700
O	-0.87648000	-2.72070800	1.71535000
O	-0.41333500	-0.28301100	-2.16162100
C	-1.47417100	-0.05659600	-3.09186500
O	-0.32623900	1.87149400	-1.21186800
C	0.70505700	2.33293300	-2.09468800
H	-3.16127100	-1.92506600	1.96629500
H	-5.11958900	-0.41171200	1.60547600
H	-4.86892200	1.57262300	0.11957300
H	-2.70652600	2.00626200	-1.01201000
H	2.66154800	-1.90105000	0.39370700
H	1.57290400	-3.00334400	1.38580400
H	-1.56494100	1.00388700	-3.35150000
H	-1.20860600	-0.62492100	-3.98617900
H	-2.43539300	-0.41584100	-2.70697900
H	0.28143400	3.17704600	-2.64804100
H	1.57906700	2.66143800	-1.52836000
H	1.00427500	1.55277200	-2.79779800
C	3.14293800	-0.15450300	2.37979800
C	2.48483500	-1.31472700	2.74580500
O	4.40675500	-0.00607500	2.03346100
C	5.35352300	-1.10644900	2.16000700
C	5.91795200	-1.18172500	3.56932700
H	2.60143600	0.77830400	2.25964300
H	1.52263100	-1.18870800	3.22786700
H	3.04832900	-2.18631200	3.06042200
H	6.12935600	-0.86154300	1.43305300
H	4.87367400	-2.03789400	1.85013400
H	6.67438400	-1.97239200	3.61172600
H	5.14085300	-1.41119500	4.30466600
H	6.39207200	-0.23477800	3.84428900

TS β -exo

C	-0.80871800	-0.51167300	-0.03382800
C	0.65011200	0.02260200	-0.14515600
C	1.54121500	-0.18992300	0.97686600
C	1.04206100	-0.43104500	2.31677900
C	-0.42159700	-0.67475100	2.49381600
C	-0.92103000	-0.88562500	3.78774400
C	-2.27730900	-1.11418600	3.99480300
C	-3.15201700	-1.13085400	2.90254100
C	-2.66358800	-0.91891100	1.61408700
C	-1.30096800	-0.68605500	1.39942000
O	1.01527000	0.52220200	-1.21623900
C	2.91927700	0.02418400	0.80645200
O	1.79785700	-0.39124200	3.30546500
O	-0.83789200	-1.81938400	-0.58291900
C	-0.51420500	-1.95785800	-1.97273200
O	-1.70712500	0.26738300	-0.79971800
C	-1.79173100	1.65002700	-0.46417100
H	-0.22024200	-0.86546900	4.61583700
H	-2.65553800	-1.27851600	4.99995500
H	-4.21288700	-1.30883700	3.05587500
H	-3.33619100	-0.92571500	0.76263400
H	3.29017600	0.07019700	-0.21236000
H	3.58804600	-0.41026000	1.54013700
H	0.54327400	-1.75228500	-2.16872100
H	-0.73370700	-3.00068200	-2.21353000

H	-1.12896500	-1.29860000	-2.59063900
H	-2.55968400	2.07176300	-1.11661200
H	-2.09436000	1.79461900	0.58101300
H	-0.84291400	2.16628400	-0.64493500
C	3.48282100	2.06909000	2.52210600
C	3.45159700	2.00153400	1.14300200
O	4.50975700	1.87413200	3.32815500
C	5.85494200	1.70218500	2.79635000
C	6.51460000	3.04531500	2.52920300
H	2.57218300	2.21921100	3.09339200
H	2.58100200	2.42164000	0.65409700
H	4.37116000	2.03954300	0.56955200
H	5.81580600	1.06986800	1.90597500
H	6.37370000	1.15382900	3.58412200
H	5.98777800	3.60759500	1.75234800
H	7.54399100	2.87998100	2.19425500
H	6.54104500	3.64867800	3.44158300

Cycloadduct α -exo

C	-0.20073500	0.41568000	-0.69016000
C	0.88495500	-0.14442700	0.23958700
C	0.67202600	-1.11076700	1.16545300
C	-0.66835600	-1.64775800	1.38949900
C	-1.81548700	-0.97784900	0.70985000
C	-3.11737000	-1.34755400	1.07181400
C	-4.21601600	-0.68138400	0.53748400
C	-4.01249500	0.37642700	-0.35248900
C	-2.71786900	0.74703700	-0.72054700
C	-1.60908800	0.06470000	-0.20824000
O	2.08912400	0.38138600	-0.05700900
C	1.81650300	-1.67732100	1.96432500
O	-0.85051700	-2.59979000	2.15641500
O	0.12562800	-0.22135600	-1.92407300
C	-0.72974600	0.00892900	-3.04596400
O	-0.18539100	1.82341100	-0.78754600
C	0.90215400	2.47986900	-1.45500400
H	-3.24066300	-2.15315000	1.78810600
H	-5.22310700	-0.97168900	0.82282500
H	-4.86137500	0.91876100	-0.75937400
H	-2.56635100	1.57959600	-1.39754800
H	2.11892000	-2.65052000	1.55654500
H	1.48195600	-1.88044200	2.98665300
H	-0.88419900	1.07789200	-3.22762300
H	-0.21046000	-0.42895600	-3.90122500
H	-1.70147300	-0.48130400	-2.92268500
H	0.47227400	3.36844000	-1.92602100
H	1.67237700	2.78088800	-0.73985300
H	1.34916900	1.83962400	-2.21747400
C	3.30449600	-0.05878700	0.62373100
C	2.98764100	-0.68985200	1.98142500
O	4.10280500	-0.77999800	-0.25971900
C	3.63763100	-2.03259300	-0.80400000
C	4.44059100	-3.20159700	-0.24951600
H	3.85924000	0.86930300	0.77536400
H	2.74107100	0.13598800	2.65955100
H	3.90443100	-1.15181300	2.35982900
H	3.78251300	-1.95825100	-1.88732900
H	2.56553500	-2.15982300	-0.63283700
H	4.14315200	-4.13056600	-0.74948500
H	4.28438500	-3.32734800	0.82695100
H	5.51033400	-3.04559000	-0.42422700

Cycloadduct β -exo

C	-1.10906900	-0.68924200	0.96941400
C	0.21851800	0.08760800	0.72275500
C	1.13182600	0.30253800	1.82987500
C	0.73141200	0.04947900	3.11163500
C	-0.61236700	-0.44280600	3.46000200
C	-1.00514000	-0.58551200	4.80025600
C	-2.28474900	-1.03906500	5.11395200
C	-3.18437400	-1.35491000	4.09350600
C	-2.79705400	-1.21790900	2.75915400
C	-1.52052900	-0.75995300	2.43486700
O	0.49577400	0.42665200	-0.43044000
C	2.49657900	0.86997600	1.54204800
O	1.51135400	0.24475200	4.19494100
O	-0.90101200	-2.04069800	0.59809800
C	-0.58745000	-2.31404100	-0.77506200
O	-2.15267200	-0.19602100	0.15486500
C	-2.47257100	1.18558400	0.30710300
H	-0.30335300	-0.33901900	5.58817300
H	-2.57840900	-1.14478700	6.15430500
H	-4.18306400	-1.70799400	4.33415100
H	-3.48617700	-1.45989200	1.95676000
H	2.41813000	1.59162000	0.72270600
H	3.16550000	0.08049100	1.17753000
H	0.42044200	-1.97826900	-1.03866700
H	-0.64600300	-3.40109900	-0.86646800
H	-1.31111500	-1.84655600	-1.44707200
H	-3.32924000	1.36966900	-0.34472600
H	-2.75314900	1.42351300	1.34123100
H	-1.64070800	1.82769000	-0.00228900
C	2.86692000	0.78334100	4.09242000
C	3.07152400	1.55525700	2.78780900
O	3.78625200	-0.21292600	4.40668900
C	4.01960000	-1.27294400	3.46392400
C	4.79070700	-2.36277200	4.18915500
H	2.92351000	1.46861500	4.94018000
H	2.57578800	2.52444900	2.91718300
H	4.14212900	1.75636300	2.67974200
H	4.59995800	-0.89476700	2.61296800
H	3.06587200	-1.66146300	3.08740000
H	5.73727500	-1.97282400	4.57780600
H	5.01228000	-3.18571400	3.50148800
H	4.20712400	-2.75652600	5.02746400

10/33a reaction

33a

C	1.32127200	1.35944500	0.03159000
C	2.54899400	1.05336000	0.47259700
C	0.09544400	0.55121200	0.15260500
C	0.06286100	-0.71099100	0.77672700
C	-1.12416100	-1.43352500	0.86553500
C	-2.31039800	-0.91538800	0.33352200
C	-2.29581000	0.33395800	-0.28910200
C	-1.10539100	1.05664900	-0.37717300
H	1.18348300	2.31226800	-0.48003500
H	3.37987500	1.73626000	0.32282200
H	2.77743300	0.12660500	0.99273600
H	0.97256200	-1.13133900	1.19591800
H	-1.12600000	-2.40563100	1.35159400

H	-3.23471700	-1.48205900	0.40461600
H	-3.21009500	0.74737200	-0.70646500
H	-1.10075900	2.02967900	-0.86337400

TS α -endo

C	0.69260800	-1.71800600	-1.08094200
C	0.88652900	-1.40461100	0.43188200
C	-0.29765400	-1.42034000	1.26782400
C	-1.62933500	-1.25527800	0.70817500
C	-1.74427800	-1.06411900	-0.77248700
C	-2.98402500	-0.67545200	-1.29746600
C	-3.12602400	-0.39786000	-2.65415500
C	-2.01606000	-0.49750600	-3.49723200
C	-0.77827700	-0.89009000	-2.98442400
C	-0.63027500	-1.18459800	-1.62499800
O	2.02287900	-1.25801400	0.88834000
C	-0.13526700	-1.50891700	2.66845100
O	-2.63819500	-1.18360400	1.43090300
O	0.70506000	-3.14911000	-1.05567100
C	0.47433500	-3.82109600	-2.29583100
O	1.70483900	-1.18806100	-1.89624500
C	3.04439800	-1.67572800	-1.73943100
H	-3.82179400	-0.58529100	-0.61390900
H	-4.09099300	-0.09588200	-3.05156700
H	-2.11205800	-0.27089000	-4.55558300
H	0.08318600	-0.96518000	-3.63778400
H	0.83370500	-1.84664000	3.02051000
H	-0.98890900	-1.89776200	3.21690500
H	0.68579300	-4.87542300	-2.10371300
H	-0.56469900	-3.71501300	-2.62805900
H	1.14266600	-3.45614300	-3.08324300
H	3.49160400	-1.66698600	-2.73834000
H	3.61571600	-1.02804500	-1.07119900
H	3.05299200	-2.69458100	-1.34654700
C	0.78994700	1.00040800	3.15941200
C	-0.26269100	0.19732600	3.59138700
C	0.80558800	1.79924900	1.96967100
C	-0.31090200	1.88911600	1.10236400
C	-0.23729600	2.64520200	-0.06518900
C	0.93592900	3.33263400	-0.38395000
C	2.04806900	3.26522100	0.46880300
C	1.98633700	2.50585900	1.62654900
H	1.72113500	0.96226900	3.72197800
H	-0.19843400	-0.17786300	4.60944200
H	-1.27422800	0.42109400	3.26218000
H	-1.24023400	1.39337900	1.35710900
H	-1.09894500	2.70386800	-0.72317900
H	0.98657200	3.92587500	-1.29245600
H	2.95765500	3.80316400	0.21902900
H	2.84939600	2.44015700	2.28376500

TS β -endo

C	-1.41105800	-0.44342900	0.09141400
C	-0.64107700	-0.66541300	-1.24320200
C	0.74413000	-1.08865900	-1.20920800
C	1.44245600	-1.39644900	0.03349600
C	0.65498700	-1.36575400	1.30404100
C	1.27921800	-1.77968100	2.49073700
C	0.58197000	-1.78474700	3.69371000
C	-0.75565300	-1.37334700	3.72137600
C	-1.38176900	-0.95848500	2.54748400

C	-0.68649200	-0.95370200	1.33294700
O	-1.23468300	-0.41120800	-2.30029400
C	1.44046000	-1.22153300	-2.42829800
O	2.64254500	-1.70960400	0.04442100
O	-2.72172700	-0.97452000	0.01101500
C	-2.82039300	-2.36270100	-0.29587300
O	-1.55233200	0.95226300	0.30706000
C	-2.38038100	1.69486700	-0.60069500
H	2.31579200	-2.09586300	2.43931200
H	1.07289900	-2.10849900	4.60723500
H	-1.30791500	-1.37546900	4.65710600
H	-2.41853000	-0.63848000	2.56066100
H	0.83255600	-1.36949800	-3.31580600
H	2.37486100	-1.77024900	-2.39996400
H	-2.28778900	-2.97879800	0.43992200
H	-3.88468600	-2.60482900	-0.25870800
H	-2.43800300	-2.58227300	-1.29942700
H	-3.35406500	1.21684700	-0.72717400
H	-2.50619300	2.67348300	-0.13113700
H	-1.90619600	1.81324700	-1.57939400
C	3.09746000	0.93252000	-2.29178900
C	2.06954500	0.51842100	-3.12989800
C	2.95322900	1.60937600	-1.03529300
C	4.11188300	1.88297500	-0.26529900
C	4.01165100	2.49137600	0.97602400
C	2.75020200	2.82916100	1.48948400
C	1.59609100	2.56846500	0.74781200
C	1.69095100	1.97613000	-0.50917200
H	4.11226400	0.64334800	-2.56067800
H	2.35472100	0.18517600	-4.12399800
H	1.09659200	0.99957600	-3.08002900
H	5.08483400	1.60087400	-0.65896300
H	4.90714600	2.69750400	1.55464600
H	2.67249700	3.29878400	2.46594200
H	0.61853700	2.82217200	1.14492800
H	0.78922300	1.81364800	-1.08620000

Cycloadduct α -endo

C	0.75076000	-1.71678400	-1.04515400
C	1.01237800	-1.67255300	0.46474800
C	0.04788400	-1.52848700	1.40636000
C	-1.34170000	-1.29743600	1.01618900
C	-1.63121800	-1.04530400	-0.42703100
C	-2.91384900	-0.61242600	-0.78697800
C	-3.20312900	-0.27729700	-2.10637500
C	-2.19726900	-0.35796300	-3.07272500
C	-0.91788400	-0.79254600	-2.72152100
C	-0.62644300	-1.15494400	-1.40215400
O	2.31580400	-1.87509200	0.73682500
C	0.38028200	-1.63113800	2.87395500
O	-2.24461800	-1.25994000	1.85936800
O	0.86237700	-3.10854500	-1.32667300
C	0.59266100	-3.54949300	-2.65977200
O	1.67159800	-0.93745000	-1.78449800
C	3.03046400	-1.38129000	-1.92002500
H	-3.66462100	-0.53289000	-0.00775700
H	-4.19931200	0.05936000	-2.37883400
H	-2.40483000	-0.07836000	-4.10181400
H	-0.13733000	-0.83622900	-3.47207300
H	-0.42665200	-2.16311000	3.38716000
H	0.42291300	-0.63057400	3.32574900
H	0.88864500	-4.60051800	-2.68231600
H	-0.47118800	-3.46734000	-2.90643100

H	1.17955800	-2.99466300	-3.39960500
H	3.34507000	-1.09044900	-2.92645300
H	3.67106700	-0.89427300	-1.18044400
H	3.11086300	-2.46392800	-1.80941200
C	2.77533300	-1.78458400	2.11060200
C	1.71416100	-2.35714300	3.05870900
C	3.20989000	-0.36237500	2.44429900
C	2.96341700	0.72422700	1.59740100
C	3.38559900	2.00890400	1.95292200
C	4.06378500	2.22282900	3.15288000
C	4.32368300	1.14062900	3.99842000
C	3.90094100	-0.14036000	3.64542000
H	3.65750800	-2.43201000	2.11902500
H	2.06968800	-2.27982400	4.09041600
H	1.59543400	-3.42337700	2.83240900
H	2.44977000	0.57350500	0.65414800
H	3.18455800	2.84156900	1.28425000
H	4.39308600	3.22157100	3.42584800
H	4.85947000	1.29246200	4.93150000
H	4.11817400	-0.97573800	4.30711300

Cycloadduct β -endo

C	-0.56570000	0.30001500	-0.35062800
C	0.91831000	0.32647700	-0.82437400
C	1.96387500	-0.08235700	0.09521800
C	1.64043300	-0.71034200	1.26597600
C	0.25929900	-1.02631700	1.66620400
C	-0.00634400	-1.77725100	2.82224000
C	-1.31912900	-2.08153800	3.17697700
C	-2.37887100	-1.63727100	2.38337600
C	-2.11958500	-0.88542400	1.23578100
C	-0.80921200	-0.58229700	0.86771400
O	1.16956300	0.77614100	-1.94513700
C	3.40395900	0.11305000	-0.30616600
O	2.55489900	-1.12719500	2.16733700
O	-1.44000200	-0.01986800	-1.41346700
C	-1.21619200	-1.27015800	-2.06186600
O	-0.90924400	1.60346000	0.08564200
C	-0.86722300	2.66124200	-0.88302800
H	0.81908300	-2.12004300	3.43496600
H	-1.51322900	-2.66530800	4.07212200
H	-3.40349000	-1.87250100	2.65680200
H	-2.93400300	-0.53205800	0.61186200
H	3.49959200	-0.04024600	-1.38549600
H	3.71895800	1.14832700	-0.11472900
H	-1.27561800	-2.10779600	-1.35510400
H	-2.01334300	-1.37235100	-2.80135300
H	-0.24727400	-1.29082700	-2.57238200
H	-1.42332700	2.39389800	-1.78450400
H	-1.34428300	3.51269000	-0.39215200
H	0.15949700	2.92502800	-1.15624600
C	3.96120300	-0.83437700	1.95888000
C	4.29472400	-0.86442000	0.46232200
H	4.46327500	-1.66835900	2.45892800
H	4.13406500	-1.88535200	0.09607600
H	5.35444700	-0.63046800	0.32439300
C	4.35527100	0.46125000	2.65729300
C	5.71961600	0.76962500	2.77186700
C	3.41697900	1.34540300	3.19991200
C	6.13462000	1.94278800	3.40083300
H	6.46469200	0.08478900	2.37338600
C	3.83279500	2.52273600	3.82901800
H	2.35868000	1.11569300	3.14445500

C	5.19028100	2.82716500	3.92988300
H	7.19548500	2.16381700	3.48131600
H	3.08970200	3.19883700	4.24317100
H	5.51205300	3.74130000	4.42100000

10/33c reaction

33c

C	-0.59974800	0.71902200	-0.44513100
C	0.18891200	-0.30294900	-0.07558900
C	-0.52089900	2.16303100	-0.03286200
C	-0.05524900	-1.69709500	-0.60583200
C	1.36028800	-0.19258200	0.87052400
H	-1.41295800	0.49271100	-1.13740600
H	0.30081100	2.37118900	0.65773300
H	-1.45357100	2.48220400	0.45275000
H	-0.39204200	2.81277600	-0.90965700
H	0.82436100	-2.07506800	-1.14621300
H	-0.91265400	-1.73197900	-1.28582900
H	-0.24072100	-2.40565600	0.21395700
H	2.28701300	-0.52043600	0.37899700
H	1.22096300	-0.85446800	1.73672100
H	1.52110800	0.82066100	1.24606400

TS α -endo

C	-0.06811800	-0.93168800	-1.15436600
C	-0.43330700	-1.67810700	0.16077900
C	-1.76298100	-1.53522600	0.67836500
C	-2.66987000	-0.50732400	0.20724800
C	-2.11690100	0.51216500	-0.74606100
C	-2.87110700	1.66614500	-0.99479000
C	-2.36767300	2.68631300	-1.79773100
C	-1.09262400	2.55887000	-2.35454000
C	-0.33824100	1.40748600	-2.12094800
C	-0.84208700	0.37327500	-1.32473000
O	0.40584800	-2.43523000	0.67821300
C	-2.19405600	-2.46323200	1.68708000
O	-3.84564500	-0.41147900	0.60030900
O	-0.45294300	-1.89991100	-2.13602700
C	-0.31115900	-1.52640300	-3.50739600
O	1.29521300	-0.59562200	-1.24356800
C	2.26484000	-1.64831600	-1.31364900
H	-3.84942400	1.74496100	-0.53232700
H	-2.95895300	3.57939800	-1.98052000
H	-0.68387100	3.35393200	-2.97233500
H	0.65165700	1.30861500	-2.55121100
H	-1.71064900	-3.43625000	1.65244000
H	-3.27745200	-2.52191000	1.77914900
H	-0.51474000	-2.43258800	-4.08274300
H	-1.02795700	-0.74815300	-3.79355900
H	0.70363900	-1.17844700	-3.73018500
H	3.07262600	-1.27672300	-1.95240300
H	2.65530800	-1.88390300	-0.32122300
H	1.83972200	-2.55262600	-1.75409800
C	-0.51958200	-2.02562000	3.54636600
C	-1.92710600	-1.98858600	3.46078300
C	0.26335400	-0.78357100	3.33274600
C	0.20059800	-3.30788100	3.77692200
C	-2.68718200	-0.69370300	3.70226000
H	-2.40711900	-2.86250100	3.90390600
H	0.06049300	-0.06561400	4.13978000

H	1.33765800	-0.96438700	3.27014300
H	-0.08171900	-0.29562200	2.40612200
H	0.83237600	-3.52982400	2.90857500
H	-0.47795600	-4.14496400	3.95813600
H	0.87037000	-3.20037100	4.64126900
H	-2.58846900	-0.39235700	4.75203500
H	-2.32226800	0.12398100	3.07654900
H	-3.74852400	-0.82909700	3.48296700

TS β -endo

C	-0.66634000	-2.24354600	0.86730600
C	-1.03516300	-1.30917700	-0.32682200
C	-0.00977800	-1.01018000	-1.29861600
C	1.39045800	-1.25881000	-1.04966400
C	1.78712000	-1.88588600	0.24859600
C	3.14987500	-2.03189300	0.54492600
C	3.55559700	-2.59677500	1.75023600
C	2.59534300	-3.02216700	2.67467300
C	1.23834800	-2.88224600	2.38515700
C	0.82502400	-2.31180900	1.17696900
O	-2.21900800	-0.96238500	-0.44245200
C	-0.37044700	-0.44871700	-2.56283300
O	2.26381000	-0.91615800	-1.87332400
O	-1.01061800	-3.57284100	0.50874700
C	-2.39139700	-3.85367900	0.24593400
O	-1.42262100	-1.93035400	2.02164400
C	-1.29234600	-0.60273900	2.52134400
H	3.87238700	-1.69141600	-0.18954500
H	4.61358500	-2.70543200	1.97261700
H	2.90418100	-3.46373700	3.61827300
H	0.48673300	-3.20989300	3.09604700
H	-1.42788300	-0.52963700	-2.80453000
H	0.29352900	-0.69674200	-3.38538300
H	-2.73454800	-3.38620000	-0.68263700
H	-2.44677200	-4.94084100	0.15023600
H	-3.02791700	-3.52286400	1.07052400
H	-1.89394400	-0.56260000	3.43240200
H	-0.25042700	-0.36514500	2.77285300
H	-1.67291200	0.13501900	1.80661500
C	-0.36959000	1.45388200	-2.71292600
C	1.00235000	1.72646600	-2.59402100
C	-1.36873200	1.97036100	-1.69280600
C	1.90623100	1.65489300	-3.77753200
C	1.57881800	2.08047800	-1.26932200
H	-0.73399700	1.47730200	-3.74071200
H	-1.44588500	3.06214000	-1.76661100
H	-1.08399000	1.71739300	-0.66881000
H	-2.35742700	1.54370600	-1.87472600
H	2.74533900	0.98164600	-3.57564200
H	2.33039600	2.65315900	-3.96103600
H	1.38544000	1.33310100	-4.68312400
H	2.66996800	2.09630700	-1.27698600
H	1.22972300	1.36633500	-0.50800400
H	1.20674000	3.06457400	-0.94959600

Cycloadduct α -endo

C	0.27051300	-0.42091600	-1.33581700
C	1.44181100	-0.86006900	-0.44614700
C	1.31743100	-1.63702600	0.65915700
C	0.00519300	-2.09537200	1.10442000
C	-1.20234500	-1.54776100	0.41774400

C	-2.46470700	-1.83982100	0.95090600
C	-3.61175800	-1.26820400	0.40929800
C	-3.49594600	-0.37851800	-0.66203100
C	-2.24168200	-0.08507700	-1.19946300
C	-1.08618200	-0.68069700	-0.68086000
O	2.61749600	-0.44692800	-0.94348400
C	2.52953300	-2.06899200	1.44723200
O	-0.10751100	-2.88080000	2.05332600
O	0.47934700	-1.22380600	-2.49597900
C	-0.46887300	-1.13348800	-3.56089200
O	0.27265700	0.96111500	-1.62917000
C	1.31039900	1.51245600	-2.45109600
C	3.86393600	-1.04757300	-0.43054200
C	3.75929600	-1.20477400	1.10678300
C	4.95584600	-0.07451500	-0.87211800
C	4.03846600	-2.39575300	-1.14260900
C	3.71629200	0.13660700	1.85902200
H	-2.51680600	-2.50822300	1.80392400
H	-4.58740700	-1.49894100	0.82750900
H	-4.38161400	0.09270700	-1.07902100
H	-2.15759000	0.62114100	-2.01704600
H	2.73553300	-3.13143400	1.26290700
H	2.30551700	-1.99876300	2.51721100
H	-0.02926600	-1.69429000	-4.38878200
H	-1.42990300	-1.58397900	-3.28971800
H	-0.63106600	-0.09681400	-3.87535900
H	0.85571900	2.35476700	-2.98018400
H	2.14360000	1.87045400	-1.84026300
H	1.68188900	0.78230200	-3.17276100
H	4.66011500	-1.74324300	1.42728200
H	5.92914100	-0.41259100	-0.50121900
H	5.00179500	-0.02946600	-1.96477800
H	4.77146700	0.93431300	-0.49539600
H	4.10636700	-2.24187100	-2.22396800
H	3.20241900	-3.07214300	-0.94800500
H	4.96001900	-2.88108100	-0.80387700
H	4.63778400	0.71042400	1.72486300
H	2.87772400	0.76082100	1.53070500
H	3.59539600	-0.04517100	2.93242200

Cycloadduct β -endo

C	-2.26955000	-0.32766400	-0.69975900
C	-1.32492600	0.31437000	-1.76040100
C	0.09201600	0.42512800	-1.47319900
C	0.55546700	0.19708600	-0.20590000
C	-0.31939800	-0.13838900	0.93071200
C	0.19528100	-0.23765600	2.23277500
C	-0.64702800	-0.53894400	3.30113900
C	-2.01009600	-0.74751100	3.07912900
C	-2.52511400	-0.65665800	1.78451300
C	-1.69161000	-0.34700600	0.71011600
O	-1.80209100	0.63601100	-2.85234100
C	1.01919800	0.87682800	-2.57437100
O	1.85172200	0.29833200	0.13407700
O	-2.43536900	-1.69621000	-1.02973000
C	-3.05379300	-2.00686900	-2.28624400
O	-3.55443200	0.25892600	-0.73319500
C	-3.61439900	1.66426800	-0.49835500
C	2.35070300	1.40867900	-2.00819900
C	2.86974400	0.43218900	-0.92370100
C	2.19862600	2.85543500	-1.50790900
C	3.13371600	-0.97247400	-1.48303400
C	4.10550600	0.94103600	-0.18261400

H	1.25405700	-0.07623200	2.39775300
H	-0.23907400	-0.61071100	4.30526900
H	-2.66996100	-0.98290900	3.90931200
H	-3.58159700	-0.81997200	1.59837400
H	0.52069000	1.65662800	-3.15986700
H	1.19829900	0.05281000	-3.27823600
H	-2.40614500	-1.76051700	-3.13366400
H	-3.22344900	-3.08575600	-2.25804100
H	-4.00757500	-1.48541200	-2.39792500
H	-3.10298100	2.22656900	-1.28717100
H	-4.67499800	1.92491600	-0.50229700
H	-3.18548000	1.92926100	0.47661000
H	3.09553800	1.40448200	-2.81373000
H	1.52922000	2.91868300	-0.64270700
H	1.77499600	3.47861900	-2.30280300
H	3.15959600	3.29391800	-1.22403100
H	3.49680600	-1.63008800	-0.68712700
H	3.89813400	-0.92509200	-2.26597200
H	2.23296400	-1.42068200	-1.90982700
H	4.43682900	0.19877400	0.55055800
H	3.90171200	1.87533800	0.34566000
H	4.92260700	1.11179300	-0.89133500

14b/17a reaction

17 β -Z

C	1.89899000	1.88318800	1.75400300
C	1.52331000	0.41462800	1.38855800
C	0.96879000	0.17408200	0.04328900
C	0.19396000	1.27891700	-0.61184600
C	0.16674100	2.61897600	0.03784000
C	-0.65621500	3.61307600	-0.51683300
C	-0.69236900	4.88761100	0.03545200
C	0.10534200	5.18519600	1.14674600
C	0.92597000	4.20510600	1.70184500
C	0.95424000	2.91607400	1.16013700
O	1.79261200	-0.46881000	2.19466300
C	1.09997800	-0.96115800	-0.71962800
O	-0.42318500	1.09164400	-1.66091900
O	3.15633300	2.13962600	1.14905400
C	4.28089200	1.39868400	1.64700200
O	2.06448700	2.04684900	3.14079300
C	0.92556800	1.80927300	3.97151600
C	3.02550700	-4.79848300	-0.71173800
C	2.49654200	-4.21421200	-1.87351300
C	1.87062900	-2.97698200	-1.82387700
C	1.75634400	-2.25055000	-0.61200700
C	2.27296700	-2.85431700	0.55784200
C	2.89059300	-4.09743800	0.49769900
C	3.72656600	-6.13191300	-0.76241100
H	-1.25644900	3.35973200	-1.38390100
H	-1.33404000	5.65021100	-0.39607700
H	0.08740400	6.18165100	1.57898200
H	1.54869800	4.42956600	2.56125600
H	0.62722300	-0.82554200	-1.69220500
H	4.16968100	0.32141000	1.48114300
H	5.13712300	1.76522400	1.07734300
H	4.43627600	1.58580300	2.71229200
H	1.24667200	2.04899100	4.98729800
H	0.08583500	2.45983300	3.69978600
H	0.60972500	0.76313700	3.92861900
H	2.57171400	-4.74034200	-2.82167900

H	1.46620200	-2.54768100	-2.73672000
H	2.16263300	-2.34659800	1.50497000
H	3.27032300	-4.54317800	1.41385600
H	3.34124900	-6.75743400	-1.57377100
H	3.61783500	-6.67755900	0.18020700
H	4.80242300	-5.99692800	-0.93780600

17 β -E

C	1.88015100	1.92676700	1.65600900
C	1.43277100	0.53408000	1.13254800
C	0.74424100	0.45545400	-0.19210300
C	0.10360700	1.67600900	-0.73157600
C	0.15163100	2.92706700	0.08667300
C	-0.63815900	4.01356100	-0.32459100
C	-0.62430100	5.20757900	0.38663600
C	0.19131500	5.33333600	1.51704300
C	0.98167800	4.26248000	1.92988800
C	0.95883800	3.05405400	1.22682900
O	1.77070600	-0.45930600	1.76576800
C	0.75925900	-0.80729400	-0.74389800
O	-0.49922700	1.69648300	-1.80723900
O	3.12199400	2.20796800	1.02855000
C	4.23423100	1.36673900	1.36971900
O	2.10676200	1.91839200	3.04396000
C	1.00033200	1.57877500	3.88266500
C	-0.42967800	-3.08767300	-4.18140700
C	0.23909300	-3.65209400	-3.08366700
C	0.60067700	-2.87090300	-1.99625600
C	0.31099400	-1.48262900	-1.94564300
C	-0.35870000	-0.92094300	-3.05868800
C	-0.71229300	-1.71211000	-4.14388600
C	-0.85196700	-3.93524400	-5.35374900
H	-1.25527000	3.89538100	-1.20839900
H	-1.24267200	6.04011600	0.06392700
H	0.21166600	6.26575900	2.07404200
H	1.62121100	4.35229900	2.80151900
H	1.26547400	-1.50126900	-0.07355900
H	4.09050000	0.33680600	1.02459400
H	5.08996900	1.80565500	0.85276000
H	4.41179700	1.36551100	2.44769600
H	1.35739300	1.70095900	4.90731900
H	0.14910000	2.25058400	3.71874700
H	0.68602100	0.54230300	3.72957700
H	0.47930600	-4.71211100	-3.08732800
H	1.12169700	-3.33228000	-1.16147200
H	-0.58873900	0.13398200	-3.05102100
H	-1.22171500	-1.25309800	-4.98776000
H	-0.19721500	-4.80346700	-5.47731200
H	-0.84913600	-3.36006900	-6.28510600
H	-1.87274800	-4.31411700	-5.20911500

TS β -exo

C	1.69144300	1.70210800	2.02322800
C	1.15562800	0.37513500	1.40106600
C	0.79756900	0.36845300	0.01130300
C	0.32061100	1.58634100	-0.61195900
C	0.55726900	2.89328300	0.07697800
C	0.13582800	4.07604400	-0.54830800
C	0.35629000	5.31151300	0.05290500
C	1.00169800	5.37518300	1.29292300
C	1.41876900	4.20286300	1.92207200

C	1.19614100	2.95908700	1.32247700
O	1.11639300	-0.62526500	2.13810900
C	0.58769000	-0.83168800	-0.77159000
O	-0.30673300	1.57000700	-1.69320900
O	3.10095100	1.72949500	1.86700100
C	3.84914000	0.68003400	2.49367600
O	1.44425400	1.75824800	3.41677600
C	0.07899300	1.71386600	3.82209700
C	3.25343200	-4.24160800	-1.11785600
C	2.84107700	-3.48798100	-2.22416600
C	1.97067200	-2.41012100	-2.07340400
C	1.49183700	-2.02613700	-0.80706800
C	1.89049200	-2.79427300	0.30125300
C	2.75407100	-3.87585100	0.14115500
C	4.21301100	-5.39734900	-1.27053300
H	-0.36151800	3.99806900	-1.50927500
H	0.02827300	6.22297300	-0.43930200
H	1.17714000	6.33644600	1.76828100
H	1.91172600	4.24100400	2.88810300
H	0.34355300	-0.53151500	-1.78781000
H	3.68820500	-0.28603400	2.00327200
H	4.89670500	0.97121400	2.38566700
H	3.59854100	0.59136100	3.55385000
H	0.08463800	1.81503800	4.91002600
H	-0.49792100	2.54266500	3.39160800
H	-0.38980400	0.76243700	3.55088000
H	3.19921500	-3.74975300	-3.21712800
H	1.66578200	-1.84830700	-2.95327300
H	1.52148000	-2.53170600	1.28367400
H	3.04350200	-4.45386800	1.01625400
H	5.24438600	-5.08350100	-1.06085400
H	4.19559500	-5.80122000	-2.28787100
H	3.97649700	-6.20928600	-0.57437400
C	-2.07623500	-0.82644900	-0.90974800
C	-1.12968900	-1.61440500	-0.25436100
O	-2.68757500	-1.08827700	-2.03865600
C	-2.51424200	-2.38310000	-2.69134100
C	-3.39778000	-2.38741700	-3.92116700
H	-2.33545500	0.16350600	-0.54708500
H	-1.01749700	-1.44212300	0.81138700
H	-1.03632900	-2.65257900	-0.55349900
H	-2.79818800	-3.16287500	-1.97799400
H	-1.45730900	-2.49847400	-2.94648700
H	-4.44877700	-2.25540500	-3.64732000
H	-3.29183500	-3.34778200	-4.43545900
H	-3.10861700	-1.59060100	-4.61274900

TS β -endo

C	1.12952200	1.72895700	1.46180400
C	0.62642900	0.31843900	1.01386800
C	0.38249700	0.11917000	-0.38900600
C	-0.06140400	1.23205400	-1.20093200
C	0.01251700	2.61823000	-0.64249000
C	-0.45861700	3.68909900	-1.41481000
C	-0.37640600	4.99466500	-0.93872700
C	0.18467200	5.24134300	0.31863000
C	0.65651800	4.18033400	1.09184800
C	0.56631400	2.86701800	0.62131700
O	0.53009200	-0.56546400	1.88094000
C	0.37676800	-1.15779000	-1.07609200
O	-0.53596700	1.05464300	-2.34461500
O	2.53274000	1.78216300	1.25616900
C	3.32534300	0.82500800	1.96999700

O	0.92736000	1.94812900	2.84431700
C	-0.41562400	1.92812700	3.31921800
C	3.12077900	-4.46384400	-0.43752500
C	3.00385600	-3.80705500	-1.66952400
C	2.10519000	-2.75568400	-1.83946700
C	1.30160100	-2.30086900	-0.77829700
C	1.40473000	-2.97188900	0.45196000
C	2.29850600	-4.02942000	0.61210200
C	4.10710600	-5.59035100	-0.24133000
H	-0.88175900	3.47089200	-2.38966500
H	-0.74478200	5.81887400	-1.54334400
H	0.25447900	6.25808300	0.69556300
H	1.09085500	4.36129700	2.06982600
H	0.37517700	-0.95358700	-2.14428400
H	3.15573700	-0.19624800	1.61087100
H	4.36256300	1.10780000	1.77613900
H	3.12674100	0.86636500	3.04434100
H	-0.36529900	2.21531800	4.37243100
H	-1.04502800	2.65209400	2.78594200
H	-0.85377400	0.92885100	3.23872400
H	3.61660000	-4.12620700	-2.50947900
H	2.03029000	-2.27347000	-2.81127400
H	0.78989800	-2.65197700	1.28270600
H	2.35452800	-4.53240900	1.57514200
H	4.32328900	-6.10267400	-1.18446700
H	3.73266500	-6.33044200	0.47387500
H	5.06154400	-5.21507000	0.15173600
C	-2.27968400	-1.06023100	-1.41367700
C	-1.34150900	-2.04107300	-1.07872200
O	-2.91380900	-0.28740600	-0.57336100
C	-2.93416000	-0.59833900	0.86057100
C	-3.72138300	0.50333000	1.53747700
H	-2.46669900	-0.77626500	-2.44404700
H	-1.15191800	-2.76629700	-1.86400000
H	-1.37573800	-2.46216300	-0.07936600
H	-3.41612100	-1.57499200	0.96947200
H	-1.90835600	-0.65983600	1.22772500
H	-3.77738100	0.29644500	2.61091600
H	-4.74003100	0.55813600	1.14194400
H	-3.23382800	1.47257500	1.39670000

Cycloadduct β -exo

C	1.75275500	1.65574900	0.52204400
C	1.68092500	0.15579800	0.09988500
C	0.38939200	-0.49991700	-0.03646600
C	-0.75363400	0.19366700	0.26054400
C	-0.75727200	1.51805600	0.90726200
C	-1.95429000	2.09106800	1.36635000
C	-1.94025800	3.32682600	2.00961500
C	-0.73341200	4.00493800	2.19611300
C	0.45740400	3.44402800	1.73146900
C	0.45398400	2.20375200	1.09407300
O	2.73753900	-0.40405000	-0.19663000
C	0.34870500	-1.91416500	-0.58935300
O	-1.99990100	-0.26262500	0.02615600
O	1.97785100	2.43729900	-0.63697000
C	3.19608900	2.22681400	-1.36537000
O	2.84606100	1.88158600	1.38949100
C	2.86148300	1.11725900	2.59346000
C	2.89336900	-4.83036100	1.43870300
C	2.84144000	-4.75438400	0.04143300
C	2.04800300	-3.80199600	-0.60156600
C	1.27682100	-2.89359800	0.12991800

C	1.31595900	-2.97473600	1.52859100
C	2.11219100	-3.92292600	2.16958800
C	3.77718500	-5.83766600	2.13770400
H	-2.88796900	1.56132700	1.22013100
H	-2.87109700	3.75898800	2.36520100
H	-0.71906500	4.96866000	2.69707200
H	1.40113700	3.96305500	1.86315900
H	0.67882400	-1.87800600	-1.63451100
H	3.17390300	1.29373400	-1.93676600
H	3.26351100	3.07441300	-2.05176200
H	4.06048900	2.22096500	-0.69781000
H	3.73490400	1.45629300	3.15451900
H	1.96021300	1.29346400	3.19462000
H	2.95974800	0.04509700	2.38943500
H	3.43083500	-5.44797500	-0.55453800
H	2.03179800	-3.76568500	-1.68886600
H	0.72198500	-2.28535200	2.12462600
H	2.12571600	-3.96085500	3.25694000
H	3.99706200	-6.69348200	1.49109800
H	3.30920200	-6.21420400	3.05398600
H	4.73845300	-5.39203500	2.42699400
C	-2.22238100	-1.47533500	-0.75473600
C	-1.09345700	-2.47545300	-0.52502700
O	-2.56692500	-1.15220000	-2.06277300
C	-1.54903300	-0.72041600	-2.98256600
C	-2.25205700	-0.25394500	-4.24585700
H	-3.14735800	-1.86749900	-0.32894600
H	-1.25633200	-2.88475600	0.47789000
H	-1.21285700	-3.30722800	-1.22643400
H	-0.87155300	-1.55344600	-3.20724400
H	-0.96214200	0.09531800	-2.54481800
H	-2.84886000	-1.06425100	-4.67736400
H	-1.51325200	0.06511400	-4.98847800
H	-2.91559900	0.58973700	-4.03064800

Cycloadduct β -endo

C	2.53764600	2.15603900	0.83471200
C	2.21470000	0.75922700	0.21688800
C	0.83229200	0.37429300	-0.01874100
C	-0.17665600	1.22651400	0.35011100
C	0.03105600	2.43406800	1.16525900
C	-1.06075600	3.15609800	1.67286800
C	-0.84919600	4.27400300	2.47701600
C	0.45221700	4.68506500	2.77520700
C	1.54019100	3.97785400	2.26021500
C	1.33825900	2.85230700	1.46224900
O	3.16349300	0.05563900	-0.13337200
C	0.55144500	-0.95655500	-0.70307100
O	-1.46465000	1.02890700	0.01245000
O	2.93663600	3.02816600	-0.20646400
C	4.11399300	2.69059100	-0.95394500
O	3.62419900	2.06703400	1.73522200
C	3.46201200	1.16748400	2.83003100
C	2.39897800	-4.46195000	1.13640600
C	2.42822000	-4.26483300	-0.24983300
C	1.86010400	-3.12917900	-0.83035900
C	1.24053000	-2.15142200	-0.04556600
C	1.19790300	-2.35109900	1.34098400
C	1.76945500	-3.48366300	1.91995600
C	3.04448900	-5.67270600	1.77030500
H	-2.06817600	2.83383900	1.43658500
H	-1.69970500	4.82343200	2.87001300
H	0.62015200	5.55675100	3.40122600

H	2.55607600	4.29249200	2.47545000
H	0.92323700	-0.89714500	-1.73456600
H	3.93329900	1.86334400	-1.64729100
H	4.35758400	3.59391300	-1.51852200
H	4.94375200	2.43251000	-0.29215200
H	4.36389300	1.26693300	3.43777700
H	2.58867700	1.42910100	3.44137100
H	3.37084300	0.12968100	2.49028300
H	2.90382800	-5.00810600	-0.88622500
H	1.90171100	-3.00217000	-1.91009200
H	0.71773800	-1.61087400	1.97715100
H	1.72405100	-3.61131100	2.99956600
H	2.49855400	-5.99644000	2.66312100
H	4.07523800	-5.45749800	2.08278600
H	3.08673500	-6.51531400	1.07220400
C	-1.72965500	0.06066200	-1.05469100
C	-0.97340100	-1.21907100	-0.74524500
O	-3.10082800	-0.03367100	-1.18941100
C	-3.82723100	-0.70195300	-0.13835800
C	-5.30070000	-0.39647100	-0.34060200
H	-1.37019500	0.51912600	-1.98269200
H	-1.30449300	-1.60516500	0.22402000
H	-1.20692000	-1.97484900	-1.50189100
H	-3.64511400	-1.78252700	-0.19040600
H	-3.48256200	-0.34011300	0.83722800
H	-5.89577200	-0.90484000	0.42535600
H	-5.63638300	-0.74222900	-1.32391000
H	-5.48726600	0.67984400	-0.26886300

Michael-type reaction

TS1 α

C	-0.42134500	-0.42401100	-0.73332800
C	-1.65116000	-0.88575600	-1.23908900
C	-2.86542500	-1.16615400	0.39962900
C	-4.11479400	-1.26503200	-0.17820200
C	1.93695100	-0.88325600	0.22839100
C	0.61252400	-1.38713500	-0.41810500
C	-0.25725400	1.00155200	-0.50873400
C	1.11269200	1.50311900	-0.18735800
C	1.34879900	2.88581300	-0.20012400
C	2.61721300	3.38916800	0.07038900
C	3.66449000	2.50863200	0.36330200
C	3.43457700	1.13347000	0.38714900
C	2.16422700	0.62053300	0.10646300
O	0.47135700	-2.60712700	-0.57319000
O	-1.20773500	1.79861100	-0.61095200
O	3.04972800	-1.61761000	-0.24400700
C	3.25714000	-1.61069100	-1.65420200
O	1.86240900	-1.10931800	1.62684000
C	1.77333800	-2.46645200	2.08076300
H	0.51880000	3.54603600	-0.42917300
H	2.79335500	4.46108600	0.05328100
H	4.65784400	2.89411900	0.57604800
H	4.23978900	0.44434800	0.61980900
H	-1.68439600	-1.90280600	-1.61261400
H	-2.27698400	-0.16581300	-1.75346500
H	3.37835200	-0.59025800	-2.04016300
H	4.18157100	-2.16667900	-1.82566600
H	2.43614100	-2.10606700	-2.18402100
H	2.55788600	-3.08481900	1.63804900
H	1.91207100	-2.41278500	3.16338600

H	0.79739300	-2.90876800	1.85724800
O	-4.94531700	-0.28989200	-0.49155800
C	-4.67586500	1.08151400	-0.06119000
C	-5.14126200	1.30778100	1.36826800
H	-4.48080100	-2.21755500	-0.55549200
H	-2.41568200	-2.09246300	0.73909900
H	-2.58256800	-0.27090600	0.93862700
H	-5.25562200	1.68200100	-0.76408500
H	-3.61397500	1.30242700	-0.20292100
H	-6.20585000	1.07619500	1.47040100
H	-4.99038700	2.36056900	1.62962400
H	-4.57954700	0.69626800	2.08083100

ZW α

C	2.03596600	-0.82439800	0.16420000
C	0.67187600	-1.41493900	-0.30812000
C	-0.43318300	-0.53449200	-0.48706400
C	-0.35589700	0.87716300	-0.31124700
C	0.99170800	1.49234200	-0.09008400
C	1.11454500	2.88878000	-0.08216800
C	2.35743200	3.49043100	0.09753900
C	3.49448800	2.69507800	0.27410500
C	3.37767800	1.30489100	0.27431000
C	2.13250300	0.69609900	0.08872100
O	0.61100700	-2.65321700	-0.45628800
C	-1.75820400	-1.10553800	-0.82772200
O	-1.37133500	1.62015000	-0.36088300
O	3.12033000	-1.43865400	-0.51756900
C	3.08688900	-1.36218600	-1.93796200
O	2.21926000	-1.11324000	1.54122100
C	2.27994500	-2.48871100	1.93534200
H	0.21667200	3.48219400	-0.22096800
H	2.44323700	4.57386200	0.09901600
H	4.46832900	3.15690100	0.41361000
H	4.25341300	0.67894800	0.41320300
H	-1.66739900	-2.13603300	-1.17189400
H	-2.27383400	-0.50238300	-1.57862700
H	3.05105500	-0.32164300	-2.28785600
H	4.01477300	-1.82048600	-2.28906300
H	2.23499700	-1.91403500	-2.35102000
H	2.98075300	-3.04998000	1.31245100
H	2.63630700	-2.47330700	2.96906900
H	1.29847500	-2.97063600	1.89134700
C	-4.04542900	-1.39834600	0.09724300
C	-2.69653800	-1.10083900	0.51358600
O	-4.90940100	-0.56895200	-0.35102200
C	-4.69044500	0.90585900	-0.34159600
C	-5.31140100	1.48916200	0.91201600
H	-4.39310100	-2.42833800	0.01643200
H	-2.32120100	-1.88270400	1.17424700
H	-2.58794800	-0.11176800	0.95775400
H	-5.21288700	1.22126000	-1.24456200
H	-3.62151800	1.11049500	-0.43456700
H	-6.37016900	1.22604700	0.98870000
H	-5.22875500	2.57968000	0.85876800
H	-4.79168500	1.15108000	1.81369400

TS2 α

C	0.38561000	0.22601000	0.45843600
C	1.82240700	0.24724800	0.78269400

C	2.76663000	0.57814600	-0.55275900
C	3.62897300	-0.56517900	-0.68009000
C	-1.75564000	-1.08044500	-0.09103200
C	-0.27369200	-1.03302700	0.38873400
C	-0.25482500	1.47487600	0.18159900
C	-1.74206900	1.47127100	-0.01207800
C	-2.42207300	2.69404000	-0.09309100
C	-3.80565100	2.72785500	-0.24674700
C	-4.52429000	1.53012800	-0.32305200
C	-3.85247300	0.30953800	-0.25054100
C	-2.46370600	0.27093900	-0.09073000
O	0.28543600	-2.12652400	0.62523400
O	0.37594600	2.55553300	0.13456100
O	-2.49983600	-2.04878800	0.63380400
C	-2.50662400	-1.89951900	2.04903400
O	-1.79465400	-1.48855800	-1.45082600
C	-1.27904100	-2.78402100	-1.77515600
H	-1.83852100	3.60693000	-0.03068400
H	-4.32478300	3.68090800	-0.30529400
H	-5.60450100	1.54750500	-0.44142200
H	-4.40067500	-0.62518900	-0.31181100
H	2.11998800	-0.70946700	1.21547800
H	2.09641800	1.05294600	1.46619700
H	-2.89352900	-0.91711200	2.35169600
H	-3.17438200	-2.67470900	2.43315900
H	-1.50667400	-2.04331800	2.47319900
H	-1.70916400	-3.55610800	-1.13206900
H	-1.57996400	-2.95943700	-2.81168600
H	-0.18799100	-2.82227000	-1.69736400
O	4.77315800	-0.76423900	-0.13173300
C	5.49857300	0.28289600	0.61963000
C	6.48531800	0.97349800	-0.30061600
H	3.27475200	-1.45672700	-1.19630700
H	2.10364200	0.64545100	-1.41216700
H	3.27279700	1.52817000	-0.39474700
H	5.99411700	-0.28499900	1.40669400
H	4.77607000	0.96341000	1.06892600
H	7.17015000	0.24942700	-0.75062900
H	7.07184400	1.68396600	0.29076200
H	5.97543600	1.52571000	-1.09564200

TS1 β

C	0.27764100	0.87983400	0.58924700
C	1.49683900	1.41207800	1.04890800
C	2.73879100	1.47993400	-0.59230300
C	3.97495600	1.67017900	-0.00977800
C	-1.19664000	-1.16284700	-0.00400600
C	0.12530600	-0.55504200	0.54942400
C	-0.75998900	1.79335200	0.13079500
C	-2.11902200	1.22216300	-0.11933900
C	-3.19279600	2.10078700	-0.32617000
C	-4.47818000	1.61086700	-0.53305100
C	-4.70070600	0.22929800	-0.53840400
C	-3.63662200	-0.65009800	-0.34230800
C	-2.34329700	-0.16351800	-0.12584100
O	1.03363100	-1.33963000	0.86774700
O	-0.55461300	3.00936800	-0.00574200
O	-1.58045900	-2.30780300	0.73360000
C	-1.76427900	-2.12114800	2.13468600
O	-0.97137400	-1.59187600	-1.33686500
C	-0.03288800	-2.65389100	-1.55179600
H	-2.99136600	3.16691300	-0.31646700

H	-5.30529100	2.29802600	-0.68811300
H	-5.70184100	-0.16132200	-0.69894400
H	-3.79997500	-1.72276300	-0.35160900
H	2.11379400	0.77048500	1.66718500
H	1.52252500	2.47044900	1.28108100
H	-2.51739600	-1.35077100	2.34483200
H	-2.11844500	-3.07876200	2.52271500
H	-0.82433100	-1.85744600	2.63234200
H	-0.24467700	-3.50781200	-0.90395300
H	-0.16564000	-2.94205900	-2.59758700
H	0.99861300	-2.32602400	-1.38963600
O	4.81003200	0.75527200	0.44383200
C	4.56099400	-0.66356100	0.19884600
C	5.03884300	-1.07568500	-1.18432300
H	4.32302100	2.66854400	0.24643200
H	2.47654600	0.51838500	-1.01490200
H	2.28122300	2.34666100	-1.05588800
H	3.50060400	-0.87730400	0.36330700
H	5.14168600	-1.15761600	0.97947900
H	4.47686900	-0.57246300	-1.97674900
H	4.90086000	-2.15577200	-1.30166200
H	6.10177800	-0.84822000	-1.30996300

Zwß

C	-1.15402400	-1.16019900	-0.03475500
C	0.18916400	-0.47189000	0.33813800
C	0.27242900	0.94022100	0.36899400
C	-0.82706400	1.81063000	0.07060500
C	-2.18060200	1.18038400	-0.09358800
C	-3.30266300	2.01122200	-0.22026700
C	-4.57806300	1.46784900	-0.34756900
C	-4.74308100	0.07855300	-0.34896100
C	-3.63052700	-0.75381900	-0.22891600
C	-2.34748100	-0.21196900	-0.09837100
O	1.17704700	-1.22286100	0.54584100
C	1.59627500	1.53484100	0.67131900
O	-0.71329400	3.05215900	-0.01539800
O	-1.42034000	-2.25664000	0.83105100
C	-1.43595200	-1.96267800	2.22304700
O	-1.07280200	-1.70061200	-1.34366500
C	-0.11321100	-2.73448900	-1.58944200
H	-3.14461500	3.08482100	-0.21411900
H	-5.44184500	2.12046900	-0.44326000
H	-5.73538300	-0.35400100	-0.44575900
H	-3.74769300	-1.83279200	-0.23084400
H	2.09109300	1.00743500	1.49007800
H	1.50991500	2.59620000	0.90448300
H	-2.17103700	-1.18358100	2.46579000
H	-1.72425400	-2.88892400	2.72620900
H	-0.44719600	-1.65270400	2.58079600
H	-0.17632800	-3.52352200	-0.83591500
H	-0.37694100	-3.14070100	-2.56996300
H	0.90908200	-2.34559100	-1.61423900
C	3.90303900	1.71610000	-0.23248500
C	2.56008600	1.38653400	-0.64338800
O	4.75185400	0.93031100	0.31323300
C	4.52276800	-0.53642600	0.44674400
C	5.15860300	-1.24549100	-0.73238900
H	4.25676300	2.74710300	-0.24634800
H	2.45363200	0.35857500	-0.98840900
H	2.20229600	2.09924300	-1.38679000
H	3.45126400	-0.72540400	0.54428300

H	5.02957800	-0.76343900	1.38450100
H	4.65654400	-0.99570200	-1.67201500
H	5.06674600	-2.32475500	-0.57228400
H	6.22047400	-0.99781900	-0.81698700

TS2 β

C	0.37868700	0.27747400	0.44273600
C	1.81374200	0.33792500	0.77703000
C	2.78191000	-0.26519600	-0.43349200
C	3.61372200	0.84596800	-0.81074000
C	-1.71109000	-1.12320000	-0.09268600
C	-0.22374600	-1.00543200	0.34918300
C	-0.31977100	1.50526700	0.20678400
C	-1.80516900	1.42877100	-0.00192300
C	-2.54020500	2.62011900	-0.07719800
C	-3.92222900	2.59352400	-0.24356400
C	-4.58602400	1.36560900	-0.33683600
C	-3.86043000	0.17646100	-0.26804200
C	-2.47217000	0.19870700	-0.09752700
O	0.40585300	-2.06924500	0.54610800
O	0.24275300	2.62355000	0.20412200
O	-2.39643900	-2.10371300	0.67509800
C	-2.36818700	-1.92111700	2.08577700
O	-1.77209600	-1.56203100	-1.44135200
C	-1.23853600	-2.85389700	-1.75225300
H	-1.99896000	3.55746500	0.00008800
H	-4.48290500	3.52299300	-0.29840100
H	-5.66486000	1.33554000	-0.46490700
H	-4.36538300	-0.78154400	-0.34100100
H	2.08419200	-0.29757000	1.62296200
H	2.09583200	1.36856200	1.00191000
H	-2.78774800	-0.94906100	2.37817600
H	-2.98969300	-2.71480300	2.50782000
H	-1.35083900	-2.01184700	2.48328800
H	-1.64396800	-3.62196700	-1.08845000
H	-1.55502900	-3.05265700	-2.77994700
H	-0.14630000	-2.87111600	-1.69217600
O	4.76083600	1.17789800	-0.33995900
C	5.52191000	0.32343900	0.59825500
C	6.46949500	-0.56692100	-0.18067100
H	3.22906700	1.60187600	-1.49458700
H	3.31447400	-1.13799900	-0.06204400
H	2.13293600	-0.54670800	-1.25981400
H	4.81962600	-0.23012000	1.22089100
H	6.04879400	1.05289900	1.21263800
H	5.92692200	-1.28125500	-0.80706400
H	7.08170700	-1.12916800	0.53167800
H	7.13342400	0.02979100	-0.81219600