Supporting Information for the Paper

Gold-catalyzed tuning of reactivity in allenes: 9-*endo* hydroarylation *versus* formal 5-*exo* hydroalkylation

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General Methods: ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance AVIII-700 with cryoprobe, Bruker AMX-500, Bruker Avance-300, Varian VRX-300S or Bruker AC-200. NMR spectra were recorded in $CDCl_3$ solutions, except otherwise stated. Chemical shifts are given in ppm relative to TMS (^{1}H, 0.0 ppm), or $CDCl_3$ (^{13}C, 76.9 ppm). Low and high resolution mass spectra were taken on an AGILENT 6520 Accurate-Mass QTOF LC/MS spectrometer using the electronic impact (EI) or electrospray modes (ES) unless otherwise stated. IR spectra were recorded on a Bruker Tensor 27 spectrometer. Specific rotation $[\alpha]_D$ is given in 10^{-1} deg cm^2 g^{-1} at 20 °C,

and the concentration (*c*) is expressed in g per 100 mL. All commercially available compounds were used without further purification.

Starting (aryloxy)allenol-tethered 2-azetidinones were prepared from 4-oxoazetidine-2-carbaldehydes via regiocontrolled indium-mediated Barbier-type carbonyl–allenylation reaction in aqueous media using our methodology: B. Alcaide, P. Almendros, C. Aragoncillo, M. C. Redondo and M. R. Torres, *Chem. Eur. J.,* 2006, **12**, 1539.

Preparation of Allenyl Acetate (+)-1a. Triethylamine (0.94 mmol) and acetic anhydride (0.47 mmol) were sequentially added dropwise via syringe to a solution of the corresponding α-allenic alcohol (119 mg, 0.39 mmol) and DMAP (cat) in dichloromethane (4 mL) at 0 ^{o}C under argon. The resulting mixture was allowed to warm to room temperature and stirred for 2 h. The crude mixture was diluted with CH_2Cl_2 (10 mL) and washed with saturated aqueous ammonium chloride (3 x 5 mL) and brine (3 x 5 mL). The organic layer was dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue eluting with ethyl acetate/hexanes (1:2) gave 78 mg (58%) of analytically pure α-allenic acetate (+)-**1a** as a colorless oil; $[\alpha]_D$ = +7.7 (*c* = 0.2 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.96 (d, 3H, *J* = 6.7 Hz, Me), 1.00 (d, 3H, *J* = 6.7 Hz, Me), 1.82 (t, 3H, *J* = 3.2 Hz, Me), 2.03 (m, 1H, CH isobut), 2.13 (s, 3H, COMe), 2.96 (dd, 1H, *J* = 13.8, 6.1 Hz, NCH*H*), 3.33 (dd, 1H, *J* = 13.7, 8.6 Hz, NC*H*H), 4.26 (dd, 1H, *J* = 6.7, 5.0 Hz, H4), 4.78 (m, 2H, =CH_2), 5.28 (d, 1H, *J* = 5.0 Hz, H3), 5.60 (dt, 1H, *J* = 6.7, 2.0 Hz, OCH), 7.04 (t, 1H, *J* = 7.3 Hz, Ar), 7.09 (d, 2H, *J* = 7.7 Hz, Ar), 7.32 (m, 2H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 206.9 (C=*C*=CH_2), 169.7 (COMe), 166.6 (CO), 157.7, 129.5 (Ar, 2CH), 122.3 (Ar, CH), 115.8 (Ar, 2CH), 97.6, 80.0 (CH, H3), 77.6 (C=*C*H_2), 72.4 (OCH), 58.5 (CH, H4), 49.4 (CH_2 isobut), 27.0 (CH isobut), 21.0 (Me), 20.4 (Me), 20.2 (Me), 16.4 (Me); IR ($CHCl_3$): ν = 2995, 1944, 1757, 1725 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{25}NO_4$ $[M]^+$: 343.1784; found: 343.1797.

General Procedure for the Synthesis of Methoxy Allenes 1b–h and 4a–e. Tetrabutyl ammonium iodide (cat), 50% aqueous sodium hydroxide (18 mL) and dimethyl sulfate (0.60 mmol) were sequentially added at room temperature to a solution of the corresponding α-allenol (0.92 mmol) in dichloromethane (18 mL). The reaction was stirred until disappearance of the starting material (TLC). Then aqueous ammonia (30%) was added (2.5 mL), before being partitioned between dichloromethane and water. The aqueous phase was extracted with dichloromethane (3 x 15 mL), the combined organic extracts were dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue using ethyl acetate/hexanes mixtures gave analytically pure compounds. Spectroscopic and analytical data for some representative pure forms of **1** and **4** follow.

Methoxy Allene (+)-1b. From 355 mg (1.18 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (4:1) as eluent gave the methoxy allene (+)-**1b** (167 mg, 45%) as a colorless oil; $[\alpha]_D$ = +11.2 (*c* = 0.3 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.92 (d, 3H, *J* = 6.7 Hz, Me), 0.96 (d, 3H, *J* = 6.7 Hz, Me), 1.70 (t, 3H, *J* = 3.2 Hz, Me), 2.06 (m, 1H, CH isobut), 3.14 (dd, 1H, *J* = 13.6, 6.3 Hz, NCH*H*), 3.26 (dd, 1H, *J* = 13.4, 8.2 Hz, NC*H*H), 3.33 (s, 3H, OMe), 4.00 (m, 1H, OCH), 4.02 (d, 1H, *J* = 5.9 Hz, H4), 4.41 (m, 1H, =CH*H*), 4.62 (m, 1H, =C*H*H), 5.22 (d, 1H, *J* = 4.1 Hz, H3), 7.00 (t, 1H, *J* = 7.3 Hz, Ar), 7.02 (d, 2H, *J* = 6.7 Hz, Ar), (m, 3H, Ar), 7.28 (m, 2H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 208.3 (C=*C*=CH_2), 166.6 (CO), 158.0, 129.4 (Ar, 2CH), 121.9 (Ar, CH), 115.6 (Ar, 2CH), 94.7, 82.6 (CH, H3), 79.7 (OCH), 74.9 (C=*C*H_2), 59.2 (CH, H4), 55.7 (OMe), 49.7 (NCH_2), 27.0 (CH isobut), 20.4 (Me), 20.2 (Me), 14.4 (Me); IR ($CHCl_3$): ν = 2992, 1947, 1756 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{25}NO_3$ $[M]^+$: 315.1834; found: 315.1832.

Methoxy Allene (+)-1c. From 322 mg (0.89 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (4:1) as eluent gave the

methoxy allene (+)-**1c** (216 mg, 65%) as a colorless oil; $[\alpha]_D$ = +16.7 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.92 (d, 3H, *J* = 6.7 Hz, Me), 0.98 (d, 3H, *J* = 6.7 Hz, Me), 2.08 (m, 1H, CH isobut), 3.20 (dd, 1H, *J* = 13.6, 6.3 Hz, NCH*H*), 3.32 (dd, 1H, *J* = 13.4, 8.3 Hz, NC*H*H), 3.41 (s, 3H, OMe), 4.19 (dd, 1H, *J* = 9.1, 4.8 Hz, H4), 4.59 (d, 1H, *J* = 9.1 Hz, OCH), 4.83 (d, 1H, *J* = 12.4 Hz, =CH*H*), 5.00 (d, 1H, *J* = 12.5 Hz, =C*H*H), 5.14 (d, 1H, *J* = 4.8 Hz, H3), 6.80 (d, 2H, *J* = 7.7 Hz, Ar), 6.96 (t, 1H, *J* = 7.3 Hz, Ar), 7.23 (m, 3H, Ar), 7.35 (t, 2H, *J* = 7.0 Hz, Ar), 7.46 (d, 2H, *J* = 7.0 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 210.5 (C=*C*=CH_2), 166.7 (CO), 157.9, 134.0, 129.2 (Ar, 2CH), 128.6 (Ar, CH), 127.2 (Ar, 3CH), 121.9 (Ar, CH), 115.7 (Ar, 3CH), 102.6, 81.5 (CH, H3), 79.6 (OCH), 78.1 (C=*C*H_2), 59.6 (CH, H4), 55.6 (OMe), 49.8 (NCH_2), 27.1 (CH isobut), 20.5 (Me), 20.2 (Me); IR ($CHCl_3$): ν = 2999, 1944, 1753 cm^{-1}; HRMS (ES): calcd for $C_{24}H_{27}NO_3$ $[M]^+$: 377.1991; found: 377.1997.

Methoxy Allene (+)-1d. From 57 mg (0.17 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (3:1) as eluent gave the methoxy allene (+)-**1d** (31 mg, 52%) as a colorless oil; $[\alpha]_D$ = +15.0 (*c* = 0.1 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.63 (t, 3H, *J* = 3.2 Hz, Me), 3.17 (s, 3H, OMe), 3.91 (dd, 1H, *J* = 9.2, 4.8 Hz, H4), 4.03 (d, 1H, *J* = 9.2 Hz, OCH), 4.32 (m, 1H, =CH*H*), 4.46 (d, 1H, *J* = 14.6 Hz, NCH*H*), 4.57 (m, 1H, =C*H*H), 4.69 (d, 1H, *J* = 14.6 Hz, NC*H*H), 5.19 (d, 1H, *J* = 4.8 Hz, H3), 7.00 (t, 1H, *J* = 7.7 Hz, Ar), 7.02 (d, 2H, *J* = 8.0 Hz, Ar), 7.30 (m, 3H, Ar), 7.36 (m, 4H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 208.3 (C=*C*=CH_2), 166.6 (CO), 136.4, 129.3 (Ar, 2CH), 128.6 (Ar, 3CH) , 128.5 (Ar, 2CH), 127.5, 122.0 (Ar, CH), 115.6 (Ar, 2CH), 94.5, 82.4 (CH, H3), 79.9 (OCH), 74.9 (C=*C*H_2), 58.6 (CH, H4), 55.6 (OMe), 45.9 (NCH_2), 14.9 (Me); IR ($CHCl_3$): ν = 2996, 1945, 1759 cm^{-1}; HRMS (ES): calcd for $C_{22}H_{23}NO_3$ $[M]^+$: 349.1678; found: 349.1689.

Methoxy Allene (+)-1e. From 215 mg (0.54 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (3:1) as eluent gave the

methoxy allene (+)-**1e** (120 mg, 54%) as a colorless oil; $[\alpha]_D$ = +8.7 (*c* = 0.1 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.18 (s, 1H, OMe), 4.00 (dd, 1H, *J* = 9.4, 4.8 Hz, H4), 4.39 (d, 1H, *J* = 14.6 Hz, NCH*H*), 4.47 (d, 1H, *J* = 9.3 Hz OCH), 4.59 (d, 1H, *J* = 12.5 Hz, =CH*H*), 4.69 (d, 1H, *J* = 14.6 Hz, NC*H*H), 4.84 (d, 1H, *J* = 12.5 Hz, =C*H*H), 5.00 (d, 1H, *J* = 5.0 Hz, H3), 6.70 (d, 2H, *J* = 7.9 Hz, Ar), 6.88 (t, 1H, *J* = 7.3 Hz, Ar), 7.18 (m, 6H, Ar), 7.25 (m, 6H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 210.6 (C=*C*=CH_2), 166.2 (CO), 157.8, 136.2, 134.2, 129.2 (Ar, 2CH), 128.6 (Ar, 4CH), 128.5 (Ar, 2CH), 128.4 (Ar, CH), 127.5 (Ar, CH), 127.2 (Ar, 2CH), 121.9 (Ar, CH), 115.7 (Ar, 2CH), 102.1, 81.6 (CH, H3), 79.9 (OCH), 77.9 (C=*C*H_2), 58.6 (CH, H4), 55.5 (OMe), 46.1 (NCH_2); IR ($CHCl_3$): ν = 2993, 1946, 1756 cm^{-1}; HRMS (ES): calcd for $C_{27}H_{25}NO_3$ $[M]^+$: 411.1834; found: 411.1846.

Methoxy Allene (+)-1f. From 314 mg (1.09 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (4:1) as eluent gave the methoxy allene (+)-**1f** (210 mg, 64%) as a colorless oil; $[\alpha]_D$ = +15.2 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.30 (d, 3H, *J* = 6.6 Hz, Me), 1.39 (d, 3H, *J* = 6.6 Hz, Me), 1.70 (t, 3H, *J* = 3.2 Hz, Me), 3.34 (s, 3H, OMe), 3.90 (sept, 1H, *J* = 6.1 Hz, NCH), 3.92 (m, 1H, OCH), 4.01 (t, 1H, *J* = 4.7 Hz, H4), 4.40 (m, 1H,=CH*H*), 4.61 (m, 1H, =C*H*H), 5.14 (d, 1H, *J* = 4.5 Hz, H3), 6.99 (t, 1H, *J* = 7.3 Hz, Ar), 7.03 (d, 2H, *J* = 7.7 Hz, Ar), 7.28 (m, 2H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 208.5 (C=*C*=CH_2), 165.8 (CO), 158.0, 129.8 (Ar, 2CH), 121.9 (Ar, CH) , 115.7 (Ar, 2CH), 94.5, 82.5 (CH, H3), 79.1 (OCH), 74.8 (C=*C*H_2), 58.6 (CH, H4), 55.6 (OMe), 46.0 (NCH), 21.2 (Me), 19.9 (Me), 14.3 (Me); IR ($CHCl_3$): ν = 2998, 1948, 1753 cm^{-1}; HRMS (ES): calcd for $C_{18}H_{23}NO_3$ $[M]^+$: 301.1678; found: 301.1684.

Methoxy Allene (+)-1g. From 259 mg (0.74 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (4:1) as eluent gave the methoxy allene (+)-**1g** (240 mg, 89%) as a colorless oil; $[\alpha]_D$ = +11.9 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR

(300 MHz, $CDCl_3$): δ = 1.34 (d, 3H, *J* = 6.7 Hz, Me), 1.40 (d, 3H, *J* = 6.8 Hz, Me), 3.43 (s, 3H, OMe), 3.95 (sept, 1H, *J* = 6.9 Hz, NCH), 4.21 (dd, 1H, *J* = 9.2, 5.0 Hz, H4), 4.51 (d, 1H, *J* = 9.2 Hz, OCH), 4.82 (d, 1H, *J* = 12.4 Hz, =CH*H*), 5.00 (d, 1H, *J* = 12.4 Hz, =C*H*H), 5.05 (d, 1H, *J* = 5.0 Hz, H3), 6.78 (d, 2H, *J* = 7.7 Hz, Ar), 6.96 (t, 1H, *J* = 7.3 Hz, Ar), 7.23 (m, 3H, Ar), 7.34 (t, 2H, *J* = 7.0 Hz, Ar), 7.47 (d, 2H, *J* = 7.1 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 210.7 (C=*C*=CH_2), 165.9 (CO), 157.9, 134.7, 129.2 (Ar, 2CH), 128.5 (Ar, 3CH), 127.2 (Ar, 2CH), 121.8 (Ar, CH), 115.7 (Ar, 2CH), 102.5, 81.5 (CH, H3), 79.1 (OCH), 78.0 (C=*C*H_2), 59.2 (CH, H4), 55.6 (OMe), 46.1 (NCH), 21.4 (Me), 20.0 (Me); IR ($CHCl_3$): ν = 2995, 1945, 1748 cm^{-1}; HRMS (ES): calcd for $C_{23}H_{25}NO_3$ $[M]^+$: 363.1834; found: 363.1836.

Methoxy Allene (+)-1h. From 105 mg (0.29 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (3:1) as eluent gave the methoxy allene (+)-**1h** (52 mg, 49%) as a colorless oil; $[\alpha]_D$ = +9.0 (*c* = 0.1 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.76 (s, 3H, Me), 3.38 (s, 3H, OMe), 3.91 (d, 1H, *J* = 15.2 Hz, NCH*H*), 4.21 (dd, 1H, *J* = 9.2, 4.8 Hz, H4), 4.14 (d, 1H, *J* = 15.4 Hz, NC*H*H), 4.61 (d, 1H, *J* = 9.2 Hz, OCH), 4.78 (d, 1H, *J* = 12.4 Hz, =CH*H*), 4.94 (d, 2H, *J* = 13.6 Hz, =CH_2), 4.98 (d, 1H, *J* = 12.5 Hz, =C*H*H), 5.17 (d, 1H, *J* = 4.8 Hz, H3), 6.81 (d, 2H, *J* = 7.7 Hz, Ar), 6.97 (t, 1H, *J* = 7.4 Hz, Ar), 7.28 (m, 5H, Ar), 7.46 (d, 2H, *J* = 7.3 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 210.5 (C=*C*=CH_2), 166.5 (CO), 157.8, 139.6, 134.4, 129.2 (Ar, 2CH), 128.5 (Ar, 2CH), 127.2 (Ar, 3CH), 121.9 (Ar, CH), 115.7 (Ar, 2CH), 113.2 (C=*C*H_2), 102.4, 81.3 (CH, H3), 79.8 (OCH), 78.1 (C=*C*H_2), 58.8 (CH, H4), 55.4 (OMe), 47.8 (NCH_2), 20.6 (Me); IR ($CHCl_3$): ν = 2997, 1946, 1758 cm^{-1}; HRMS (ES): calcd for $C_{24}H_{25}NO_3$ $[M]^+$: 375.1834; found: 375.1832.

Allenes **4** were prepared from 3-*O*-(aryl) glucofuranosides through selective removal of the 5,6-*O*-isopropylidene group, oxidation, and carbonyl–allenylation. For the synthesis of related

starting glucofuranosides see: N. D. Adhikary and P. Chattopadhyay, *Eur. J. Org. Chem.,* 2011, 7346.

Methoxy Allene (–)-4a. From 150 mg (0.47 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave the methoxy allene (–)-**4a** (124 mg, 79%) as a colorless oil; $[\alpha]_D$ = –22.1 (*c* = 0.1 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.23 (s, 3H, Me), 1.44 (s, 3H, Me), 1.66 (t, 3H, *J* = 3.0 Hz, Me), 3.08 (s, 3H, OMe), 4.01 (d, 1H, *J* = 9.5 Hz, OCH), 4.23 (dd, 1H, *J* = 9.5, 2.9 Hz, H4), 4.53 (d, 1H, *J* = 3.8 Hz, H2), 4.68 (m, 2H, =CH_2), 4.69 (m, 1H, H3), 5.88 (d, 1H, *J* = 3.8 Hz, H1), 6.91 (t, 1H, *J* = 7.4 Hz, Ar), 6.93 (d, 2H, *J* = 8.0 Hz, Ar), 7.23 (t, 2H, *J* = 7.2 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 208.6 (C=*C*=CH_2), 157.3, 129.6 (Ar, 2CH), 121.5 (Ar, CH) , 115.5 (Ar, 2CH), 111.9, 105.1 (CH, H1), 95.2, 82.2 (CH, H2), 79.8 (CH, H3), 78.9 (CH, H4), 78.8 (OCH), 74.4 (C=*C*H_2), 56.0 (OMe), 26.8 (Me), 26.3 (Me), 12.6 (Me); IR ($CHCl_3$): ν = 2990, 1941 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{24}O_5$ $[M]^+$: 332.1624; found: 332.1624.

Methoxy Allene (–)-4b. From 174 mg (0.52 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave the methoxy allene (–)-**4b** (135 mg, 75%) as a colorless oil; $[\alpha]_D$ = –16.9 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.01 (t, 3H, *J* = 7,3 Hz, Me), 1.23 (s, 3H, Me), 1.45 (s, 3H, Me), 1.98 (m, 2H, CH_2), 3.08 (s, 3H, OMe), 4.04 (d, 1H, *J* = 9.6 Hz, OCH), 4.26 (dd, 1H, *J* = 9.5, 2.9 Hz, H4), 4.54 (d, 1H, *J* = 3.8 Hz, H2), 4.71 (d, 1H, *J* = 3.1 Hz, H3), 4.81 (m, 2H, =CH_2), 5.88 (d, 1H, *J* = 3.8 Hz, H1), 6.93 (t, 1H, *J* = 7.7 Hz, Ar), 6.94 (d, 2H, *J* = 7.7 Hz, Ar), 7.24 (t, 2H, *J* = 7.1 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 207.9 (C=*C*=CH_2), 157.3, 129.6 (Ar, 2CH), 121.5 (Ar, CH), 115.5 (Ar, 2CH), 111.9, 105.1 (CH, H1), 102.4, 82.1 (CH, H2), 79.8 (CH, H3), 79.2 (CH, H4), 78.9 (OCH), 76.9 (C=*C*H_2), 56.1 (OMe), 26.8 (Me), 26.4 (Me), 18.8 (CH_2), 12.0 (Me); IR ($CHCl_3$): ν = 2996, 1945 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{26}O_5$ $[M]^+$: 346.1780; found: 346.1792.

Methoxy Allene (–)-4c. From 267 mg (0.63 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave the methoxy allene (–)-**4c** (221 mg, 80%) as a colorless oil; $[\alpha]_D = -27.9$ (*c* = 0.5 in $CHCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ = 1.21 (s, 3H, Me), 1.36 (s, 3H, Me), 3.13 (s, 3H, OMe), 4.04 (d, 1H, *J* = 11.9 Hz, OC*H*H), 4.13 (d, 1H, *J* = 9.5 Hz, OCH), 4.18 (dt, 1H, *J* = 11.9, 2.3 Hz, OCH*H*), 4.39 (dd, 1H, *J* = 9.5, 3.0 Hz, H4), 4.47 (d, 1H, *J* = 11.9 Hz, OC*H*HAr), 4.52 (d, 1H, *J* = 4.0 Hz, H2), 4.55 (d, 1H, *J* = 12.0 Hz, OCH*H*Ar), 4.72 (d, 1H, *J* = 3.0 Hz, H3), 4.90 (q, 2H, *J* = 11.1 Hz, $=CH_2$), 5.87 (d, 1H, *J* = 3.8 Hz, H1), 6.92 (t, 1H, *J* = 7.5 Hz, Ar), 6.93 (d, 2H, *J* = 8.5 Hz, Ar), 7.18 (m, 2H, Ar), 7.24 (m, 3H, Ar), 7.29 (t, 2H, *J* = 7.0 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 208.9 (C=*C*=CH_2), 157.2, 138.3, 129.6 (Ar, 2CH), 128.2 (Ar, 2CH), 127.9 (Ar, 2CH), 127.4 (Ar,CH), 121.5 (Ar,CH), 115.5 (Ar, 2CH), 112.0, 105.2 (CH, H1), 98.6, 82.1 (CH, H2), 80.5 (CH, H3), 79.8 (CH, H4), 77.3 (OCH), 77.1 (C=*C*H_2), 71.7 (O*C*H_2Ar), 67.7 (O*C*H_2), 56.7 (OMe), 26.7 (Me), 26.4 (Me); IR ($CHCl_3$): ν = 3000, 1947 cm^{-1}; HRMS (ES): calcd for $C_{26}H_{30}O_6$ $[M]^+$: 438.2042; found: 438.2051.

Methoxy Allene (–)-4d. From 283 mg (0.71 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave the methoxy allene (–)-**4d** (225 mg, 77%) as a colorless oil; $[\alpha]_D = -22.3$ (*c* = 0.5 in $CHCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ = 1.32 (s, 3H, Me), 1.52 (s, 3H, Me), 1.73 (t, 3H, *J* = 3.0 Hz, Me), 3.14 (s, 3H, OMe), 4.02 (d, 1H, *J* = 9.5 Hz, OCH), 4.30 (dd, 1H, *J* = 9.5, 3.1 Hz, H4), 4.58 (d, 1H, *J* = 3.8 Hz, H2), 4.73 (d, 1H, *J* = 2.9 Hz, H3), 4.77 (m, 2H, $=CH_2$), 5.96 (d, 1H, *J* = 3.8 Hz, H1), 6.90 (d, 2H, *J* = 9.1 Hz, Ar), 7.41 (d, 2H, *J* = 9.1 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 208.7 (C=*C*=CH_2), 156.5, 132.5 (Ar, 2CH), 117.3 (Ar, 2CH), 113.9, 112.1, 105.1 (CH, H1), 95.1, 82.2 (CH, H2), 80.3 (CH, H3), 78.8 (CH, H4), 78.8 (OCH), 74.6 (C=*C*H_2), 56.0 (OMe), 26.8 (Me), 26.4 (Me), 12.6 (Me); IR ($CHCl_3$): ν = 2995, 1945 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{23}BrO_5$ $[M]^+$: 410.0729; found: 410.0738.

Methoxy Allene (–)-4e. From 85 mg (0.17 mmol) of the corresponding α-allenic alcohol, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave the methoxy allene (–)-**4e** (85 mg, 99%) as a colorless oil; $[\alpha]_D = -12.3$ ($c = 0.1$ in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.21 (s, 3H, Me), 1.36 (s, 3H, Me), 3.11 (s, 3H, OMe), 4.02 (m, 1H, OC*H*H), 4.06 (d, 1H, *J* = 9.6 Hz, OCH), 4.17 (dt, 1H, *J* = 11.8, 2.5 Hz, OCH*H*), 4.39 (dd, 1H, *J* = 9.5, 3.0 Hz, H4), 4.45 (d, 1H, *J* = 11.8 Hz, OC*H*HAr), 4.47 (d, 1H, *J* = 3.5 Hz, H2), 4.54 (d, 1H, *J* = 11.9 Hz, OCH*H*Ar), 4.65 (d, 1H, *J* = 3.0 Hz, H3), 4.89 (q, 2H, *J* = 11.2 Hz, =CH_2), 5.87 (d, 1H, *J* = 3.8 Hz, H1), 6.82 (d, 2H, *J* = 9.1 Hz, Ar), 7.21 (m, 2H, Ar), 7.27 (m, 3H, Ar), 7.33 (d, 2H, *J* = 9.1 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 209.3 (C=*C*=CH_2), 156.8, 138.7, 132.9 (Ar, 2CH), 128.7 (Ar, 2CH), 128.3 (Ar, 2CH), 127.9 (Ar,CH), 117.6 (Ar, 2CH), 114.2, 112.5, 105.6 (CH, H1), 98.8, 82.5 (CH, H2), 80.9 (CH, H3), 80.7 (CH, H4), 77.3 (OCH), 77.2 (C=*C*H_2), 72.1 (O*C*H_2), 68.1 (O*C*H_2Ar), 57.0 (OMe), 27.1 (Me), 26.8 (Me); IR ($CHCl_3$): ν = 2998, 1947 cm^{-1}; HRMS (ES): calcd for $C_{26}H_{29}BrO_6$ $[M]^+$: 516.1184; found: 516.1169.

General Procedure for the Gold-Catalyzed Hydroarylation of Allenyl-Tethered Arenes 1. Preparation of Nine-Membered Fused β-Lactams 3. $[(Ph_3P)AuNTf_2]$ (0.05 mmol) was added to a stirred solution of the corresponding allene **1** (1.0 mmol) in 1,2-dichloroethane (13.0 mL) under argon. The resulting mixture was stirred at room temperature (**1a**) or at 110 °C under μwave irradiation (**1b–h**), until disappearance of the starting material (TLC). After filtration through a pad of Celite, the mixture was extracted with ethyl acetate (3 x 5 mL), and the combined extracts were washed twice with brine. The organic layer was dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue eluting with ethyl acetate/hexanes mixtures gave analytically pure adducts **3**.

Preparation of Diene (–)-2a and Benzocycle (+)-3a. From 80 mg (0.23 mmol) of allene (+)-**1a**, and after chromatography of the residue using hexanes/ethyl acetate (2:1) as eluent, 27 mg

(34%) of the less polar compound (–)-**2a** and 11 mg (13%) of the more polar compound (+)-**3a** were obtained.

Diene (–)-2a. Colorless oil; $[\alpha]_D$ = –3.5 (*c* = 0.2 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.87 (t, 6H, *J* = 6.4 Hz, 2Me), 1.74 (m, 1H, CH isobut), 1.84 (d, 3H, *J* = 1.2 Hz, Me), 2.03 (s, 3H, COMe), 2.76 (dd, 1H, *J* = 13.9, 6.7 Hz, NCH*H*), 3.07 (dd, 1H, *J* = 14.0, 7.6 Hz, NC*H*H), 4.64 (dd, 1H, *J* = 9.6, 4.4 Hz, H4), 4.81 (d, 1H, *J* = 2.0 Hz, =CH*H*), 5.03 (d, 1H, *J* = 2.2 Hz, =C*H*H), 5.26 (d, 1H, *J* = 4.5 Hz, H3), 5.67 (d, 1H, *J* = 9.6 Hz, =CH), 6.85 (d, 2H, *J* = 7.7 Hz, Ar), 6.92 (t, 1H, *J* = 7.3 Hz, Ar), 7.18 (t, 2H, *J* = 7.4 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 168.6 (COMe), 165.8 (CO), 157.3, 153.2, 135.3, 129.5 (Ar, 2CH), 122.2 (Ar, CH), 121.0 (=CH), 115.5 (Ar, 2CH), 104.1 (=CH_2), 81.7 (CH, H3), 56.5 (CH, H4), 48.4 (NCH_2), 27.5 (CH isobut), 20.3 (2Me), 13.7 (Me); IR ($CHCl_3$): ν = 1758 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{25}NO_4$ $[M]^+$: 343.1784; found: 343.1797.

Benzocycle (+)-3a. Colorless oil; $[\alpha]_D$ = +16.8 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.95 (d, 3H, *J* = 6.7 Hz, Me), 0,99 (d, 3H, *J* = 6.7 Hz, Me), 1.80 (t, 3H, *J* = 2.6 Hz, Me), 2.03 (m, 1H, CH isobut), 2.11 (s, 3H, COMe), 2.67 (m, 2H, CH_2Ar), 2.95 (dd, 1H, *J* = 13.7, 6.0 Hz, NCH*H*), 3.32 (dd, 1H, *J* = 13.8, 8.6 Hz, NC*H*H), 4.34 (dd, 1H, *J* = 7.2, 5.1 Hz, H4), 5.26 (m, 1H, OCH), 5.29 (d, 1H, *J* = 5.1 Hz, H3), 7.03 (t, 1H, *J* = 7.3 Hz, =CH), 7.10 (d, 2H, *J* = 7.9 Hz, Ar), 7.30 (t, 2H, *J* = 7.6 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 169.7 (COMe), 166.4 (CO), 157.6, 129.6 (Ar, 2CH), 122.5 (=CH), 122.0 (=C), 115.8 (Ar, 2CH), 115.7, 79.9 (CH, H3), 71.1 (OCH), 57.9 (CH, H4), 49.6 (CH_2 isobut), 27.0 (CH isobut), 22.0 (CH_2Ar), 21.1 (Me), 20.4 (Me), 20.1 (Me), 3.5 (Me); IR ($CHCl_3$): ν = 1757 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{25}NO_4$ $[M]^+$: 343.1784; found: 343.1797.

Benzocycle (+)-3b. From 68 mg (0.215 mmol) of allene (+)-**1b**, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave tricycle (+)-**3b** (50 mg, 72%) as a colorless oil; $[\alpha]_D$ = +25.9 (*c* = 0.8 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.93 (d, 3H, *J* =

6.7 Hz, Me), 0.98 (d, 3H, *J* = 6.7 Hz, Me), 1.81 (t, 3H, *J* = 2.6 Hz, Me), 2.08 (m, 1H, CH isobut), 2.58 (m, 2H, CH_2Ar), 3.10 (dd, 1H, *J* = 13.6, 6.3 Hz, NCH*H*), 3.28 (dd, 1H, *J* = 13.6, 8.3 Hz, NC*H*H), 3.47 (s, 3H, OMe), 3.67 (dt, 1H, *J* = 8.4, 4.2 Hz, OCH), 4.12 (dd, 1H, *J* = 8,5, 5.1 Hz, H4), 5.23 (d, 1H, *J* = 5.1 Hz, H3), 7.03 (t, 1H, *J* = 7.3 Hz, =CH), 7.13 (d, 2H, *J* = 7.7 Hz, Ar), 7.31 (m, 2H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 167.2 (CO), 158.1, 130.0 (Ar, 2CH), 122.8 (=CH), 121.0 (=C), 116.3 (Ar, 2CH), 115.7, 80.1 (CH, H3), 79.7 (OCH), 59.6 (CH, H4), 57.4 (OMe), 50.1 (NCH_2), 27.3 (CH isobut), 20.8 (2Me), 20.6 (CH_2Ar), 4.1 (Me); IR ($CHCl_3$): ν = 1756 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{25}NO_3$ $[M]^+$: 315.1834; found: 315.1844.

Benzocycle (+)-3c. From 50 mg (0.132 mmol) of allene (+)-**1c**, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave tricycle (+)-**3c** (30 mg, 60%) as a colorless oil; $[\alpha]_D$ = +24.1 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR (700 MHz, $CDCl_3$): δ = 0.92 (d, 3H, *J* = 6.6 Hz, Me), 0.97 (d, 3H, *J* = 6.6 Hz, Me), 2.08 (m, 1H, CH isobut), 2.78 (dd, 1H, *J* = 17.5, 4.5 Hz, CH*H*Ar), 2.94 (dd, 1H, *J* = 17.5, 4.2 Hz, C*H*HAr), 3.11 (dd, 1H, *J* = 13.6, 6.2 Hz, NCH*H*), 3.32 (dd, 1H, *J* = 13.2, 8.3 Hz, NC*H*H), 3.54 (s, 3H, OMe), 3.81 (dt, 1H, *J* = 8.5, 4.4 Hz, OCH), 4.17 (dd, 1H, *J* = 8.3, 5.1 Hz, H4), 5.27 (d, 1H, *J* = 5.0 Hz, H3), 7.04 (t, 1H, *J* = 7.3 Hz, =CH), 7.16 (d, 2H, *J* = 7.6 Hz, Ar), 7.31 (m, 5H, Ar), 7.41 (m, 2H, Ar); ^{13}C NMR (175 MHz, $CDCl_3$): δ = 166.7 (CO), 157.7, 131.7 (Ar, 2CH) ,129.7 (Ar, 3CH), 128.7, 128.3 (Ar, 2CH), 124.0 (=C), 122.4 (=CH), 115.9 (Ar, 2CH), 115.7, 79.7 (CH, H3), 79.3 (OCH), 59.4 (CH, H4), 57.4 (OMe), 49.7 (NCH_2), 27.0 (CH isobut), 21.4 (CH_2Ar), 20.5 (Me), 20.2 (Me); IR ($CHCl_3$): ν = 1757 cm^{-1}; HRMS (ES): calcd for $C_{24}H_{27}NO_3$ $[M]^+$: 377.1991; found: 377.2001.

Benzocycle (+)-3d. From 50 mg (0.16 mmol) of allene (+)-**1d**, and after chromatography of the residue using hexanes/ethyl acetate (7:1) as eluent gave tricycle (+)-**3d** (30 mg, 58%) as a colorless oil; $[\alpha]_D$ = +28.0 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.75 (d, 3H, *J* = 2.5 Hz, Me), 2.42 (d, 1H, *J* = 17.4 Hz, CH*H*Ar), 2.61 (d, 1H, *J* = 17.4 Hz, C*H*HAr), 3.28 (s, 3H,

OMe), 3.65 (m, 1H, OCH), 4.04 (dd, 1H, *J* = 8,6, 5.1 Hz, H4), 4.46 (d, 1H, *J* = 14.8 Hz, NCH*H*), 4.64 (d, 1H, *J* = 14.8 Hz, NC*H*H), 5.20 (d, 1H, *J* = 5.1 Hz, H3), 7.03 (t, 1H, *J* = 7.3 Hz, =CH), 7.13 (d, 2H, *J* = 8.6 Hz, Ar), 7.31 (m, 4H, Ar), 7.53 (m, 3H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 166.3 (CO), 157.4, 130.0 (Ar, 2CH), 129.02 (Ar, 2CH), 128.8 (Ar, 2CH), 127.9 (Ar, CH), 122.4 (=CH), 121.8 (=C), 116.0 (Ar, 2CH), 115.6, 79.5 (CH, H3), 77.6 (OCH), 59.3 (CH, H4), 57.3 (OMe), 46.3 (NCH_2), 20.6 (CH_2Ar), 14.5 (Me); IR ($CHCl_3$): ν = 1758 cm^{-1}; HRMS (ES): calcd for $C_{22}H_{23}NO_3$ $[M]^+$: 349.1678; found: 349.1671.

Benzocycle (+)-3e. From 44 mg (0.108 mmol) of allene (+)-**1e**, and after chromatography of the residue using hexanes/ethyl acetate (7:1) as eluent gave tricycle (+)-**3e** (30 mg, 69%) as a colorless oil; $[\alpha]_D$ = +16.6 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.67 (dd, 1H, *J* = 17.5, 4.5 Hz, CH*H*Ar), 2.88 (dd, 1H, *J* = 17.5, 4.0 Hz, C*H*HAr), 3.37 (s, 3H, OMe), 3.80 (dt, 1H, *J* = 8.6, 4.2 Hz, OCH), 4.09 (dd, 1H, *J* = 8.6, 5.0 Hz, H4), 4.45 (d, 1H, *J* = 14.6 Hz, NCH*H*), 4.71(d, 1H, *J* = 14.8 Hz, NC*H*H), 5.23 (d, 1H, *J* = 5.1 Hz, H3), 7.04 (t, 1H, *J* = 7.3 Hz, =CH), 7.15 (d, 2H, *J* = 7.7 Hz, Ar), 7.29 (m, 6H, Ar), 7.35 (m, 6H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 166.3 (CO), 157.6, 136.1, 131.6 (Ar, 2CH), 129.6 (Ar, 2CH), 128.7 (Ar, 4CH), 128.5 (Ar, 2CH), 128.2 (Ar, 2CH), 127.9, 127.6, 123.4 (=C),122.5 (=CH), 115.9 (Ar, 2CH), 80.0 (CH, H3), 79.1 (OCH), 58.7 (CH, H4), 57.1 (OMe), 46.0 (NCH_2), 21.3 (CH_2Ar); IR ($CHCl_3$): ν = 1758 cm^{-1}; HRMS (ES): calcd for $C_{27}H_{25}NO_3$ $[M]^+$: 411.1834; found: 411.1835.

Benzocycle (+)-3f. From 46 mg (0.16 mmol) of allene (+)-**1f**, and after chromatography of the residue using hexanes/ethyl acetate (7:1) as eluent gave tricycle (+)-**3f** (32 mg, 65%) as a colorless oil; $[\alpha]_D$ = +16.4 (*c* = 0.2 in $CHCl_3$); ^{1}H NMR (700 MHz, $CDCl_3$): δ = 1.30 (d, 3H, *J* = 6.7 Hz, Me), 1.39 (d, 3H, *J* = 6.9 Hz, Me), 1.80 (t, 3H, *J* = 2.6 Hz, Me), 2.52 (d, 1H, *J* = 16.9 Hz, CH*H*Ar), 2.71 (d, 1H, *J* = 16.4 Hz, C*H*HAr), 3.48 (s, 3H, OMe), 3.62 (dt, 1H, *J* = 8.7, 4.0 Hz, OCH), 3.88 (sept, 1H, *J* = 6.7 Hz, NCH), 4.14 (dd, 1H, *J* = 8,8, 5.1 Hz, H4), 5.15 (d, 1H, *J* = 5.1

Hz, H3), 7.02 (t, 1H, *J* = 7.4 Hz, =CH), 7.13 (d, 2H, *J* = 8.0 Hz, Ar), 7.30 (t, 2H, *J* = 7.4 Hz, Ar); ^{13}C NMR (175 MHz, $CDCl_3$): δ = 165.9 (CO), 157.7, 129.5 (Ar, 2CH), 122.3 (=CH), 120.0 (=C), 116.0 (Ar, 2CH), 115.9, 79.3 (CH, H3), 79.1 (OCH), 58.6 (CH, H4), 56.9 (OMe), 46.2 (NCH), 21.2 (Me), 20.1 (Me), 19.8 (CH_2Ar), 3.7 (Me); IR ($CHCl_3$): ν = 1751 cm^{-1}; HRMS (ES): calcd for $C_{18}H_{23}NO_3$ $[M]^+$: 301.1678; found: 301.1674.

Benzocycle (+)-3g. From 60 mg (0.165 mmol) of allene (+)-**1g**, and after chromatography of the residue using hexanes/ethyl acetate (7:1) as eluent gave tricycle (+)-**3g** (36 mg, 59%) as a colorless oil; $[\alpha]_D$ = +17.9 (*c* = 0.5 in $CHCl_3$); ^{1}H NMR (700 MHz, $CDCl_3$): δ = 1.31 (d, 3H, *J* = 6.7 Hz, Me), 1.39 (d, 3H, *J* = 6.9 Hz, Me), 2.77 (dd, 1H, *J* = 17.7, 4.1 Hz, CH*H*Ar), 2.98 (dd, 1H, *J* = 17.7, 4.0 Hz, C*H*HAr), 3.55 (s, 3H, OMe), 3.76 (dt, 1H, *J* = 8.7, 4.1 Hz, OCH), 3.90 (sept, 1H, *J* = 6.7 Hz, NCH), 4.19 (dd, 1H, *J* = 8.5, 5.2 Hz, H4), 5.19 (d, 1H, *J* = 5.2 Hz, H3), 7.03 (t, 1H, *J* = 7.2 Hz, =CH), 7.15 (d, 2H, *J* = 8.0 Hz, Ar), 7.30 (m, 5H, Ar), 7.41 (m, 2H, Ar); ^{13}C NMR (175 MHz, $CDCl_3$): δ = 165.9 (CO), 157.7, 131.6 (Ar, 2CH) , 129. (Ar, 2CH), 128.2 (Ar, 2CH), 127.9 (Ar, CH), 127.8, 123.4 (=C),122.3 (=CH), 115.9 (Ar, 2CH), 115.8, 79.2 (CH, H3), 79.1 (OCH), 58.7 (CH, H4), 57.1 (OMe), 46.2 (NCH), 21.3 (Me), 20.9 (CH_2Ar), 20.0 (Me); IR ($CHCl_3$): ν = 1752 cm^{-1}; HRMS (ES): calcd for $C_{23}H_{25}NO_3$ $[M]^+$: 363.1834; found: 363.1840.

Benzocycle (+)-3h. From 30 mg (0.08 mmol) of allene (+)-**1h**, and after chromatography of the residue using hexanes/ethyl acetate (4:1) as eluent gave tricycle (+)-**3h** (19 mg, 63%) as a colorless oil; $[\alpha]_D$ = +14.8 (*c* = 0.4 in $CHCl_3$); ^{1}H NMR (700 MHz, $CDCl_3$): δ = 1.76 (s, 3H, Me), 2.73 (dd, 1H, *J* = 17.7, 4.7 Hz, CH*H*Ar), 2.91 (dd, 1H, *J* = 17.6, 4.5 Hz, C*H*HAr), 3.52 (s, 3H, OMe), 3.80 (m, 1H, OCH), 3.83 (d, 1H, *J* = 14.9 Hz, NCH*H*), 4.09 (d, 1H, *J* = 15.0 Hz, NC*H*H), 4.16 (dd, 1H, *J* = 7.9, 5.0 Hz, H4), 4.94 (d, 2H, *J* = 13.9 Hz, =CH_2), 5.29 (d, 1H, *J* = 5.1 Hz, H3), 7.04 (t, 1H, *J* = 7.3 Hz, =CH), 7.15 (d, 2H, *J* = 7.7 Hz, Ar), 7.30 (m, 5H, Ar), 7.40 (m, 2H, Ar); ^{13}C NMR (175 MHz, $CDCl_3$): δ = 166.6 (CO), 157.8, 157.7, 139.4, 131.6 (Ar, 2CH), 129.6. (Ar, 2CH),

128.2 (Ar, 2CH), 127.9 (Ar, CH), 123.4 (=C),122.4 (=CH), 118.1, 115.9 (Ar, 2CH), 113.2 (C=*C*H_2), 79.9 (CH, H3), 79.0 (OCH), 59.1 (CH, H4), 57.4 (OMe), 47.8 (NCH_2), 21.5 (CH_2Ar), 20.6 (Me); IR ($CHCl_3$): ν = 1758 cm^{-1}; HRMS (ES): calcd for $C_{24}H_{25}NO_3$ $[M]^+$: 375.1834; found: 375.1836.

General Procedure for the Gold-Catalyzed Hydroalkylation of Allenyl-Tethered Arenes 4. Preparation of Cyclopenta[*b*]furans 5. $[(Ph_3P)AuNTf_2]$ (0.05 mmol) was added to a stirred solution of the corresponding allene **4** (1.0 mmol) in 1,2-dichloroethane (13.0 mL) under argon. The resulting mixture was stirred at room temperature until disappearance of the starting material (TLC). After filtration through a pad of Celite, the mixture was extracted with ethyl acetate (3 x 5 mL), and the combined extracts were washed twice with brine. The organic layer was dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue eluting with ethyl acetate/hexanes mixtures gave analytically pure adducts **5**.

Fused Cyclopentene (+)-5a. From 156 mg (0.47 mmol) of allene (–)-**4a**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave tricycle (+)-**5a** (73 mg, 46%) as a colorless oil; $[\alpha]_D$ = +55.9 (*c* = 0.9 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.43 (s, 3H, Me), 1.53 (s, 3H, Me), 1.88 (s, 3H, Me), 2.19 (s, 3H, Me), 3.35 (s, 3H, OMe), 4.53 (dd, 1H, *J* = 6.7, 2.3 Hz, H4), 5.00 (d, 1H, *J* = 2.5 Hz, H2), 5.09 (d, 1H, *J* = 6.9 Hz, OCH), 6.15 (s, 1H, H1), 6.96 (t, 1H, *J* = 7.3 Hz, Ar), 6.97 (d, 2H, *J* = 7.8 Hz, Ar), 7.24 (m, 2H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 157.9, 147.6, 147.2, 129.3 (Ar, 2CH), 121.4 (Ar, CH) , 116.3 (Ar, 2CH), 114.8, 112.7 (CH, H1), 112.0, 104.3 (CH, H2), 83.7 (CH, H4), 74.4 (OCH), 55.2 (OMe), 27.6 (Me), 27.2 (Me), 11.4 (Me), 9.8 (Me); IR ($CHCl_3$): ν = 1072 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{24}O_5$ $[M]^+$: 315.1624; found: 332.1614.

Fused Cyclopentene (+)-5b. From 126 mg (0.36 mmol) of allene (–)-**4b**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave tricycle (+)-**5b** (46

mg, 34%) as a colorless oil; $[\alpha]_D$ = +33.3 (*c* = 0.2 in $CHCl_3$); ^1H NMR (700 MHz, $CDCl_3$): δ = 1.07 (t, 3H, *J* = 7,6 Hz, Me), 1.41 (s, 3H, Me), 1.53 (s, 3H, Me), 2.19 (s, 1H, Me), 2.29 (q, 2H, *J* = 9.6 Hz, CH_2), 3.34 (s, 3H, OMe), 4.53 (dd, 1H, *J* = 7.0, 2.5 Hz, H4), 5.00 (d, 1H, *J* = 2.5 Hz, H2), 5.09 (d, 1H, *J* = 6.9 Hz, OCH), 6.20 (s, 1H, H1), 6.94 (t, 1H, *J* = 7.3 Hz, Ar), 6.98 (d, 2H, *J* = 7.7 Hz, Ar), 7.24 (t, 2H, *J* = 7.4 Hz, Ar); ^{13}C NMR (175 MHz, $CDCl_3$): δ = 157.8, 146.9, 146.7, 129.1 (Ar, 2CH), 121.3 (Ar, CH), 121.2, 116.2 (Ar, 2CH), 111.8, 111.0 (CH, H1), 104.2 (CH, H2), 83.4 (CH, H4), 74.4 (OCH), 55.1 (OMe), 27.4 (Me), 27.0 (Me), 17.8 (CH_2), 14.6 (Me), 11.4 (Me); IR ($CHCl_3$): ν = 1074 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{26}O_5$ $[M]^+$: 346.1780; found: 346.1777.

Fused Cyclopentene (+)-5c. From 150 mg (0.34 mmol) of allene (–)-**4c**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave tricycle (+)-**5c** (73 mg, 48%) as a colorless oil; $[\alpha]_D$ = +34.9 (*c* = 0.5 in $CHCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ = 1.34 (s, 3H, Me), 1.45 (s, 3H, Me), 2.16 (s, 3H, Me), 3.26 (s, 3H, OMe), 4.22 (d, 2H, *J* = 11.9 Hz, OCH_2), 4.35 (m, 2H, OCH_2Ar), 4.47 (dd, 1H, *J* = 6.7, 2.5 Hz, H4), 4.94 (d, 1H, *J* = 2.5 Hz, H2), 5.06. (d, 1H, *J* = 6.7 Hz, OCH), 6.27 (s, 1H, H1), 6.87 (t, 1H, *J* = 7.2 Hz, Ar), 6.89 (d, 2H, *J* = 7.7 Hz, Ar), 7.16 (m, 2H, Ar), 7.22 (m, 3H, Ar), 7.27 (m, 2H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 157.8, 150.3, 147.9, 138.0, 129.3 (Ar, 2CH), 128.3 (Ar, 2CH), 127.8 (Ar, 2CH), 127.6 (Ar,CH), 121.6 (Ar,CH), 116.3, 116.4 (Ar, 2CH), 112.0, 111.6 (CH, H1), 104.2 (CH, H2), 83.5 (OCH), 79.4 (CH, H4), 71.5 (OCH_2Ar), 63.2 (OCH_2), 55.2 (OMe), 27.6 (Me), 27.2 (Me), 11.9 (Me); IR ($CHCl_3$): ν = 1071 cm^{-1}; HRMS (ES): calcd for $C_{26}H_{30}O_6$ $[M]^+$: 438.2042; found: 438.2034.

Fused Cyclopentene (+)-5d. From 118 mg (0.29 mmol) of allene (–)-**4d**, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave tricycle (+)-**5d** (40 mg, 35%) as a colorless oil; $[\alpha]_D$ = +32.1 (*c* = 0.4 in $CHCl_3$); ^1H NMR (300 MHz, $CDCl_3$): δ = 1.43 (s, 3H, Me), 1.52 (s, 3H, Me), 1.88 (s, 3H, Me), 2.18 (s, 3H, Me), 3.33 (s, 3H, OMe), 4.50 (dd, 1H, *J* = 7.1, 2.4 Hz, H4), 4.95 (d, 1H, *J* = 2.3 Hz, H2), 5.01 (d, 1H, *J* = 6.9 Hz, OCH), 6.13 (s, 1H,

H1), 6.84 (d, 2H, J = 9.1 Hz, Ar), 7.33 (d, 2H, J = 9.1 Hz, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 157.0, 148.0, 146.5, 132.2 (Ar, 2CH), 118.3 (Ar, 2CH), 117.2, 113.9, 112.9 (CH, H1), 111.7, 104.5 (CH, H2), 83.5 (CH, H4), 74.9 (OCH), 55.2 (OMe), 27.8 (Me), 26.9 (Me), 11.4 (Me), 9.9 (Me); IR ($CHCl_3$): ν = 1079 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{23}BrO_5$ $[M]^+$: 410.0729; found: 410.0744.

Fused Cyclopentene (+)-5e. From 68 mg (0.13 mmol) of allene (–)-**4e**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave tricycle (+)-**5e** (27 mg, 41%) as a colorless oil; $[\alpha]_D$ = +41.5 (c = 0.2 in $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.53 (s, 3H, Me), 1.57 (s, 3H, Me), 2.24 (s, 3H, Me), 3.33 (s, 3H, OMe), 4.30 (m, 2H, OCH_2), 4.44 (m, 2H, OCH_2Ar), 4.53 (dd, 1H, J = 7.4, 2.4 Hz, H4), 4.98 (d, 1H, J = 2.3 Hz, H2), 5.05 (d, 1H, J = 7.0 Hz, OCH), 6.34 (s, 1H, H1), 6.85 (d, 2H, J = 9.1 Hz, Ar), 7.29 (m, 2H, Ar), 7.32 (m, 3H, Ar), 7.36 (m, 2H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 156.9, 150.6, 147.5, 138.0, 132.4 (Ar, 2CH), 127.9 (Ar, 2CH), 127.8 (Ar, 2CH), 127.7 (Ar, CH), 118.4 (Ar, 2CH), 117.1, 114.0, 112.2, 111.9 (CH, H1), 104.2 (CH, H2), 83.4 (OCH), 77.5 (CH, H4), 71.6 (OCH_2Ar), 63.2 (OCH_2), 55.2 (OMe), 27.6 (Me), 27.1 (Me), 11.8 (Me); IR ($CHCl_3$): ν = 1074 cm^{-1}; HRMS (ES): calcd for $C_{26}H_{29}BrO_6$ $[M]^+$: 516.1148; found: 516.1154.

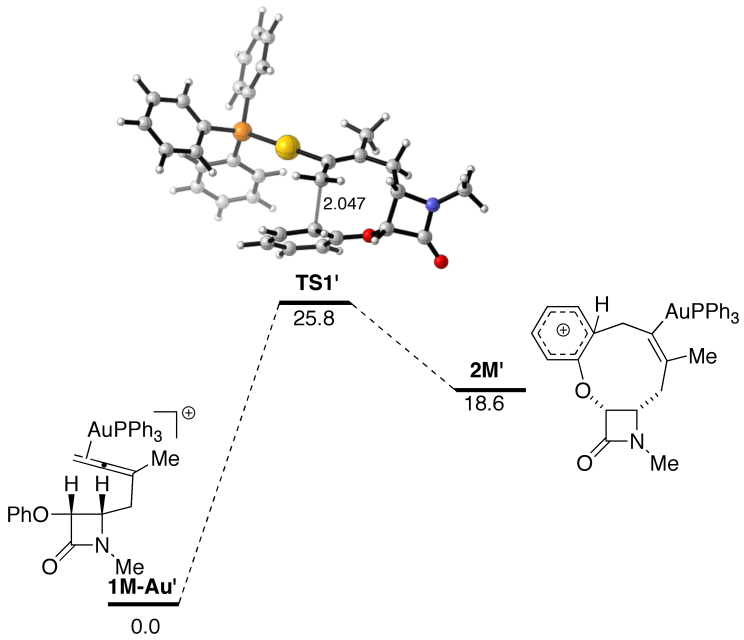

Figure 1S. Energy profile for the reaction between allenyl-β-lactam **1M** and [(PPh_3)AuNTf_2] catalyst. Relative free energies (ΔG, 298 K) have been computed at the PCM(CH_2Cl_2)-M06/def2-SVP//PCM(CH_2Cl_2)-B3LYP/def2-SVP level.

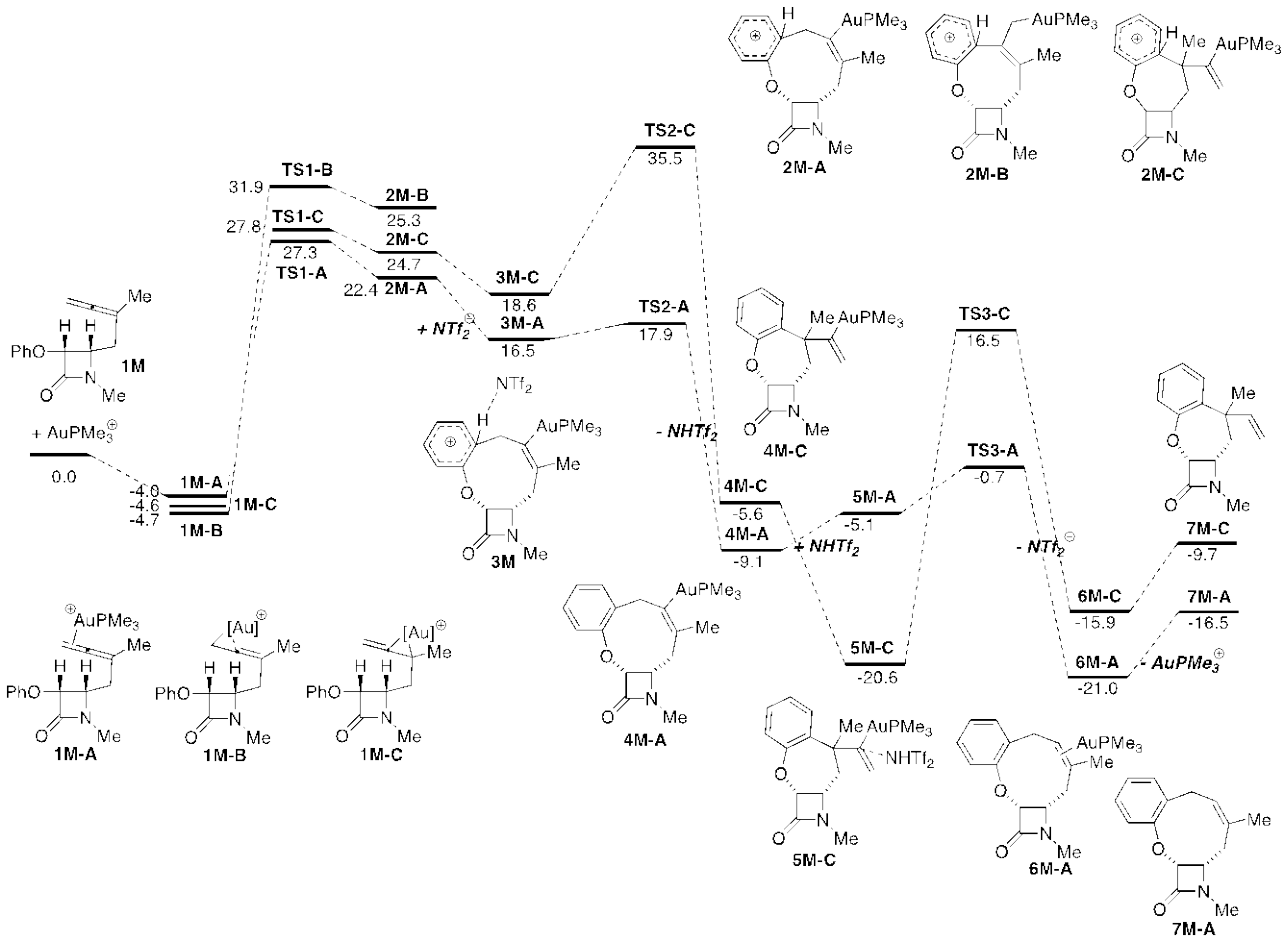

Figure 2S. Energy profile for the reaction between allenyl-β-lactam **1M** and [(PMe_3)AuNTf_2] catalyst. Relative free energies (ΔG, 298 K) have been computed at the PCM(CH_2Cl_2)-B3LYP/def2-SVP level.

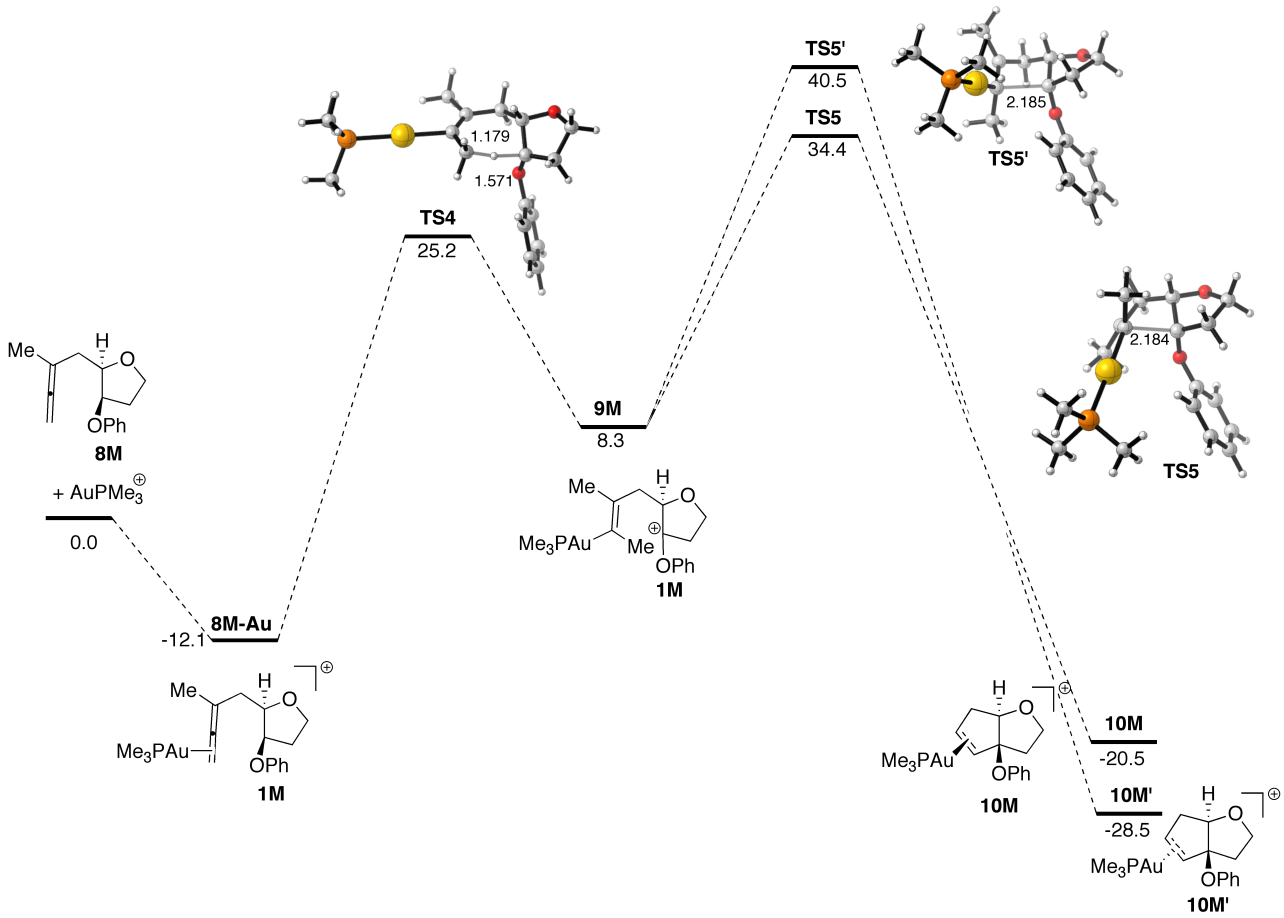

Figure 3S. Energy profile for the reaction between allenyl species **8M** and [(PMe_3)$AuNTf_2$] catalyst. Relative free energies (ΔG, 298 K) have been computed at the PCM(CH_2Cl_2)-M06/def2-SVP//PCM(CH_2Cl_2)-B3LYP/def2-SVP level.

Computational Details

All the calculations reported in this paper were obtained with the GAUSSIAN 09 suite of programs.[1] Geometry optimizations were performed using the B3LYP[2] hybrid functional in combination with the double-ζ quality plus polarization def2-SVP basis set[3] for all atoms and the Polarizable Continuum Model (PCM, using CH_2Cl_2 as solvent)[4] to take into account solvent effects. This level is denoted PCM(CH_2Cl_2)-B3LYP/def2-SVP. Reactants and products were characterized by frequency calculations,[5] and have positive definite Hessian matrices. Transition structures (TS's) show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the Intrinsic Reaction Coordinate (IRC) method.[6] Single point energy calculations were computed using the dispersion-corrected meta-hybrid M06 functional, which has been recommended for transition metal containing species,[7] with the same PCM/def2-SVP combination on the PCM-B3LYP/def2-SVP optimized geometries. This level is denoted PCM(CH_2Cl_2)-M06/def2-SVP//PCM(CH_2Cl_2)-B3LYP/def2-SVP.

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Cartesian coordinates (in Å) and total energies (in a. u., non corrected zero-point vibrational energies included) of all the stationary points discussed in the text. All calculations have been performed at the PCM(CH_2Cl_2)-B3LYP/def2-SVP + ΔZPVE level.

Profile in Figure 1 (main text).

1M: E= -786.110736

C	0.159094000	2.450434000	0.341882000
C	1.513889000	2.111897000	0.197955000
C	2.501508000	3.103720000	0.286008000
C	2.119246000	4.432955000	0.504591000
C	0.772753000	4.779061000	0.645894000
C	-0.204458000	3.778051000	0.569189000
O	1.789793000	0.787098000	-0.006806000
C	2.982619000	0.417637000	-0.648424000
C	3.089746000	-1.113798000	-0.941742000
C	1.957795000	-2.012924000	-0.463337000
C	0.739474000	-2.069289000	-1.368649000
C	0.666150000	-1.424514000	-2.513891000
C	0.577960000	-0.788639000	-3.658329000
C	-0.404253000	-2.926607000	-0.868105000
C	4.250272000	0.211080000	0.225463000
O	4.974007000	0.918076000	0.897232000
N	4.293990000	-1.111039000	-0.091395000
C	5.291009000	-2.120668000	0.162412000
H	5.747682000	-2.473847000	-0.777964000
H	4.864255000	-2.987850000	0.692166000
H	6.074895000	-1.676302000	0.792094000
H	2.349504000	-3.041278000	-0.352945000
H	1.640221000	-1.699405000	0.545420000
H	0.173404000	0.229424000	-3.720427000
H	0.905684000	-1.247480000	-4.599598000
H	3.557728000	2.836217000	0.227812000
H	3.173820000	1.053118000	-1.530027000
H	3.330247000	-1.327427000	-1.997134000
H	2.892462000	5.202588000	0.575253000
H	0.485122000	5.818585000	0.819572000
H	-1.261547000	4.033854000	0.679834000
H	-0.590606000	1.659767000	0.267945000
H	-1.243356000	-2.944740000	-1.577073000
H	-0.774211000	-2.548417000	0.100643000
H	-0.066098000	-3.963918000	-0.699959000

1M-Au: E= -1382.604105

C	0.247313000	2.714473000	0.203032000
C	1.573707000	2.263543000	0.133200000
C	2.635284000	3.176838000	0.193283000
C	2.354506000	4.543143000	0.315103000
C	1.036349000	5.001916000	0.386336000
C	-0.015748000	4.078929000	0.334446000
O	1.753794000	0.906373000	0.027517000
C	2.907131000	0.415609000	-0.604123000
C	2.913371000	-1.136476000	-0.797377000
C	1.752008000	-1.944845000	-0.208728000
C	0.589140000	-2.166052000	-1.179753000
Au	-1.386374000	-1.073719000	-0.313044000
P	-3.233022000	-0.583758000	1.040879000
C	-3.993710000	-2.098385000	1.730495000
C	0.136260000	-1.183786000	-1.998262000
C	0.012432000	-0.375701000	-3.030476000
C	0.156131000	-3.605628000	-1.384445000
C	4.180645000	0.184654000	0.255530000
O	4.960828000	0.883223000	0.866623000
N	4.138897000	-1.155413000	0.015129000

C	5.091608000	-2.203571000	0.288869000
C	-4.567512000	0.276073000	0.131835000
C	-2.827315000	0.475299000	2.475648000
H	5.499898000	-2.622919000	-0.646103000
H	4.640032000	-3.020225000	0.874763000
H	5.915445000	-1.769157000	0.872299000
H	2.129679000	-2.939683000	0.072552000
H	1.411012000	-1.468595000	0.722012000
H	-0.761884000	0.392694000	-3.095796000
H	0.710001000	-0.464033000	-3.872038000
H	3.667832000	2.823809000	0.187184000
H	3.123023000	0.974093000	-1.530689000
H	3.101742000	-1.439913000	-1.841907000
H	3.184321000	5.252830000	0.365259000
H	0.828555000	6.069758000	0.485289000
H	-1.051362000	4.424630000	0.387735000
H	-0.560107000	1.981012000	0.145286000
H	-0.717877000	-3.691545000	-2.042555000
H	-0.057368000	-4.099315000	-0.424210000
H	1.000114000	-4.145809000	-1.848219000
H	-5.425637000	0.446950000	0.800032000
H	-4.198282000	1.241079000	-0.243856000
H	-4.884875000	-0.340699000	-0.721160000
H	-2.079215000	-0.030111000	3.103247000
H	-2.408480000	1.429310000	2.124853000
H	-3.733749000	0.668937000	3.069578000
H	-4.869277000	-1.835286000	2.343647000
H	-4.307225000	-2.758000000	0.908683000
H	-3.257602000	-2.628635000	2.351621000

TS1: E= -1382.557542

C	-4.699571000	0.479538000	0.245188000
N	-4.603673000	-0.812990000	-0.174782000
C	-5.582489000	-1.717051000	-0.728302000
C	-0.775469000	-1.100166000	-1.053073000
C	-2.294333000	-1.214709000	-1.031433000
C	0.122431000	-0.885187000	-0.026063000
C	-0.316992000	-0.868637000	1.347539000
C	-0.733975000	1.001189000	2.068667000
C	-1.252232000	1.728937000	0.944190000
O	-2.399206000	1.419410000	0.331066000
C	-3.267610000	0.427333000	0.827910000
C	-3.187291000	-1.004496000	0.192097000
C	0.493340000	1.471236000	2.653196000
C	1.219451000	2.487998000	2.077901000
C	0.710744000	3.131569000	0.924020000
C	-0.505425000	2.763440000	0.363951000
C	-0.281571000	-1.246424000	-2.471247000
O	-5.584507000	1.301211000	0.206693000
Au	2.178662000	-0.617413000	-0.339118000
P	4.509408000	-0.343389000	-0.673107000
H	-5.699695000	-2.608347000	-0.090109000
H	-5.306618000	-2.042898000	-1.744290000
H	-6.543653000	-1.186704000	-0.779324000
H	-2.527590000	-2.224043000	-1.419677000
H	-2.659978000	-0.534829000	-1.821302000
H	0.438578000	-1.050136000	2.112827000
H	-1.277277000	-1.315773000	1.615685000
H	-1.443878000	0.537913000	2.757444000
H	-3.286831000	0.415278000	1.927145000
H	-3.065843000	-1.807701000	0.937036000
H	0.847917000	0.982577000	3.563747000
H	2.165082000	2.814196000	2.513676000
H	1.280159000	3.944803000	0.467198000
H	-0.905953000	3.267741000	-0.516583000
H	0.809363000	-1.353757000	-2.518221000
H	-0.564814000	-0.353879000	-3.059044000

H	-0.752474000	-2.108514000	-2.972294000
C	5.358350000	0.655513000	0.613042000
H	6.435506000	0.734021000	0.399221000
H	4.919557000	1.663621000	0.642278000
H	5.216335000	0.181882000	1.595597000
C	4.941700000	0.482199000	-2.255462000
H	4.532049000	-0.099792000	-3.094045000
H	4.497149000	1.488021000	-2.277386000
H	6.033857000	0.562938000	-2.368049000
C	5.446034000	-1.922522000	-0.714689000
H	6.517528000	-1.735576000	-0.886054000
H	5.316551000	-2.450067000	0.241637000
H	5.053829000	-2.559031000	-1.521404000

2M: E= -1382.565914

C	5.322579000	0.107485000	-0.111614000
N	5.034573000	-1.218741000	-0.191859000
C	5.871139000	-2.388822000	-0.082141000
C	1.135724000	-1.435390000	0.464777000
C	2.655019000	-1.635354000	0.506333000
C	0.388665000	-0.629674000	-0.330674000
C	0.985112000	0.232404000	-1.430116000
C	1.247917000	1.722167000	-0.967481000
C	2.067575000	1.865995000	0.272782000
O	3.216081000	1.258802000	0.444620000
C	3.882724000	0.476549000	-0.543987000
C	3.606111000	-1.062414000	-0.540488000
C	-0.009002000	2.518742000	-0.956019000
C	-0.366290000	3.331732000	0.075350000
C	0.472702000	3.403729000	1.225295000
C	1.652951000	2.688358000	1.330846000
C	0.501972000	-2.280882000	1.553056000
O	6.321759000	0.730237000	0.161041000
Au	-1.685384000	-0.440567000	-0.141902000
P	-4.052904000	-0.259947000	0.052323000
H	5.858325000	-2.970385000	-1.018743000
H	5.546957000	-3.041126000	0.744457000
H	6.899164000	-2.055014000	0.116054000
H	2.835632000	-2.725717000	0.517776000
H	3.003238000	-1.289211000	1.497350000
H	0.285681000	0.323990000	-2.272832000
H	1.900351000	-0.176431000	-1.869337000
H	1.860224000	2.166031000	-1.786673000
H	3.828074000	0.965343000	-1.526960000
H	3.390959000	-1.458489000	-1.546434000
H	-0.630395000	2.446795000	-1.851671000
H	-1.285638000	3.917460000	0.038341000
H	0.177900000	4.051292000	2.055336000
H	2.287232000	2.758120000	2.215131000
H	-0.585720000	-2.135222000	1.604525000
H	0.930443000	-2.039796000	2.542690000
H	0.699959000	-3.354534000	1.383241000
C	-4.864670000	0.723200000	-1.271181000
H	-5.953949000	0.765334000	-1.115841000
H	-4.458191000	1.745374000	-1.269426000
H	-4.654278000	0.264760000	-2.248720000
C	-4.628678000	0.525720000	1.610643000
H	-4.259145000	-0.052757000	2.470083000
H	-4.223576000	1.546314000	1.676530000
H	-5.728446000	0.567016000	1.645531000
C	-4.927785000	-1.875322000	0.013046000
H	-6.015257000	-1.734119000	0.112139000
H	-4.711668000	-2.384412000	-0.937757000
H	-4.566305000	-2.507125000	0.837755000

3M: E= -3208.797590

C	-2.534858000	3.582166000	0.045070000
N	-1.890723000	4.012701000	-1.072995000
C	-2.175548000	5.091370000	-1.985833000
C	1.721245000	2.432144000	-0.768519000
C	0.540713000	3.390330000	-0.954653000
C	1.723707000	1.089328000	-0.573267000
C	0.459815000	0.245641000	-0.561603000
C	-0.080755000	-0.038706000	0.894360000
C	-0.300430000	1.150495000	1.751639000
O	-0.932299000	2.227023000	1.340933000
C	-1.646231000	2.319588000	0.108058000
C	-0.898322000	2.916295000	-1.125652000
C	0.638706000	-1.143826000	1.562357000
C	1.034721000	-1.099098000	2.866692000
C	0.792893000	0.083434000	3.619566000
C	0.148753000	1.184571000	3.081511000
C	3.008471000	3.235583000	-0.775262000
O	-3.457912000	4.021053000	0.692886000
Au	3.470166000	-0.004210000	-0.221792000
P	5.452605000	-1.273261000	0.150647000
H	-2.405796000	4.706242000	-2.993430000
H	-1.328199000	5.791997000	-2.061035000
H	-3.050328000	5.637821000	-1.606095000
H	0.767543000	4.016343000	-1.837354000
H	0.558648000	4.098032000	-0.104510000
H	0.655942000	-0.751121000	-0.980294000
H	-0.355874000	0.639097000	-1.174429000
H	-2.187920000	1.388935000	-0.101458000
H	-1.030379000	2.297903000	-2.026913000
H	0.805748000	-2.040565000	0.961030000
H	1.535694000	-1.948011000	3.333972000
H	1.118068000	0.124433000	4.662583000
H	-0.039526000	2.082010000	3.671888000
H	3.889716000	2.601460000	-0.606044000
H	2.991300000	4.018612000	0.004690000
H	3.140721000	3.761792000	-1.738004000
N	-2.856269000	-1.056244000	-0.096012000
S	-3.330974000	-0.989158000	-1.645036000
S	-3.685117000	-1.788519000	1.095362000
O	-4.761187000	-1.186803000	-1.885001000
O	-2.647082000	0.151170000	-2.271106000
O	-4.606388000	-2.846186000	0.676956000
O	-2.741513000	-2.033523000	2.190278000
C	-2.493315000	-2.494734000	-2.394194000
C	-4.774878000	-0.398099000	1.735664000
F	-4.020047000	0.638500000	2.106560000
F	-5.459484000	-0.831295000	2.791304000
F	-5.625804000	0.003297000	0.797343000
F	-2.767394000	-2.548007000	-3.694913000
F	-2.930912000	-3.605475000	-1.809528000
F	-1.171107000	-2.416293000	-2.234610000
H	-1.112206000	-0.460200000	0.691187000
C	6.736750000	-1.061375000	-1.147723000
H	7.016621000	0.000257000	-1.214574000
H	7.631752000	-1.660091000	-0.916692000
H	6.328748000	-1.375977000	-2.119591000
C	6.332173000	-0.868584000	1.713325000
H	7.241825000	-1.479743000	1.821851000
H	6.607117000	0.196544000	1.711525000
H	5.664539000	-1.054347000	2.567531000
C	5.203564000	-3.092333000	0.236815000
H	4.754875000	-3.444309000	-0.703825000
H	6.160446000	-3.612020000	0.400748000
H	4.515897000	-3.329543000	1.061875000

TS2: E= -3208.798034

C	-2.619551000	3.733406000	-0.194965000

N	-1.793122000	4.280189000	-1.127281000
C	-1.914266000	5.468426000	-1.933753000
C	1.733022000	2.599395000	-0.516256000
C	0.584541000	3.599281000	-0.677904000
C	1.697193000	1.243476000	-0.479911000
C	0.415554000	0.427512000	-0.650717000
C	-0.211257000	0.046426000	0.716570000
C	-0.712803000	1.079231000	1.603297000
O	-1.267581000	2.223637000	1.193125000
C	-1.747005000	2.458934000	-0.119708000
C	-0.805564000	3.179918000	-1.139042000
C	0.408336000	-1.088597000	1.374673000
C	0.440867000	-1.240410000	2.740646000
C	-0.097079000	-0.218844000	3.551857000
C	-0.670534000	0.916006000	2.997031000
C	3.028294000	3.366559000	-0.324038000
O	-3.643835000	4.112847000	0.327478000
Au	3.400740000	0.082060000	-0.129458000
P	5.330335000	-1.266011000	0.242056000
H	-1.956597000	5.216399000	-3.006936000
H	-1.071553000	6.159244000	-1.768023000
H	-2.846101000	5.979088000	-1.652304000
H	0.926203000	4.371090000	-1.392001000
H	0.473199000	4.140304000	0.280762000
H	0.642552000	-0.524047000	-1.151345000
H	-0.318691000	0.904288000	-1.301765000
H	-2.244470000	1.570565000	-0.529193000
H	-0.773615000	2.679523000	-2.120834000
H	0.817169000	-1.867388000	0.726212000
H	0.878330000	-2.131281000	3.194046000
H	-0.075616000	-0.324572000	4.639530000
H	-1.094444000	1.704295000	3.620772000
H	3.878453000	2.697486000	-0.131312000
H	2.948437000	4.074635000	0.521261000
H	3.263732000	3.976433000	-1.215470000
N	-2.593315000	-1.136403000	-0.095723000
S	-2.952324000	-1.254172000	-1.702061000
S	-3.557094000	-1.767241000	1.093639000
O	-4.363027000	-1.510707000	-1.970472000
O	-2.249145000	-0.168362000	-2.386974000
O	-4.371092000	-2.895741000	0.656092000
O	-2.736044000	-1.850076000	2.298310000
C	-2.041752000	-2.819594000	-2.212294000
C	-4.750653000	-0.350852000	1.431643000
F	-4.058819000	0.738242000	1.764429000
F	-5.539034000	-0.695745000	2.442365000
F	-5.488132000	-0.089271000	0.362045000
F	-2.205120000	-2.998225000	-3.516918000
F	-2.524409000	-3.865353000	-1.556011000
F	-0.741672000	-2.697810000	-1.945278000
H	-1.345769000	-0.532472000	0.367646000
C	6.636773000	-1.086194000	-1.039323000
H	6.958064000	-0.035300000	-1.087592000
H	7.505741000	-1.722209000	-0.808738000
H	6.227382000	-1.370394000	-2.020016000
C	6.208073000	-0.919564000	1.819824000
H	7.091956000	-1.567330000	1.929610000
H	6.524471000	0.133867000	1.836398000
H	5.523848000	-1.090545000	2.663974000
C	5.011132000	-3.075824000	0.298446000
H	4.565602000	-3.397589000	-0.654471000
H	5.944155000	-3.634478000	0.471196000
H	4.300348000	-3.297573000	1.108142000

4M: E= -1382.185841

C	-2.363859000	3.186832000	-0.947248000
C	-2.226286000	1.953519000	-0.297601000

C	-1.171678000	1.721275000	0.611371000
C	-0.287128000	2.788413000	0.847481000
C	-0.415830000	4.022992000	0.204938000
C	-1.457747000	4.220593000	-0.705740000
C	-0.925426000	0.372365000	1.270168000
Au	1.766270000	-0.452828000	0.108383000
P	4.123505000	-0.165114000	-0.103848000
O	-3.151707000	0.990077000	-0.638393000
C	-3.841215000	0.304575000	0.370247000
C	-3.496809000	-1.207121000	0.608570000
C	-2.521911000	-1.860963000	-0.364869000
C	-1.011046000	-1.615382000	-0.330634000
C	-0.337396000	-2.606090000	-1.263880000
C	-5.244211000	-0.202997000	-0.042134000
O	-6.266253000	0.299585000	-0.459109000
N	-4.911751000	-1.482943000	0.283640000
C	-5.696878000	-2.688996000	0.341752000
H	-5.700485000	-3.112862000	1.360521000
H	-5.320068000	-3.456772000	-0.354337000
H	-6.729457000	-2.438354000	0.059143000
H	-2.675460000	-2.952797000	-0.276188000
H	-2.867453000	-1.614933000	-1.386753000
H	-0.234042000	0.546778000	2.108047000
H	-1.844875000	0.002283000	1.738834000
H	-3.884584000	0.892873000	1.301578000
H	-3.263012000	-1.461226000	1.656348000
H	0.533101000	2.632913000	1.554312000
H	0.296311000	4.825031000	0.414454000
H	-1.574519000	5.178623000	-1.218673000
H	-3.199457000	3.310960000	-1.639507000
H	0.745474000	-2.432690000	-1.335968000
H	-0.764077000	-2.546327000	-2.282339000
H	-0.498440000	-3.646279000	-0.924708000
C	-0.301740000	-0.664723000	0.328186000
C	4.629931000	1.184456000	-1.246103000
H	4.204579000	2.136619000	-0.896112000
H	5.726834000	1.270782000	-1.293985000
H	4.235836000	0.977534000	-2.252021000
C	5.022578000	-1.639664000	-0.735882000
H	4.632206000	-1.906728000	-1.729122000
H	6.103329000	-1.442086000	-0.810450000
H	4.853644000	-2.488088000	-0.056401000
C	4.993102000	0.241609000	1.465304000
H	4.824683000	-0.562902000	2.196430000
H	6.074914000	0.360410000	1.296863000
H	4.584340000	1.176491000	1.876445000

5M: E= -3208.833584

C	3.295667000	-4.154640000	0.971041000
C	2.932371000	-2.814028000	0.795269000
C	1.757663000	-2.293281000	1.377843000
C	0.987603000	-3.171278000	2.159703000
C	1.343450000	-4.510402000	2.345400000
C	2.500679000	-5.007613000	1.738966000
C	1.282046000	-0.871116000	1.129554000
Au	-1.131772000	-1.572671000	-0.601017000
P	-3.243331000	-2.617724000	-0.925796000
O	3.762442000	-2.055814000	-0.003310000
C	4.282409000	-0.859779000	0.510969000
C	3.780093000	0.498249000	-0.088930000
C	2.876554000	0.435541000	-1.317634000
C	1.430569000	-0.065449000	-1.289992000
C	0.827445000	0.111710000	-2.672703000
C	5.670616000	-0.456766000	-0.041107000
O	6.771532000	-0.963553000	-0.090559000
N	5.194260000	0.756426000	-0.436425000
C	5.859894000	1.917240000	-0.969144000

H	5.715357000	2.794406000	-0.315587000
H	5.495504000	2.170323000	-1.978802000
H	6.935135000	1.696117000	-1.032205000
H	2.861909000	1.451605000	-1.752904000
H	3.397884000	-0.182938000	-2.072070000
H	0.474459000	-0.668329000	1.849523000
H	2.069170000	-0.149624000	1.377760000
H	4.281742000	-0.863853000	1.613490000
H	3.401394000	1.216090000	0.654348000
H	0.076284000	-2.786180000	2.626213000
H	0.716491000	-5.162092000	2.959003000
H	2.792814000	-6.052380000	1.871683000
H	4.215387000	-4.504229000	0.497000000
H	-0.207106000	-0.255268000	-2.720890000
H	1.419928000	-0.429192000	-3.432525000
H	0.834405000	1.174411000	-2.974074000
C	0.731189000	-0.660198000	-0.285214000
N	-0.776785000	2.177649000	0.202573000
S	-2.461708000	2.298215000	0.127441000
S	0.271227000	3.359072000	0.803999000
O	-2.919867000	1.326879000	-0.852371000
O	-2.836095000	3.699616000	0.085980000
O	1.518406000	2.684279000	1.126008000
O	-0.437468000	4.211201000	1.740223000
C	0.623076000	4.399730000	-0.731321000
C	-2.986866000	1.643236000	1.821344000
F	-2.388243000	0.483699000	2.061730000
F	-4.299883000	1.470366000	1.793745000
F	-2.662524000	2.516436000	2.756837000
F	1.510760000	5.321480000	-0.394768000
F	-0.488243000	4.972519000	-1.156192000
F	1.121575000	3.622578000	-1.685236000
H	-0.330888000	1.274970000	-0.098465000
C	-3.377452000	-4.347467000	-0.319234000
H	-3.162779000	-4.372659000	0.759312000
H	-4.386003000	-4.750922000	-0.499693000
H	-2.636081000	-4.974467000	-0.836134000
C	-3.765404000	-2.718967000	-2.685400000
H	-3.030477000	-3.310359000	-3.251145000
H	-4.758089000	-3.186955000	-2.776030000
H	-3.800139000	-1.705625000	-3.111931000
C	-4.632959000	-1.742427000	-0.100340000
H	-4.652927000	-0.698926000	-0.446273000
H	-5.595767000	-2.228277000	-0.322700000
H	-4.466710000	-1.742211000	0.987043000

TS3: E= -3208.828771

C	2.811275000	-4.022970000	1.152504000
C	2.621744000	-2.652859000	0.936572000
C	1.521911000	-1.969718000	1.495618000
C	0.645028000	-2.718491000	2.300292000
C	0.827666000	-4.085638000	2.527139000
C	1.912870000	-4.744014000	1.940937000
C	1.231273000	-0.504418000	1.215515000
Au	-1.029292000	-1.397472000	-0.680306000
P	-2.917081000	-2.724573000	-1.113610000
O	3.542853000	-2.028299000	0.121505000
C	4.207011000	-0.892910000	0.607001000
C	3.885086000	0.490890000	-0.051368000
C	2.996470000	0.481677000	-1.291860000
C	1.504630000	0.191810000	-1.247845000
C	0.890996000	0.426347000	-2.611494000
C	5.641817000	-0.684876000	0.063801000
O	6.672015000	-1.323389000	0.051951000
N	5.321703000	0.561888000	-0.385003000
C	6.129958000	1.616668000	-0.941969000
H	6.083627000	2.525002000	-0.317579000

H	5.811876000	1.878773000	-1.964751000
H	7.171105000	1.265533000	-0.979983000
H	3.110993000	1.466763000	-1.778409000
H	3.425009000	-0.237958000	-2.014183000
H	0.442121000	-0.194293000	1.916656000
H	2.091234000	0.125340000	1.468134000
H	4.190743000	-0.857438000	1.708391000
H	3.579073000	1.281055000	0.651523000
H	-0.209986000	-2.206791000	2.751244000
H	0.123737000	-4.633305000	3.158512000
H	2.069728000	-5.812818000	2.106589000
H	3.680127000	-4.500595000	0.694698000
H	-0.206682000	0.387361000	-2.581565000
H	1.236556000	-0.349475000	-3.317055000
H	1.205132000	1.395802000	-3.030353000
C	0.717605000	-0.228898000	-0.205570000
N	-0.799572000	2.014693000	0.227797000
S	-2.462441000	2.104184000	0.226246000
S	0.165221000	3.270235000	0.744453000
O	-2.956670000	1.119325000	-0.731269000
O	-2.946047000	3.478589000	0.205246000
O	1.486052000	2.714083000	1.020746000
O	-0.504546000	4.139322000	1.702312000
C	0.396355000	4.292825000	-0.822868000
C	-2.919442000	1.425587000	1.925853000
F	-2.373712000	0.223880000	2.105686000
F	-4.241257000	1.317498000	1.983554000
F	-2.495291000	2.243855000	2.875764000
F	1.038646000	5.407039000	-0.498606000
F	-0.771765000	4.593748000	-1.368685000
F	1.125636000	3.602181000	-1.696897000
H	-0.205255000	0.920288000	-0.094532000
C	-2.752752000	-4.505003000	-0.699489000
H	-2.506616000	-4.610575000	0.367191000
H	-3.689480000	-5.042729000	-0.914085000
H	-1.935693000	-4.943491000	-1.290938000
C	-3.458446000	-2.707619000	-2.867487000
H	-2.655035000	-3.107799000	-3.503052000
H	-4.366845000	-3.315743000	-2.999916000
H	-3.665079000	-1.671582000	-3.173296000
C	-4.388644000	-2.159008000	-0.173062000
H	-4.570154000	-1.098847000	-0.401745000
H	-5.275832000	-2.757005000	-0.432956000
H	-4.187566000	-2.250486000	0.904483000

6M: E= -1382.636496

C	0.216057000	3.029137000	0.918350000
C	0.757569000	2.037253000	0.094859000
C	0.520696000	2.032755000	-1.295021000
C	-0.266712000	3.068823000	-1.823000000
C	-0.813469000	4.063989000	-1.008225000
C	-0.573907000	4.041732000	0.369010000
C	1.082610000	0.954360000	-2.206575000
Au	-1.072033000	-0.687110000	-0.355331000
P	-2.860979000	-0.550554000	1.127236000
O	1.469831000	1.028599000	0.715114000
C	2.805132000	0.808899000	0.343594000
C	3.173437000	-0.547519000	-0.354310000
C	2.100626000	-1.636420000	-0.440233000
C	0.958658000	-1.563549000	-1.447281000
C	0.456784000	-2.936676000	-1.849728000
C	3.741796000	0.338268000	1.482194000
O	4.075291000	0.762030000	2.565152000
N	4.104396000	-0.765713000	0.765766000
C	5.122907000	-1.761545000	0.992115000
H	5.863227000	-1.763976000	0.174623000

H	4.693744000	-2.772913000	1.082288000
H	5.634722000	-1.515118000	1.933159000
H	2.627387000	-2.583945000	-0.643152000
H	1.655827000	-1.773499000	0.560652000
H	0.916509000	1.280066000	-3.242948000
H	2.171763000	0.894865000	-2.095856000
H	3.226729000	1.683345000	-0.177313000
H	3.699437000	-0.433770000	-1.317675000
H	-0.455820000	3.087887000	-2.899820000
H	-1.423265000	4.855335000	-1.449922000
H	-0.991000000	4.817133000	1.015995000
H	0.433098000	2.989843000	1.987704000
H	-0.461319000	-2.895278000	-2.451398000
H	0.286637000	-3.581507000	-0.974261000
H	1.242273000	-3.422313000	-2.455380000
C	0.478633000	-0.446416000	-2.106512000
H	-0.264340000	-0.656375000	-2.885939000
C	-2.345604000	-0.676510000	2.877631000
H	-1.642129000	0.135370000	3.110945000
H	-3.224550000	-0.601091000	3.536125000
H	-1.844767000	-1.640860000	3.044209000
C	-4.103922000	-1.868108000	0.871927000
H	-3.631824000	-2.850049000	1.018832000
H	-4.932160000	-1.749122000	1.587314000
H	-4.494346000	-1.810844000	-0.154248000
C	-3.766583000	1.032045000	0.982391000
H	-4.163127000	1.135901000	-0.037758000
H	-4.598058000	1.056192000	1.703477000
H	-3.079324000	1.866559000	1.183322000

7M: E= -786.142182

C	-2.396005000	-1.579316000	-0.946191000
C	-1.518258000	-0.708502000	-0.289880000
C	-1.998778000	0.261591000	0.615968000
C	-3.385000000	0.303489000	0.839513000
C	-4.268568000	-0.562831000	0.189811000
C	-3.770623000	-1.505708000	-0.713890000
C	-1.084736000	1.277226000	1.287670000
O	-0.185187000	-0.826379000	-0.621287000
C	0.769840000	-0.976537000	0.393217000
C	1.788529000	0.193332000	0.632636000
C	1.755410000	1.355333000	-0.355736000
C	0.625493000	2.369002000	-0.339454000
C	0.898275000	3.529917000	-1.270670000
C	2.011307000	-1.814790000	0.001158000
O	2.211040000	-2.937482000	-0.409113000
N	2.846356000	-0.791205000	0.337210000
C	4.283044000	-0.712746000	0.410444000
H	4.617411000	-0.467647000	1.432893000
H	4.686288000	0.045731000	-0.280922000
H	4.692900000	-1.693503000	0.129567000
H	2.704515000	1.911087000	-0.243299000
H	1.795762000	0.930693000	-1.376017000
H	-1.677598000	1.799220000	2.054317000
H	-0.280301000	0.775233000	1.837179000
H	0.315429000	-1.352501000	1.324247000
H	1.834915000	0.549840000	1.675879000
H	-3.777355000	1.047340000	1.539015000
H	-5.341251000	-0.497621000	0.387224000
H	-4.447261000	-2.190315000	-1.231379000
H	-1.972173000	-2.311808000	-1.636427000
H	0.056901000	4.236777000	-1.305336000
H	1.091827000	3.174418000	-2.298378000
H	1.801741000	4.084046000	-0.959629000
C	-0.541506000	2.315969000	0.328790000
H	-1.243608000	3.135752000	0.133476000

Profile in Figure 1S (supplementary material)

1M-Au': E= -1957.230070

C	1.935938000	2.582728000	0.030457000
C	3.158169000	1.907410000	-0.113105000
C	4.331540000	2.625779000	-0.380874000
C	4.264774000	4.017557000	-0.522544000
C	3.051310000	4.696709000	-0.390698000
C	1.888003000	3.970362000	-0.105487000
C	1.604723000	-1.531316000	-2.982517000
C	1.433508000	-1.940049000	-1.741454000
Au	-0.240583000	-1.053294000	-0.515724000
P	-2.168765000	0.109866000	0.167130000
C	-3.523721000	-1.042170000	0.606719000
O	3.116116000	0.543851000	0.034414000
C	4.207350000	-0.232738000	-0.385877000
C	3.991163000	-1.769339000	-0.193570000
C	2.680386000	-2.256459000	0.431618000
C	1.604470000	-2.635400000	-0.587250000
C	0.929884000	-3.976324000	-0.375241000
C	5.388948000	-0.404934000	0.608975000
O	6.243813000	0.312258000	1.081487000
N	5.137327000	-1.738716000	0.727501000
C	5.891644000	-2.798093000	1.352091000
C	-2.801228000	1.191339000	-1.170532000
C	-1.879032000	1.177100000	1.627023000
H	6.285333000	-3.502756000	0.600028000
H	5.279383000	-3.359819000	2.075902000
H	6.736094000	-2.342595000	1.888054000
H	2.893172000	-3.162503000	1.019487000
H	2.307982000	-1.506278000	1.144215000
H	1.013540000	-0.730009000	-3.432283000
H	2.368598000	-2.009424000	-3.607444000
H	5.295266000	2.119226000	-0.434554000
H	4.533411000	0.045908000	-1.402322000
H	4.214343000	-2.346356000	-1.107854000
H	5.183441000	4.572964000	-0.728357000
H	3.011508000	5.782859000	-0.499423000
H	0.931937000	4.487238000	0.010281000
H	1.036798000	2.005889000	0.255037000
H	0.127551000	-4.162776000	-1.100030000
H	0.530325000	-4.065821000	0.646377000
H	1.700523000	-4.758218000	-0.493451000
C	-4.372814000	-0.794625000	1.697776000
C	-5.413109000	-1.683157000	1.988013000
C	-5.612685000	-2.816771000	1.194854000
C	-4.767990000	-3.067286000	0.107260000
C	-3.724105000	-2.187445000	-0.185075000
H	-4.226273000	0.086618000	2.324954000
H	-6.068552000	-1.486100000	2.839520000
H	-6.425314000	-3.509557000	1.426167000
H	-4.918241000	-3.954273000	-0.512497000
H	-3.063218000	-2.393639000	-1.031384000
C	-2.428359000	2.466698000	1.716620000
C	-2.202482000	3.243542000	2.857527000
C	-1.432659000	2.740925000	3.910476000
C	-0.882812000	1.456681000	3.824348000
C	-1.100141000	0.677791000	2.686450000
H	-3.030863000	2.869830000	0.900471000
H	-2.630777000	4.246576000	2.920195000
H	-1.256017000	3.352231000	4.798634000
H	-0.276571000	1.062469000	4.643094000
H	-0.660209000	-0.320954000	2.623309000
C	-4.175321000	1.294846000	-1.441414000
C	-4.624918000	2.144603000	-2.457266000
C	-3.711370000	2.893867000	-3.204106000
C	-2.341129000	2.793567000	-2.937077000

C	-1.884842000	1.943455000	-1.927900000
H	-4.898185000	0.713909000	-0.865706000
H	-5.695076000	2.218028000	-2.664239000
H	-4.066192000	3.554708000	-3.998572000
H	-1.623241000	3.374880000	-3.520240000
H	-0.812215000	1.869022000	-1.731119000

TS1': E= -1957.185058

C	-2.636309000	-2.324131000	1.373141000
C	-3.420831000	-1.806145000	0.333565000
C	-3.029471000	-1.995669000	-1.035407000
C	-1.903617000	-2.854546000	-1.289631000
C	-1.139060000	-3.358398000	-0.263375000
C	-1.513091000	-3.083937000	1.074462000
C	-2.456925000	-0.138874000	-1.677994000
C	-1.875300000	0.681102000	-0.644119000
Au	0.178354000	0.436746000	-0.320638000
P	2.517929000	0.146708000	0.030556000
C	3.371495000	1.728107000	0.421944000
O	-4.467122000	-1.060717000	0.703013000
C	-5.372316000	-0.531364000	-0.238095000
C	-5.183075000	0.959656000	-0.686114000
C	-4.151052000	1.818258000	0.047860000
C	-2.647172000	1.577566000	0.068055000
C	-2.001561000	2.515446000	1.057693000
C	-6.722568000	-0.061658000	0.352693000
O	-7.611818000	-0.577205000	0.987522000
N	-6.551928000	1.180334000	-0.181211000
C	-7.437336000	2.315923000	-0.272027000
C	3.400842000	-0.546900000	-1.426790000
C	2.906134000	-0.990024000	1.422778000
H	-7.606041000	2.599415000	-1.323920000
H	-7.037589000	3.188198000	0.270166000
H	-8.398651000	2.033474000	0.179459000
H	-4.288321000	2.854972000	-0.313371000
H	-4.462937000	1.861607000	1.106146000
H	-1.780178000	-0.547389000	-2.429171000
H	-3.419935000	0.140213000	-2.112435000
H	-3.806759000	-1.987479000	-1.802306000
H	-5.531604000	-1.220004000	-1.080142000
H	-5.127385000	1.085075000	-1.779725000
H	-1.655375000	-3.080185000	-2.329406000
H	-0.266333000	-3.979587000	-0.470474000
H	-0.911160000	-3.485461000	1.893282000
H	-2.934662000	-2.124134000	2.403265000
H	-0.907875000	2.519105000	0.970781000
H	-2.263664000	2.208301000	2.086957000
H	-2.378162000	3.544842000	0.937376000
C	4.354356000	1.829730000	1.419828000
C	4.975342000	3.057786000	1.671957000
C	4.624203000	4.190033000	0.931199000
C	3.643934000	4.095824000	-0.063269000
C	3.015655000	2.873872000	-0.313410000
H	4.638967000	0.953658000	2.005774000
H	5.737297000	3.126791000	2.452132000
H	5.110756000	5.147856000	1.131114000
H	3.361954000	4.978628000	-0.642155000
H	2.243258000	2.811533000	-1.084769000
C	4.032889000	-1.829015000	1.413601000
C	4.297160000	-2.662900000	2.504788000
C	3.442775000	-2.665703000	3.611806000
C	2.317870000	-1.833635000	3.626571000
C	2.046752000	-1.003552000	2.535812000
H	4.707157000	-1.837064000	0.554730000
H	5.175242000	-3.313024000	2.487669000
H	3.651309000	-3.319239000	4.462412000
H	1.645148000	-1.834457000	4.487622000

H	1.159832000	-0.364549000	2.547182000
C	4.636488000	-0.047005000	-1.868413000
C	5.269229000	-0.616354000	-2.978922000
C	4.677659000	-1.687810000	-3.653695000
C	3.445580000	-2.190038000	-3.219030000
C	2.806574000	-1.620017000	-2.115904000
H	5.109885000	0.788794000	-1.349637000
H	6.229571000	-0.218259000	-3.315458000
H	5.173875000	-2.130072000	-4.521027000
H	2.977188000	-3.025140000	-3.745550000
H	1.839752000	-2.012710000	-1.789614000

2M′ : E= -1957.193583

C	-3.273198000	2.666099000	-1.290297000
C	-3.652118000	1.818366000	-0.239116000
C	-2.819026000	1.688742000	0.994317000
C	-1.588926000	2.526469000	0.982262000
C	-1.266916000	3.362364000	-0.042099000
C	-2.116809000	3.419456000	-1.184834000
C	-2.502899000	0.204875000	1.439963000
C	-1.884734000	-0.627275000	0.329910000
Au	0.182927000	-0.389597000	0.151063000
P	2.563389000	-0.145777000	0.013363000
C	3.287958000	-0.914720000	-1.493576000
O	-4.779687000	1.173275000	-0.411862000
C	-5.414201000	0.358656000	0.571182000
C	-5.081892000	-1.169271000	0.555106000
C	-4.119740000	-1.698496000	-0.505070000
C	-2.607876000	-1.447566000	-0.472362000
C	-1.953182000	-2.259880000	-1.572910000
C	-6.841980000	-0.059529000	0.143753000
O	-7.864576000	0.527895000	-0.120011000
N	-6.506296000	-1.375082000	0.216557000
C	-7.303565000	-2.573170000	0.116140000
C	3.454679000	-0.915659000	1.427433000
C	3.119116000	1.609129000	-0.025065000
H	-7.272839000	-3.146255000	1.057647000
H	-6.957412000	-3.221399000	-0.704631000
H	-8.341785000	-2.274790000	-0.085485000
H	-4.262371000	-2.794187000	-0.526806000
H	-4.487250000	-1.354380000	-1.489717000
H	-1.803297000	0.311022000	2.280634000
H	-3.401010000	-0.241011000	1.878042000
H	-3.439162000	2.104080000	1.822594000
H	-5.375170000	0.841203000	1.557897000
H	-4.843485000	-1.564725000	1.555940000
H	-0.956916000	2.464136000	1.871129000
H	-0.364209000	3.973164000	-0.006548000
H	-1.849982000	4.085340000	-2.009841000
H	-3.915841000	2.723910000	-2.169408000
H	-0.874738000	-2.063352000	-1.642288000
H	-2.408892000	-2.036810000	-2.554340000
H	-2.098307000	-3.341897000	-1.402694000
C	4.332006000	-0.316849000	-2.218274000
C	4.855494000	-0.950550000	-3.350218000
C	4.344708000	-2.183687000	-3.766103000
C	3.304573000	-2.784867000	-3.048407000
C	2.774695000	-2.152923000	-1.920993000
H	4.739651000	0.645910000	-1.903800000
H	5.666874000	-0.476333000	-3.907788000
H	4.754400000	-2.675598000	-4.651726000
H	2.898977000	-3.746900000	-3.370837000
H	1.956938000	-2.626069000	-1.370854000
C	4.149834000	2.096006000	0.794117000
C	4.525537000	3.442534000	0.727741000
C	3.881243000	4.310646000	-0.157659000

C	2.852817000	3.831379000	-0.978171000
C	2.468089000	2.490681000	-0.907825000
H	4.663682000	1.427986000	1.487673000
H	5.327899000	3.811066000	1.371485000
H	4.178011000	5.361071000	-0.208734000
H	2.346861000	4.505522000	-1.673729000
H	1.657250000	2.126476000	-1.544512000
C	4.716229000	-1.516383000	1.279776000
C	5.359932000	-2.081445000	2.385046000
C	4.753446000	-2.050564000	3.644761000
C	3.496880000	-1.455161000	3.798862000
C	2.847403000	-0.895087000	2.695709000
H	5.199953000	-1.548566000	0.301538000
H	6.339459000	-2.549044000	2.258946000
H	5.257958000	-2.495190000	4.506135000
H	3.015817000	-1.433477000	4.779681000
H	1.859591000	-0.443779000	2.820500000

Profile in Figure 2S (supplementary material)

1M-B: E= -1382.606165

C	-5.362186000	-0.271767000	0.080812000
N	-4.985126000	-1.569229000	0.271910000
C	-5.737369000	-2.798643000	0.235122000
C	-1.113061000	-1.551429000	-0.009960000
C	-2.568798000	-1.816349000	-0.377316000
C	-0.392884000	-0.846241000	-0.856284000
C	0.128749000	-0.109928000	-1.855993000
C	-1.789135000	2.005536000	1.268349000
C	-2.403020000	1.983505000	0.008092000
O	-3.324018000	1.050143000	-0.386974000
C	-3.976711000	0.238553000	0.546335000
C	-3.589613000	-1.284692000	0.636023000
C	-0.855791000	3.008700000	1.561781000
C	-0.521163000	3.978136000	0.613235000
C	-1.133091000	3.942221000	-0.646975000
C	-2.069666000	2.954087000	-0.950703000
C	-0.585492000	-2.140219000	1.274648000
O	-6.399590000	0.237697000	-0.276509000
Au	1.934198000	-0.339887000	-0.496705000
P	4.056305000	-0.293188000	0.493538000
H	-5.737696000	-3.294250000	1.220657000
H	-5.333965000	-3.501251000	-0.512287000
H	-6.773290000	-2.554092000	-0.039255000
H	-2.694615000	-2.911910000	-0.442263000
H	-2.796390000	-1.401519000	-1.369068000
H	0.472371000	-0.585424000	-2.783933000
H	-0.010142000	0.979329000	-1.873060000
H	-2.020690000	1.252035000	2.022313000
H	-4.044503000	0.718072000	1.535235000
H	-3.349174000	-1.620437000	1.658748000
H	-0.386810000	3.023518000	2.549084000
H	0.205758000	4.757458000	0.852610000
H	-0.886307000	4.696434000	-1.398564000
H	-2.566131000	2.919484000	-1.922684000
H	0.495683000	-1.983172000	1.383284000
H	-0.791228000	-3.222556000	1.304747000
H	-1.086691000	-1.687638000	2.145296000
C	4.028065000	0.210007000	2.251888000
H	5.051909000	0.213180000	2.656180000
H	3.594725000	1.216446000	2.340478000
H	3.410981000	-0.496185000	2.825539000
C	5.181752000	0.879236000	-0.346903000
H	5.287986000	0.593723000	-1.403350000
H	4.762443000	1.894094000	-0.292722000
H	6.170022000	0.863994000	0.137731000
C	4.901741000	-1.914882000	0.453526000

H	5.897331000	-1.829997000	0.915671000
H	4.304226000	-2.654808000	1.005059000
H	5.008779000	-2.248756000	-0.588418000

1M-C: E= -1382.605160

C	2.930518000	2.296498000	-0.480981000
N	1.665780000	2.336074000	-0.986124000
C	0.950113000	3.379222000	-1.678749000
C	0.021922000	-1.189651000	-0.839177000
C	0.760041000	0.014967000	-1.408632000
C	-0.986721000	-1.756377000	-1.551926000
C	-1.600063000	-2.497261000	-2.452450000
C	5.399663000	0.492814000	0.923343000
C	4.592613000	-0.462332000	0.290859000
O	3.346821000	-0.187089000	-0.216724000
C	2.645338000	0.943545000	0.228380000
C	1.211788000	1.070022000	-0.392833000
C	6.658290000	0.112384000	1.405572000
C	7.119197000	-1.197839000	1.255563000
C	6.308895000	-2.140047000	0.609131000
C	5.049017000	-1.779747000	0.130541000
C	0.622050000	-1.895137000	0.357289000
O	3.863418000	3.066701000	-0.549122000
Au	-2.215452000	-0.503835000	-0.143880000
P	-3.968944000	0.530596000	1.023545000
H	0.122363000	3.771538000	-1.063701000
H	0.540312000	3.022003000	-2.637145000
H	1.656112000	4.196158000	-1.883645000
H	0.135932000	0.497729000	-2.173576000
H	1.648767000	-0.386045000	-1.926002000
H	-1.005617000	-3.125491000	-3.126986000
H	-2.686784000	-2.522327000	-2.563957000
H	5.075033000	1.531090000	1.000332000
H	2.663992000	1.021723000	1.329129000
H	0.429472000	1.234667000	0.369920000
H	7.286580000	0.860971000	1.895129000
H	8.104132000	-1.483079000	1.632032000
H	6.658096000	-3.167679000	0.479532000
H	4.407304000	-2.506154000	-0.372553000
H	0.027908000	-2.766873000	0.658613000
H	0.731672000	-1.219717000	1.218956000
H	1.636011000	-2.224756000	0.078240000
C	-5.025190000	1.556949000	-0.060509000
H	-5.833502000	2.019310000	0.526482000
H	-4.415279000	2.343180000	-0.528209000
H	-5.460921000	0.927413000	-0.849450000
C	-3.373165000	1.643125000	2.348283000
H	-2.776748000	1.068415000	3.071081000
H	-2.743278000	2.430901000	1.911178000
H	-4.229343000	2.104435000	2.864153000
C	-5.088025000	-0.665118000	1.837707000
H	-5.890381000	-0.127529000	2.366144000
H	-5.528944000	-1.330744000	1.081929000
H	-4.518056000	-1.270615000	2.556865000

TS1-B: E= -1382.549912

C	5.367884000	-0.396632000	0.100815000
N	4.945580000	-1.678853000	-0.096135000
C	5.652103000	-2.936447000	-0.071184000
C	1.106552000	-1.591448000	0.712028000
C	2.611871000	-1.792751000	0.788472000
C	0.396713000	-0.461040000	0.541241000
C	-0.845748000	0.036914000	1.030805000
C	1.307871000	0.911132000	-0.642452000
C	2.146032000	1.458814000	0.390798000
O	3.358125000	0.966986000	0.674891000

C	3.977441000	0.146681000	-0.298373000
C	3.532826000	-1.344663000	-0.350004000
C	0.257665000	1.750992000	-1.154416000
C	-0.124103000	2.877073000	-0.468291000
C	0.569983000	3.247279000	0.718597000
C	1.699190000	2.564755000	1.138974000
C	0.338926000	-2.854616000	1.073612000
O	6.429600000	0.086385000	0.415607000
Au	-2.534755000	-0.954897000	0.079415000
P	-4.434323000	-1.952198000	-0.869911000
H	5.567560000	-3.455833000	-1.039850000
H	5.272922000	-3.601695000	0.721576000
H	6.712029000	-2.725170000	0.127917000
H	2.781681000	-2.871851000	0.915959000
H	2.979682000	-1.319699000	1.716807000
H	-0.943934000	-0.077822000	2.121222000
H	-1.121945000	1.050988000	0.723738000
H	1.740455000	0.211257000	-1.353335000
H	3.991081000	0.649607000	-1.277820000
H	3.176092000	-1.692496000	-1.334348000
H	-0.257670000	1.444374000	-2.066813000
H	-0.947893000	3.497367000	-0.826440000
H	0.241790000	4.127006000	1.277444000
H	2.295405000	2.906288000	1.986625000
H	-0.746748000	-2.740469000	0.967926000
H	0.555938000	-3.130952000	2.120952000
H	0.677523000	-3.693036000	0.442038000
C	-5.020147000	-1.134494000	-2.403059000
H	-5.913926000	-1.646726000	-2.791747000
H	-5.265594000	-0.084550000	-2.187200000
H	-4.224424000	-1.161767000	-3.161537000
C	-5.887536000	-1.950557000	0.248018000
H	-5.640308000	-2.493350000	1.171871000
H	-6.148696000	-0.914297000	0.507494000
H	-6.748121000	-2.432846000	-0.241013000
C	-4.196772000	-3.710639000	-1.332390000
H	-5.122576000	-4.122636000	-1.762954000
H	-3.384589000	-3.789913000	-2.069524000
H	-3.920428000	-4.289835000	-0.439367000

TS1-C: E= -1382.557279

C	-2.297207000	3.195906000	-0.457027000
N	-1.580321000	3.017889000	0.689660000
C	-1.169321000	3.945051000	1.716350000
C	-1.554069000	-0.876871000	1.237794000
C	-1.796209000	0.618821000	1.454393000
C	-0.141930000	-1.350199000	1.329624000
C	0.125448000	-2.353013000	2.201924000
C	-1.913522000	-1.083061000	-0.798215000
C	-3.129740000	-0.357883000	-1.043300000
O	-3.193553000	0.973341000	-1.029263000
C	-2.005345000	1.742163000	-0.901389000
C	-1.227112000	1.611850000	0.442563000
C	-1.939656000	-2.507990000	-0.989731000
C	-3.116174000	-3.172588000	-1.235517000
C	-4.318941000	-2.429539000	-1.357119000
C	-4.334905000	-1.045096000	-1.263117000
C	-2.645000000	-1.700373000	1.887968000
O	-2.890111000	4.138213000	-0.924865000
Au	1.502780000	-0.529776000	0.319250000
P	3.447765000	0.291509000	-0.758702000
H	-0.070907000	4.036533000	1.749336000
H	-1.528905000	3.633214000	2.709994000
H	-1.601444000	4.927139000	1.478938000
H	-1.349824000	0.832458000	2.442826000
H	-2.875026000	0.806232000	1.557578000
H	-0.634340000	-2.858060000	2.809518000

H	1.151762000	-2.690347000	2.375027000
H	-0.967475000	-0.582693000	-1.015158000
H	-1.393834000	1.659497000	-1.813774000
H	-0.143042000	1.465126000	0.305195000
H	-0.999930000	-3.054109000	-0.882993000
H	-3.134488000	-4.258287000	-1.341732000
H	-5.257485000	-2.957763000	-1.543187000
H	-5.253813000	-0.471446000	-1.391718000
H	-2.525804000	-2.777846000	1.731416000
H	-3.643983000	-1.396228000	1.548681000
H	-2.607273000	-1.503334000	2.973491000
C	3.772091000	2.075151000	-0.468643000
H	4.698325000	2.389496000	-0.973948000
H	2.929742000	2.668213000	-0.853993000
H	3.866433000	2.259193000	0.611643000
C	3.443537000	0.117992000	-2.586424000
H	3.335067000	-0.943260000	-2.854159000
H	2.593788000	0.675263000	-3.007235000
H	4.380829000	0.507183000	-3.013289000
C	4.987682000	-0.550860000	-0.222234000
H	5.860403000	-0.136374000	-0.750026000
H	5.119517000	-0.417744000	0.861516000
H	4.909389000	-1.626831000	-0.436182000

2M-B: E= -1382.560856

C	-5.577142000	-0.464570000	0.607545000
N	-5.016602000	-1.707284000	0.603480000
C	-5.600093000	-3.026535000	0.573814000
C	-1.527912000	-0.971138000	-1.041720000
C	-2.898963000	-1.526122000	-0.705088000
C	-0.918721000	0.180955000	-0.628211000
C	0.306063000	0.712055000	-1.275070000
C	-1.492171000	1.035580000	0.602218000
C	-2.633680000	1.720950000	-0.064968000
O	-3.826625000	1.171552000	-0.148481000
C	-4.186262000	0.176644000	0.813273000
C	-3.613041000	-1.249720000	0.617904000
C	-0.466937000	1.972738000	1.148823000
C	-0.408669000	3.261976000	0.729522000
C	-1.360735000	3.740560000	-0.234185000
C	-2.450099000	2.993406000	-0.639761000
C	-0.819536000	-1.792504000	-2.102285000
O	-6.713215000	-0.062702000	0.531960000
Au	2.104730000	0.039391000	-0.339875000
P	4.143423000	-0.695910000	0.622360000
H	-5.294909000	-3.612461000	1.456112000
H	-5.309627000	-3.577093000	-0.335584000
H	-6.693154000	-2.914167000	0.581608000
H	-2.843888000	-2.622212000	-0.799309000
H	-3.584097000	-1.207662000	-1.516368000
H	0.355427000	0.419504000	-2.332596000
H	0.361504000	1.806763000	-1.238182000
H	-1.806188000	0.339843000	1.386356000
H	-4.063394000	0.585396000	1.827080000
H	-3.044885000	-1.633406000	1.481955000
H	0.248886000	1.574420000	1.870009000
H	0.357142000	3.943057000	1.104012000
H	-1.259070000	4.762545000	-0.608901000
H	-3.231283000	3.412352000	-1.275798000
H	0.248379000	-1.924148000	-1.864709000
H	-0.863744000	-1.297979000	-3.089177000
H	-1.275252000	-2.786090000	-2.212186000
C	5.182586000	0.655738000	1.305830000
H	6.119708000	0.255704000	1.723379000
H	5.417432000	1.374994000	0.507502000
H	4.626490000	1.180055000	2.096850000
C	5.246072000	-1.563741000	-0.562174000

H	4.728602000	-2.447341000	-0.963807000
H	5.487295000	-0.889653000	-1.397207000
H	6.177815000	-1.879586000	-0.067893000
C	3.956074000	-1.874944000	2.018434000
H	4.940964000	-2.186974000	2.399435000
H	3.387690000	-1.395714000	2.829067000
H	3.401057000	-2.761135000	1.677451000

2M-C: E= -1382.562262

C	-2.649493000	2.965422000	-0.643519000
N	-2.055248000	2.955072000	0.581555000
C	-1.946120000	3.967887000	1.603811000
C	-1.555876000	-0.904954000	1.156285000
C	-1.988367000	0.565495000	1.424427000
C	-0.074565000	-1.115596000	1.536758000
C	0.234072000	-1.791584000	2.660843000
C	-1.682920000	-1.246082000	-0.446148000
C	-2.900762000	-0.688237000	-1.085016000
O	-3.093876000	0.601140000	-1.215490000
C	-2.063529000	1.567698000	-0.966840000
C	-1.455003000	1.613595000	0.460288000
C	-1.509491000	-2.704629000	-0.643323000
C	-2.465491000	-3.486334000	-1.211494000
C	-3.685294000	-2.887157000	-1.655320000
C	-3.910236000	-1.523648000	-1.591729000
C	-2.539385000	-1.800146000	1.934710000
O	-3.334867000	3.767047000	-1.231551000
Au	1.511744000	-0.368567000	0.395995000
P	3.403422000	0.410954000	-0.819719000
H	-0.895175000	4.265316000	1.755076000
H	-2.355967000	3.614660000	2.563440000
H	-2.521006000	4.845221000	1.276465000
H	-1.663819000	0.810542000	2.447375000
H	-3.088741000	0.628691000	1.423651000
H	-0.508638000	-2.249803000	3.325099000
H	1.273739000	-1.909288000	2.982909000
H	-0.789256000	-0.735778000	-0.863657000
H	-1.349633000	1.546872000	-1.803955000
H	-0.353190000	1.640796000	0.456791000
H	-0.582434000	-3.135726000	-0.258459000
H	-2.323440000	-4.562205000	-1.321851000
H	-4.460190000	-3.526043000	-2.087499000
H	-4.819693000	-1.071491000	-1.989204000
H	-2.248107000	-2.858679000	1.913220000
H	-3.560503000	-1.712296000	1.533770000
H	-2.579284000	-1.483197000	2.987043000
C	3.726461000	2.212022000	-0.654817000
H	4.622515000	2.502052000	-1.224906000
H	2.859506000	2.776322000	-1.028888000
H	3.874922000	2.461415000	0.406176000
C	3.323665000	0.126354000	-2.632615000
H	3.207073000	-0.949739000	-2.828302000
H	2.454869000	0.655102000	-3.051236000
H	4.240419000	0.487789000	-3.123824000
C	4.978768000	-0.382318000	-0.308672000
H	5.820737000	0.008588000	-0.900532000
H	5.159674000	-0.184446000	0.758018000
H	4.904595000	-1.469904000	-0.454835000

3M-C: E= -3208.795330

C	3.554261000	-2.372149000	2.261484000
N	4.292391000	-1.471670000	1.553635000
C	5.635335000	-0.978255000	1.734653000
C	2.215690000	-1.271312000	-1.783086000
C	3.436162000	-1.447902000	-0.831088000
C	2.009484000	0.220074000	-2.123460000

C	2.224987000	0.655483000	-3.380787000
C	0.847307000	-1.785914000	-1.042516000
C	1.026887000	-3.078238000	-0.330731000
O	1.793682000	-3.190027000	0.725348000
C	2.297289000	-2.040257000	1.423997000
C	3.215780000	-1.075597000	0.627200000
C	-0.268171000	-1.785333000	-2.019629000
C	-0.918218000	-2.923484000	-2.384839000
C	-0.552523000	-4.162474000	-1.778927000
C	0.395670000	-4.251008000	-0.773887000
C	2.486698000	-2.162800000	-3.010591000
O	3.806904000	-3.104304000	3.189797000
Au	1.441876000	1.657462000	-0.712126000
P	0.857305000	3.434209000	0.761015000
H	6.086491000	-1.519610000	2.577984000
H	5.633864000	0.100715000	1.963022000
H	6.250617000	-1.147697000	0.836353000
H	4.256946000	-0.841529000	-1.245100000
H	3.776419000	-2.495782000	-0.864319000
H	2.506364000	0.005504000	-4.218388000
H	2.129316000	1.715980000	-3.635313000
H	1.460363000	-1.582459000	1.971159000
H	2.925741000	-0.017636000	0.737082000
H	-0.526656000	-0.820395000	-2.459901000
H	-1.721869000	-2.900893000	-3.121382000
H	-1.066543000	-5.075108000	-2.093342000
H	0.614106000	-5.193142000	-0.269789000
H	1.726067000	-2.042064000	-3.793080000
H	2.524875000	-3.226119000	-2.729008000
H	3.463676000	-1.908442000	-3.447423000
C	1.014328000	3.061848000	2.551893000
H	0.775766000	3.952771000	3.153773000
H	0.312974000	2.252032000	2.798528000
H	2.041788000	2.737604000	2.774067000
C	-0.852188000	4.073019000	0.572098000
H	-0.995319000	4.421195000	-0.461419000
H	-1.570209000	3.265624000	0.773654000
H	-1.029672000	4.909375000	1.266543000
C	1.918756000	4.915575000	0.510694000
H	1.633595000	5.722183000	1.204080000
H	2.972049000	4.646176000	0.678733000
H	1.811145000	5.272061000	-0.524416000
H	0.634943000	-0.999647000	-0.294035000
N	-2.124812000	-0.410961000	0.094890000
S	-2.933168000	0.704652000	-0.753428000
O	-2.163278000	1.100407000	-1.940683000
O	-3.614523000	1.744631000	0.028302000
S	-1.786983000	-0.329837000	1.659464000
O	-1.611857000	1.020483000	2.212204000
O	-0.760071000	-1.344387000	1.946020000
C	-4.314945000	-0.358662000	-1.451477000
F	-5.002199000	-0.932775000	-0.466599000
F	-5.134866000	0.414981000	-2.158646000
F	-3.824720000	-1.307905000	-2.247439000
C	-3.314532000	-0.997246000	2.526559000
F	-3.077502000	-1.069792000	3.834747000
F	-4.354855000	-0.194814000	2.317446000
F	-3.605907000	-2.212874000	2.071061000

TS2-C: E= -3208.774412

C	3.076136000	-2.867616000	2.122307000
N	3.872343000	-2.031988000	1.397806000
C	5.280503000	-1.736124000	1.477681000
C	1.615509000	-1.620820000	-1.805670000
C	2.849654000	-1.919790000	-0.900663000
C	1.597971000	-0.123130000	-2.181270000
C	1.696111000	0.255875000	-3.471924000

C	0.221305000	-2.092918000	-1.204421000
C	0.131196000	-3.111921000	-0.172535000
O	1.057039000	-3.345576000	0.768094000
C	1.816533000	-2.329096000	1.408647000
C	2.792301000	-1.489642000	0.549804000
C	-0.834281000	-2.130250000	-2.199349000
C	-1.913774000	-2.980410000	-2.128844000
C	-1.980038000	-3.909449000	-1.072110000
C	-0.983568000	-3.966357000	-0.109279000
C	1.848729000	-2.548816000	-3.033948000
O	3.304999000	-3.672949000	2.997593000
Au	1.544147000	1.428383000	-0.781374000
P	1.577904000	3.308637000	0.680285000
H	5.716003000	-2.358162000	2.272555000
H	5.451577000	-0.674373000	1.723297000
H	5.796201000	-1.963983000	0.530287000
H	3.716688000	-1.447156000	-1.388547000
H	3.041606000	-3.004647000	-0.908861000
H	1.754406000	-0.443051000	-4.315449000
H	1.717620000	1.313519000	-3.754357000
H	1.151938000	-1.749542000	2.060395000
H	2.664830000	-0.400200000	0.659680000
H	-0.769753000	-1.388976000	-2.996827000
H	-2.703886000	-2.937870000	-2.879400000
H	-2.831417000	-4.591077000	-0.999259000
H	-1.027642000	-4.680298000	0.714208000
H	1.110710000	-2.399337000	-3.832087000
H	1.798159000	-3.604457000	-2.725047000
H	2.846830000	-2.370938000	-3.461867000
C	1.986136000	2.923590000	2.429990000
H	2.008513000	3.842461000	3.036549000
H	1.221684000	2.238996000	2.823630000
H	2.969124000	2.432079000	2.479559000
C	0.010573000	4.257625000	0.781310000
H	-0.236745000	4.651550000	-0.215551000
H	-0.796465000	3.581838000	1.095822000
H	0.106156000	5.093995000	1.491429000
C	2.829981000	4.567627000	0.197705000
H	2.830657000	5.411914000	0.904802000
H	3.828488000	4.106276000	0.181114000
H	2.601788000	4.940291000	-0.811858000
H	-0.592042000	-1.159170000	-0.551697000
N	-1.621000000	-0.299760000	0.090093000
S	-2.315861000	0.884759000	-0.844695000
O	-1.698765000	0.852514000	-2.166663000
O	-2.508783000	2.140952000	-0.121680000
S	-1.477950000	-0.155356000	1.734986000
O	-0.872466000	1.096456000	2.187666000
O	-0.938250000	-1.438060000	2.193127000
C	-4.076692000	0.252206000	-1.177259000
F	-4.886654000	0.604762000	-0.186808000
F	-4.492342000	0.819234000	-2.302416000
F	-4.101068000	-1.067565000	-1.314232000
C	-3.228444000	-0.146922000	2.455237000
F	-3.113775000	-0.436874000	3.744393000
F	-3.797707000	1.040004000	2.319830000
F	-3.970105000	-1.073830000	1.858594000

4M-C: E= -1382.180042

C	-3.270620000	-2.128072000	1.097310000
N	-2.891304000	-2.438494000	-0.173909000
C	-3.252956000	-3.530002000	-1.041551000
C	-1.522515000	1.066620000	-1.344482000
C	-2.352597000	-0.255254000	-1.340312000
C	-0.095083000	0.762070000	-1.870418000
C	0.236239000	1.008176000	-3.153877000
C	-1.423198000	1.772968000	0.031072000

C	-2.104063000	1.414110000	1.214335000
O	-2.927024000	0.305566000	1.306625000
C	-2.287393000	-0.934679000	1.136955000
C	-1.944151000	-1.317267000	-0.332801000
C	-0.631652000	2.938263000	0.100051000
C	-0.531602000	3.719528000	1.250924000
C	-1.233349000	3.349199000	2.402974000
C	-2.008607000	2.192513000	2.378487000
C	-2.311423000	2.030667000	-2.271882000
O	-4.062766000	-2.633126000	1.864566000
Au	1.362037000	-0.015538000	-0.596667000
P	3.085553000	-0.854131000	0.815568000
H	-3.978513000	-4.163602000	-0.511460000
H	-2.372215000	-4.141025000	-1.303339000
H	-3.716909000	-3.169539000	-1.974707000
H	-2.292500000	-0.674373000	-2.357437000
H	-3.410791000	-0.011402000	-1.156758000
H	-0.450886000	1.455228000	-3.884274000
H	1.229720000	0.765239000	-3.545622000
H	-1.454846000	-1.060330000	1.851033000
H	-0.907386000	-1.658188000	-0.484252000
H	-0.079138000	3.239164000	-0.792906000
H	0.091545000	4.617378000	1.246273000
H	-1.170563000	3.949628000	3.313992000
H	-2.563846000	1.859278000	3.258062000
H	-1.769160000	2.972002000	-2.439809000
H	-3.286486000	2.273593000	-1.821646000
H	-2.505013000	1.569326000	-3.252386000
C	2.524535000	-1.387054000	2.483814000
H	3.371336000	-1.752632000	3.085401000
H	2.052203000	-0.537568000	2.998888000
H	1.779836000	-2.190055000	2.380189000
C	4.424704000	0.356316000	1.165534000
H	4.888744000	0.670354000	0.218910000
H	3.995376000	1.243348000	1.654215000
H	5.193310000	-0.084550000	1.819448000
C	3.978173000	-2.321658000	0.159679000
H	4.761906000	-2.649802000	0.860211000
H	3.263836000	-3.142990000	0.001378000
H	4.437018000	-2.067725000	-0.807244000

5M-C: E= -3208.858007

C	5.971702000	-0.403218000	-0.614807000
N	5.274189000	-0.284730000	-1.781307000
C	5.707341000	-0.054389000	-3.136688000
C	1.885546000	-1.971572000	-0.716759000
C	3.172198000	-1.672727000	-1.527962000
C	0.711584000	-1.066668000	-1.094026000
C	0.626243000	-0.153111000	-2.113835000
C	2.058835000	-1.987554000	0.829140000
C	3.290383000	-1.882687000	1.516353000
O	4.504039000	-1.707228000	0.878974000
C	4.659889000	-0.488640000	0.200245000
C	3.936400000	-0.402409000	-1.175762000
C	0.915181000	-2.208037000	1.627724000
C	0.980541000	-2.321989000	3.017143000
C	2.212269000	-2.222582000	3.669504000
C	3.359214000	-1.999716000	2.912278000
C	1.415776000	-3.395819000	-1.153334000
O	7.156281000	-0.412218000	-0.363383000
Au	0.764942000	1.180038000	-0.235087000
P	0.829941000	2.974592000	1.262674000
H	6.805058000	0.004669000	-3.137986000
H	5.300511000	0.892717000	-3.529868000
H	5.399284000	-0.874186000	-3.806224000
H	2.905945000	-1.661090000	-2.596794000
H	3.860711000	-2.519620000	-1.395253000

H	1.473414000	0.087020000	-2.761345000
H	-0.359657000	0.208502000	-2.426703000
H	4.488411000	0.373292000	0.867902000
H	3.336303000	0.512427000	-1.313186000
H	-0.062874000	-2.318957000	1.156138000
H	0.064306000	-2.499254000	3.585226000
H	2.280408000	-2.316398000	4.756003000
H	4.343236000	-1.914904000	3.378011000
H	0.446020000	-3.654889000	-0.707330000
H	2.159659000	-4.142834000	-0.837809000
H	1.313844000	-3.445843000	-2.248645000
C	-0.029034000	2.611581000	2.837806000
H	0.020519000	3.487025000	3.503326000
H	-1.080043000	2.368310000	2.627365000
H	0.445115000	1.749349000	3.328058000
C	0.017142000	4.470246000	0.592163000
H	0.527950000	4.787049000	-0.328252000
H	-1.029467000	4.233040000	0.355906000
H	0.053795000	5.283971000	1.332784000
C	2.525475000	3.488101000	1.721112000
H	2.488159000	4.347127000	2.408370000
H	3.043122000	2.650657000	2.210823000
H	3.080353000	3.769072000	0.814438000
H	-0.235754000	-1.339170000	-0.619011000
N	-2.692192000	-0.502842000	-0.537273000
S	-3.137870000	-2.051168000	-0.531968000
O	-2.047774000	-2.818233000	0.092701000
O	-3.730165000	-2.549741000	-1.774733000
S	-3.411167000	0.660698000	-1.398355000
O	-4.698850000	0.319222000	-2.010865000
O	-2.418293000	1.390845000	-2.201579000
C	-4.520006000	-2.148432000	0.736967000
F	-5.582299000	-1.462248000	0.323584000
F	-4.866873000	-3.422718000	0.908930000
F	-4.111214000	-1.651482000	1.902908000
C	-3.843942000	1.867464000	-0.023350000
F	-4.476946000	2.913005000	-0.547539000
F	-4.631790000	1.286826000	0.876684000
F	-2.739278000	2.305878000	0.595284000

TS3-C: E= -3208.803465

C	5.657038000	-0.667221000	-0.274747000
N	5.085788000	-0.640396000	-1.512069000
C	5.662034000	-0.569442000	-2.830887000
C	1.488475000	-1.996223000	-0.653460000
C	2.888350000	-1.888262000	-1.330930000
C	0.525452000	-0.912679000	-1.252470000
C	0.354555000	-0.862387000	-2.596315000
C	1.537346000	-1.900384000	0.895137000
C	2.697590000	-1.801771000	1.698036000
O	3.981104000	-1.734706000	1.186101000
C	4.269307000	-0.603799000	0.405302000
C	3.688560000	-0.629610000	-1.038343000
C	0.314940000	-1.994351000	1.592467000
C	0.229310000	-2.000608000	2.984292000
C	1.394643000	-1.911168000	3.751251000
C	2.620595000	-1.807445000	3.099734000
C	0.976042000	-3.420390000	-1.008802000
O	6.810176000	-0.704939000	0.097117000
Au	0.625945000	1.008582000	-0.236163000
P	1.039636000	3.064494000	0.804077000
H	6.756211000	-0.548118000	-2.725536000
H	5.338326000	0.344020000	-3.358211000
H	5.385344000	-1.443469000	-3.443505000
H	2.746999000	-1.984478000	-2.417919000
H	3.494888000	-2.752555000	-1.021081000
H	0.830605000	-1.560300000	-3.299323000

H	-0.324627000	-0.132082000	-3.046328000
H	4.086841000	0.330755000	0.962962000
H	3.151040000	0.286477000	-1.334154000
H	-0.605088000	-2.091425000	1.019304000
H	-0.748970000	-2.084108000	3.463646000
H	1.350358000	-1.919190000	4.843127000
H	3.557270000	-1.731611000	3.656135000
H	-0.043567000	-3.587704000	-0.646335000
H	1.639301000	-4.181563000	-0.568458000
H	0.975201000	-3.565149000	-2.100725000
C	0.142210000	3.300191000	2.385613000
H	0.358310000	4.294174000	2.806486000
H	-0.937326000	3.200702000	2.209964000
H	0.455227000	2.523583000	3.098615000
C	0.585471000	4.512658000	-0.224981000
H	1.157666000	4.486944000	-1.163692000
H	-0.485591000	4.465643000	-0.465372000
H	0.803001000	5.448832000	0.312253000
C	2.802245000	3.335098000	1.232749000
H	2.935150000	4.326132000	1.693275000
H	3.130556000	2.560075000	1.940270000
H	3.417700000	3.270357000	0.323834000
H	-0.945659000	-0.702511000	-0.896094000
N	-2.265801000	-0.616403000	-0.845892000
S	-3.153970000	-2.022380000	-0.715216000
O	-2.200844000	-3.088474000	-0.420467000
O	-4.155524000	-2.191470000	-1.757600000
S	-2.939174000	0.810369000	-1.394398000
O	-4.292853000	0.640288000	-1.905823000
O	-1.922034000	1.512057000	-2.174792000
C	-4.122052000	-1.784493000	0.885775000
F	-4.851654000	-0.672981000	0.814754000
F	-4.921432000	-2.827443000	1.048761000
F	-3.289783000	-1.694871000	1.916195000
C	-3.148646000	1.857619000	0.202092000
F	-2.529782000	3.021760000	0.030052000
F	-4.436316000	2.074553000	0.407541000
F	-2.628141000	1.243086000	1.259004000

6M-C: E= -1382.627501

C	-3.253089000	-1.921230000	1.414962000
N	-2.850781000	-2.420446000	0.209658000
C	-3.175011000	-3.646388000	-0.476736000
C	-1.605410000	0.885243000	-1.512160000
C	-2.385309000	-0.434731000	-1.283326000
C	-0.221898000	0.660596000	-2.126563000
C	0.302155000	-0.496065000	-2.644365000
C	-1.499586000	1.817826000	-0.271031000
C	-2.169104000	1.620490000	0.959590000
O	-2.965288000	0.524668000	1.224347000
C	-2.299999000	-0.711058000	1.268165000
C	-1.939052000	-1.313247000	-0.120891000
C	-0.763142000	3.015580000	-0.390810000
C	-0.686787000	3.963972000	0.629137000
C	-1.365187000	3.745220000	1.830805000
C	-2.098456000	2.572287000	1.987317000
C	-2.388063000	1.662855000	-2.618150000
O	-4.036845000	-2.316990000	2.247556000
Au	1.486311000	-0.252286000	-0.677027000
P	3.024555000	-0.480031000	1.072876000
H	-3.887918000	-4.206063000	0.145136000
H	-2.276178000	-4.266887000	-0.631448000
H	-3.642068000	-3.452051000	-1.456184000
H	-2.362382000	-1.013891000	-2.219564000
H	-3.440252000	-0.176650000	-1.114806000
H	-0.222769000	-1.453332000	-2.597761000
H	1.164134000	-0.446978000	-3.317127000

H	-1.472486000	-0.699598000	1.998267000
H	-0.891581000	-1.647687000	-0.208322000
H	-0.243924000	3.237091000	-1.324787000
H	-0.106080000	4.876403000	0.476578000
H	-1.323715000	4.479340000	2.638733000
H	-2.644696000	2.360203000	2.908599000
H	-1.877863000	2.592588000	-2.906149000
H	-3.387173000	1.925919000	-2.240317000
H	-2.506462000	1.040224000	-3.518166000
C	2.984552000	0.923462000	2.244710000
H	3.742197000	0.774786000	3.029484000
H	3.193113000	1.858652000	1.705970000
H	1.988698000	0.991619000	2.705540000
C	4.745314000	-0.576506000	0.460169000
H	4.847994000	-1.440214000	-0.212416000
H	4.987711000	0.339604000	-0.097370000
H	5.440417000	-0.685411000	1.306805000
C	2.762485000	-1.983431000	2.081111000
H	3.518845000	-2.035378000	2.879261000
H	1.759488000	-1.956107000	2.530576000
H	2.843505000	-2.874723000	1.442694000
H	0.318619000	1.582054000	-2.365661000

7M-C: E= -786.130732

C	-2.595588000	-1.400333000	-0.127326000
N	-2.876066000	-0.066843000	-0.088119000
C	-4.108132000	0.646021000	0.135795000
C	0.730961000	1.393648000	0.392159000
C	-0.765683000	1.113352000	0.678976000
C	0.908575000	2.384653000	-0.762588000
C	0.018909000	3.267361000	-1.228158000
C	1.581748000	0.120593000	0.114355000
C	1.121177000	-1.216169000	0.143264000
O	-0.191600000	-1.567308000	0.392849000
C	-1.133964000	-1.115333000	-0.545770000
C	-1.516188000	0.388934000	-0.429759000
C	2.962714000	0.288964000	-0.122373000
C	3.840428000	-0.778490000	-0.309254000
C	3.356540000	-2.088703000	-0.262355000
C	1.998190000	-2.296127000	-0.040773000
C	1.302769000	2.068469000	1.674463000
O	-3.268651000	-2.387481000	0.076210000
H	-4.902036000	-0.092284000	0.318313000
H	-4.383353000	1.252855000	-0.743596000
H	-4.039192000	1.311032000	1.012634000
H	-1.259829000	2.074561000	0.890917000
H	-0.845921000	0.517161000	1.599895000
H	-1.000918000	3.352474000	-0.843221000
H	0.292331000	3.958502000	-2.030459000
H	-0.882917000	-1.452375000	-1.566292000
H	-1.483349000	0.940349000	-1.382128000
H	3.376702000	1.298898000	-0.144679000
H	4.901186000	-0.583459000	-0.483808000
H	4.027610000	-2.939660000	-0.401845000
H	1.573876000	-3.301580000	-0.002137000
H	2.344919000	2.390893000	1.539207000
H	1.269453000	1.367944000	2.523897000
H	0.706005000	2.957780000	1.929401000
H	1.905165000	2.392093000	-1.215675000

Profile in Figure 3S (supplementary material)

8M: E= -731.988494

C	4.384494000	-0.862969000	0.132935000
C	3.682584000	-0.222359000	1.155570000
C	2.362116000	0.207261000	0.967500000

C	1.729678000	-0.013653000	-0.267386000
C	2.437086000	-0.655547000	-1.301388000
C	3.750197000	-1.075106000	-1.099239000
O	0.452295000	0.348594000	-0.558590000
C	-0.370884000	0.965107000	0.428598000
C	-1.827375000	0.965740000	-0.082228000
O	-1.932442000	2.159309000	-0.848074000
C	-1.254791000	3.171184000	-0.120290000
C	-0.067525000	2.474281000	0.585519000
C	-2.271853000	-0.206366000	-0.941684000
C	-2.434326000	-1.541873000	-0.239426000
C	-2.349324000	-1.694886000	1.065252000
C	-2.264874000	-1.871160000	2.363194000
C	-2.732344000	-2.717097000	-1.147975000
H	-2.479122000	1.040010000	0.813302000
H	-0.946294000	3.955644000	-0.826799000
H	-1.935783000	3.626948000	0.625014000
H	0.891229000	2.710203000	0.103612000
H	0.006614000	2.767631000	1.642668000
H	1.844157000	0.712319000	1.782757000
H	1.931114000	-0.816813000	-2.255845000
H	4.163366000	-0.045055000	2.121419000
H	4.284516000	-1.574176000	-1.912126000
H	5.414169000	-1.192338000	0.289730000
H	-3.239254000	0.067207000	-1.400002000
H	-1.560827000	-0.322954000	-1.774883000
H	-3.639040000	-2.521120000	-1.746368000
H	-1.904416000	-2.872120000	-1.861147000
H	-2.882756000	-3.646620000	-0.581875000
H	-3.142170000	-1.779028000	3.015863000
H	-1.312678000	-2.117698000	2.849731000
H	-0.288809000	0.409403000	1.374549000

8M-Au: E= -1328.487264

C	2.839460000	-2.203854000	0.089213000
O	3.966984000	-2.984197000	0.453175000
C	4.921708000	-2.817167000	-0.583310000
C	4.821694000	-1.338082000	-1.005850000
C	3.426273000	-0.894878000	-0.498563000
H	2.291826000	-2.712206000	-0.731350000
H	5.909560000	-3.097639000	-0.191285000
H	4.682639000	-3.484888000	-1.434210000
H	5.589186000	-0.729561000	-0.507511000
H	4.936993000	-1.209324000	-2.091348000
O	3.500468000	0.076399000	0.539482000
C	3.742528000	1.384549000	0.248080000
C	4.003736000	1.879566000	-1.039678000
C	3.719106000	2.271088000	1.340559000
C	4.227905000	3.251110000	-1.220723000
H	4.045467000	1.213911000	-1.901591000
C	3.946172000	3.631878000	1.144348000
H	3.519894000	1.867815000	2.335862000
C	4.200626000	4.133765000	-0.139673000
H	4.432029000	3.625073000	-2.227538000
H	3.924405000	4.308230000	2.002954000
H	4.379698000	5.200553000	-0.291457000
C	1.947339000	-2.074374000	1.314348000
H	1.782583000	-3.088132000	1.718980000
H	2.491418000	-1.512956000	2.087819000
C	0.584579000	-1.425129000	1.131019000
C	-0.108850000	-1.023207000	2.410449000
H	-0.162740000	-1.888026000	3.091628000
H	0.479462000	-0.242579000	2.919960000
H	-1.124783000	-0.643385000	2.238871000
C	0.064591000	-1.267457000	-0.067787000
C	-0.281888000	-1.196859000	-1.368279000
H	-0.704022000	-2.069179000	-1.884527000

H	0.069809000	-0.370615000	-2.000374000
H	2.785339000	-0.511429000	-1.307987000
Au	-2.122974000	-0.283480000	-0.393877000
P	-4.184836000	0.682527000	0.144119000
C	-4.456889000	2.283307000	-0.697848000
H	-4.429883000	2.136024000	-1.786934000
H	-5.433320000	2.701590000	-0.408868000
H	-3.659531000	2.985099000	-0.413793000
C	-5.606527000	-0.376885000	-0.305612000
H	-6.548528000	0.117277000	-0.022301000
H	-5.600094000	-0.559602000	-1.389714000
H	-5.526843000	-1.340382000	0.218118000
C	-4.359326000	1.023842000	1.933230000
H	-5.345025000	1.471137000	2.133464000
H	-4.261313000	0.086666000	2.499491000
H	-3.569791000	1.718614000	2.253372000

TS4: E= -1328.432735

C	2.544071000	-2.284191000	-0.133018000
O	3.757941000	-3.009260000	-0.031001000
C	4.495272000	-2.693774000	-1.221053000
C	4.203536000	-1.194176000	-1.530068000
C	3.110404000	-0.927037000	-0.523400000
H	1.958239000	-2.667753000	-0.990770000
H	5.558962000	-2.873163000	-1.020961000
H	4.167891000	-3.341198000	-2.052064000
H	5.066921000	-0.542134000	-1.341347000
H	3.875385000	-1.033061000	-2.566841000
O	3.186003000	-0.022790000	0.410018000
C	3.885694000	1.189517000	0.311773000
C	3.953778000	1.914866000	-0.878350000
C	4.449535000	1.651042000	1.501703000
C	4.633045000	3.137662000	-0.869313000
H	3.475046000	1.555802000	-1.790250000
C	5.125829000	2.871884000	1.489666000
H	4.356400000	1.054233000	2.410441000
C	5.220163000	3.614669000	0.306410000
H	4.693965000	3.720639000	-1.790716000
H	5.578995000	3.244287000	2.410856000
H	5.746937000	4.571233000	0.303150000
C	1.692976000	-2.315333000	1.112516000
H	1.567435000	-3.375714000	1.389918000
H	2.240191000	-1.850279000	1.951117000
C	0.305973000	-1.684237000	0.975069000
C	-0.580577000	-2.095245000	2.132008000
H	-0.733475000	-3.189365000	2.141443000
H	-0.107759000	-1.839608000	3.097214000
H	-1.564179000	-1.607763000	2.093422000
C	-0.120139000	-0.859850000	-0.009129000
C	0.594945000	-0.348352000	-1.206122000
H	0.274798000	-0.810104000	-2.155512000
H	0.553123000	0.747600000	-1.306068000
H	1.758351000	-0.536728000	-1.222281000
Au	-2.084823000	-0.088872000	-0.070230000
P	-4.294010000	0.771241000	-0.128396000
C	-4.383473000	2.595617000	-0.314227000
H	-3.892840000	2.891627000	-1.253035000
H	-5.430674000	2.935576000	-0.327474000
H	-3.854955000	3.073883000	0.523367000
C	-5.325374000	0.118466000	-1.499987000
H	-6.336711000	0.552753000	-1.465643000
H	-4.854095000	0.366118000	-2.462425000
H	-5.395262000	-0.975845000	-1.415124000
C	-5.266954000	0.413296000	1.386724000
H	-6.283637000	0.827361000	1.303252000
H	-5.328372000	-0.675124000	1.532734000
H	-4.763259000	0.856459000	2.258378000

9M: E= -1328.456595

C	3.134339000	-2.132254000	-0.520313000
O	4.275512000	-2.904403000	-0.203478000
C	5.440134000	-2.092999000	-0.333074000
C	4.986464000	-0.694353000	0.130983000
C	3.566095000	-0.730186000	-0.280779000
H	2.877223000	-2.204563000	-1.600362000
H	6.234707000	-2.517231000	0.292722000
H	5.785792000	-2.058254000	-1.382335000
H	5.021571000	-0.619495000	1.235341000
H	5.533627000	0.168583000	-0.276836000
O	2.767022000	0.234300000	-0.476596000
C	3.108559000	1.604108000	-0.254393000
C	3.089759000	2.436048000	-1.368221000
C	3.357406000	2.051702000	1.038700000
C	3.373390000	3.790604000	-1.172339000
H	2.863702000	2.031761000	-2.356000000
C	3.633025000	3.412300000	1.211309000
H	3.314711000	1.372786000	1.891858000
C	3.645701000	4.276341000	0.111671000
H	3.376162000	4.466982000	-2.029508000
H	3.830437000	3.794120000	2.214979000
H	3.861383000	5.336852000	0.256950000
C	1.912441000	-2.611324000	0.323311000
H	1.895324000	-3.698555000	0.137446000
H	2.178257000	-2.476447000	1.378995000
C	0.581286000	-1.993065000	-0.046156000
C	0.064725000	-2.456691000	-1.391195000
H	0.756434000	-2.197197000	-2.215312000
H	-0.048839000	-3.555573000	-1.420712000
H	-0.909068000	-2.002936000	-1.623758000
C	-0.103326000	-1.130465000	0.754406000
C	0.405584000	-0.669952000	2.104674000
H	0.446954000	0.432242000	2.146771000
H	-0.294318000	-0.969061000	2.904699000
H	1.402612000	-1.046761000	2.390010000
Au	-1.959931000	-0.332059000	0.237493000
P	-4.079301000	0.622090000	-0.292558000
C	-5.173821000	0.895566000	1.158946000
H	-4.672739000	1.565391000	1.873185000
H	-6.131240000	1.343142000	0.849539000
H	-5.365226000	-0.065824000	1.658060000
C	-3.989390000	2.272427000	-1.098272000
H	-4.997826000	2.660735000	-1.309601000
H	-3.460570000	2.974404000	-0.436753000
H	-3.426697000	2.189360000	-2.039890000
C	-5.108164000	-0.377544000	-1.442681000
H	-6.072652000	0.116941000	-1.637178000
H	-4.570867000	-0.512193000	-2.393123000
H	-5.290269000	-1.368626000	-1.001616000

TS5: E= -1328.408347

C	3.067483000	-1.858081000	-0.118957000
O	4.360531000	-1.386292000	-0.419424000
C	4.172113000	-0.676145000	-1.669656000
C	2.641282000	-0.284050000	-1.804467000
C	2.225280000	-0.626068000	-0.393538000
H	2.795772000	-2.609670000	-0.872793000
H	4.810372000	0.217413000	-1.646043000
H	4.472441000	-1.317505000	-2.513283000
H	2.502243000	0.765810000	-2.081962000
H	2.135317000	-0.918578000	-2.542811000
O	2.370786000	0.342201000	0.528420000
C	2.167995000	1.702279000	0.304900000

C	1.072470000	2.195100000	-0.407787000
C	3.099175000	2.559382000	0.896733000
C	0.923927000	3.580727000	-0.538129000
H	0.340130000	1.510827000	-0.840291000
C	2.932542000	3.939721000	0.763513000
H	3.939368000	2.134322000	1.448755000
C	1.847541000	4.454015000	0.044217000
H	0.072651000	3.975970000	-1.097391000
H	3.658176000	4.615354000	1.222210000
H	1.721387000	5.533857000	-0.060136000
C	2.625401000	-2.388174000	1.237903000
H	2.714124000	-3.483061000	1.317751000
H	3.178613000	-1.943042000	2.076771000
C	1.174629000	-1.901216000	1.256782000
C	0.737247000	-1.284242000	2.535844000
H	1.068084000	-1.904072000	3.386079000
H	1.255922000	-0.312336000	2.647751000
H	-0.344950000	-1.113144000	2.579792000
C	0.425925000	-1.777170000	0.061627000
C	0.452901000	-2.868019000	-1.010262000
H	1.214234000	-3.650511000	-0.868986000
H	-0.524702000	-3.374462000	-0.985037000
H	0.550804000	-2.453306000	-2.025360000
Au	-1.345874000	-0.643345000	-0.003313000
P	-3.379591000	0.570439000	-0.132767000
C	-3.244162000	2.197978000	-0.971529000
H	-2.873897000	2.051383000	-1.996760000
H	-4.224177000	2.698507000	-1.007148000
H	-2.530070000	2.832390000	-0.426633000
C	-4.710881000	-0.301534000	-1.047604000
H	-5.628519000	0.306543000	-1.067175000
H	-4.380319000	-0.494844000	-2.078705000
H	-4.921848000	-1.264586000	-0.560441000
C	-4.118589000	0.956166000	1.502782000
H	-5.061336000	1.512123000	1.383140000
H	-4.314485000	0.020146000	2.046218000
H	-3.411658000	1.560839000	2.089561000

TS5′: E= -1328.398119

C	-2.118930000	-2.388166000	0.536051000
O	-3.286334000	-2.477353000	1.311695000
C	-3.036480000	-1.525253000	2.380986000
C	-1.908443000	-0.518387000	1.907508000
C	-1.906187000	-0.888292000	0.438157000
H	-1.280172000	-2.762446000	1.155450000
H	-3.978252000	-0.994861000	2.575929000
H	-2.720851000	-2.061860000	3.289675000
H	-2.170414000	0.522129000	2.123870000
H	-0.943976000	-0.749896000	2.376961000
O	-2.828313000	-0.279819000	-0.325547000
C	-3.158595000	1.069092000	-0.234030000
C	-2.221850000	2.066704000	0.051608000
C	-4.494245000	1.380212000	-0.500922000
C	-2.646047000	3.399120000	0.084255000
H	-1.175811000	1.813136000	0.233655000
C	-4.901084000	2.715991000	-0.467782000
H	-5.194076000	0.573634000	-0.726380000
C	-3.980816000	3.728044000	-0.172510000
H	-1.920077000	4.184738000	0.306014000
H	-5.944939000	2.964532000	-0.672729000
H	-4.302081000	4.771562000	-0.147664000
C	-1.902302000	-2.974931000	-0.859931000
H	-1.950027000	-4.070494000	-0.890488000
H	-2.582948000	-2.536978000	-1.600827000
C	-0.476244000	-2.433045000	-0.894866000
C	0.596086000	-3.393908000	-0.528480000
H	0.237838000	-4.249801000	0.063409000

H	0.964764000	-3.810125000	-1.489072000
H	1.451655000	-2.900824000	-0.046858000
C	-0.261221000	-1.032703000	-0.992089000
C	-0.902297000	-0.318731000	-2.181408000
H	-1.037667000	0.753614000	-1.995910000
H	-0.188062000	-0.403243000	-3.017372000
H	-1.858627000	-0.742072000	-2.519461000
Au	1.506563000	-0.134293000	-0.302103000
P	3.483804000	0.938045000	0.451914000
C	3.545676000	1.258684000	2.258782000
H	3.453373000	0.307777000	2.803802000
H	4.494122000	1.745406000	2.534487000
H	2.706431000	1.909771000	2.544137000
C	5.013244000	-0.015466000	0.101320000
H	5.901127000	0.526920000	0.461211000
H	4.958389000	-0.994516000	0.599454000
H	5.100685000	-0.178790000	-0.982859000
C	3.779949000	2.578386000	-0.317212000
H	4.710521000	3.025869000	0.064625000
H	3.853600000	2.461641000	-1.408361000
H	2.935786000	3.246910000	-0.093090000

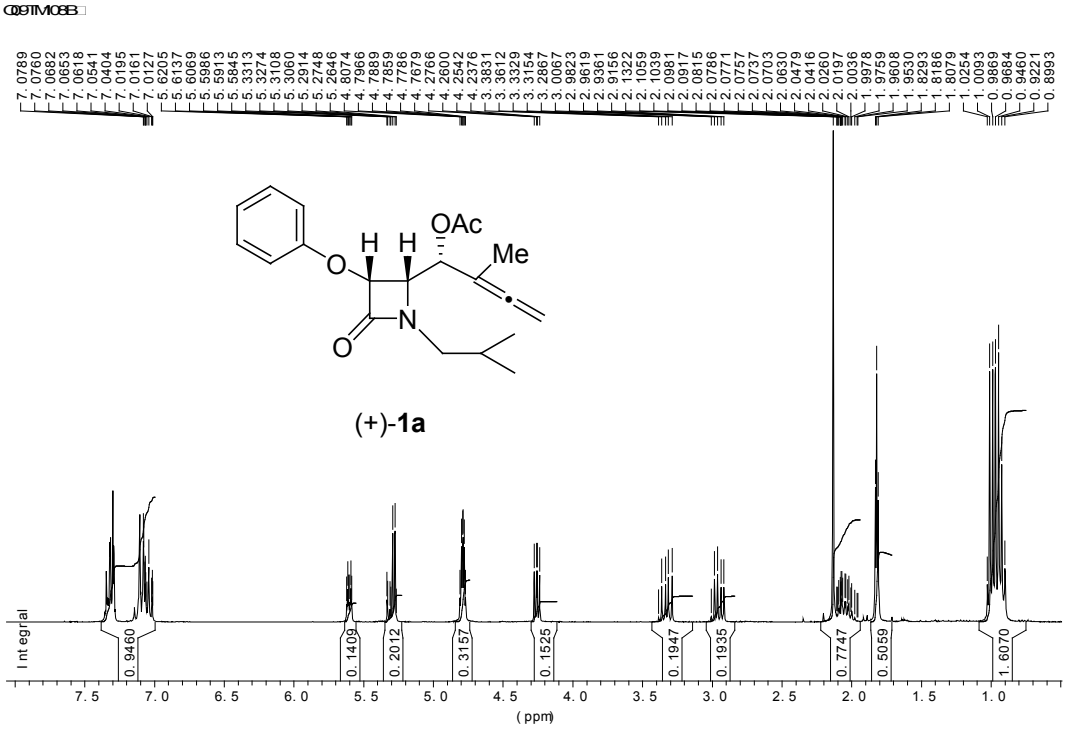
10M: E= -1328.498708

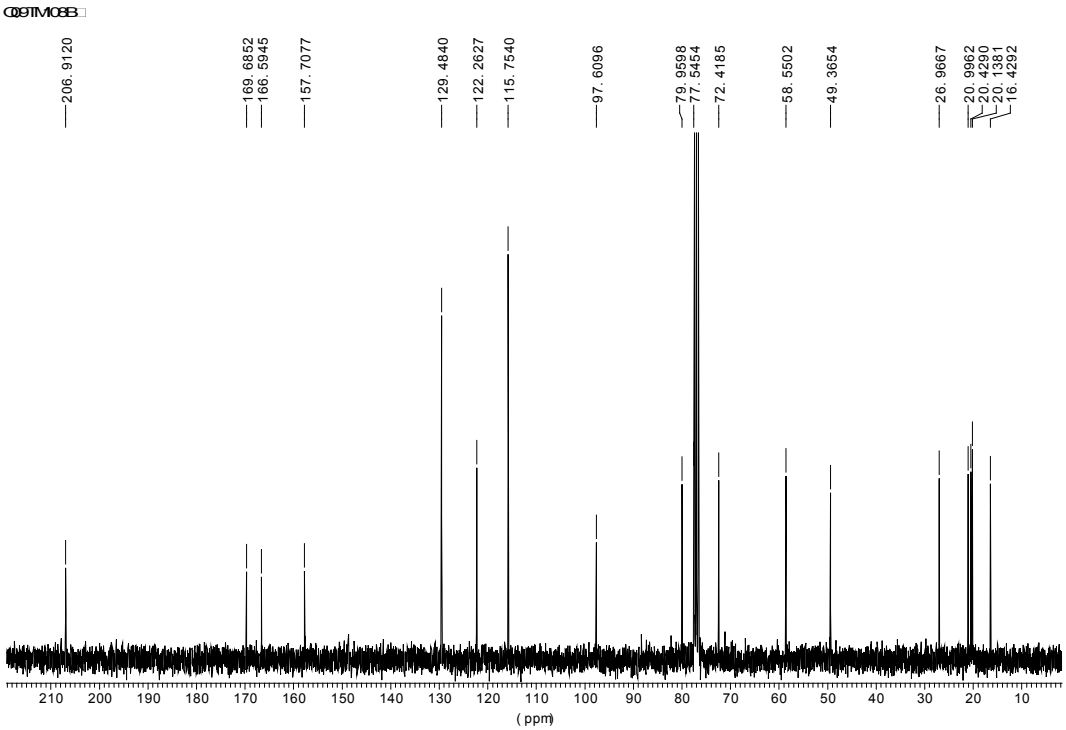
C	-2.807326000	-1.542079000	-0.740047000
O	-3.791293000	-0.873951000	-1.469322000
C	-4.472110000	-0.049681000	-0.494162000
C	-3.576955000	0.013894000	0.792756000
C	-2.248066000	-0.496576000	0.232647000
H	-3.276695000	-2.324511000	-0.105174000
H	-4.623878000	0.943951000	-0.941140000
H	-5.459717000	-0.482686000	-0.263779000
H	-3.537948000	1.025171000	1.215175000
H	-3.952023000	-0.664683000	1.571707000
O	-1.652097000	0.525406000	-0.595483000
C	-1.419515000	1.805909000	-0.167719000
C	-1.156474000	2.165146000	1.162796000
C	-1.393290000	2.787575000	-1.171640000
C	-0.873567000	3.500580000	1.476343000
H	-1.174690000	1.418759000	1.956411000
C	-1.100743000	4.112809000	-0.847523000
H	-1.606520000	2.487434000	-2.199641000
C	-0.839927000	4.478744000	0.479193000
H	-0.675912000	3.771163000	2.516717000
H	-1.083755000	4.867359000	-1.638111000
H	-0.617430000	5.517688000	0.732438000
C	-1.562613000	-2.196100000	-1.333249000
H	-1.738733000	-3.185040000	-1.779611000
H	-1.076686000	-1.557298000	-2.084269000
C	-0.757687000	-2.318591000	-0.020397000
C	-0.006547000	-3.592017000	0.255935000
H	-0.739702000	-4.416629000	0.317534000
H	0.681058000	-3.839197000	-0.566739000
H	0.560014000	-3.568412000	1.196106000
C	-1.169590000	-1.369174000	0.920874000
C	-1.005327000	-1.449778000	2.413876000
H	-1.944325000	-1.829937000	2.853592000
H	-0.197849000	-2.130798000	2.713092000
H	-0.814134000	-0.467115000	2.868363000
Au	0.968929000	-0.672087000	0.070257000
P	3.016530000	0.383651000	-0.284755000
C	2.836326000	2.105201000	-0.874104000
H	2.278577000	2.691115000	-0.129465000
H	3.827817000	2.557094000	-1.030949000
H	2.275866000	2.111170000	-1.819713000
C	4.047539000	0.471952000	1.223642000
H	5.004110000	0.967879000	0.997200000
H	3.515882000	1.040203000	2.000279000

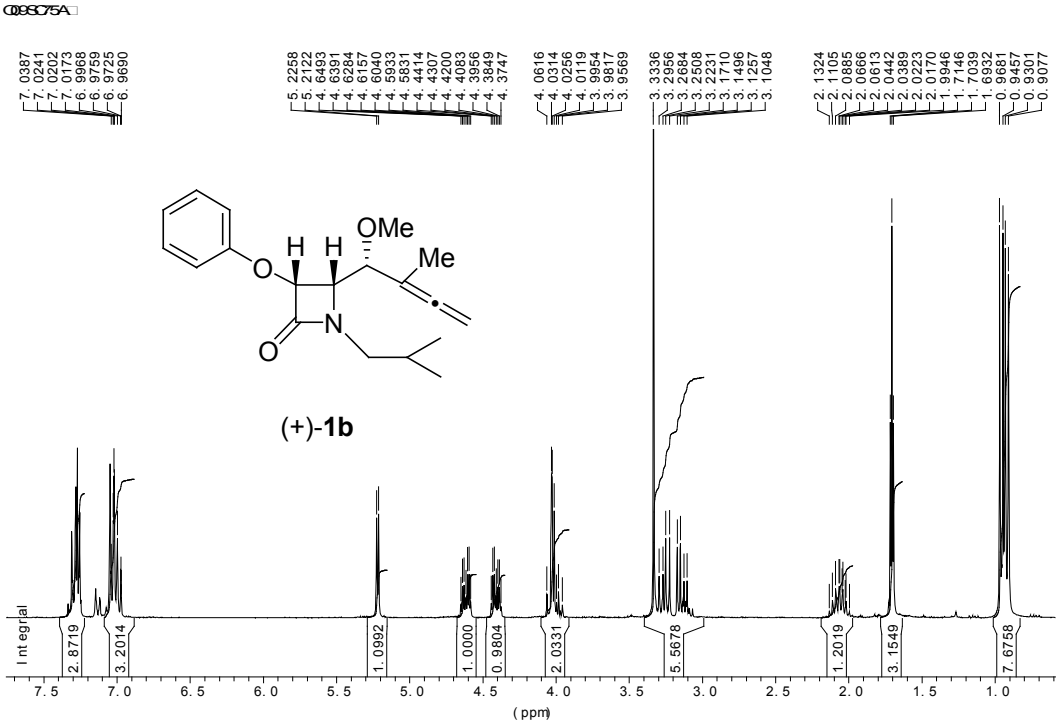
H	4.241373000	-0.544236000	1.595499000
C	4.035021000	-0.477393000	-1.536775000
H	4.990911000	0.051532000	-1.672317000
H	4.229982000	-1.507468000	-1.205500000
H	3.493260000	-0.506588000	-2.492914000

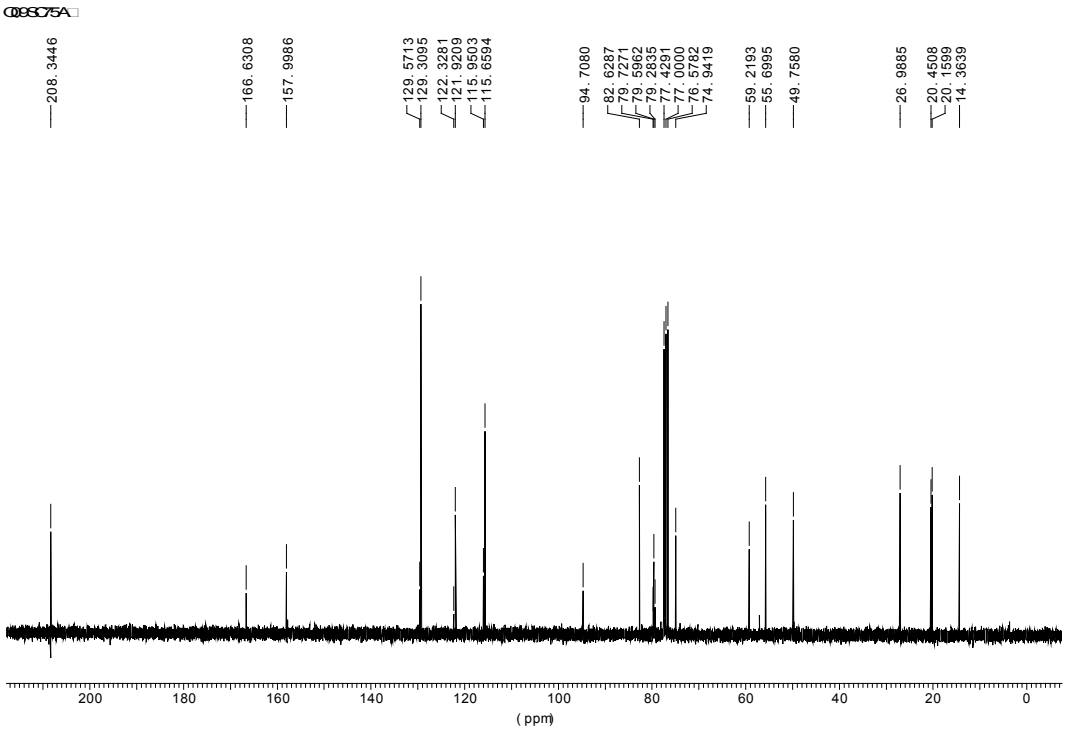
10M'： E= -1328.501607

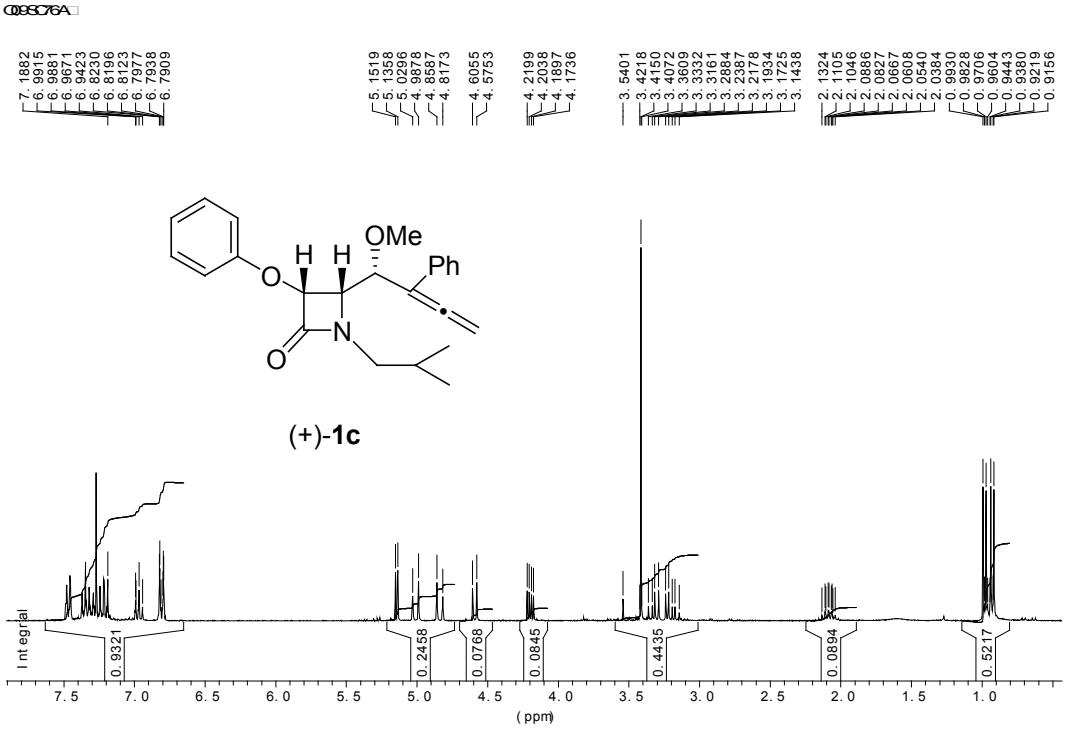
C	-0.895181000	1.690493000	0.587433000
O	-1.768226000	2.728260000	0.250285000
C	-2.114761000	2.481116000	-1.132324000
C	-1.709582000	1.004791000	-1.471739000
C	-1.515104000	0.443234000	-0.065012000
H	0.086572000	1.865759000	0.096485000
H	-3.196323000	2.649201000	-1.242902000
H	-1.583357000	3.194286000	-1.784763000
H	-2.471715000	0.501563000	-2.077185000
H	-0.758998000	0.966727000	-2.022041000
O	-2.790924000	0.262743000	0.599994000
C	-3.941759000	-0.184691000	0.010822000
C	-4.001983000	-1.192063000	-0.964906000
C	-5.132485000	0.385128000	0.491738000
C	-5.245518000	-1.612101000	-1.452399000
H	-3.092168000	-1.655409000	-1.345174000
C	-6.366302000	-0.051002000	0.007311000
H	-5.063629000	1.170081000	1.247651000
C	-6.430871000	-1.050739000	-0.970989000
H	-5.279759000	-2.395479000	-2.213925000
H	-7.284253000	0.399975000	0.393025000
H	-7.396682000	-1.388077000	-1.353870000
C	-0.598870000	1.236842000	2.007897000
H	0.170399000	1.818527000	2.535188000
H	-1.511812000	1.222957000	2.625094000
C	-0.183442000	-0.216588000	1.749697000
C	0.310025000	-1.052484000	2.893295000
H	1.129364000	-0.553330000	3.432259000
H	-0.520478000	-1.170279000	3.612522000
H	0.638406000	-2.055139000	2.590529000
C	-0.623810000	-0.674484000	0.501686000
C	-0.756864000	-2.117242000	0.085216000
H	-0.655663000	-2.234306000	-1.003467000
H	-0.014826000	-2.765537000	0.570030000
H	-1.755816000	-2.486762000	0.371411000
Au	1.653417000	-0.198009000	0.148404000
P	3.825548000	-0.030042000	-0.698812000
C	4.009102000	1.293340000	-1.948068000
H	3.722249000	2.258172000	-1.505780000
H	5.053433000	1.344332000	-2.292544000
H	3.351325000	1.083151000	-2.803588000
C	5.060357000	0.329321000	0.602171000
H	6.066340000	0.383750000	0.158302000
H	4.820329000	1.288850000	1.081763000
H	5.036849000	-0.465584000	1.361605000
C	4.385829000	-1.571888000	-1.508602000
H	5.415328000	-1.450861000	-1.879335000
H	4.353255000	-2.398595000	-0.784658000
H	3.718973000	-1.808541000	-2.349930000

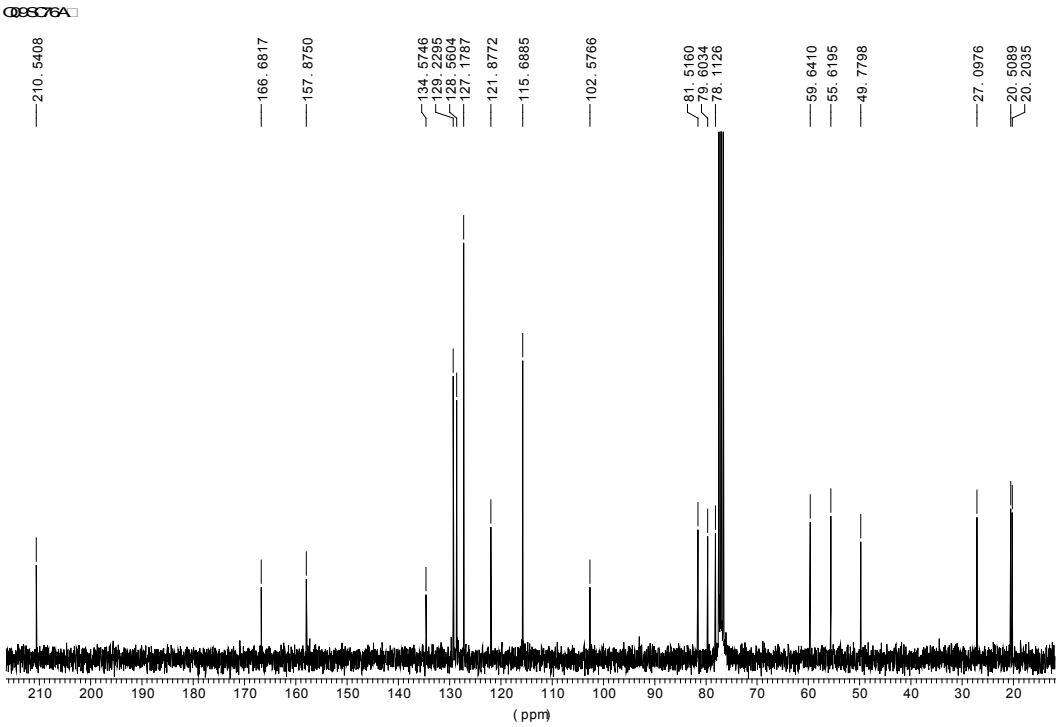

OAc
H
H
Me
O
N
O
(+)-1a
Integral
0.9460
0.1409
0.2012
0.3157
0.1525
0.1947
0.1935
0.7747
0.5059
1.6070
(ppm)

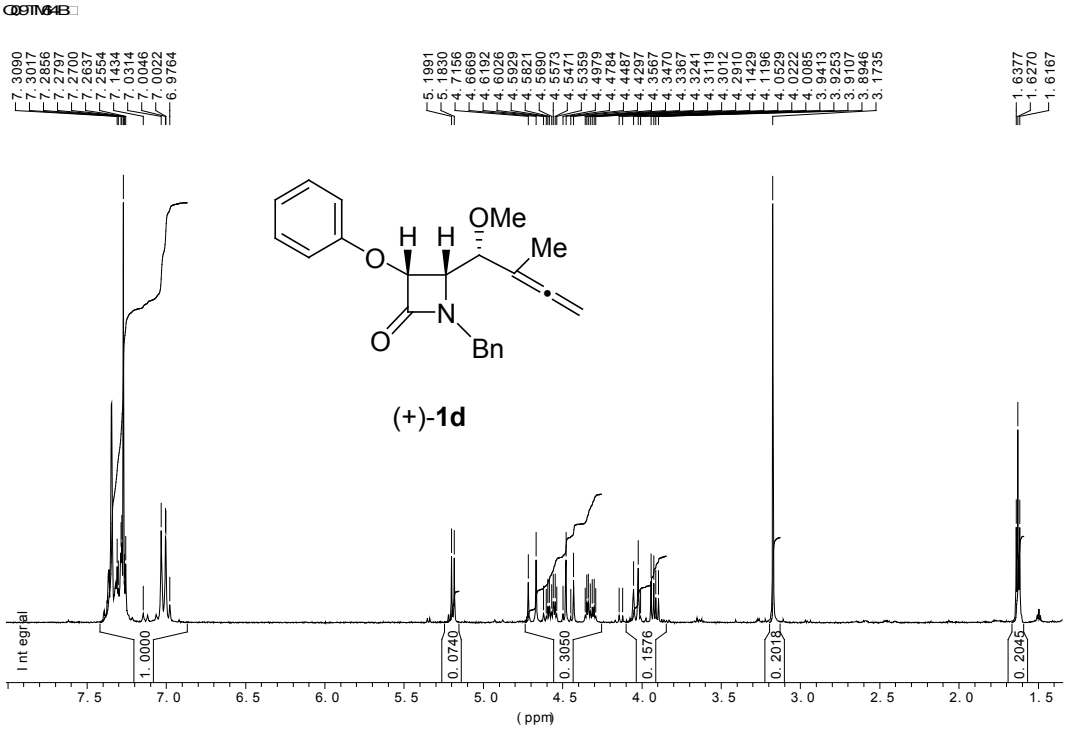

206.9120
169.6852
166.5945
157.7077
129.4840
122.2627
115.7540
97.6096
79.9598
77.5454
72.4185
58.5502
49.3654
26.9667
20.9962
20.4290
20.1381
16.4292
(ppm)

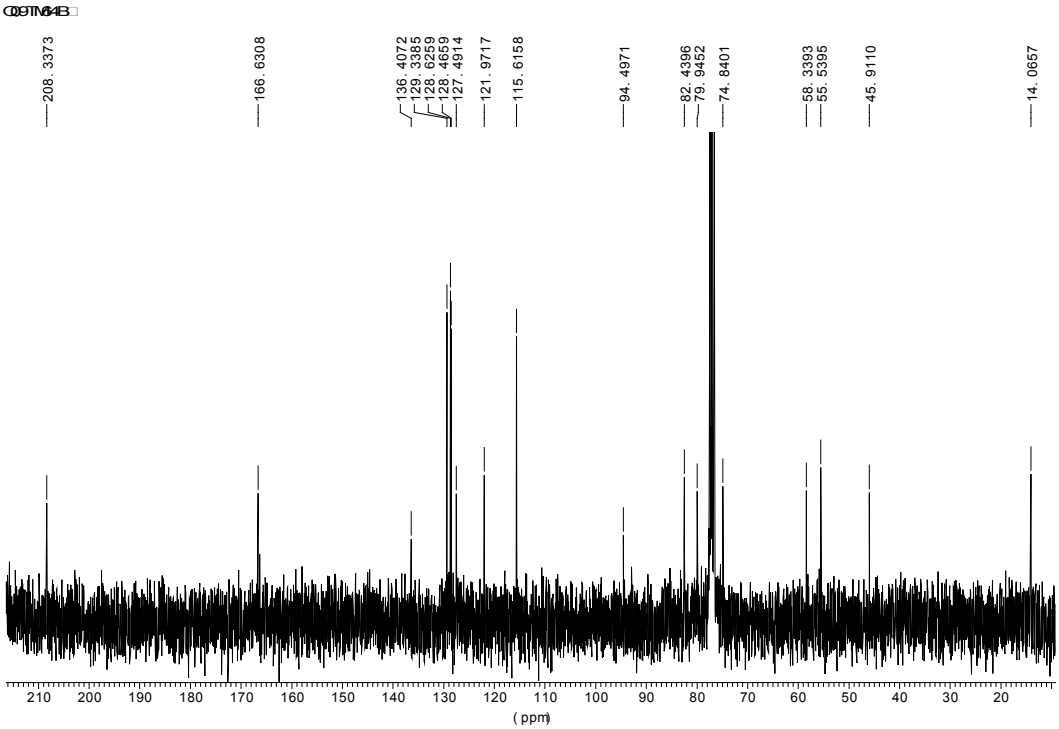

OMe
H H
Me
O
N
O
(+)-1b
Integral
2.8719
3.2014
1.0992
1.0000
0.9804
2.0331
5.5678
1.2019
3.1549
7.6758
(ppm)

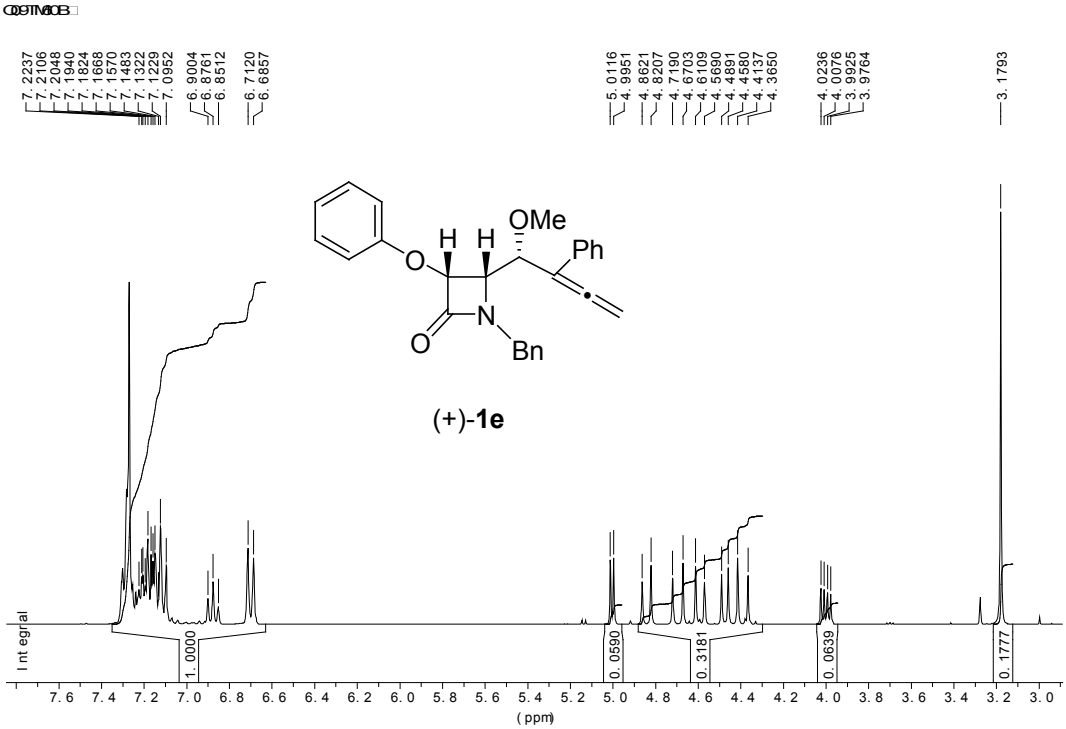

208.3446
166.6308
157.9986
129.5713
129.3095
122.3281
121.9209
115.9503
115.6594
94.7080
82.6287
79.7271
79.5962
79.2835
77.4291
77.0000
76.5782
74.9419
59.2193
55.6995
49.7580
26.9885
20.4508
20.1599
14.3639
(ppm)

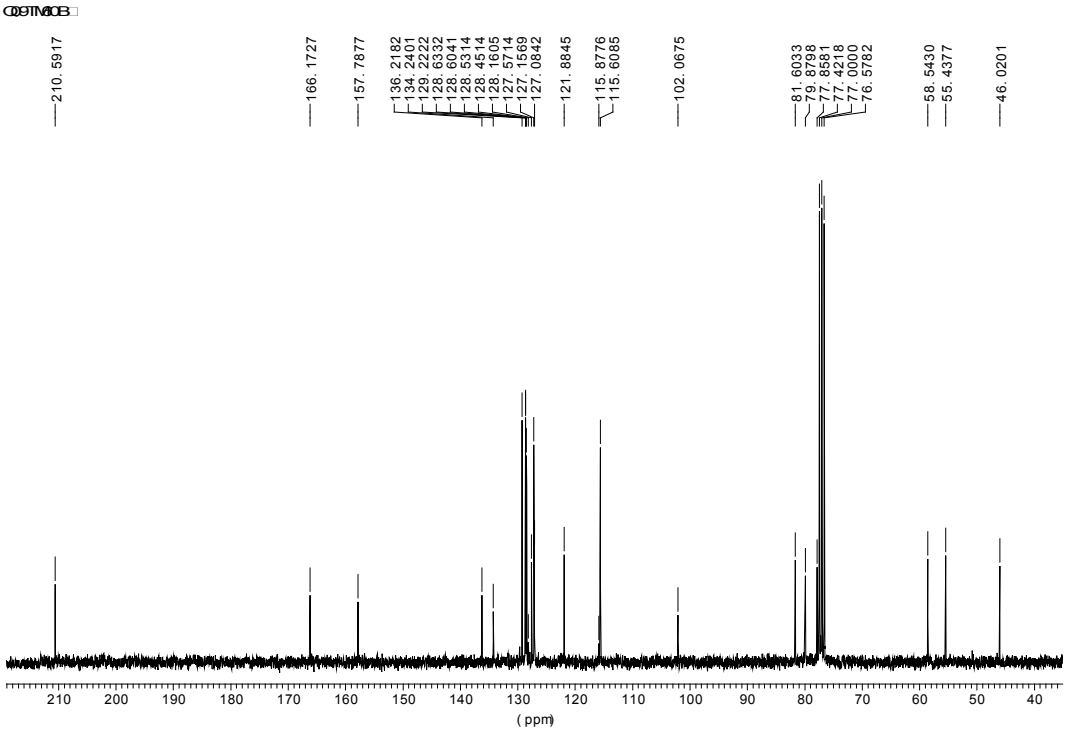

OMe
H
H
Ph
O
N
O
(+)-1c
Integral
0.9321
0.2458
0.0768
0.0845
0.4435
0.0894
0.5217
(ppm)

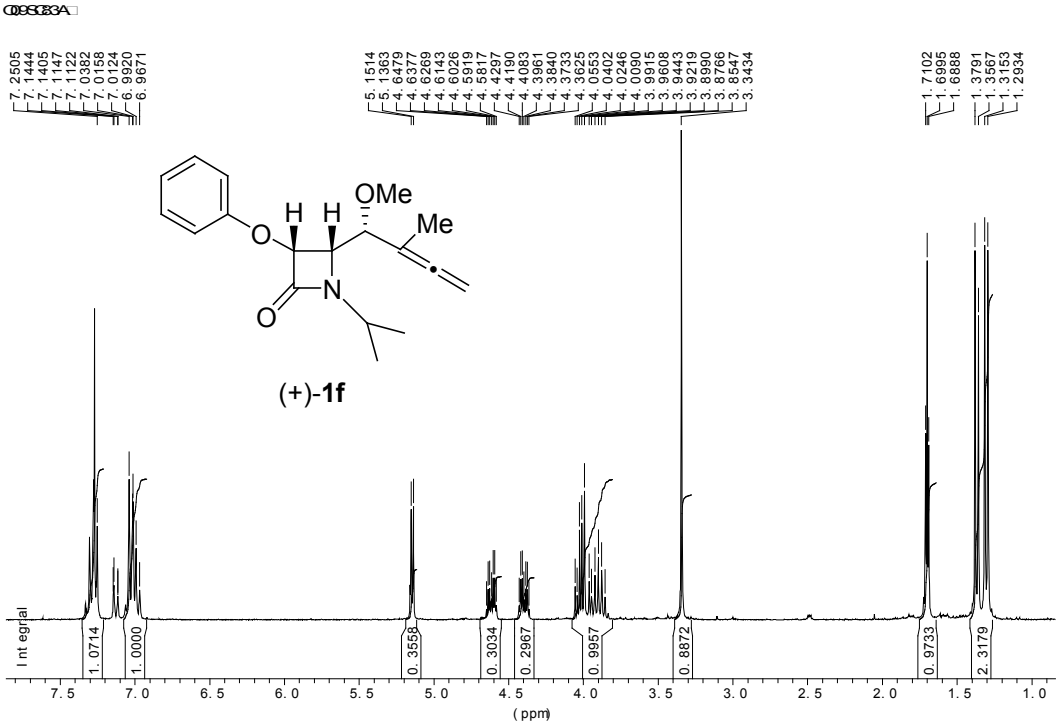

210.5408
166.6817
157.8750
134.5746
129.2295
128.5604
127.1787
121.8772
115.6885
102.5766
81.5160
79.6034
78.1126
59.6410
55.6195
49.7798
27.0976
20.5089
20.2035
(ppm)

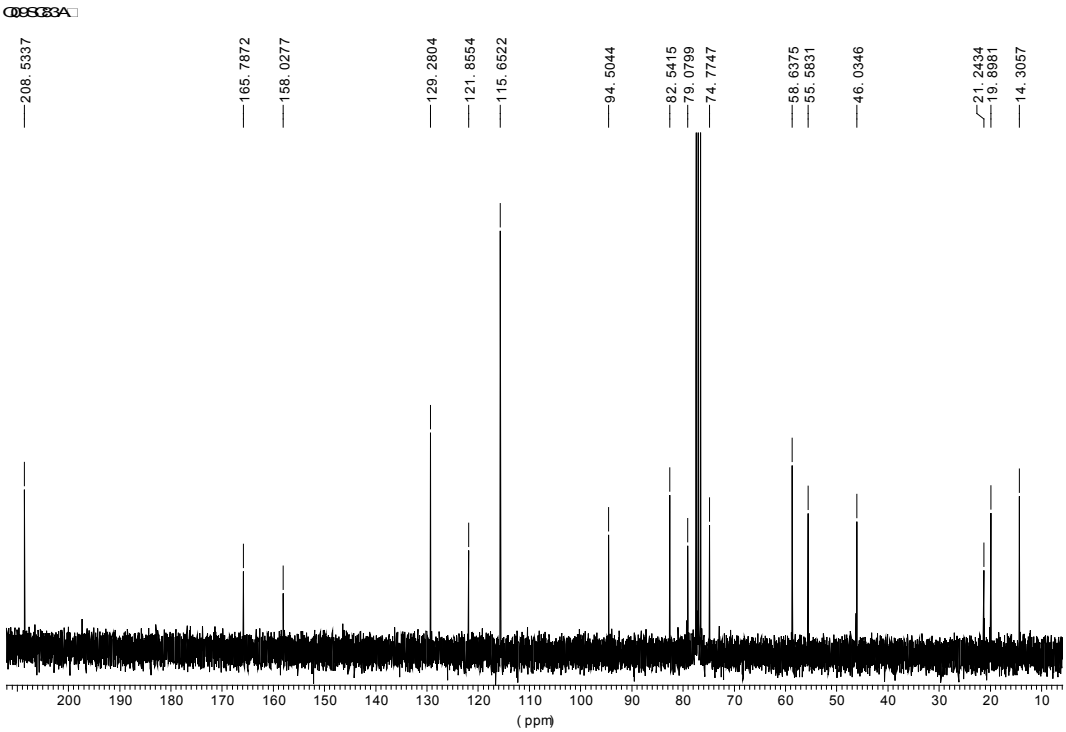

7.3090
7.3017
7.2856
7.2797
7.2700
7.2637
7.2554
7.1434
7.0314
7.0046
7.0022
6.9764
5.1991
5.1830
4.7156
4.6669
4.6192
4.6026
4.5929
4.5821
4.5690
4.5573
4.5471
4.5359
4.4979
4.4784
4.4487
4.4297
4.3567
4.3470
4.3367
4.3241
4.3119
4.3012
4.2910
4.1429
4.1196
4.0529
4.0222
4.0085
3.9413
3.9253
3.9107
3.8946
3.1735
1.6377
1.6270
1.6167
OMe
H H
Me
O
N
O
Bn
(+)-1d
Integral
1.0000
0.0740
0.3050
0.1576
0.2018
0.2045
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
(ppm)

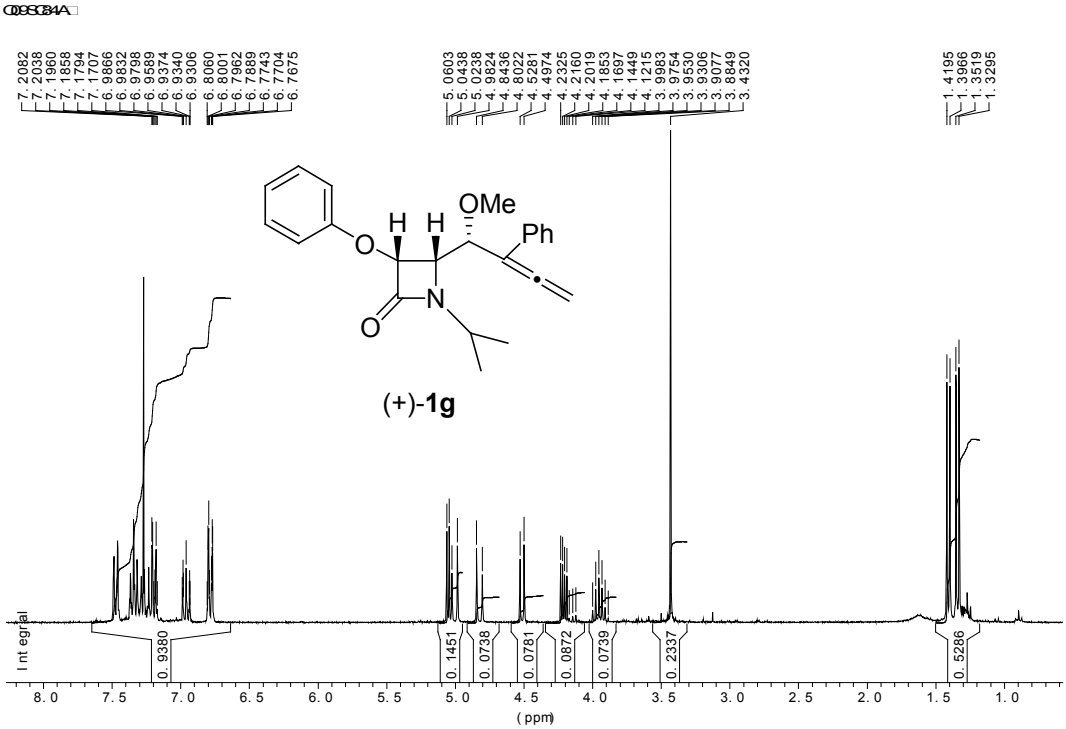

208.3373
166.6308
136.4072
129.3385
128.6259
128.4659
127.4914
121.9717
115.6158
94.4971
82.4396
79.9452
74.8401
58.3393
55.5395
45.9110
14.0657
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
(ppm)

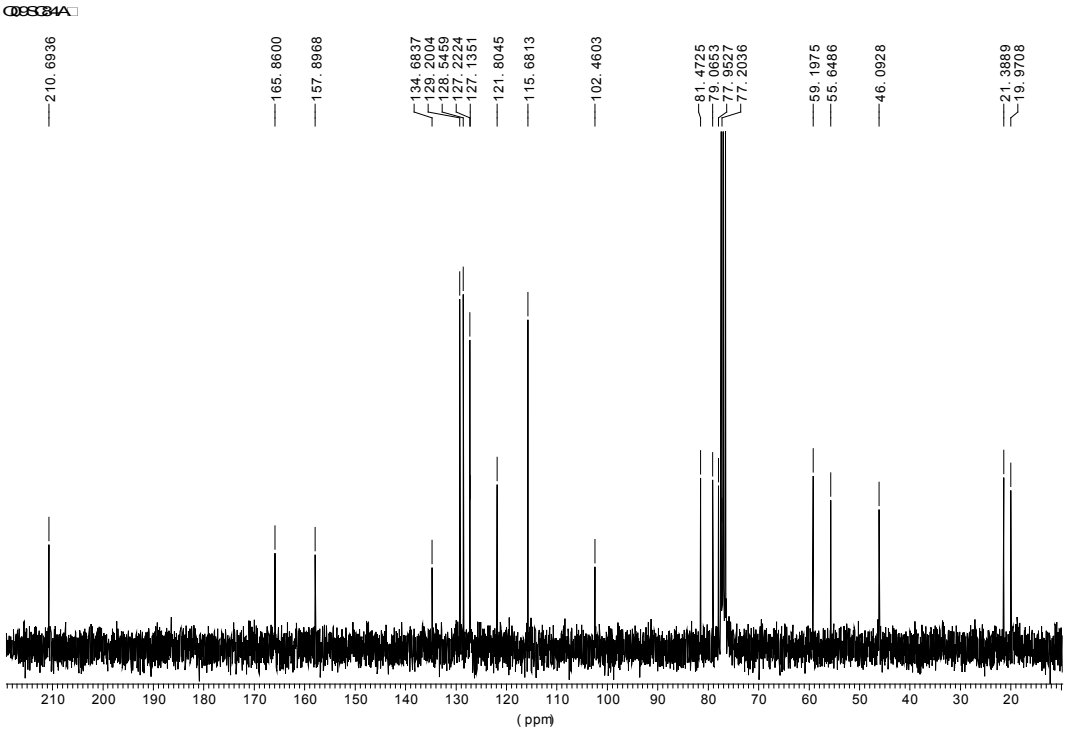

7.2237
7.2106
7.2048
7.1940
7.1824
7.1668
7.1570
7.1483
7.1322
7.1229
7.0952
6.9004
6.8761
6.8512
6.7120
6.6857
5.0116
4.9951
4.8821
4.8207
4.7190
4.6703
4.6109
4.5690
4.4891
4.4580
4.4137
4.3650
4.0236
4.0076
3.9925
3.9764
3.1793
OMe
H
H
Ph
O
N
O
Bn
(+)-1e
Integral
1.0000
0.0590
0.3181
0.0639
0.1777
7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0
(ppm)


210.5917
166.1727
157.7877
136.2182
134.2401
129.2222
128.6332
128.6041
128.5314
128.4514
128.1605
127.5714
127.1569
127.0842
121.8845
115.8776
115.6085
102.0675
81.6033
79.8798
77.8581
77.4218
77.0000
76.5782
58.5430
55.4377
46.0201
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40
(ppm)


7.2505
7.1444
7.1405
7.1147
7.1122
7.0382
7.0158
7.0124
6.9920
6.9671
5.1514
5.1363
4.6479
4.6377
4.6269
4.6143
4.6026
4.5919
4.5817
4.4297
4.4190
4.4083
4.3961
4.3840
4.3733
4.3625
4.0553
4.0402
4.0246
4.0090
3.9915
3.9608
3.9443
3.9219
3.8990
3.8766
3.8547
3.3434
1.7102
1.6995
1.6888
1.3791
1.3567
1.3153
1.2934
OMe
H
H
Me
O
N
O
(+)-1f
Integral
1.0714
1.0000
0.3558
0.3034
0.2967
0.9957
0.8872
0.9733
2.3179
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)


208.5337
165.7872
158.0277
129.2804
121.8554
115.6522
94.5044
82.5415
79.0799
74.7747
58.6375
55.5831
46.0346
21.2434
19.8981
14.3057
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)


7.2082
7.2038
7.1960
7.1858
7.1794
7.1707
6.9866
6.9832
6.9798
6.9589
6.9374
6.9340
6.9306
6.8060
6.8001
6.7962
6.7889
6.7743
6.7704
6.7675
5.0603
5.0438
5.0238
4.9824
4.8436
4.8022
4.5281
4.4974
4.2325
4.2160
4.2019
4.1853
4.1697
4.1449
4.1215
3.9983
3.9754
3.9530
3.9306
3.9077
3.8849
3.4320
1.4195
1.3966
1.3519
1.3295
OMe
H
H
Ph
O
N
O
(+)-1g
Integral
0.9380
0.1451
0.0738
0.0781
0.0872
0.0739
0.2337
0.5286
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)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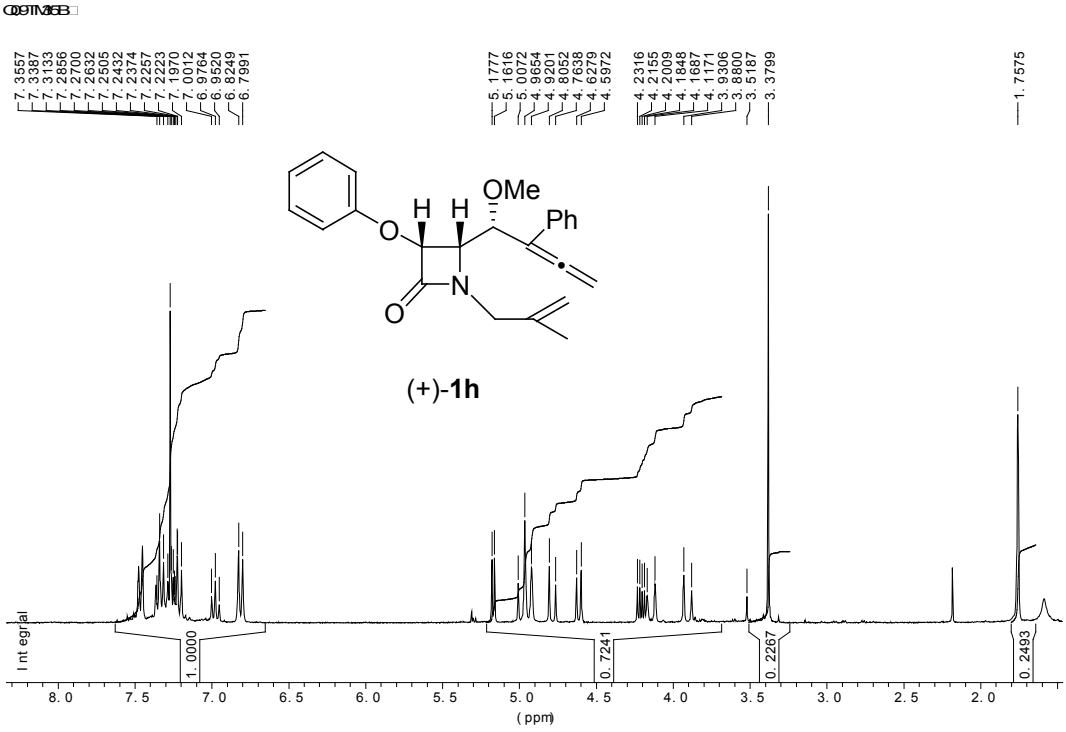
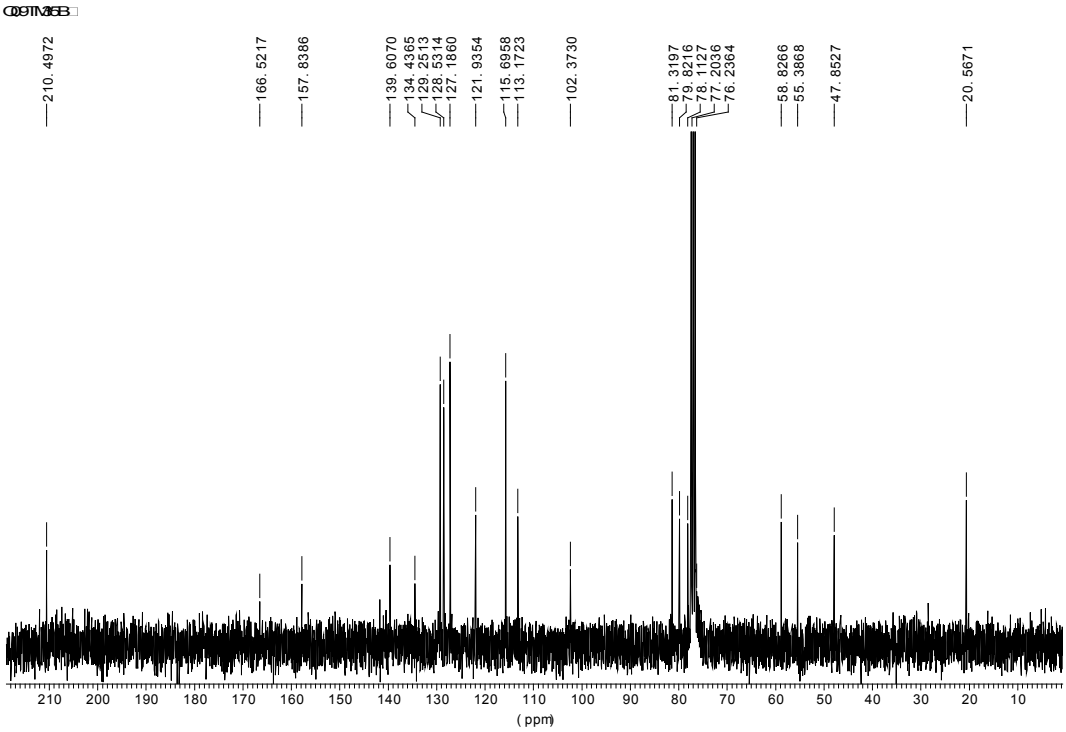
165.8600
157.8968
134.6837
129.2004
128.5459
127.2224
127.1351
121.8045
115.6813
102.4603
81.4725
79.0653
77.9527
77.2036
59.1975
55.6486
46.0928
21.3889
19.9708
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
(ppm)


7.3557
7.3387
7.3133
7.2856
7.2700
7.2632
7.2505
7.2432
7.2374
7.2257
7.2223
7.1970
7.0012
6.9764
6.9520
6.8249
6.7991
5.1777
5.1616
5.0072
4.9654
4.9201
4.8052
4.7638
4.6279
4.5972
4.2316
4.2155
4.2009
4.1848
4.1687
4.1171
3.9306
3.8800
3.5187
3.3799
1.7575
OMe
H H
Ph
O
N
O
(+)-1h
Integral
1.0000
0.7241
0.2267
0.2493
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
(ppm)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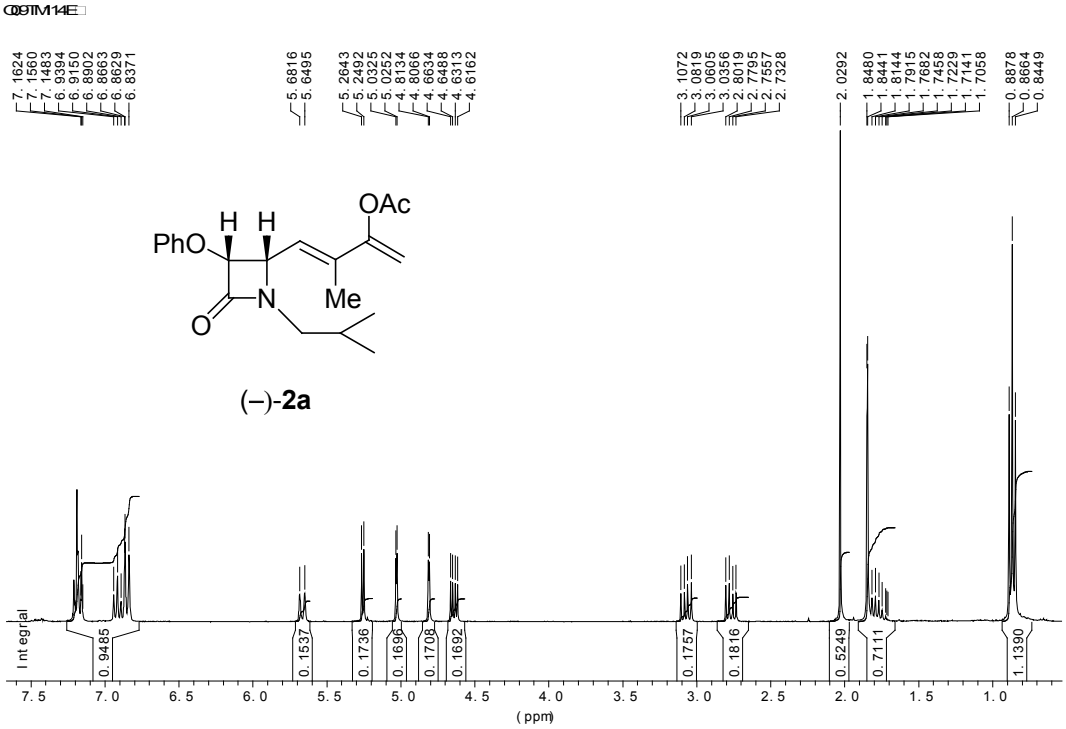
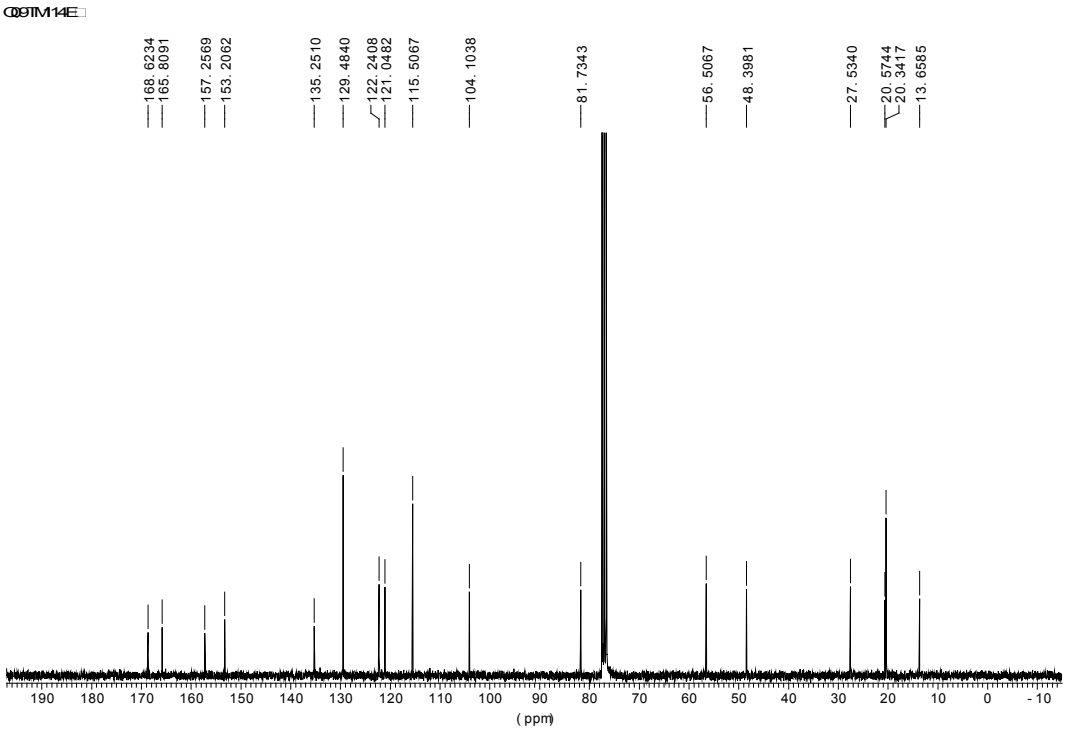
166.5217
157.8386
139.6070
134.4365
129.2513
128.5314
127.1860
121.9354
115.6958
113.1723
102.3730
81.3197
79.8216
78.1127
77.2036
76.2364
58.8266
55.3868
47.8527
20.5671
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)


7.1624
7.1560
7.1483
6.9394
6.9150
6.8902
6.8663
6.8629
6.8371
5.6816
5.6495
5.2643
5.2492
5.0325
5.0252
4.8134
4.8066
4.6634
4.6488
4.6313
4.6162
3.1072
3.0819
3.0605
3.0356
2.8019
2.7795
2.7557
2.7328
2.0292
1.8480
1.8441
1.8144
1.7915
1.7682
1.7458
1.7229
1.7141
1.7058
0.8878
0.8664
0.8449
OAc
H H
PhO
N
Me
O
(–)-2a
Integral
0.9485
0.1537
0.1736
0.1696
0.1708
0.1692
0.1757
0.1816
0.5249
0.7111
1.1390
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
(ppm)


168.6234
165.8091
157.2569
153.2062
135.2510
129.4840
122.2408
121.0482
115.5067
104.1038
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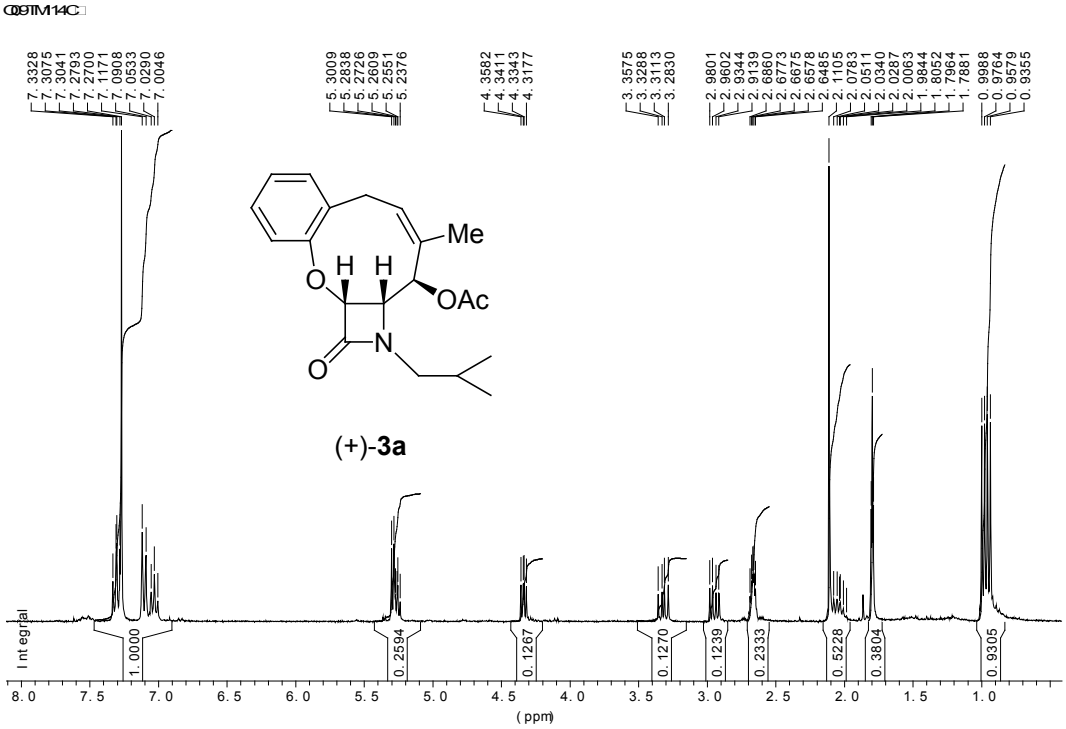
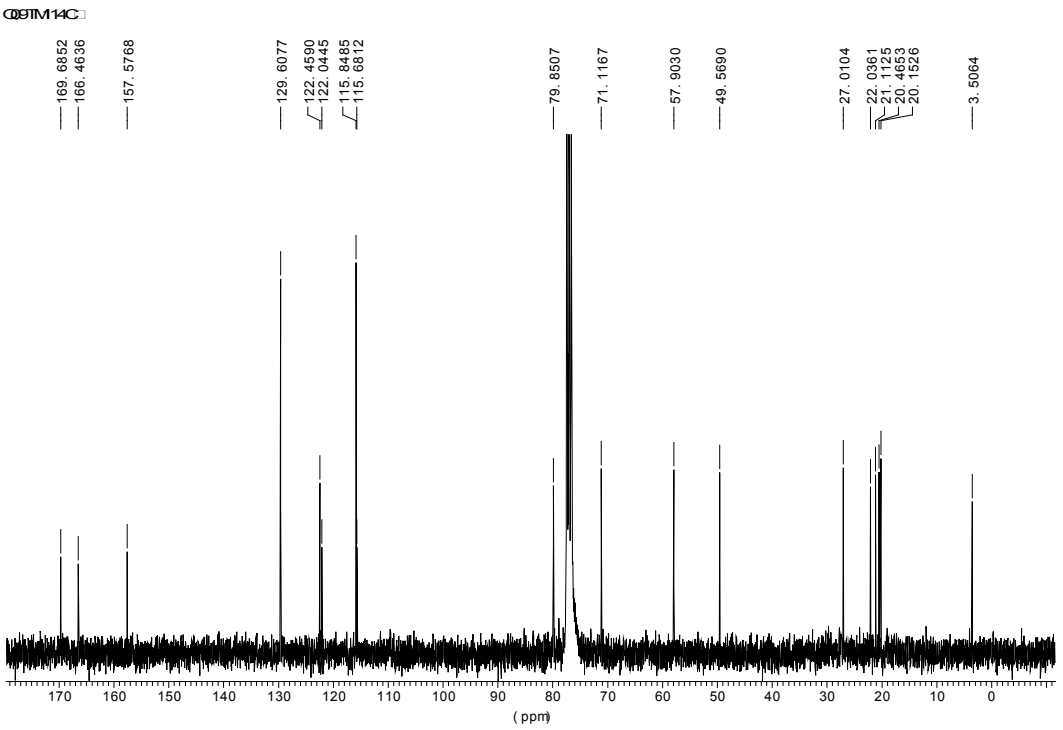
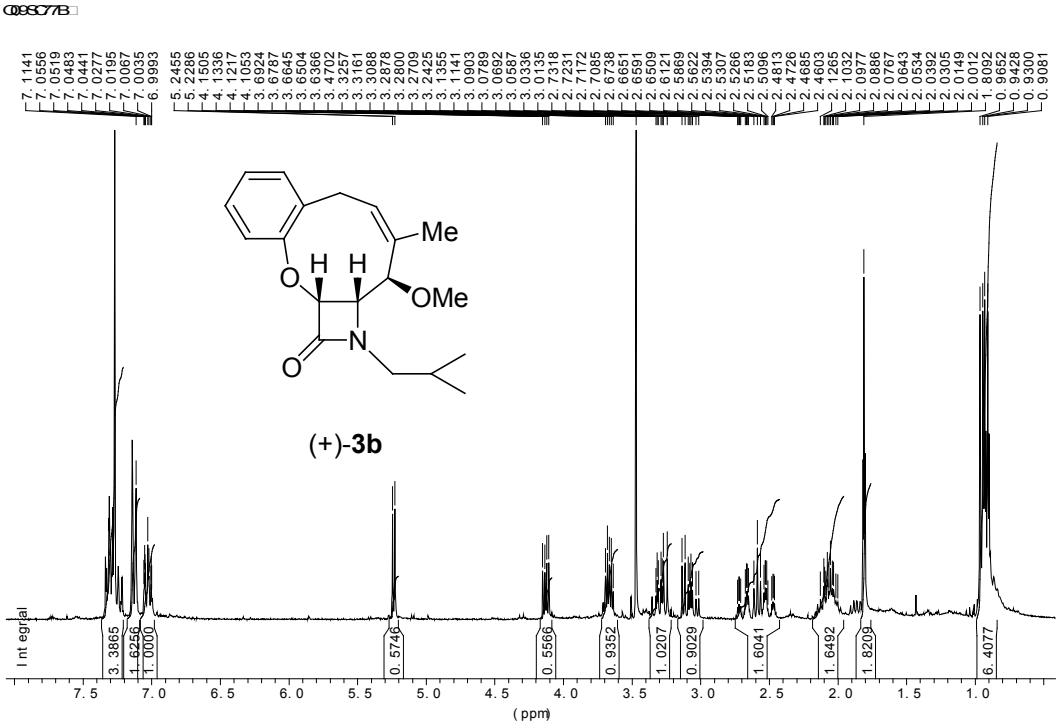
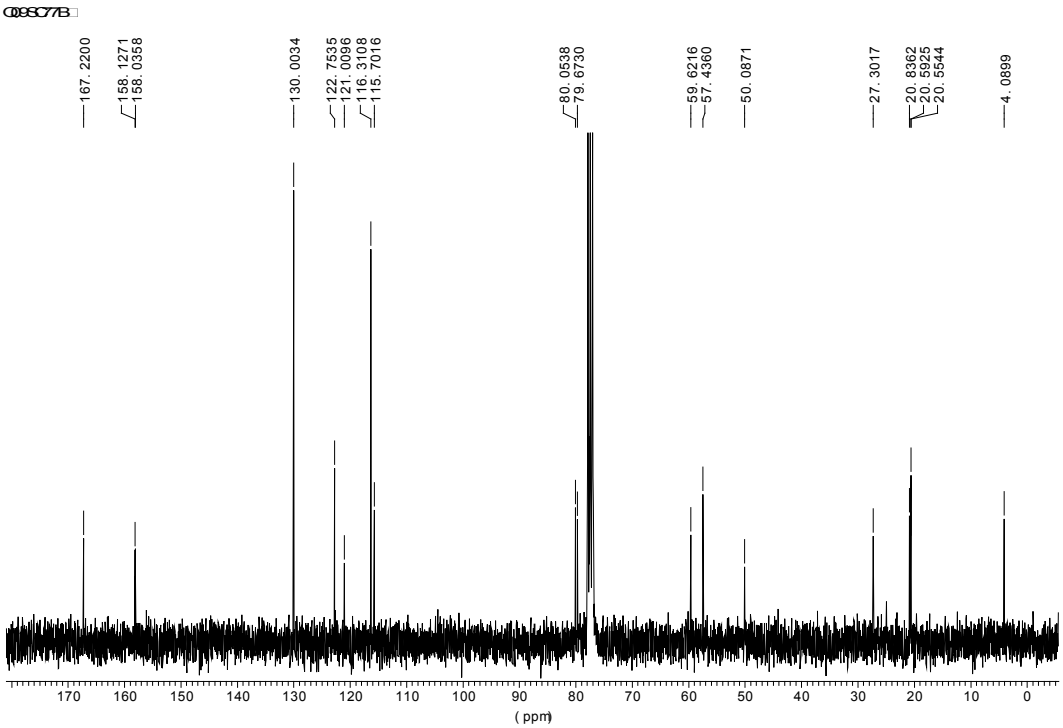
56.5067
48.3981
27.5340
20.5744
20.3417
13.6585
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)


Me
O
H
H
OAc
N
O
(+)-3a
Integral
1.0000
0.2594
0.1267
0.1270
0.1239
0.2333
0.5228
0.3804
0.9305
(ppm)


169.6852
166.4636
157.5768
129.6077
122.4590
122.0445
115.8485
115.6812
79.8507
71.1167
57.9030
49.5690
27.0104
22.0361
21.1125
20.4653
20.1526
3.5064
(ppm)


Me
O H H
OMe
N
O
(+)-3b
Integral
3.3865
1.6256
1.0000
0.5746
0.5566
0.9352
1.0207
0.9029
1.6041
1.6492
1.8209
6.4077
(ppm)


167.2200
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158.0358
130.0034
122.7535
121.0096
116.3108
115.7016
80.0538
79.6730
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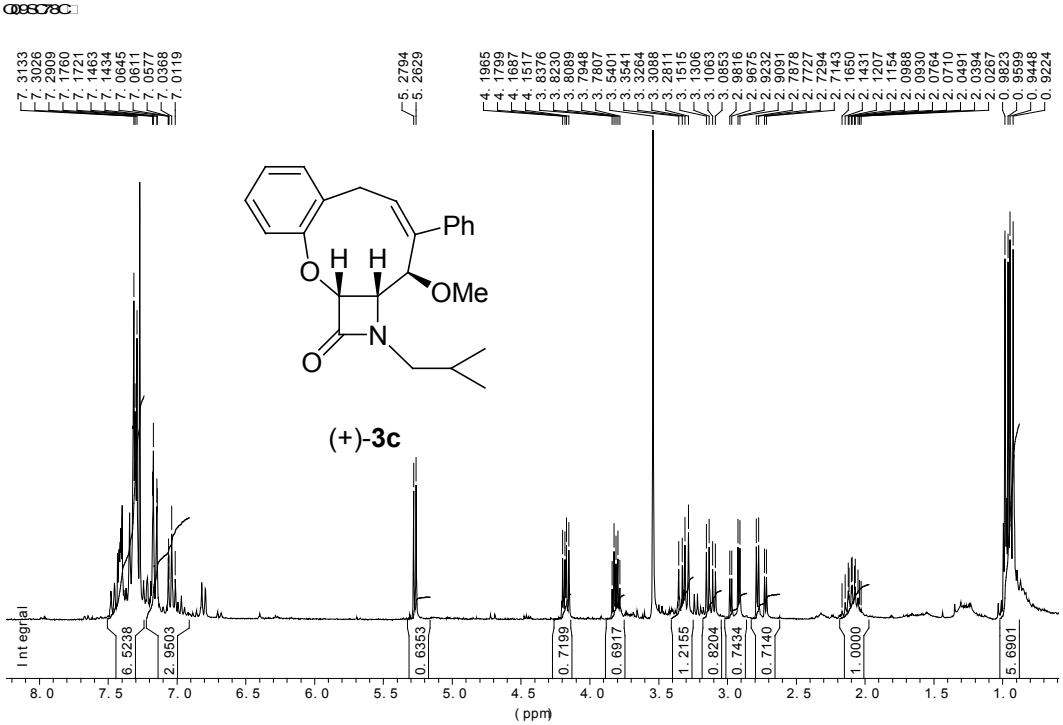
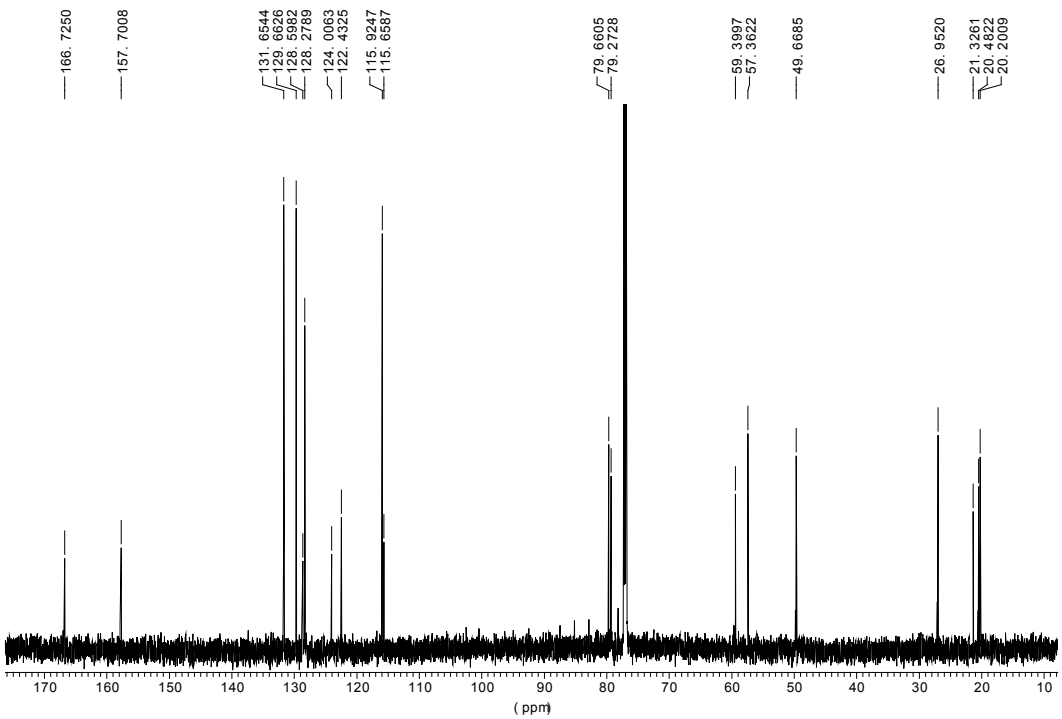
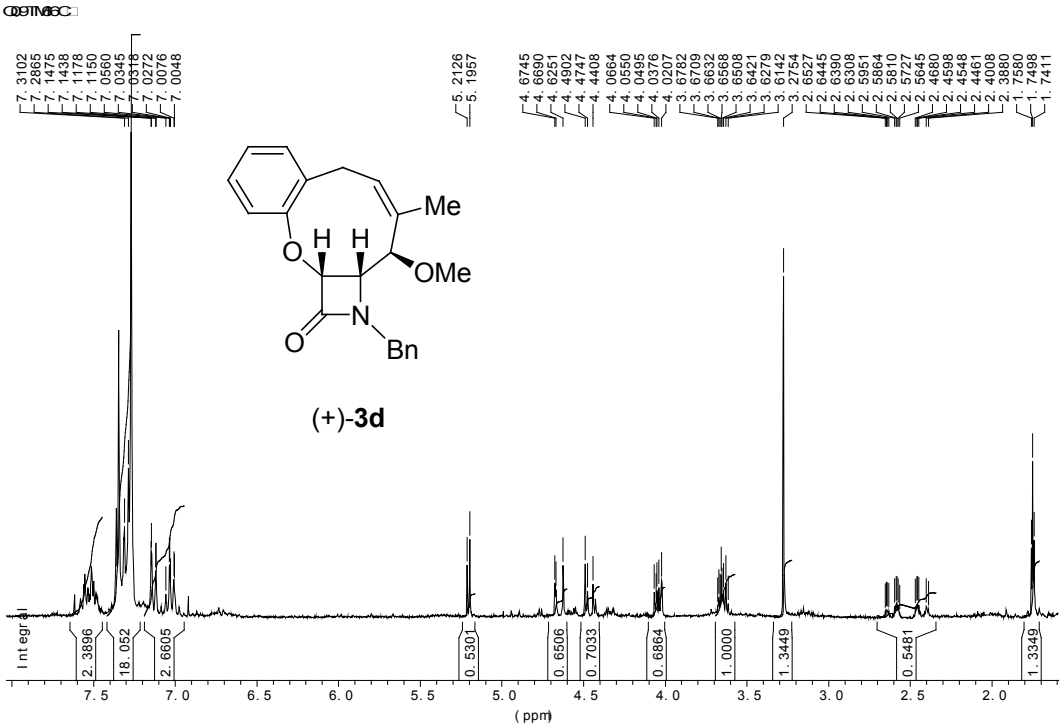
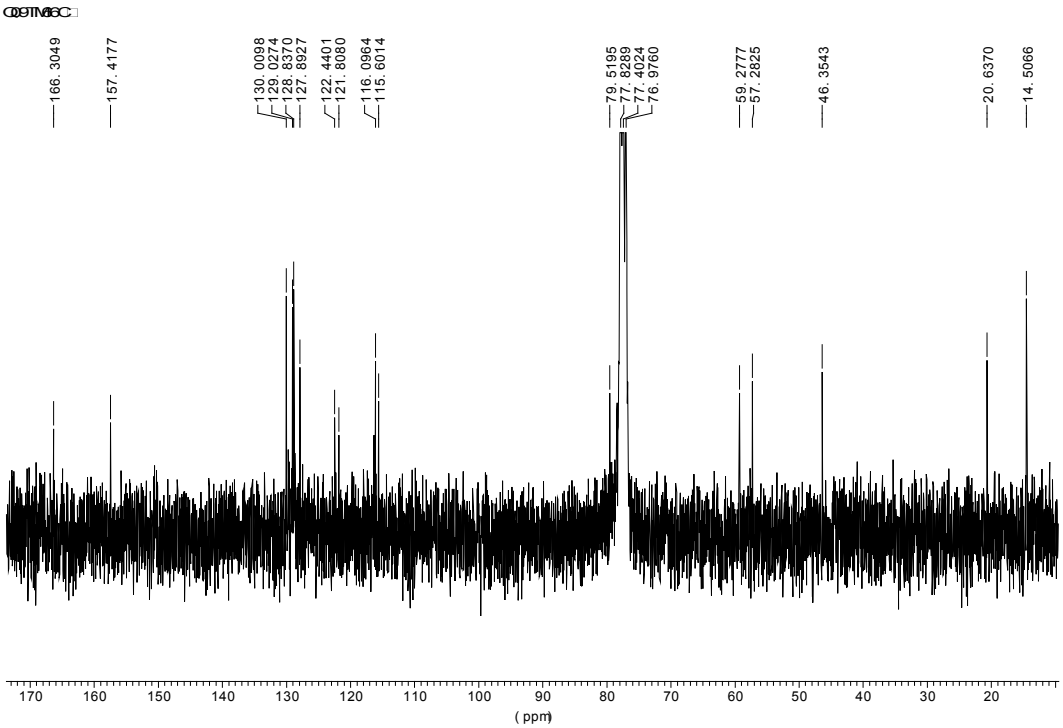
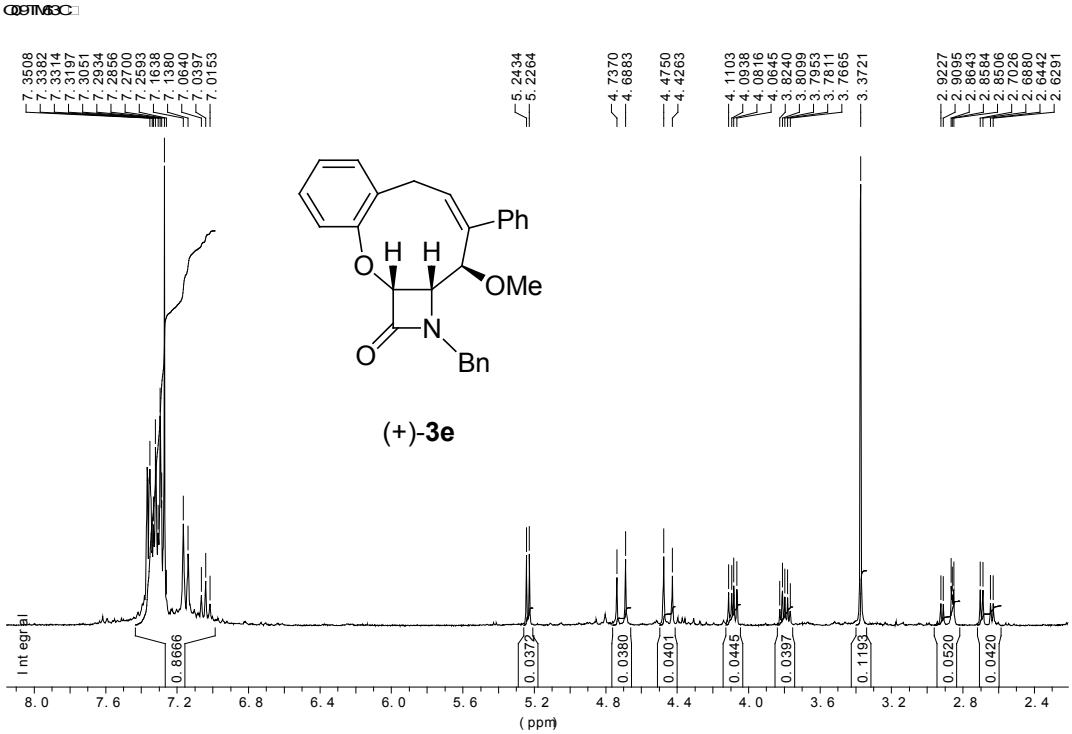
57.4360
50.0871
27.3017
20.8362
20.5925
20.5544
4.0899
(ppm)


Ph
H
H
OMe
O
N
O
(+)-3c
(ppm)


(ppm)


Me
H H
O
OMe
N
O
Bn
(+)-3d
(ppm)


(ppm)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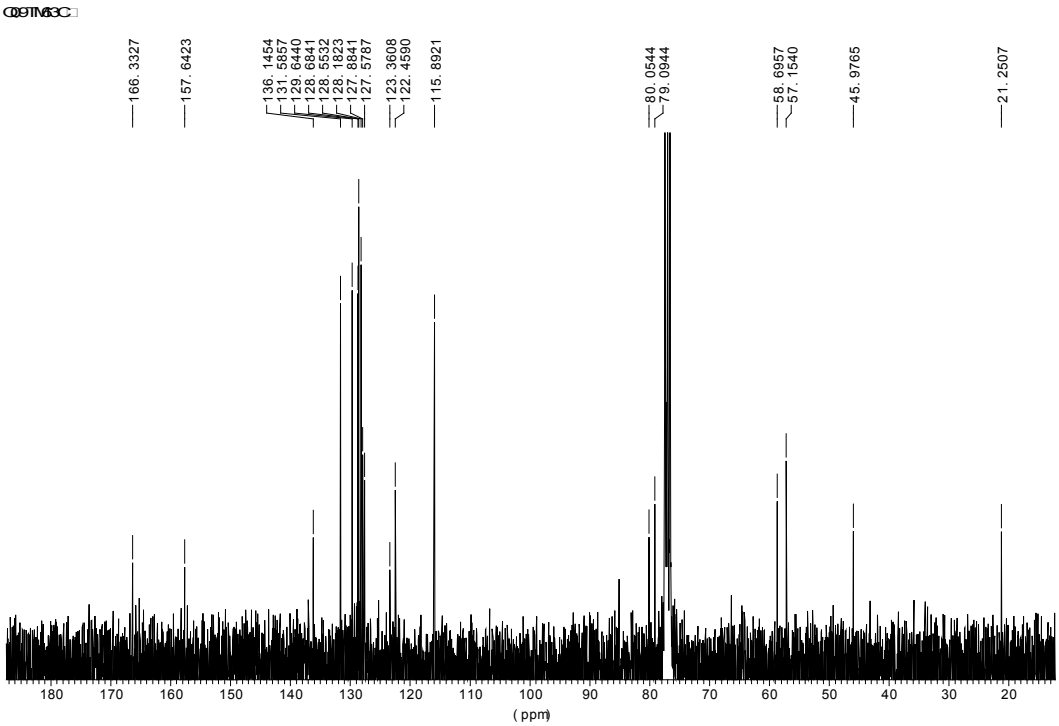
7.3382
7.3314
7.3197
7.3051
7.2934
7.2856
7.2700
7.2593
7.1638
7.1380
7.0640
7.0397
7.0153
5.2434
5.2264
4.7370
4.6883
4.4750
4.4263
4.1103
4.0938
4.0816
4.0645
3.8240
3.8099
3.7953
3.7811
3.7665
3.3721
2.9227
2.9095
2.8643
2.8584
2.8506
2.7026
2.6880
2.6442
2.6291
Ph
H H
O
OMe
N
O
Bn
(+)-3e
Integral
0.8666
0.037
0.380
0.401
0.445
0.397
1.193
0.520
0.420
8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4
(ppm)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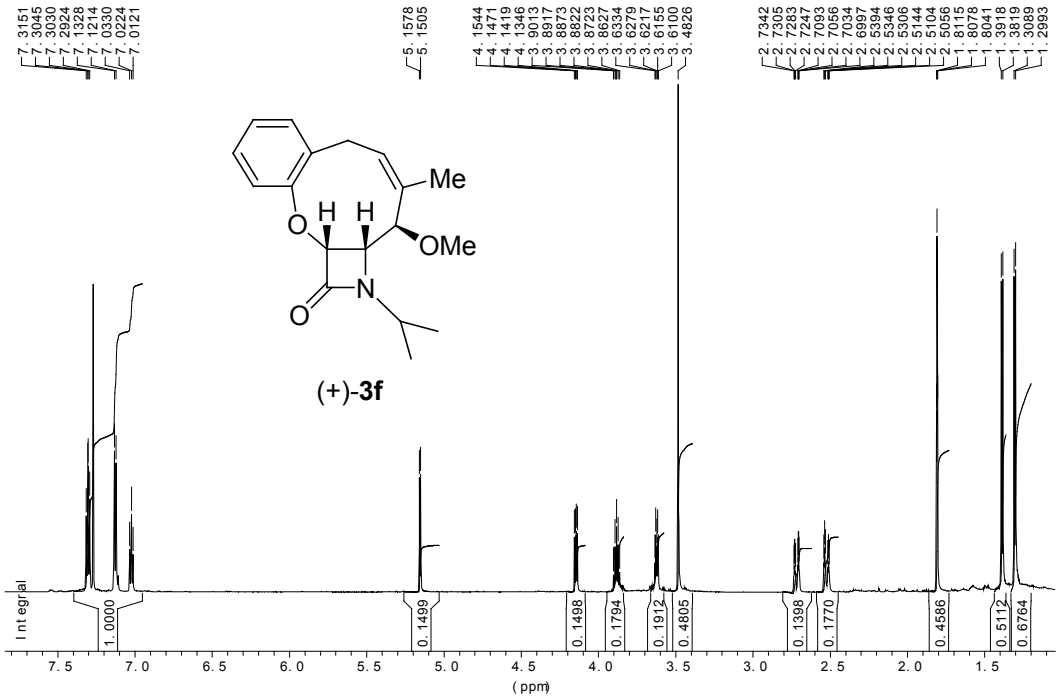
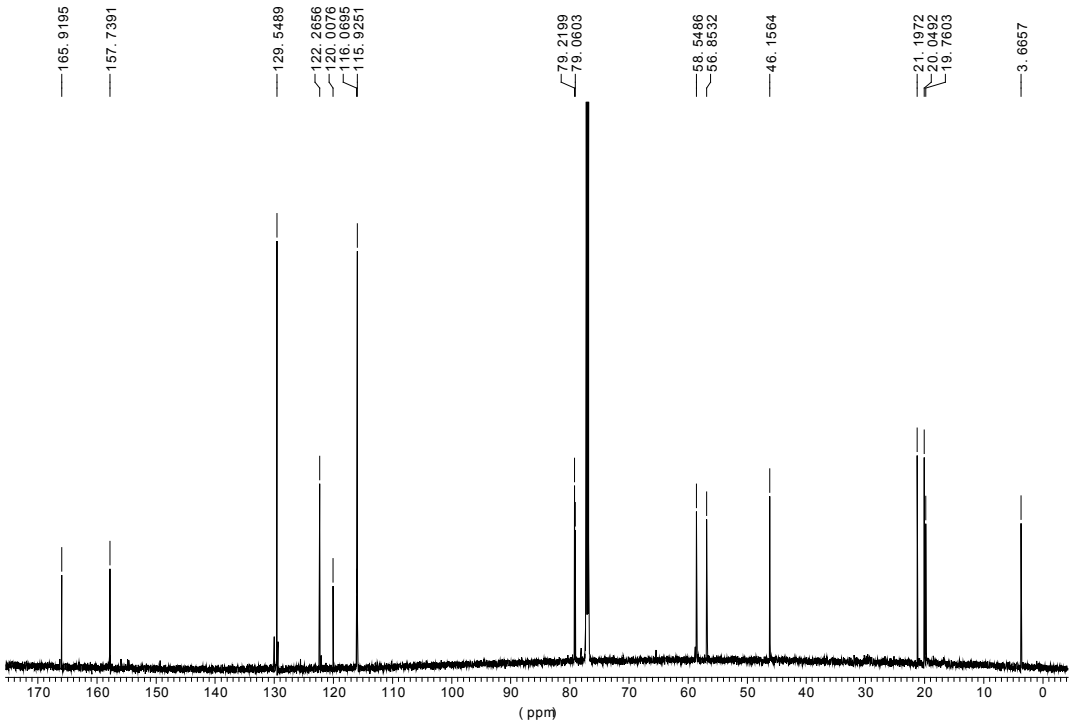
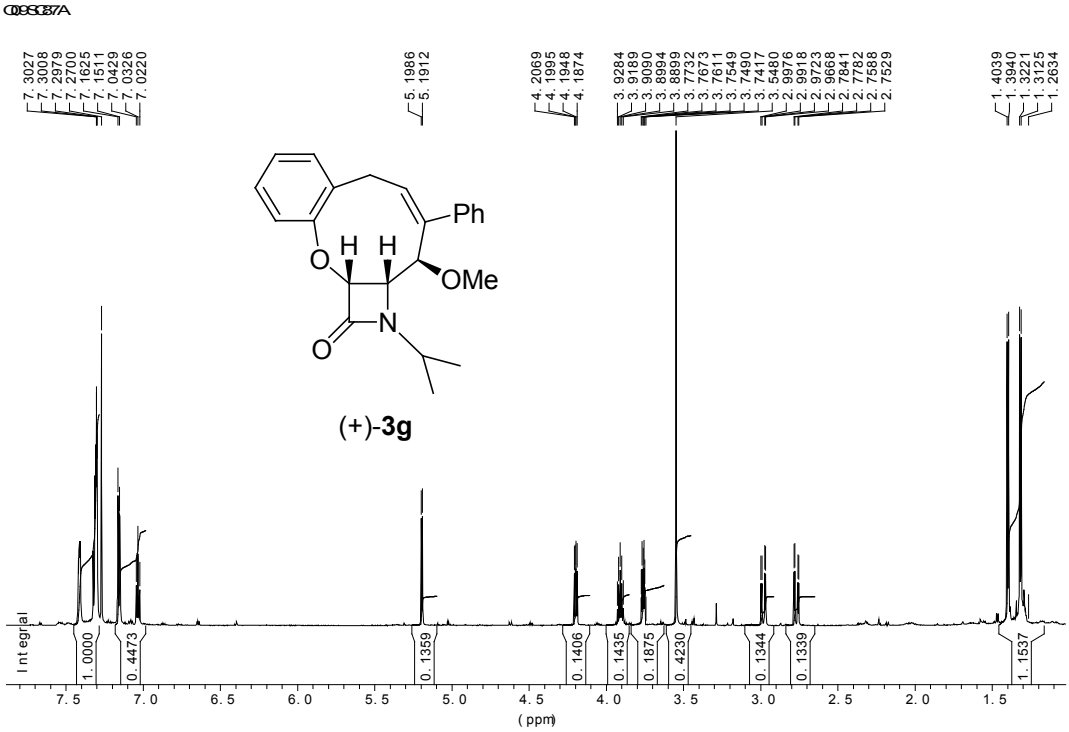
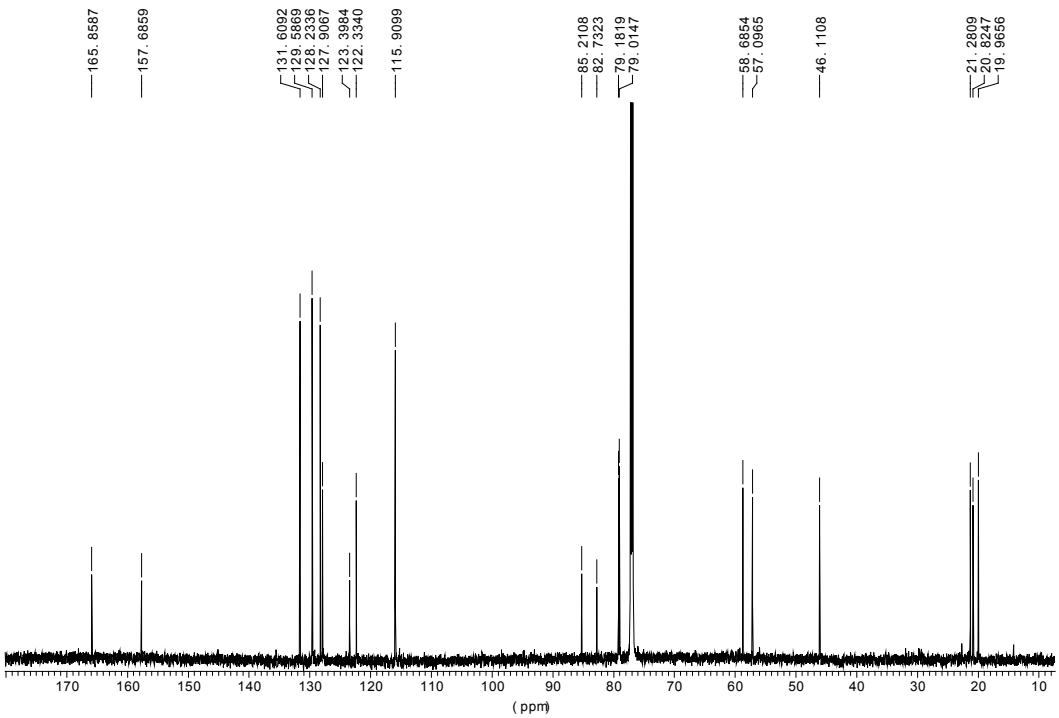
136.1454
131.5857
129.6440
128.6841
128.5532
128.1823
127.8841
127.5787
123.3608
122.4590
115.8921
80.0544
79.0944
58.6957
57.1540
45.9765
21.2507
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
(ppm)


Me
H H
O
OMe
N
O
(+)-3f
(ppm)


(ppm)


7.3027
7.3008
7.2979
7.2700
7.1625
7.1511
7.0429
7.0326
7.0220
5.1986
5.1912
4.2069
4.1995
4.1948
4.1874
3.9284
3.9189
3.9090
3.8994
3.8899
3.7732
3.7673
3.7611
3.7549
3.7490
3.7417
3.5480
2.9976
2.9918
2.9723
2.9668
2.7841
2.7782
2.7588
2.7529
1.4039
1.3940
1.3221
1.3125
1.2634
Ph
H
H
O
OMe
N
O
(+)-3g
Integral
1.0000
0.4473
0.1359
0.1406
0.1435
0.1875
0.4230
0.1344
0.1339
1.1537
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
(ppm)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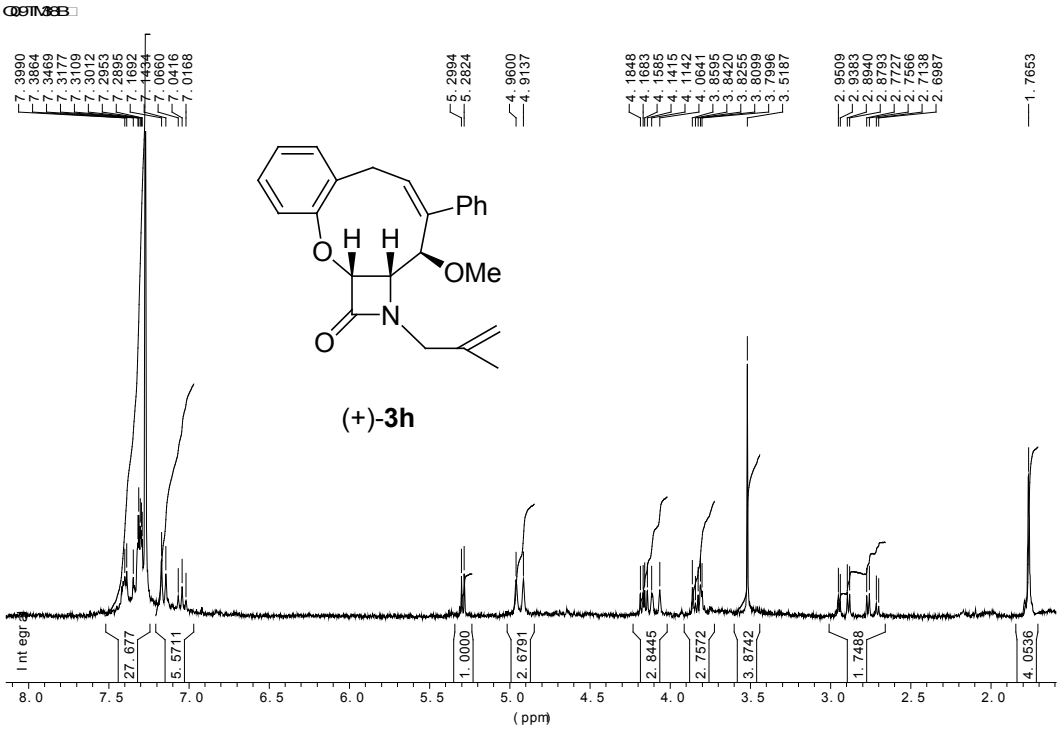
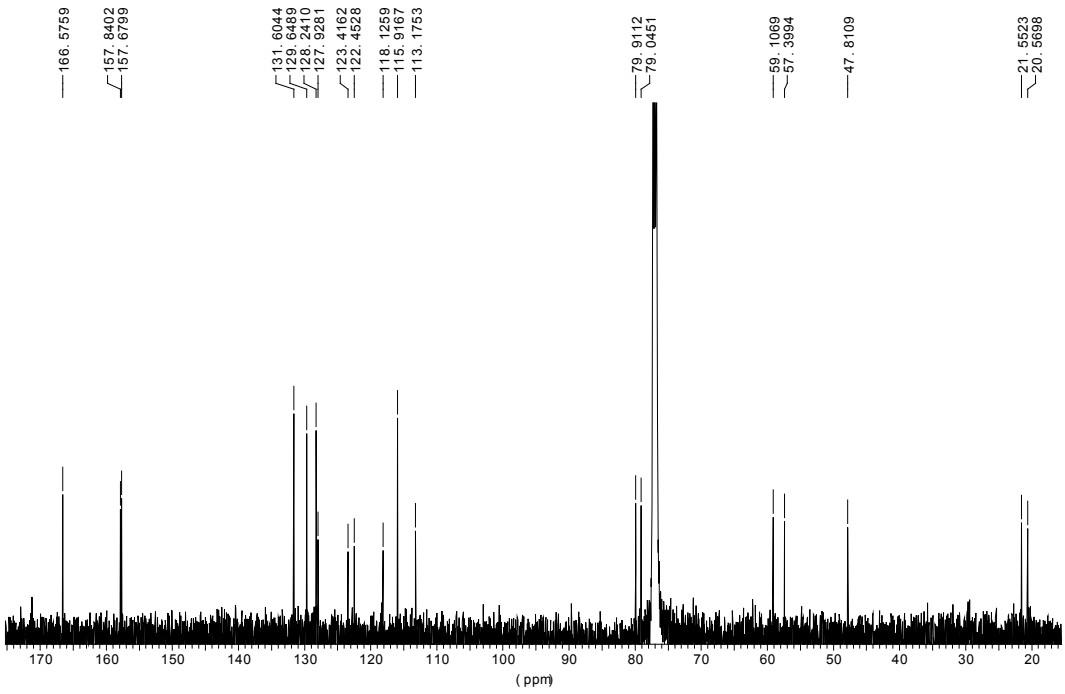
157.6859
131.6092
129.5869
128.2336
127.9067
123.3984
122.3340
115.9099
85.2108
82.7323
79.1819
79.0147
58.6854
57.0965
46.1108
21.2809
20.8247
19.9656
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)


7.3990
7.3864
7.3469
7.3177
7.3109
7.3012
7.2953
7.2895
7.1692
7.1434
7.0660
7.0416
7.0168
5.2994
5.2824
4.9600
4.9137
4.1848
4.1683
4.1585
4.1415
4.1142
4.0641
3.8595
3.8420
3.8255
3.8099
3.7996
3.5187
2.9509
2.9383
2.8940
2.8793
2.7727
2.7566
2.7138
2.6987
1.7653
Ph
O
H
H
OMe
N
O
(+)-3h
Int egral
27.677
5.5711
1.0000
2.6791
2.8445
2.7572
3.8742
1.7488
4.0536
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
(ppm)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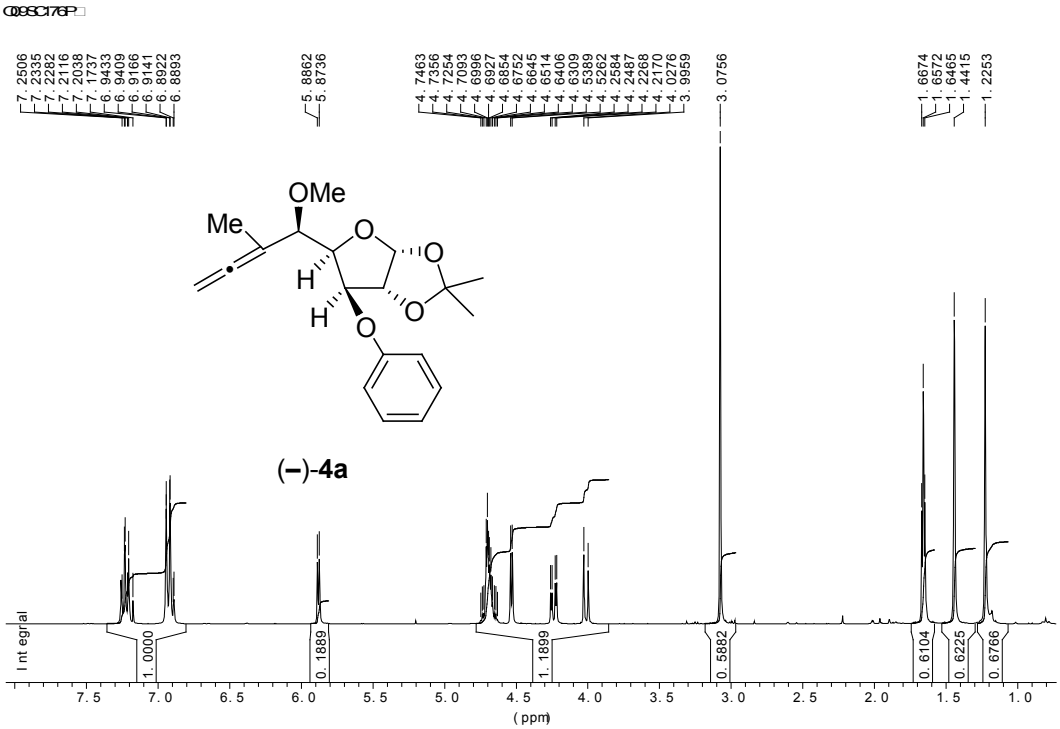
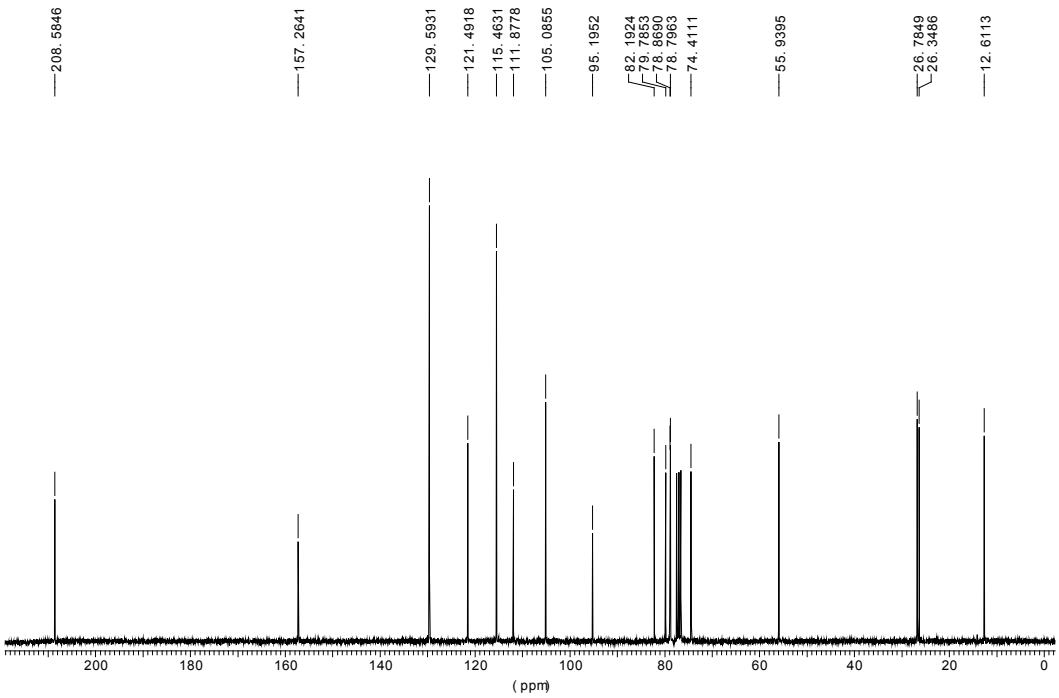
157.6799
131.6044
128.6489
128.2410
127.9281
123.4162
122.4528
118.1259
115.9167
113.1753
79.9112
79.0451
59.1069
57.3994
47.8109
21.5523
20.5698
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
(ppm)


OMe
Me
O
O
H
H
O
O
(–)-4a
7.2506
7.2335
7.2282
7.2116
7.2038
7.1737
6.9433
6.9409
6.9166
6.9141
6.8922
6.8893
5.8862
5.8736
4.7463
4.7356
4.7254
4.7093
4.6996
4.6927
4.6854
4.6752
4.6645
4.6514
4.6406
4.6309
4.5389
4.5262
4.2584
4.2487
4.2268
4.2170
4.0276
3.9959
3.0756
1.6674
1.6572
1.6465
1.4415
1.2253
Integral
1.0000
0.1889
1.1899
0.5882
0.6104
0.6225
0.6766
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)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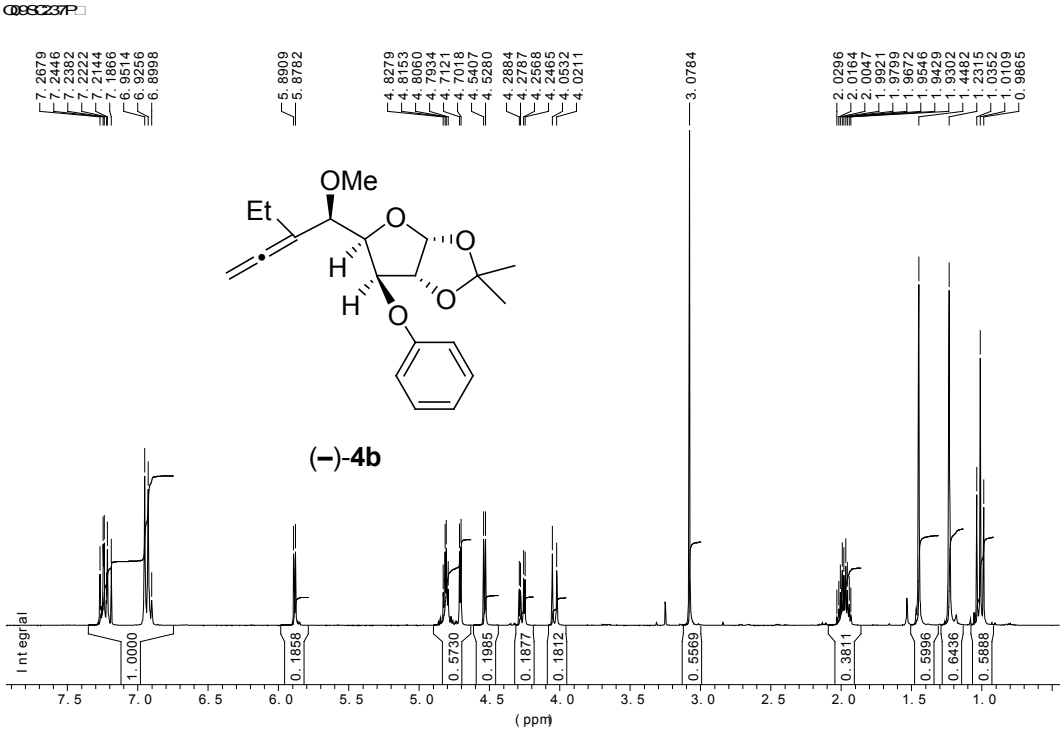
129.5931
121.4918
115.4631
111.8778
105.0855
95.1952
82.1924
79.7853
78.8690
78.7963
74.4111
55.9395
26.7849
26.3486
12.6113
200
180
160
140
120
100
80
60
40
20
0
(ppm)


Q09SC237P
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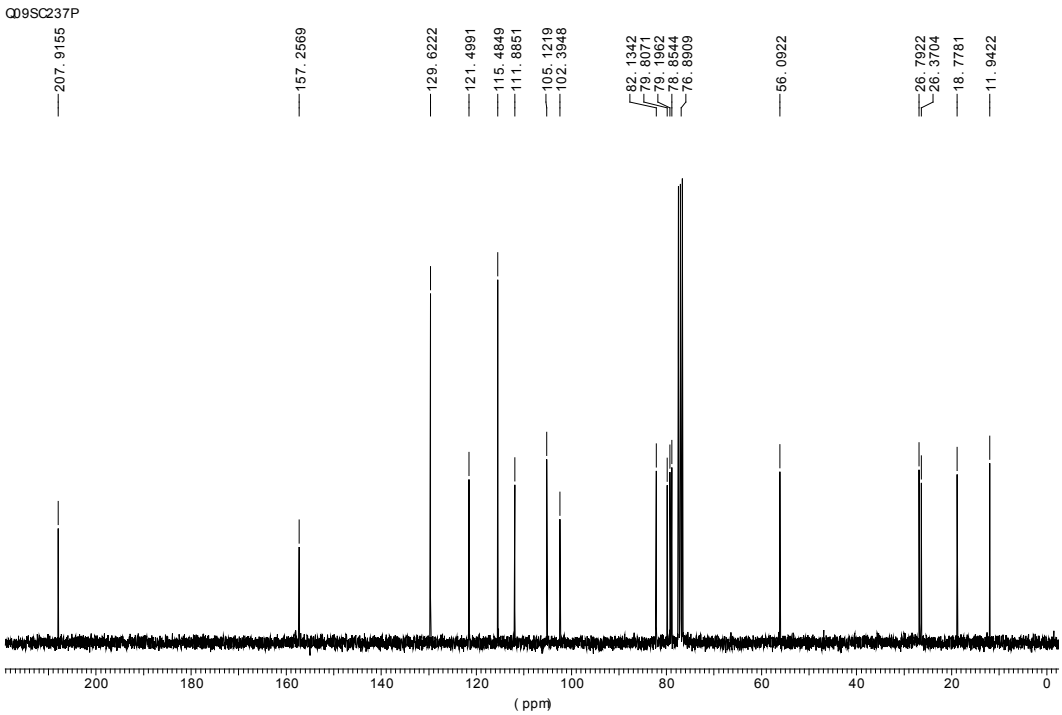
7.2446
7.2382
7.2222
7.2144
7.1866
6.9514
6.9256
6.8998
5.8909
5.8782
4.8279
4.8153
4.8060
4.7934
4.7121
4.7018
4.5407
4.5280
4.2884
4.2787
4.2568
4.2465
4.0532
4.0211
3.0784
2.0296
2.0164
2.0047
1.9921
1.9799
1.9672
1.9546
1.9429
1.9302
1.4482
1.2315
1.0352
1.0109
0.9865
OMe
Et
O
O
H
H
O
O
(−)-4b
Integral
1.0000
0.1858
0.5730
0.1985
0.1877
0.1812
0.5569
0.3811
0.5996
0.6436
0.5888
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)


Q09SC237P
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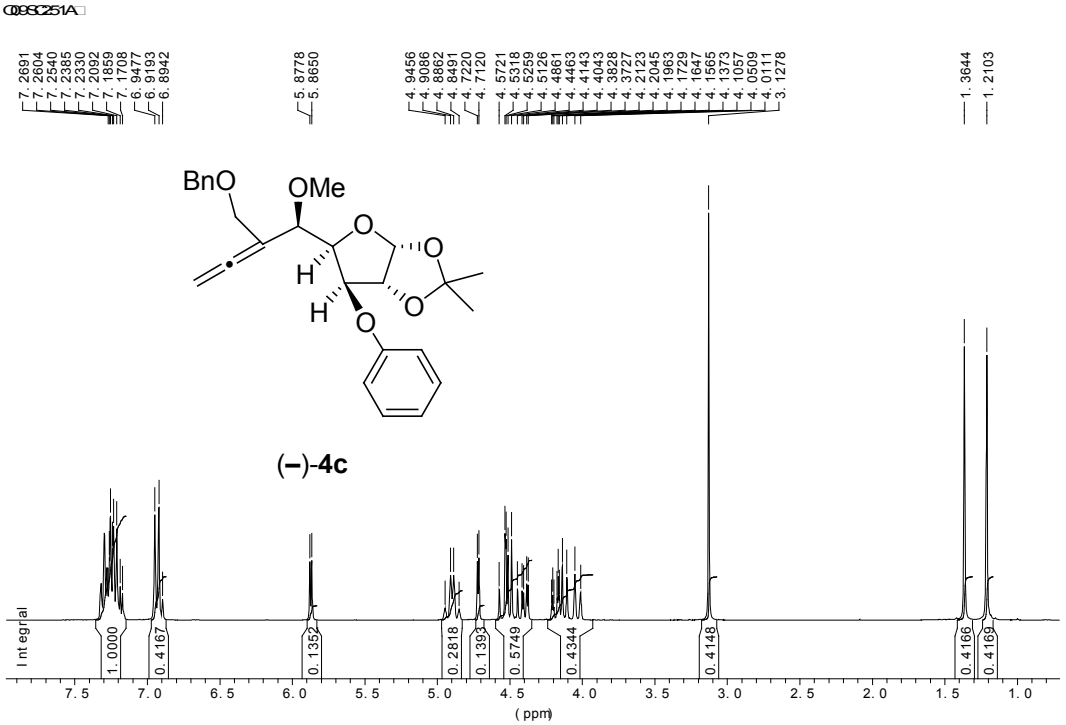
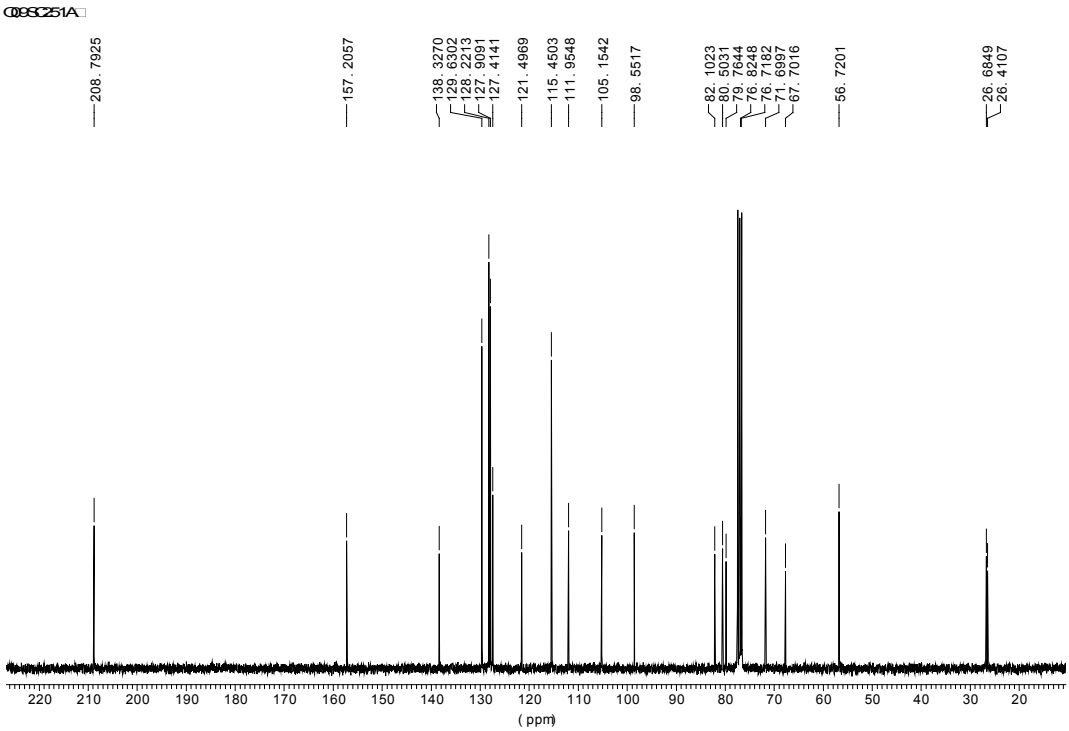
121.4991
115.4849
111.8851
105.1219
102.3948
82.1342
79.8071
79.1962
78.8544
76.8909
56.0922
26.7922
26.3704
18.7781
11.9422
200
180
160
140
120
100
80
60
40
20
0
(ppm)


7.2691
7.2604
7.2540
7.2385
7.2330
7.2092
7.1859
7.1708
6.9477
6.9193
6.8942
5.8778
5.8650
4.9456
4.9086
4.8862
4.8491
4.7220
4.7120
4.5721
4.5318
4.5258
4.5126
4.4861
4.4463
4.4143
4.4043
4.3828
4.3727
4.2123
4.2045
4.1963
4.1729
4.1647
4.1565
4.1373
4.1057
4.0509
4.0111
3.1278
1.3644
1.2103
BnO
OMe
O
O
H
H
O
O
O
(−)-4c
Integral
1.0000
0.4167
0.1352
0.2818
0.1393
0.5749
0.4344
0.4148
0.4166
0.4169
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)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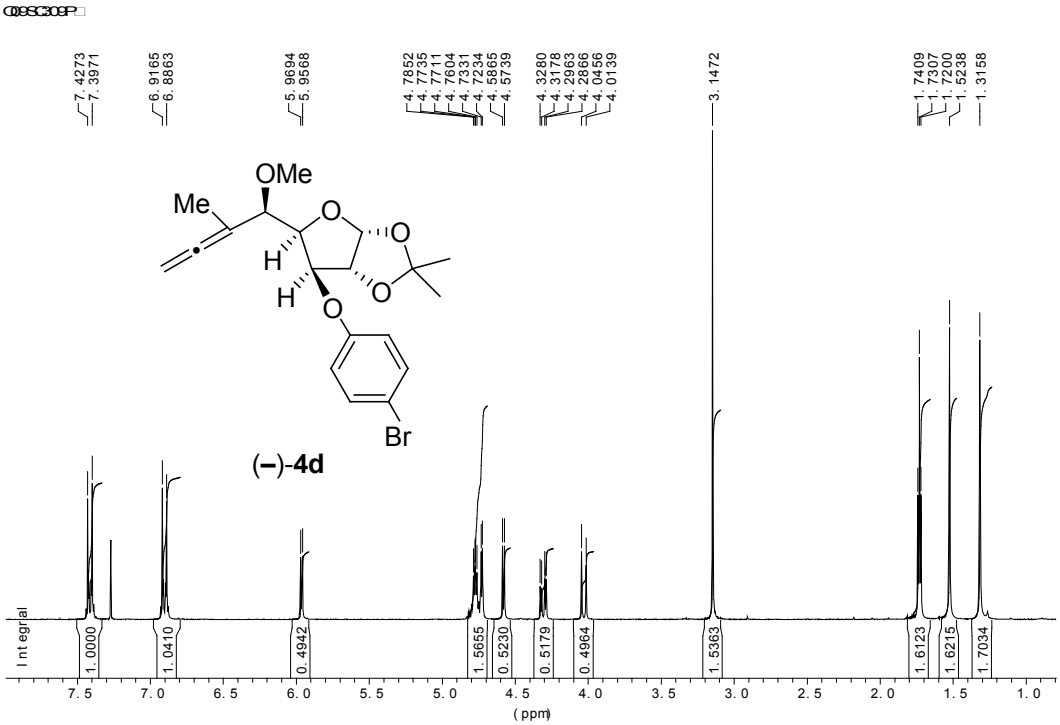
128.2213
127.9091
127.4141
121.4969
115.4503
111.9548
105.1542
98.5517
82.1023
80.5031
79.7644
76.8248
76.7182
71.6997
67.7016
56.7201
26.6849
26.4107
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
(ppm)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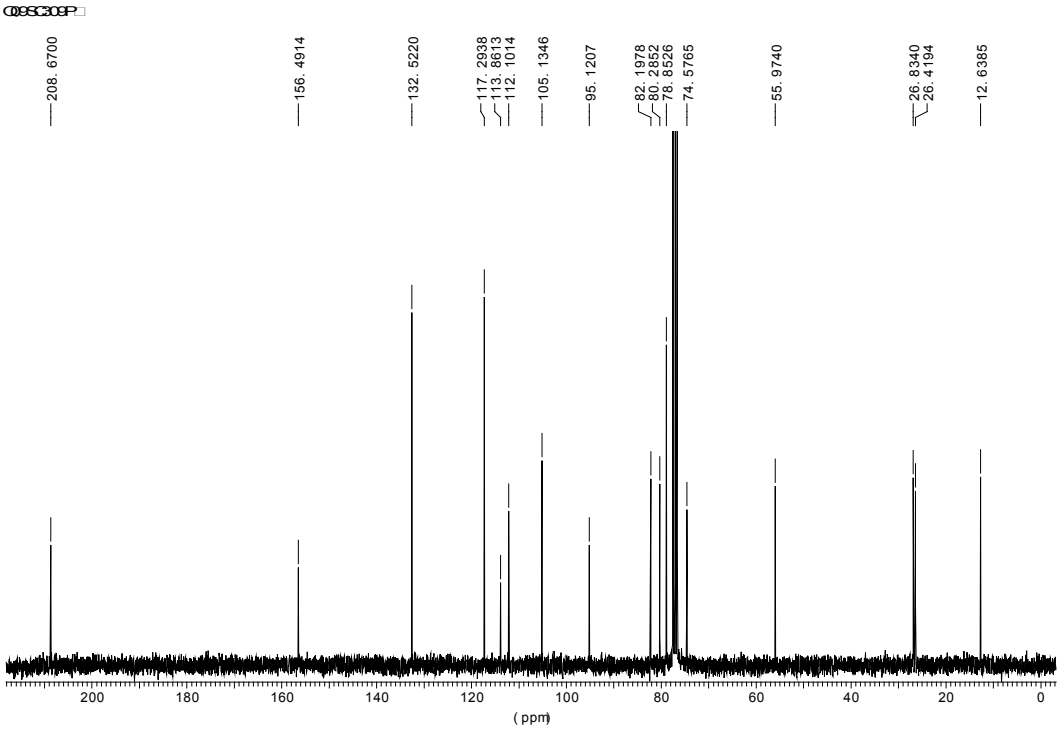
5.9694
5.9568
4.7852
4.7735
4.7711
4.7604
4.7331
4.7234
4.6865
4.5739
4.3280
4.3178
4.2963
4.2866
4.0456
4.0139
3.1472
1.7409
1.7307
1.7200
1.5238
1.3158
OMe
Me
O
O
H
H
O
O
O
Br
(–)-4d
Integral
1.0000
1.0410
0.4942
1.5655
0.5230
0.5179
0.4964
1.5363
1.6123
1.6215
1.7034
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)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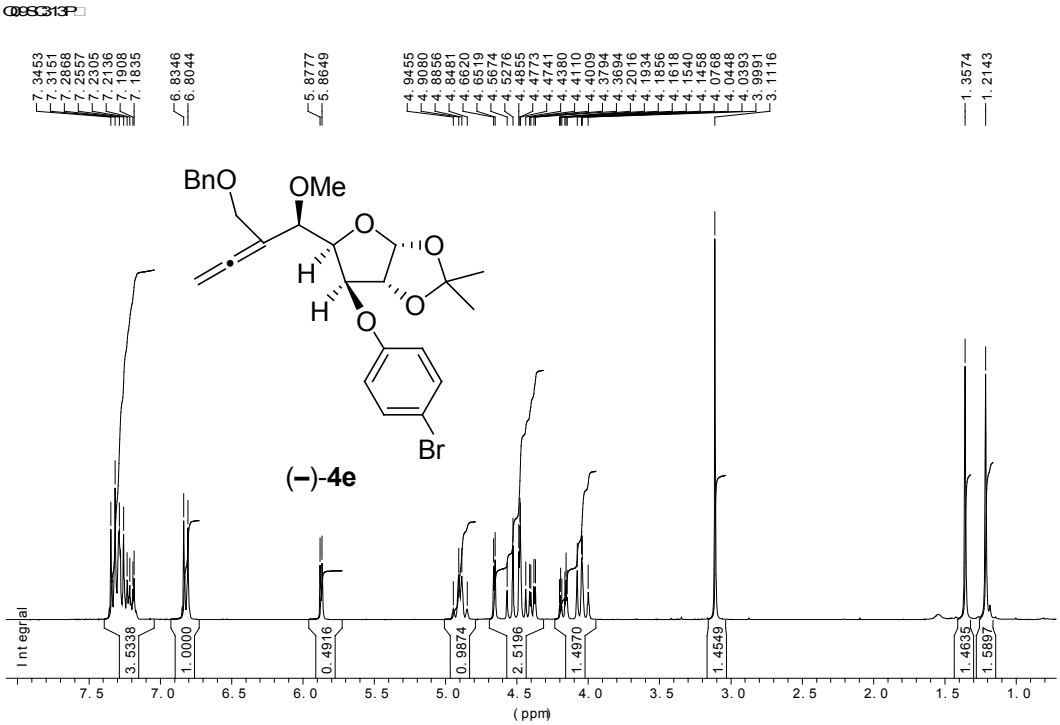
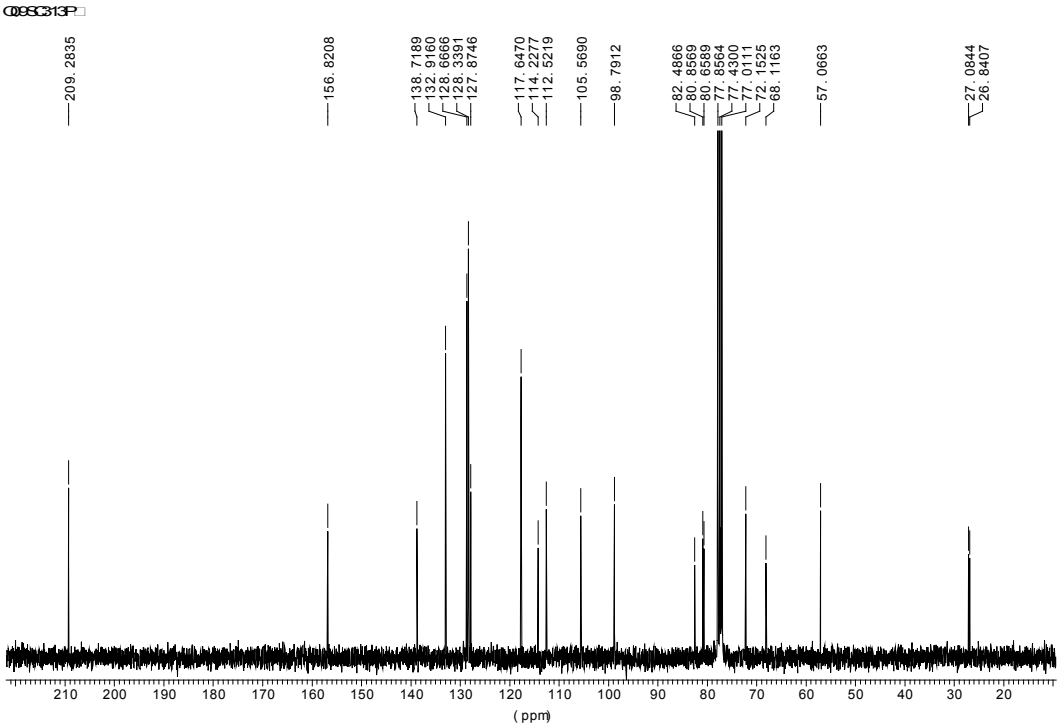
113.8613
112.1014
105.1346
95.1207
82.1978
80.2852
78.8526
74.5765
55.9740
26.8340
26.4194
12.6385
200
180
160
140
120
100
80
60
40
20
0
(ppm)


BnO
OMe
O
O
H
H
O
O
O
Br
(–)-4e
7.3453
7.3151
7.2868
7.2557
7.2305
7.2136
7.1908
7.1835
6.8346
6.8044
5.8777
5.8649
4.9455
4.9080
4.8856
4.8481
4.6620
4.6519
4.5674
4.5276
4.4855
4.4773
4.4741
4.4380
4.4110
4.4009
4.3794
4.3694
4.2016
4.1934
4.1856
4.1618
4.1540
4.1458
4.0768
4.0448
4.0393
3.9991
3.1116
1.3574
1.2143
Integral
3.5338
1.0000
0.4916
0.9874
2.5196
1.4970
1.4549
1.4635
1.5897
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)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138.7189
132.9160
128.6666
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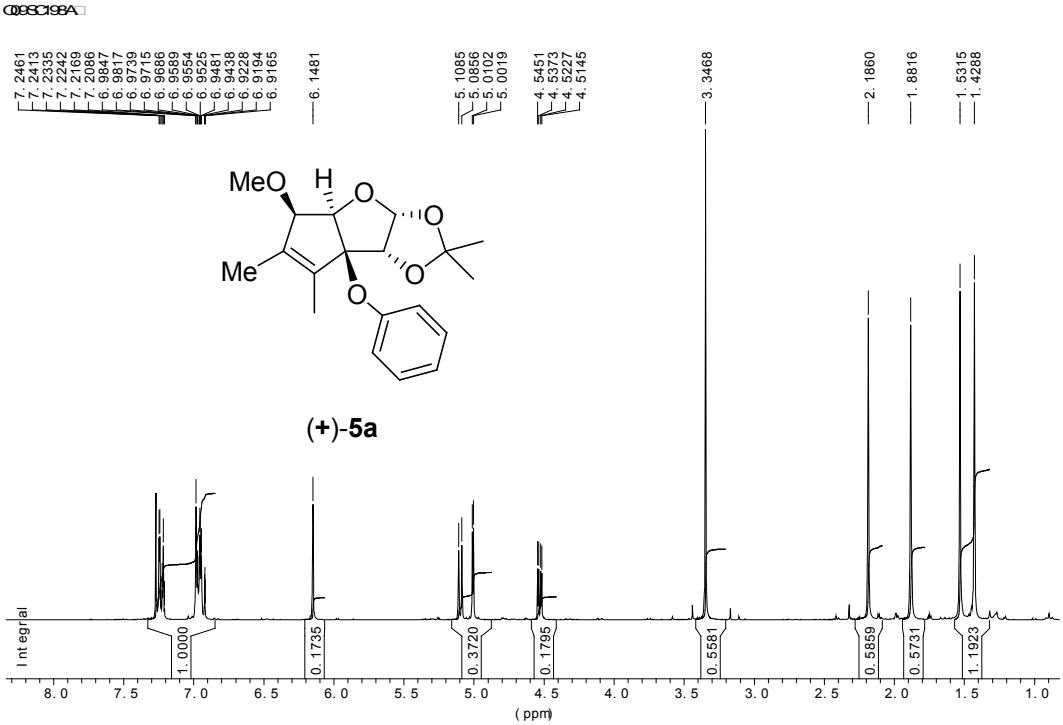
127.8746
117.6470
114.2277
112.5219
105.5690
98.7912
82.4866
80.8569
80.6589
77.8564
77.4300
77.0111
72.1525
68.1163
57.0663
27.0844
26.8407
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
(ppm)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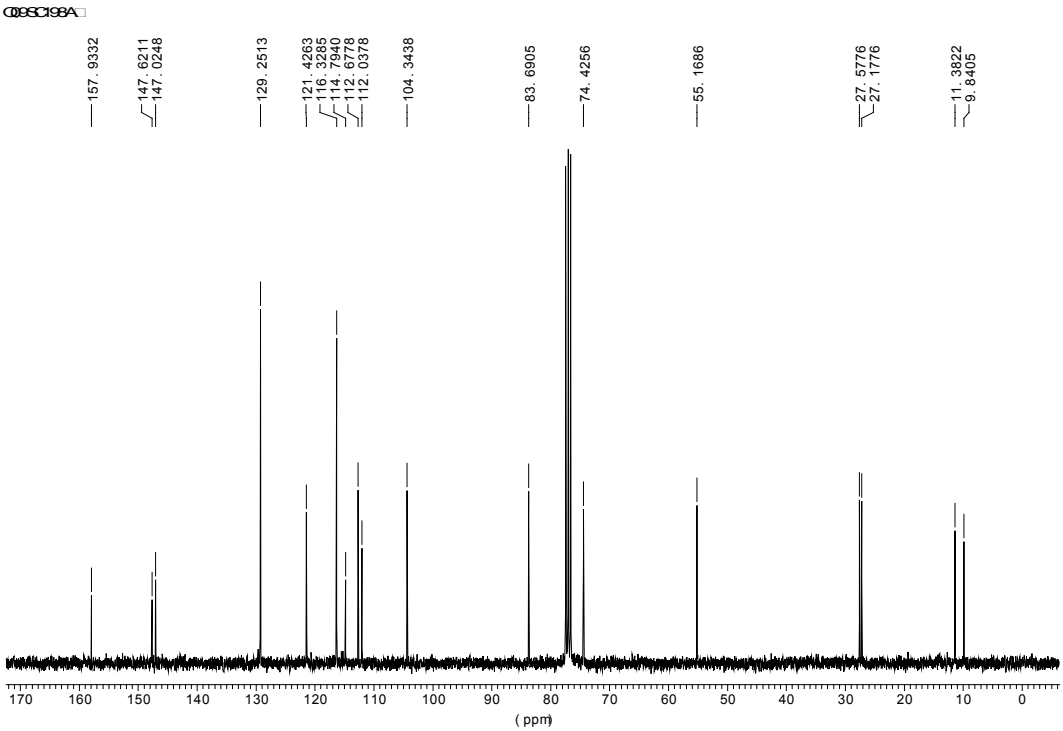
7.2335
7.2242
7.2169
7.2086
6.9847
6.9817
6.9739
6.9715
6.9686
6.9589
6.9554
6.9525
6.9481
6.9438
6.9228
6.9194
6.9165
6.1481
5.1085
5.0856
5.0102
5.0019
4.5451
4.5373
4.5227
4.5145
3.3468
2.1860
1.8816
1.5315
1.4288
MeO
H
O
O
Me
O
O
(+)-5a
Integral
1.0000
0.1735
0.3720
0.1795
0.5581
0.5859
0.5731
1.1923
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)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74.4256
55.1686
27.5776
27.1776
11.3822
9.8405
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120
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100
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60
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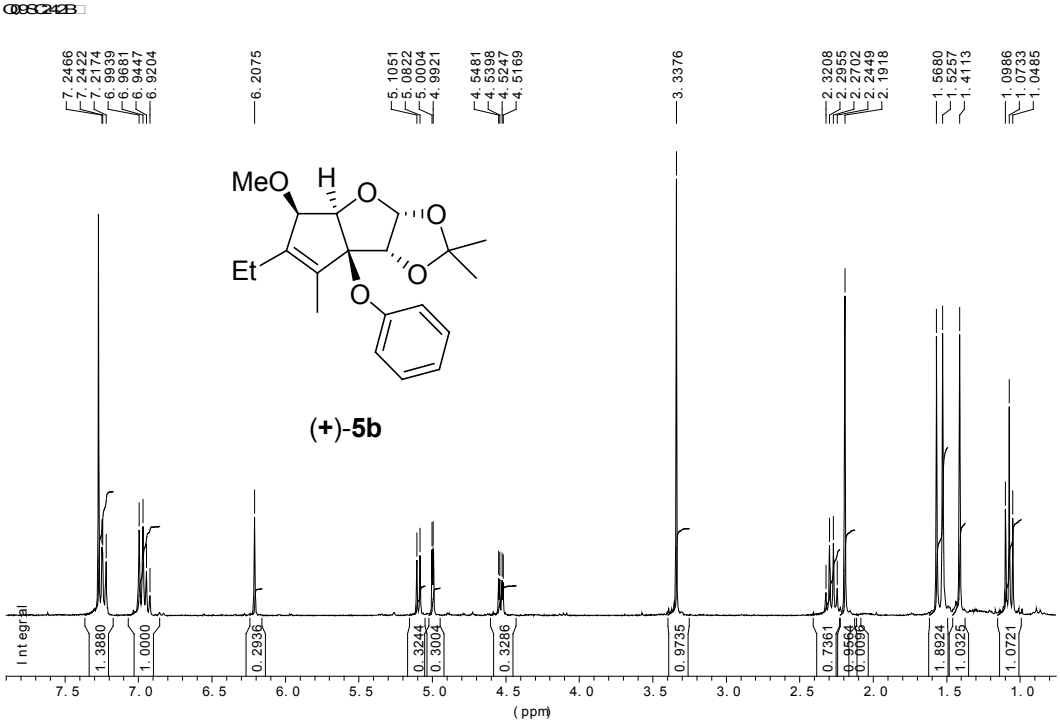
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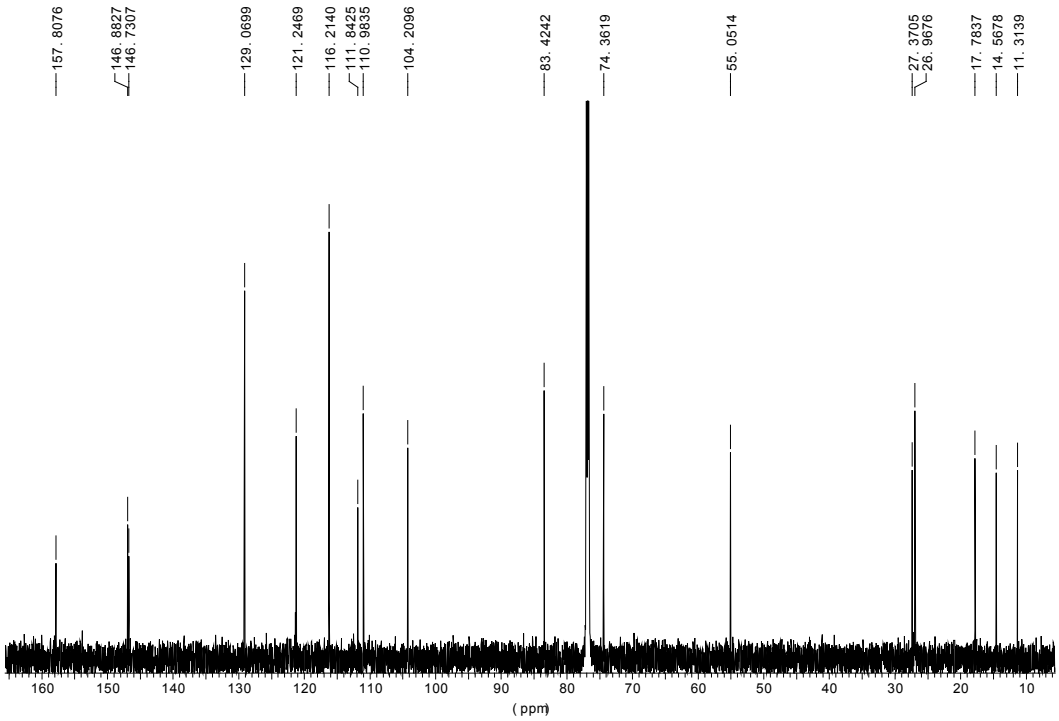
5.0822
5.0004
4.9921
4.5481
4.5398
4.5247
4.5169
3.3376
2.3208
2.2955
2.2702
2.2449
2.1918
1.5680
1.5257
1.4113
1.0986
1.0733
1.0485
MeO
H
O
O
O
Et
O
(+)-5b
Integral
1.3880
1.0000
0.2936
0.3244
0.3004
0.3286
0.9735
0.7361
0.9564
0.0098
1.8924
1.0325
1.0721
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)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55.0514
27.3705
26.9676
17.7837
14.5678
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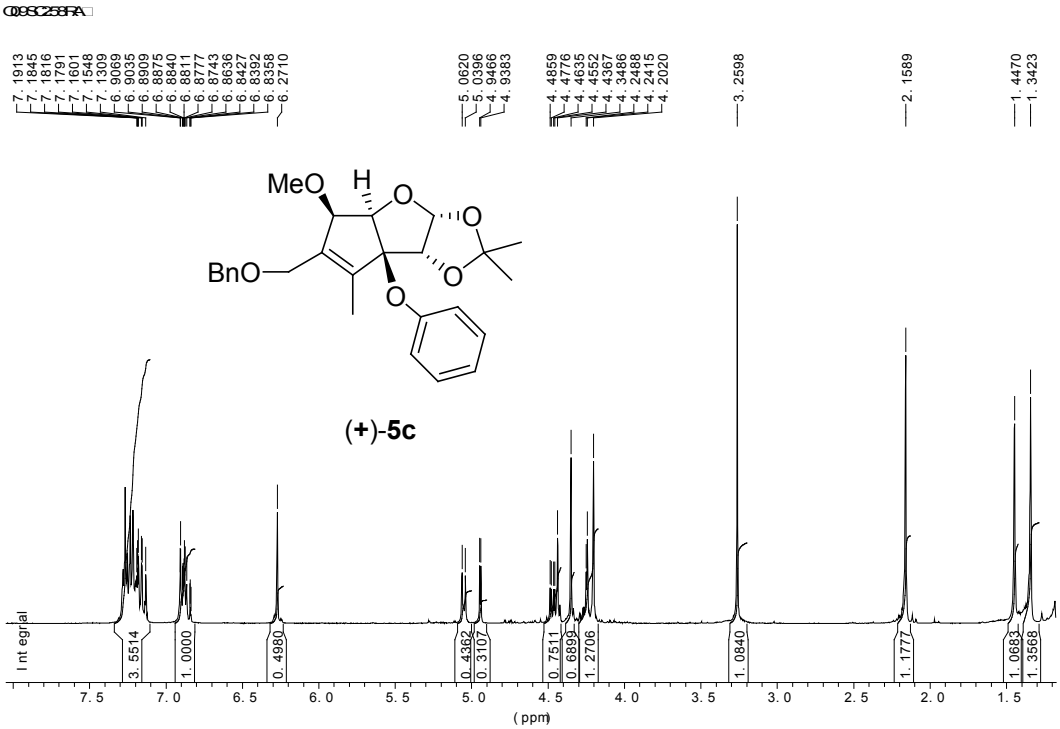
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)


MeO
H
O
O
O
O
BnO
(+)-5c
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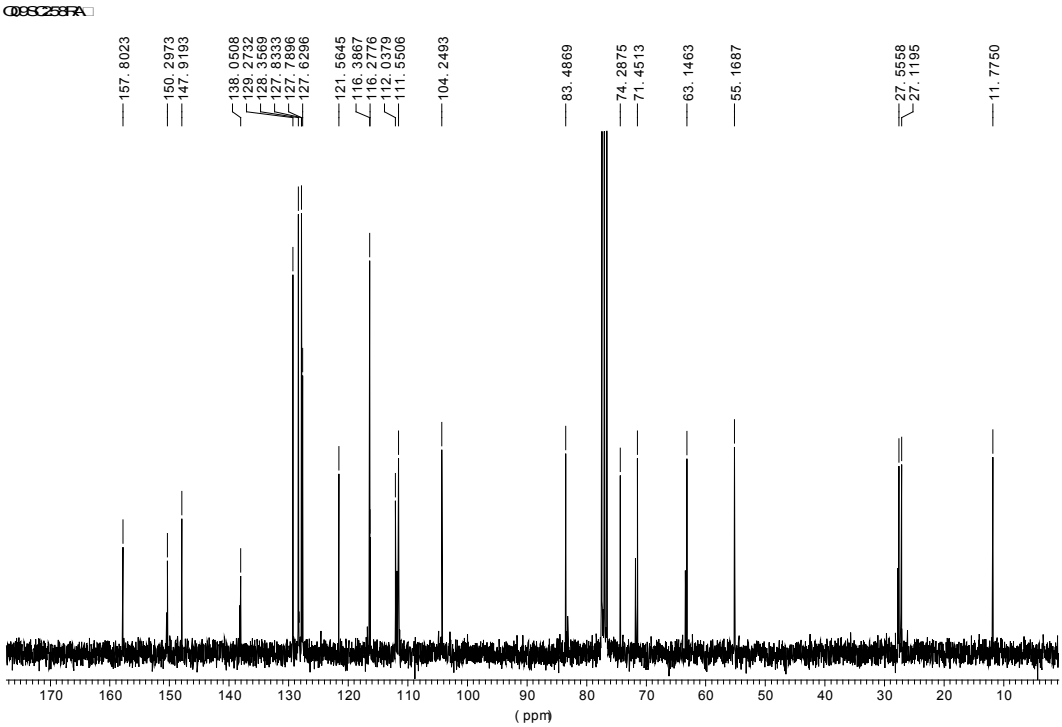
7.1548
7.1309
6.9069
6.9035
6.8909
6.8875
6.8840
6.8811
6.8777
6.8743
6.8636
6.8427
6.8392
6.8358
6.2710
5.0620
5.0396
4.9466
4.9383
4.4859
4.4776
4.4635
4.4552
4.4367
4.3486
4.2488
4.2415
4.2020
3.2598
2.1589
1.4470
1.3423
Integral
3.5514
1.0000
0.4980
0.4362
0.3107
0.7511
0.6893
1.2706
1.0840
1.1777
1.0683
1.3568
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
(ppm)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112.0379
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104.2493
83.4869
74.2875
71.4513
63.1463
55.1687
27.5558
27.1195
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150
140
130
120
110
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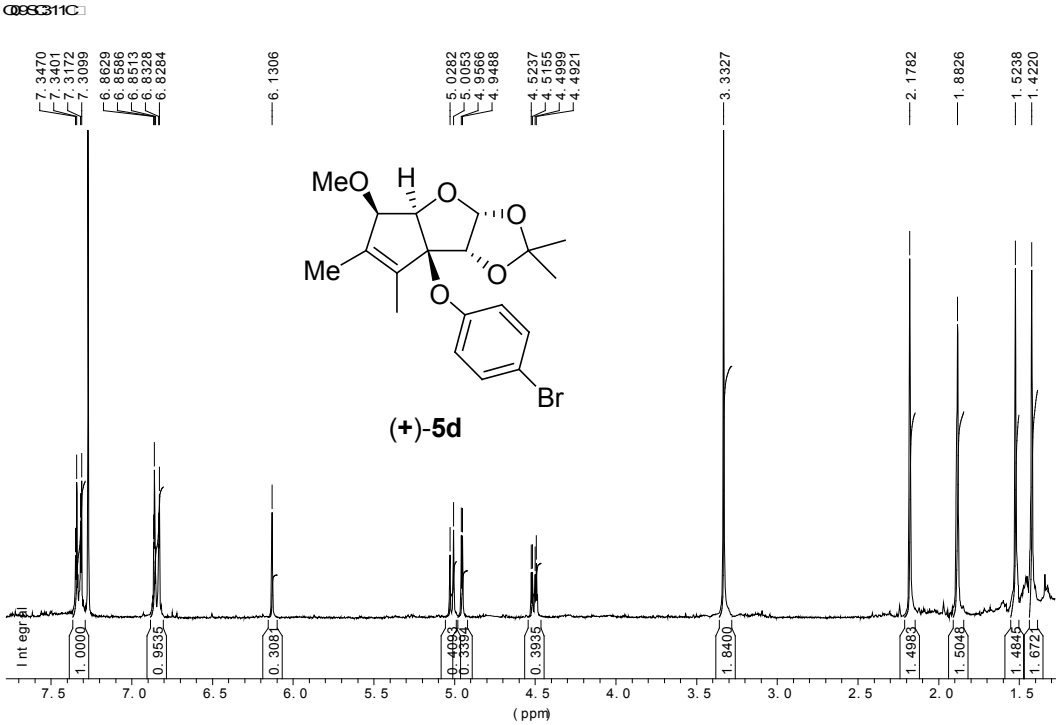
(ppm)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7.3099
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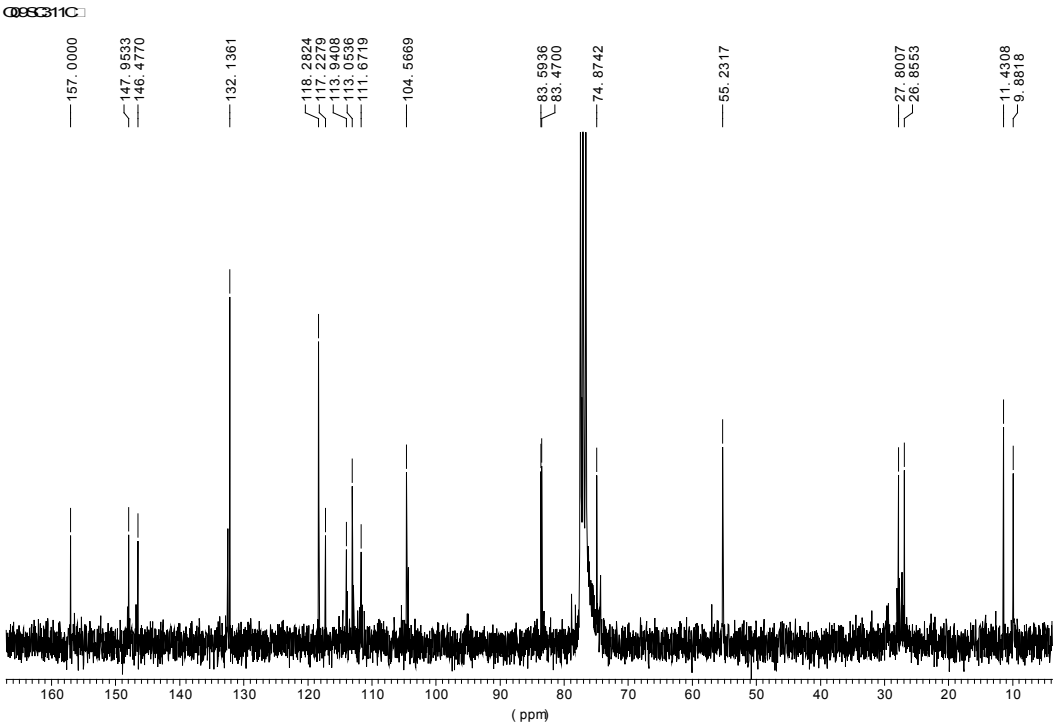
6.8586
6.8513
6.8328
6.8284
6.1306
5.0282
5.0053
4.9566
4.9488
4.5237
4.5155
4.4999
4.4921
3.3327
2.1782
1.8826
1.5238
1.4220
MeO
H
O
O
Me
O
O
Br
(+)-5d
Int egral
1.0000
0.9535
0.3081
0.4093
0.3394
0.3935
1.8400
1.4983
1.5048
1.4845
1.6721
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
(ppm)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111.6719
104.5669
83.5936
83.4700
74.8742
55.2317
27.8007
26.8553
11.4308
9.8818
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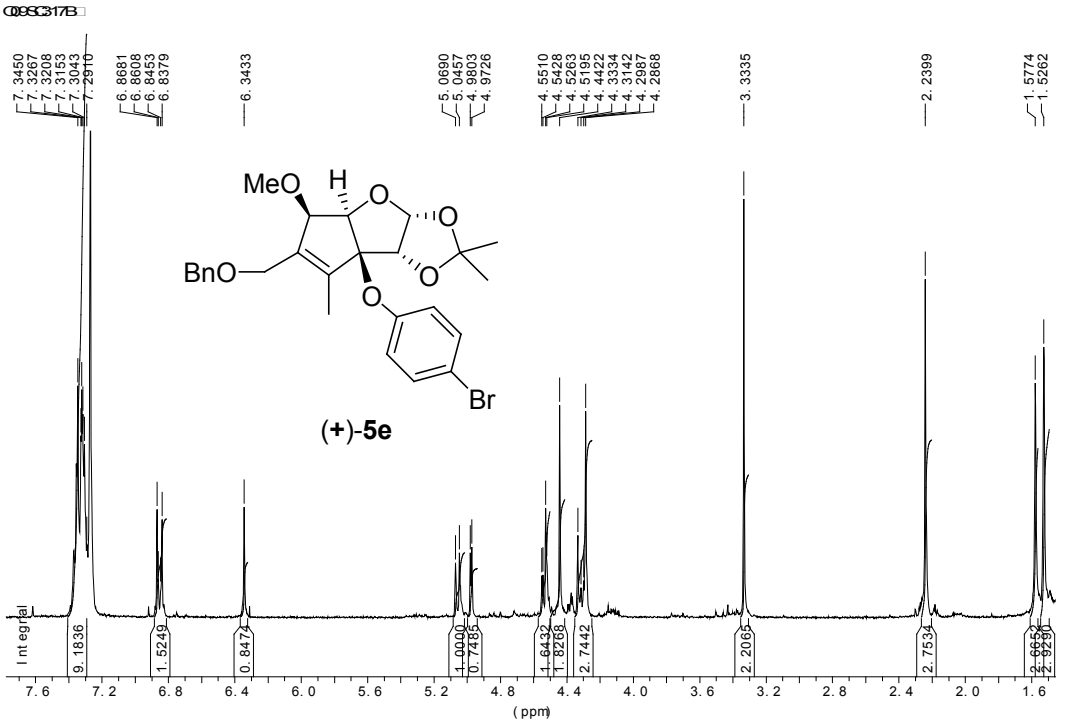
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)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6.8379
6.3433
5.0690
5.0457
4.9803
4.9726
4.5510
4.5428
4.5263
4.5195
4.4422
4.3334
4.3142
4.2987
4.2868
3.3335
2.2399
1.5774
1.5262
MeO
H
O
O
O
O
BnO
Br
(+)-5e
Integral
9.1836
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0.8474
1.0000
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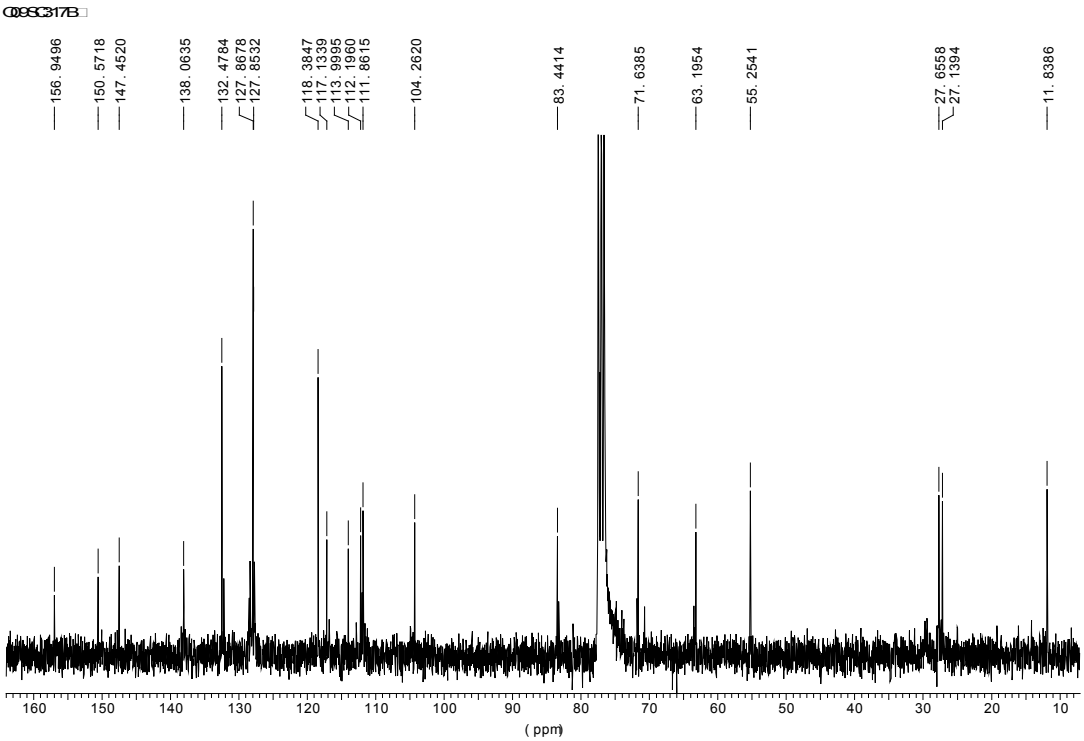
1.6433
1.8269
2.7442
2.2065
2.7534
2.6656
2.9290
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
(ppm)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104.2620
83.4414
71.6385
63.1954
55.2541
27.6558
27.1394
11.8386
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)