

Supporting Information

Rational Design and Organocatalytic Enantioselective [1+4]-Annulations of MBH Carbonates with Modified Enones

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A: Experimental section

1. General Remarks

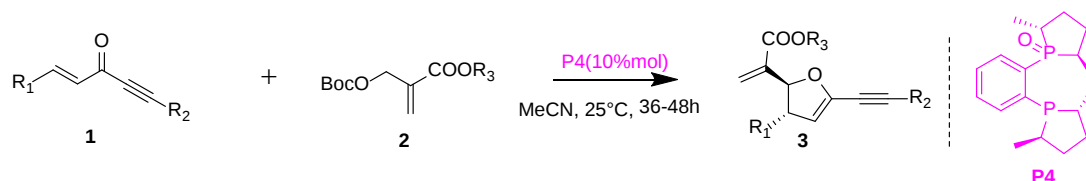
All reactions were carried out with dry, freshly distilled solvents in anhydrous conditions. All chemicals were used without further purification as commercially available unless otherwise noted. All reactions were performed under an atmosphere of dry nitrogen. Thin-layer chromatography (TLC) was performed on silica gel plates (60F-254) using UV-light (254 and 365 nm). Flash chromatography was conducted on silica gel (300–400 mesh). NMR (400 or 500 MHz for ^1H NMR, 100 or 126 MHz for ^{13}C NMR, 376 or 471 MHz for ^{19}F NMR) spectra were recorded in CDCl_3 or Acetone- d_6 with TMS as the internal standard. Chemical shifts are reported in ppm and coupling constants are given in Hz. Data for ^1H NMR are recorded as follows: chemical shift (ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quarter; m, multiplet), coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (δ , ppm). Data for ^{19}F NMR are reported in terms of chemical shift (δ , ppm). High resolution mass spectral (HRMS) analyses were measured using ESI techniques.

2. Synthesis of β,γ -unsaturated- α -ketone alkynes **1** and β,γ -unsaturated- α -ketone olefins **4**

β,γ -unsaturated- α -ketone alkynes **1** were synthesized according to the literature.¹ To a stirred solution of alkyne (1.0 eq) dissolved in THF at -78°C , was added $n\text{-BuLi}$ (2.5 M in hexane, 1.1 eq) dropwise and then stirred for 20 minutes. The solution was warmed to room temperature for another 30 minutes before returning to -78°C . A solution of aldehyde (1.0 eq) dissolved in THF was added and the reaction warmed to room temperature and stirred for 4 hours. Saturated NH_4Cl was added to quench the reaction. Then extracted with EtOAc, washed with brine, dried over Na_2SO_4 , filtered and concentrated in vacuo to afford a crude residue. To a stirred solution of the crude residue dissolved in DCM was added MnO_2 (30 eq) and stirred for 24 hours. The mixture was filtered through celite then concentrated in vacuo. Purified by silica gel chromatography to obtain the desired β,γ -unsaturated- α -ketone alkynes **1**.

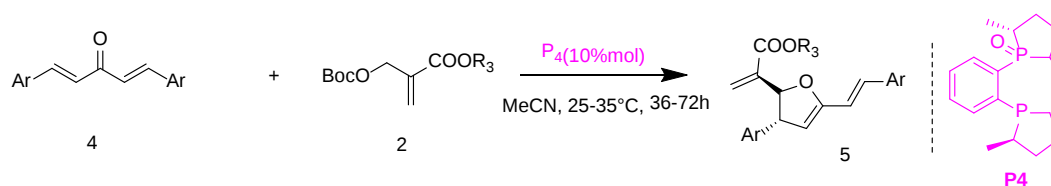
β,γ -unsaturated- α -ketone olefins **4** were synthesized according to the literature.² To a stirred solution of acetone (1.0 eq) and aldehyde (2.0 eq) dissolved in ethanol, was added 1 M NaOH aq (5.0 eq) dropwise and then stirred for 0.2–1.0 h. And then filter the suspension to afford a crude residue. Recrystallization with EtOAc to obtain the desired β,γ -unsaturated- α -ketone olefins **4**.

3. General procedure for organocatalytic enantioselective [4+1]-annulations of modified enones with MBH carbonates:



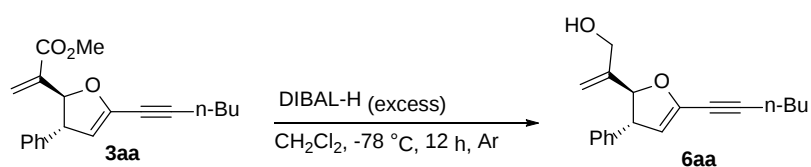
Under nitrogen atmosphere, a mixture of β,γ -unsaturated- α -ketone alkynes **1** (0.3 mmol), Morita-Baylis-Hillman carbonate **2** (0.1 mmol), catalyst **P4** (0.01 mmol) in MeCN (1.0 mL) was stirred at

25 °C in a sealed tube for 36-48 h. After removal of the solvent, the crude residue was purified by column chromatography (petroleum ether/ethyl acetate) on silica gel to give the corresponding products **3**.



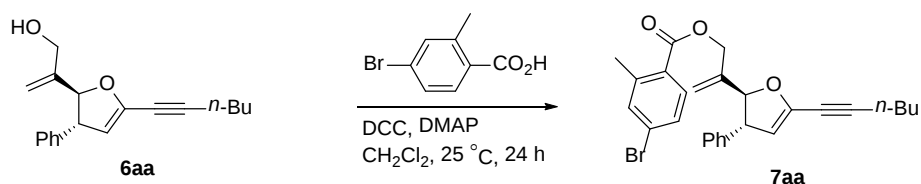
Under nitrogen atmosphere, a mixture of β,γ -unsaturated- α -ketone **4** (0.3 mmol), Morita-Baylis-Hillman carbonate **2** (0.1 mmol), catalyst **P4** (0.01 mmol) in MeCN (1.0 mL) was stirred at 25 °C-35 °C in a sealed tube for 36 h-72 h. After removal of the solvent, the crude residue was purified by column chromatography (petroleum ether/ethyl acetate) on silica gel to give the corresponding products **5**.

4. Reduction of product 3aa



To a suspension of **3aa** (0.1 mmol, 93% ee) in anhydrous dichloromethane (2.0 mL) at -78 °C, DIBAL-H (0.4 mmol) was added dropwise. Then the reaction mixture was stirred at -78 °C for 12 h. Then MeOH (1.0 mL) was added to quench the reaction. After removal the solvent under reduced pressure, the crude product was subjected to column chromatography purification to provide **6aa** as light-green oil in 86% yield (24.4 mg, 94% ee).

5. Esterification of product 6aa



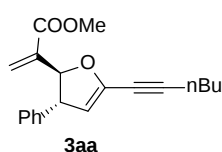
To a solution of **6aa** (0.1 mmol, 94% ee) in anhydrous dichloromethane (2.0 mL) at room temperature, 4-bromo-2-methylbenzoic acid (0.11 mmol), DCC (0.11 mmol), and DMAP (0.02 mmol) were added. Then the reaction mixture was stirred at room temperature for 24 h. After removal the solvent under reduced pressure, the crude product was subjected to column chromatography purification to provide **7aa** as yellow oil in 81% yield (38.6 mg, 91% ee).

6. Reference:

1. S. J. Heffernan, J. P. Tellam, M. E. Queru, A. C. Silvanus, D. Benito, M. F. Mahon, A. J. Hennessy, B. I. Andrews, D. R. Carbery. *Adv. Synth. Catal.* 2013, **355**, 1149-1159.
2. A. Kashyap, T. Bokosike, N. Bhuvanesh, M. Pattabiraman. *Org. Biomol. Chem.* 2018, **16**, 6870-6875.

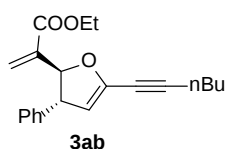
B: Characterization of the products

Methyl 2-((2S,3R)-5-(hex-1-yn-1-yl)-3-phenyl-2,3-dihydrofuran-2-yl)acrylate (3aa):



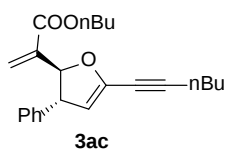
Colourless oil, 27.5 mg, 89% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.37 – 7.24 (m, 5H), 6.35 (s, 1H), 5.93 (t, J = 1.3 Hz, 1H), 5.23 (d, J = 3.0 Hz, 1H), 5.17 – 5.11 (m, 1H), 3.92 (dd, J = 5.0, 3.0 Hz, 1H), 3.74 (s, 3H), 2.40 (t, J = 7.1 Hz, 2H), 1.61 – 1.55 (m, 2H), 1.51 – 1.41 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.9, 143.1, 139.6, 139.1, 128.6, 127.6, 127.1, 124.9, 108.7, 94.2, 86.3, 70.9, 55.7, 51.8, 30.3, 22.0, 19.1, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{20}\text{H}_{23}\text{O}_3$) requires m/z 311.1642, found m/z 311.1635; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 4.197 min, t_R (major) = 6.327 min, 93% ee. $[\alpha]_D^{20}$ = 24.5356 (c = 1.00, CH_2Cl_2).

Ethyl 2-((2S,3R)-5-(hex-1-yn-1-yl)-3-phenyl-2,3-dihydrofuran-2-yl)acrylate (3ab):



Colourless oil, 25.6mg, 79.0% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.37 – 7.21 (m, 5H), 6.34 (s, 1H), 5.90 (s, 1H), 5.22 (d, J = 3.0 Hz, 1H), 5.17 (d, J = 5.1 Hz, 1H), 4.19 (qd, J = 7.1, 2.9 Hz, 2H), 3.91 (dd, J = 4.8, 3.2 Hz, 1H), 2.40 (t, J = 7.1 Hz, 2H), 1.63 – 1.56 (m, 2H), 1.45 (dd, J = 15.0, 7.4 Hz, 2H), 1.20 (t, J = 7.1 Hz, 3H), 0.94 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.5, 143.1, 139.5, 139.5, 128.6, 127.6, 127.1, 124.7, 108.8, 94.2, 86.3, 71.0, 60.9, 55.8, 30.3, 22.0, 19.1, 14.1, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{21}\text{H}_{24}\text{O}_3$) requires m/z 325.1798, found m/z 325.1796; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 3.939 min, t_R (major) = 5.820 min, 94% ee. $[\alpha]_D^{20}$ = 24.8889 (c = 1.00, CH_2Cl_2).

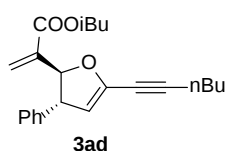
Butyl 2-((2S,3R)-5-(hex-1-yn-1-yl)-3-phenyl-2,3-dihydrofuran-2-yl)acrylate (3ac):



Colourless oil, 27.1mg; 77.0% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.35 (t, J = 7.4 Hz, 2H), 7.28 (d, J = 9.0 Hz, 3H), 6.35 (s, 1H), 5.91 (s, 1H), 5.25 (d, J = 3.0 Hz, 1H), 5.19 (d, J = 5.2 Hz, 1H), 4.16 (dq, J = 10.9, 4.2 Hz, 2H), 3.94 (dd, J = 5.0, 3.1 Hz, 1H), 2.42 (t, J = 7.1 Hz, 2H), 1.59 – 1.52 (m, 3H), 1.51 – 1.42 (m, 2H), 1.37 – 1.24 (m, 3H), 0.96 (t, J = 7.3 Hz, 3H), 0.90 (t, J = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.6, 143.1, 139.49 (d, J = 5.6 Hz), 128.6, 127.5, 127.1, 124.7, 108.9, 94.1, 86.4, 71.0, 64.8, 55.8, 30.5, 30.3, 22.0, 19.1, 19.1, 13.7, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{23}\text{H}_{29}\text{O}_3$) requires m/z 353.2111, found m/z 353.2109; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 3.752 min, t_R (major) = 5.290 min, 95% ee. $[\alpha]_D^{20}$ = 28.6667 (c = 1.00, CH_2Cl_2).

Isobutyl 2-((2S,3R)-5-(hex-1-yn-1-yl)-3-phenyl-2,3-dihydrofuran-2-yl)acrylate (3ad):

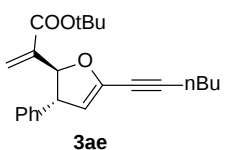
Colourless oil, 26.1mg; 74.2% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.32 (t, J = 7.5 Hz, 2H), 7.28 – 7.20 (m, 3H), 6.34 (s, 1H), 5.89 (s, 1H), 5.23 (d, J = 2.9 Hz, 1H), 5.17 (d, J = 5.2 Hz, 1H), 4.00 – 3.81 (m, 3H),



2.39 (t, $J = 7.1$ Hz, 2H), 1.93 – 1.82 (m, 1H), 1.56 (s, 2H), 1.45 (d, $J = 7.6$ Hz, 2H), 0.94 (t, $J = 7.3$ Hz, 3H), 0.87 (dd, $J = 9.8, 6.7$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.5, 143.1, 139.5, 139.4, 128.6, 127.6, 127.1, 124.8, 108.9, 94.2, 86.5, 70.9, 55.8, 30.3, 27.7, 22.0, 19.1, 19.1, 19.0, 13.6. HRMS: exact mass calculated for

$[\text{M}+\text{H}]^+$ ($\text{C}_{23}\text{H}_{29}\text{O}_3$) requires m/z 353.2111, found m/z 353.2109; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 3.644 min, t_R (major) = 5.125 min, 95% ee. $[\alpha]_D^{20} = 20.0741$ ($c = 1.00$, CH_2Cl_2).

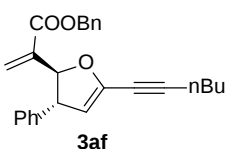
Tert-butyl 2-((2S,3R)-5-(hex-1-yn-1-yl)-3-phenyl-2,3-dihydrofuran-2-yl)acrylate (3ae):



Colourless oil, 27.5mg; 78.1% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.34 (t, $J = 7.5$ Hz, 2H), 7.27 (dd, $J = 18.3, 6.5$ Hz, 3H), 6.26 (s, 1H), 5.82 (s, 1H), 5.21 (dd, $J = 9.1, 4.2$ Hz, 2H), 3.90 (dd, $J = 5.3, 3.0$ Hz, 1H), 2.41 (t, $J = 7.1$ Hz, 2H), 1.59 (d, $J = 8.1$ Hz, 2H), 1.47 (dd, $J = 14.9, 7.3$ Hz, 2H), 1.40 (s, 9H), 0.95 (t, $J = 7.3$ Hz, 3H). ^{13}C

NMR (126 MHz, CDCl_3) δ 164.6, 143.3, 141.0, 139.4, 128.6, 127.6, 127.0, 123.8, 109.1, 94.0, 86.5, 81.4, 71.1, 56.2, 30.3, 27.9, 22.0, 19.1, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{23}\text{H}_{29}\text{O}_3$) requires m/z 353.2111, found m/z 353.2109; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 3.330 min, t_R (major) = 4.061 min, 95% ee. $[\alpha]_D^{20} = 54.1943$ ($c = 1.00$, CH_2Cl_2).

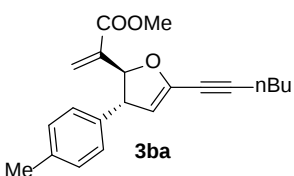
Benzyl 2-((2S,3R)-5-(hex-1-yn-1-yl)-3-phenyl-2,3-dihydrofuran-2-yl)acrylate (3af):



Light-green oil, 31.2mg; 80.8% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.35 (dt, $J = 4.4, 2.3$ Hz, 4H), 7.31 (d, $J = 6.7$ Hz, 3H), 7.27 – 7.21 (m, 3H), 6.41 (s, 1H), 5.95 (s, 1H), 5.22 (dd, $J = 15.7, 4.9$ Hz, 4H), 3.97 – 3.89 (m, 1H), 2.42 (t, $J = 7.2$ Hz, 2H), 1.59 (s, 2H), 1.49 – 1.42 (m, 2H), 0.96 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz,

CDCl_3) δ 165.3, 139.53, 139.2, 135.6, 129.0, 128.6, 128.6, 128.3, 127.5, 127.1, 125.3, 108.8, 94.2, 86.3, 66.6, 55.7, 30.3, 22.0, 19.1, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{26}\text{H}_{27}\text{O}_3$) requires m/z 387.1955, found m/z 387.1953; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 5.108 min, t_R (major) = 8.137 min, 94% ee. $[\alpha]_D^{20} = 19.5625$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-5-(hex-1-yn-1-yl)-3-(p-tolyl)-2,3-dihydrofuran-2-yl)acrylate (3ba):

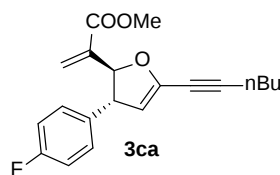


Light-green oil, 26.8mg; 82.7% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.22 – 7.09 (m, 4H), 6.33 (s, 1H), 5.91 (s, 1H), 5.21 (d, $J = 3.0$ Hz, 1H), 5.11 (d, $J = 5.1$ Hz, 1H), 3.88 (dd, $J = 4.9, 3.1$ Hz, 1H), 3.73 (s, 3H), 2.39 (t, $J = 7.1$ Hz, 2H), 2.33 (s, 3H), 1.58 (d, $J = 4.0$ Hz, 2H), 1.51 – 1.38 (m, 2H), 0.94 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.9, 140.1, 139.4, 139.2, 136.7, 129.3, 127.4, 124.8, 108.9,

94.1, 86.4, 71.0, 55.3, 51.8, 30.3, 22.0, 21.1, 19.1, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{21}\text{H}_{25}\text{O}_3$) requires m/z 325.1798, found m/z 325.1792; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) =

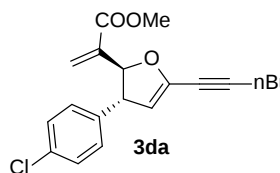
3.992 min, t_R (major) = 6.105 min, 94% ee. $[\alpha]_D^{20} = 41.6700$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-(4-fluorophenyl)-5-(hex-1-yn-1-yl)-2,3-dihydrofuran-2-yl)acrylate (3ca):



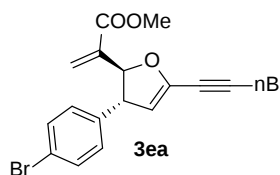
Colourless oil, 23.8mg; 72.5% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.32 – 7.19 (m, 2H), 7.03 (t, $J = 8.6$ Hz, 2H), 6.36 (s, 1H), 5.94 (s, 1H), 5.22 (d, $J = 3.0$ Hz, 1H), 5.11 (d, $J = 4.8$ Hz, 1H), 3.94 – 3.87 (m, 1H), 3.76 (s, 3H), 2.42 (t, $J = 7.1$ Hz, 2H), 1.62 (d, $J = 8.1$ Hz, 2H), 1.48 (dd, $J = 15.1, 7.3$ Hz, 2H), 0.96 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.9, 162.0 (d, $J = 245.5$ Hz), 139.8, 138.9, 138.8 (d, $J = 3.1$ Hz), 129.07 (d, $J = 8.0$ Hz), 124.9, 115.4 (d, $J = 21.4$ Hz), 108.4, 94.4, 86.3, 70.8, 54.9, 51.9, 30.2, 22.0, 19.1, 13.6. ^{19}F NMR (376 MHz, CDCl_3) δ -115.9. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{20}\text{H}_{22}\text{FO}_3$) requires m/z 329.1547, found m/z 329.1541; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 6.942 min, t_R (major) = 7.355min, 95% ee. $[\alpha]_D^{20} = 15.6405$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-(4-chlorophenyl)-5-(hex-1-yn-1-yl)-2,3-dihydrofuran-2-yl)acrylate (3da):



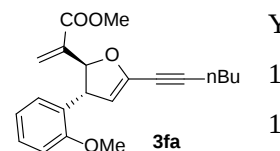
Yellow oil, 26.2mg; 76.2% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.35 – 7.20 (m, 4H), 6.36 (s, 1H), 5.95 (s, 1H), 5.21 (d, $J = 3.0$ Hz, 1H), 5.11 (d, $J = 4.8$ Hz, 1H), 3.93 – 3.84 (m, 1H), 3.76 (s, 3H), 2.42 (t, $J = 7.1$ Hz, 2H), 1.60 (d, $J = 7.5$ Hz, 2H), 1.48 (d, $J = 7.8$ Hz, 2H), 0.96 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.8, 141.7, 140.0, 138.8, 132.8, 129.0, 128.7, 125.0, 108.2, 94.5, 86.1, 70.8, 55.1, 51.9, 30.2, 22.0, 19.1, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{20}\text{H}_{22}\text{ClO}_3$) requires m/z 345.1252, found m/z 345.1245; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (major) = 6.826 min, t_R (minor) = 7.579min, 94% ee. $[\alpha]_D^{20} = 18.4328$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-(4-bromophenyl)-5-(hex-1-yn-1-yl)-2,3-dihydrofuran-2-yl)acrylate (3ea):



Yellow oil, 31.8mg; 81.7% yield. ^1H NMR (400 MHz, Acetone) δ 7.58 – 7.51 (m, 2H), 7.32 – 7.22 (m, 2H), 6.30 (s, 1H), 5.87 (t, $J = 1.3$ Hz, 1H), 5.29 (d, $J = 3.0$ Hz, 1H), 5.09 (dt, $J = 4.7, 1.2$ Hz, 1H), 4.03 – 3.98 (m, 1H), 3.75 (s, 3H), 2.44 (t, $J = 7.0$ Hz, 2H), 1.58 (dd, $J = 8.1, 7.1$ Hz, 2H), 1.50 – 1.40 (m, 2H), 0.95 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz, Acetone) δ 165.2, 142.9, 140.0, 139.5, 131.5, 129.6, 123.5, 120.3, 108.2, 93.9, 85.9, 70.9, 54.6, 51.3, 30.2, 21.7, 18.4, 12.9. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{20}\text{H}_{22}\text{BrO}_3$) requires m/z 389.0747, found m/z 389.0742; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, $\lambda = 230$ nm, retention time: t_R (major) = 7.374 min, t_R (minor) = 7.904 min, 96% ee. $[\alpha]_D^{20} = 35.5426$ ($c = 1.00$, CH_2Cl_2).

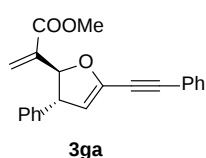
Methyl 2-((2S,3R)-5-(hex-1-yn-1-yl)-3-(2-methoxyphenyl)-2,3-dihydrofuran-2-yl)acrylate (3fa):



Yellow oil, 28.2mg; 82.9% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.32 (dd, $J = 7.5, 1.1$ Hz, 1H), 7.23 (d, $J = 7.9$ Hz, 1H), 6.98 (t, $J = 7.5$ Hz, 1H), 6.85 (d, $J = 8.2$ Hz, 1H), 6.34 (s, 1H), 5.95 (s, 1H), 5.20 (d, $J = 3.0$ Hz, 1H), 4.49 (dd, $J = 6.4, 2.8$ Hz,

1H), 3.78 (s, 3H), 3.68 (s, 3H), 2.40 (t, $J = 7.1$ Hz, 2H), 1.58 (d, $J = 7.9$ Hz, 2H), 1.46 (d, $J = 7.7$ Hz, 2H), 0.95 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.0, 156.5, 140.1, 139.2, 131.3, 128.3, 128.0, 124.7, 120.9, 110.3, 108.9, 85.8, 71.2, 55.3, 51.7, 48.2, 30.3, 27.8, 22.0, 19.1, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{21}\text{H}_{25}\text{O}_4$) requires m/z 341.1747, found m/z 341.1741; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (major) = 4.626 min, t_R (minor) = 5.307 min, 93% ee. $[\alpha]_D^{20} = 47.2381$ ($c = 1.00$, CH_2Cl_2).

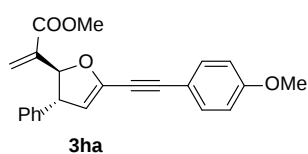
Methyl 2-((2S,3R)-3-phenyl-5-(phenylethynyl)-2,3-dihydrofuran-2-yl)acrylate (3ga):



Yellow oil, 26.8mg; 81.2% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.57 – 7.49 (m, 2H), 7.39 – 7.27 (m, 8H), 6.38 (s, 1H), 5.98 (s, 1H), 5.45 (d, $J = 3.1$ Hz, 1H), 5.22 (d, $J = 5.1$ Hz, 1H), 4.00 (dd, $J = 5.0, 3.1$ Hz, 1H), 3.75 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.8, 142.8, 139.4, 139.0, 131.8, 129.1, 128.7, 128.4, 127.6, 127.2, 125.1, 121.8,

110.8, 92.3, 86.6, 79.5, 55.9, 51.9. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{22}\text{H}_{19}\text{O}_3$) requires m/z 331.1329, found m/z 331.1321; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 5.105 min, t_R (major) = 6.278 min, 92% ee. $[\alpha]_D^{20} = 37.9624$ ($c = 1.00$, CH_2Cl_2).

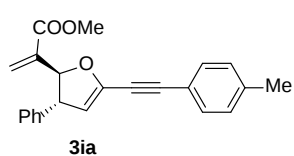
Methyl 2-((2S,3R)-5-((4-methoxyphenyl)ethynyl)-3-phenyl-2,3-dihydrofuran-2-yl)acrylate (3ha):



Yellow oil, 28.2mg; 78.3% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.47 (d, $J = 8.6$ Hz, 2H), 7.33 (dd, $J = 14.0, 7.0$ Hz, 5H), 6.87 (d, $J = 8.7$ Hz, 2H), 6.37 (s, 1H), 5.98 (s, 1H), 5.40 (d, $J = 3.0$ Hz, 1H), 5.21 (d, $J = 4.9$ Hz, 1H), 4.02 – 3.94 (m, 1H), 3.83 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.9,

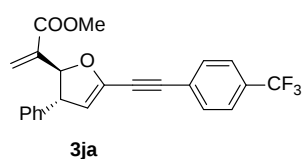
160.2, 143.0, 139.6, 139.0, 133.4, 128.7, 127.6, 127.2, 125.1, 114.1, 113.8, 110.0, 92.4, 86.5, 78.3, 55.9, 55.4, 51.9. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{23}\text{H}_{21}\text{O}_4$) requires m/z 361.1434, found m/z 361.1429; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 6.621 min, t_R (major) = 8.876 min, 92% ee. $[\alpha]_D^{20} = 26.3816$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-phenyl-5-(p-tolylethynyl)-2,3-dihydrofuran-2-yl)acrylate (3ia):

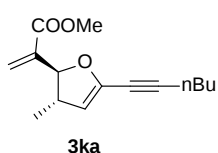


Yellow oil, 30.3mg; 88.1% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.45 (d, $J = 8.1$ Hz, 2H), 7.40 – 7.28 (m, 5H), 7.19 (d, $J = 7.9$ Hz, 2H), 6.40 (s, 1H), 6.01 (s, 1H), 5.45 (d, $J = 3.1$ Hz, 1H), 5.24 (d, $J = 5.1$ Hz, 1H), 4.02 (dd, $J = 5.0, 3.1$ Hz, 1H), 3.78 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.9,

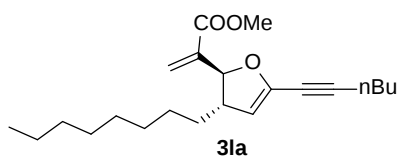
142.99, 139.5, 139.4, 139.09, 131.79, 129.29, 128.7, 127.6, 127.2, 125.1, 118.7, 110.4, 92.5, 86.6, 78.9, 55.9, 51.9, 21.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{23}\text{H}_{21}\text{O}_3$) requires m/z 345.1485, found m/z 345.1480; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 4.803 min, t_R (major) = 5.541 min, 91% ee. $[\alpha]_D^{20} = 21.5520$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-phenyl-5-((4-(trifluoromethyl)phenyl)ethynyl)-2,3-dihydrofuran-2-yl)acrylate (3ja):**(3ja):**

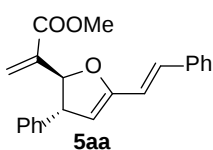
Yellow oil, 31.3mg; 78.6% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.68 – 7.59 (m, 4H), 7.36 (t, J = 7.4 Hz, 2H), 7.32 – 7.26 (m, 3H), 6.38 (s, 1H), 5.97 (s, 1H), 5.52 (d, J = 3.1 Hz, 1H), 5.23 (d, J = 5.2 Hz, 1H), 4.03 (dd, J = 5.1, 3.1 Hz, 1H), 3.76 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.8, 142.6, 138.9, 138.8, 132.0, 130.6(q, J = 32.8 Hz), 129.2, 128.8, 128.0, 127.6, 126.3 (q, J = 266.2 Hz), 125.6(q, J = 1.1 Hz), 125.4 (q, J = 3.8 Hz), 125.2, 112.1, 90.7, 86.9, 81.7, 55.9, 51.9. ^{19}F NMR (376 MHz, CDCl_3) δ -62.9. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{23}\text{H}_{18}\text{F}_3\text{O}_3$) requires m/z 399.1203, found m/z 399.1197; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 4.829 min, t_R (major) = 5.148 min, 88% ee. $[\alpha]_D^{20}$ = 9.6812(c = 1.00, CH_2Cl_2).

Methyl 2-((2S,3S)-5-(hex-1-yn-1-yl)-3-methyl-2,3-dihydrofuran-2-yl)acrylate (3ka):

Yellow oil, 18.3mg; 73.8% yield. ^1H NMR (400 MHz, CDCl_3) δ 6.28 (s, 1H), 5.89 (s, 1H), 5.11 (d, J = 2.9 Hz, 1H), 4.89 (d, J = 5.1 Hz, 1H), 3.80 (s, 3H), 2.85 – 2.72 (m, 1H), 2.37 (t, J = 7.1 Hz, 2H), 1.56 (d, J = 8.0 Hz, 2H), 1.49 – 1.37 (m, 2H), 1.25 (d, J = 6.8 Hz, 3H), 0.94 (dd, J = 8.7, 5.9 Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.2, 139.5, 138.1, 124.0, 110.5, 93.5, 85.2, 71.2, 51.8, 45.1, 30.3, 22.0, 20.8, 19.0, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{21}\text{H}_{25}\text{O}_4$) requires m/z 249.1485, found m/z 249.1482; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 3.484 min, t_R (minor) = 4.004 min, 91% ee. $[\alpha]_D^{20}$ = 18.4628(c = 1.00, CH_2Cl_2).

Methyl 2-((2S,3S)-5-(hex-1-yn-1-yl)-3-octyl-2,3-dihydrofuran-2-yl)acrylate (3la):

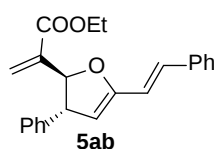
Yellow oil, 24.3mg; 73.2% yield. ^1H NMR (400 MHz, CDCl_3) δ 6.28 (s, 1H), 5.87 (s, 1H), 5.16 (d, J = 2.9 Hz, 1H), 4.95 (d, J = 4.6 Hz, 1H), 3.80 (s, 3H), 2.71 (dd, J = 8.0, 3.1 Hz, 1H), 2.38 (t, J = 7.1 Hz, 2H), 1.56 (d, J = 7.8 Hz, 2H), 1.45 (d, J = 7.7 Hz, 2H), 1.28 (s, 14H), 1.00 – 0.85 (m, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.1, 139.6, 138.4, 124.2, 108.9, 83.7, 51.8, 50.2, 35.6, 31.9, 30.3, 29.7, 29.5, 29.3, 26.6, 22.7, 22.0, 19.0, 14.1, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{22}\text{H}_{35}\text{O}_3$) requires m/z 347.2581, found m/z 347.2573; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 3.581 min, t_R (minor) = 4.093 min, 95% ee. $[\alpha]_D^{20}$ = 21.3462 (c = 1.00, CH_2Cl_2).

Methyl 2-((2S,3R)-3-phenyl-5-((E)-styryl)-2,3-dihydrofuran-2-yl)acrylate (5aa):

Colourless oil, 24.2mg, 72.9% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.50 (d, J = 7.5 Hz, 2H), 7.40 – 7.24 (m, 8H), 7.08 (d, J = 16.1 Hz, 1H), 6.74 (d, J = 16.1 Hz, 1H), 6.36 (s, 1H), 5.93 (s, 1H), 5.29 (d, J = 4.3 Hz, 1H), 5.17 (d, J = 3.1 Hz, 1H), 3.97 (t, J = 3.7 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.0, 155.2, 143.7, 139.7, 136.5, 130.8, 128.7, 128.6, 128.1, 127.6, 127.0, 126.8, 124.3, 116.7, 104.8, 86.4, 56.0, 51.8. HRMS:

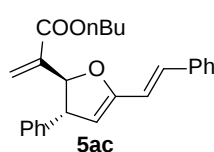
exact mass calculated for $[M+H]^+$ ($C_{22}H_{21}O_3$) requires m/z 333.1485, found m/z 333.1479; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 5.829 min, t_R (major) = 6.409 min, 97% ee. $[\alpha]^{20}_D$ = 33.9105(c = 1.00, CH_2Cl_2).

Ethyl 2-((2S,3R)-3-phenyl-5-((E)-styryl)-2,3-dihydrofuran-2-yl)acrylate (5ab):



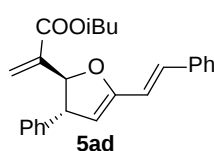
Colourless oil, 26.3mg; 76.0% yield. 1H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, J = 7.4 Hz, 2H), 7.37 – 7.25 (m, 8H), 7.05 (d, J = 16.1 Hz, 1H), 6.71 (d, J = 16.1 Hz, 1H), 6.33 (s, 1H), 5.87 (t, J = 1.3 Hz, 1H), 5.28 (d, J = 4.5 Hz, 1H), 5.13 (d, J = 3.1 Hz, 1H), 4.22 (tt, J = 7.2, 3.6 Hz, 2H), 3.98 – 3.92 (m, 1H), 1.22 (t, J = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.6, 155.2, 143.7, 140.1, 136.6, 130.8, 128.7, 128.6, 128.1, 127.6, 127.0, 126.8, 124.1, 116.7, 104.9, 86.4, 60.9, 56.1, 14.1. HRMS: exact mass calculated for $[M+H]^+$ ($C_{23}H_{23}O_3$) requires m/z 347.1642, found m/z 347.1635; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 8.827min, t_R (major) = 9.734min, 97% ee. $[\alpha]^{20}_D$ = 31.9105(c = 1.00, CH_2Cl_2).

Butyl 2-((2S,3R)-3-phenyl-5-((E)-styryl)-2,3-dihydrofuran-2-yl)acrylate (5ac):

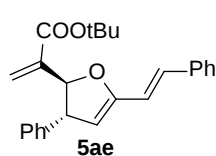


Yellow oil, 28.6mg; 76.4% yield. 1H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 7.7 Hz, 2H), 7.40 – 7.25 (m, 8H), 7.08 (d, J = 16.1 Hz, 1H), 6.73 (d, J = 16.1 Hz, 1H), 6.35 (s, 1H), 5.89 (s, 1H), 5.31 (d, J = 4.4 Hz, 1H), 5.16 (d, J = 3.1 Hz, 1H), 4.26 – 4.13 (m, 2H), 4.04 – 3.93 (m, 1H), 1.58 (dd, J = 14.8, 6.8 Hz, 2H), 1.32 (dd, J = 15.0, 7.6 Hz, 2H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.7, 155.1, 143.7, 140.1, 136.6, 130.8, 128.7, 128.6, 128.1, 127.5, 127.0, 126.8, 124.1, 116.7, 104.9, 86.5, 64.8, 56.1, 30.5, 19.2, 13.7. HRMS: exact mass calculated for $[M+H]^+$ ($C_{25}H_{27}O_3$) requires m/z 375.1955, found m/z 375.1949; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, λ = 280 nm, retention time: t_R (minor) = 8.112min, t_R (major) = 9.190min, 97% ee. $[\alpha]^{20}_D$ = 32.1160(c = 1.00, CH_2Cl_2).

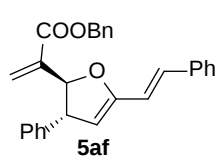
Isobutyl 2-((2S,3R)-3-phenyl-5-((E)-styryl)-2,3-dihydrofuran-2-yl)acrylate (5ad):



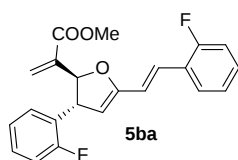
Yellow oil, 29.0mg; 77.5% yield. 1H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 7.4 Hz, 2H), 7.40 – 7.26 (m, 8H), 7.08 (d, J = 16.1 Hz, 1H), 6.73 (d, J = 16.1 Hz, 1H), 6.36 (s, 1H), 5.90 (s, 1H), 5.32 (d, J = 4.6 Hz, 1H), 5.17 (d, J = 3.1 Hz, 1H), 4.05 – 3.92 (m, 3H), 1.99 – 1.87 (m, 1H), 0.90 (dd, J = 8.2, 6.8 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.7, 155.17, 143.7, 140.1, 136.6, 130.8, 128.7, 128.6, 128.1, 127.6, 127.0, 126.8, 124.2, 116.7, 104.9, 86.5, 70.9, 56.0, 27.7, 19.1, 19.1. HRMS: exact mass calculated for $[M+H]^+$ ($C_{25}H_{27}O_3$) requires m/z 375.1955, found m/z 375.1949; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 7.205min, t_R (major) = 7.996min, 97% ee. $[\alpha]^{20}_D$ = 37.4910(c = 1.00, CH_2Cl_2).

Tert-butyl 2-((2S,3R)-3-phenyl-5-((E)-styryl)-2,3-dihydrofuran-2-yl)acrylate (5ae):

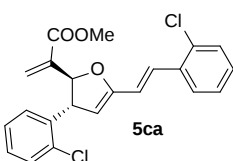
Yellow oil, 27.8mg; 74.3% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.47 (d, $J = 7.4$ Hz, 2H), 7.35 – 7.24 (m, 8H), 7.04 (d, $J = 16.0$ Hz, 1H), 6.68 (d, $J = 16.1$ Hz, 1H), 6.23 (s, 1H), 5.77 (s, 1H), 5.29 (d, $J = 4.9$ Hz, 1H), 5.11 (d, $J = 3.1$ Hz, 1H), 3.97 – 3.89 (m, 1H), 1.50 (s, 2H), 1.40 (s, 9H). ^{13}C NMR (126 MHz, CDCl_3) δ 164.8, 155.0, 143.9, 141.7, 136.6, 130.7, 128.7, 128.6, 128.1, 127.6, 127.0, 126.8, 123.2, 116.8, 105.2, 86.6, 81.4, 56.4, 28.0. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{25}\text{H}_{27}\text{O}_3$) requires m/z 375.1955, found m/z 375.1949; HPLC conditions: Daicel Chiralpak IB column, n-hexane/2-propanol = 99.5/0.5, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (major) = 6.259min, >99% ee. $[\alpha]_D^{20} = 43.0520$ ($c = 1.00$, CH_2Cl_2).

Benzyl 2-((2S,3R)-3-phenyl-5-((E)-styryl)-2,3-dihydrofuran-2-yl)acrylate (5af):

Yellow oil, 33.6mg; 82.3% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.50 (d, $J = 7.4$ Hz, 2H), 7.40 – 7.26 (m, 13H), 7.07 (d, $J = 16.1$ Hz, 1H), 6.73 (d, $J = 16.1$ Hz, 1H), 6.41 (s, 1H), 5.93 (s, 1H), 5.33 (d, $J = 4.4$ Hz, 1H), 5.25 (s, 2H), 5.15 (d, $J = 3.1$ Hz, 1H), 4.03 – 3.95 (m, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.4, 155.2, 143.5, 139.8, 136.5, 135.6, 130.8, 128.7, 128.6, 128.6, 128.3, 128.1, 127.6, 127.0, 126.8, 124.8, 116.7, 104.9, 86.4, 66.6, 55.9. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{28}\text{H}_{25}\text{O}_3$) requires m/z 409.1798, found m/z 409.1793; HPLC conditions: Daicel Chiralpak IB column, n-hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, $\lambda = 260$ nm, retention time: t_R (minor) = 5.310min, t_R (major) = 6.609min., 98% ee. $[\alpha]_D^{20} = 52.0800$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-(2-fluorophenyl)-5-((E)-2-fluorostyryl)-2,3-dihydrofuran-2-yl)acrylate (5ba):

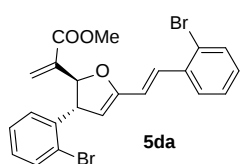
Yellow oil, 31.8mg; 86.5% yield. ^1H NMR (500 MHz, Acetone) δ 7.73 (td, $J = 7.8$, 1.4 Hz, 1H), 7.44 – 7.27 (m, 3H), 7.26 – 7.05 (m, 5H), 6.98 (d, $J = 16.2$ Hz, 1H), 6.30 (s, 1H), 5.93 (s, 1H), 5.33 (d, $J = 5.3$ Hz, 1H), 5.25 (d, $J = 3.1$ Hz, 1H), 4.35 (dd, $J = 4.9$, 3.4 Hz, 1H), 3.69 (s, 3H). ^{13}C NMR (126 MHz, Acetone) δ 165.2, 160.5 (d, $J = 249.5$ Hz), 160.1 (d, $J = 245.7$ Hz), 155.3, 140.3, 130.5, 130.4, 129.8 (d, $J = 8.6$ Hz), 129.2, 128.67 (d, $J = 8.3$ Hz), 127.67 (d, $J = 3.4$ Hz), 126.7, 124.69 (dd, $J = 13.0$, 3.5 Hz), 124.3, 124.2, 123.4, 122.7, 119.3, 119.2, 115.7 (d, $J = 22.7$ Hz), 115.2 (d, $J = 22.7$ Hz), 104.9, 85.6, 51.2, 48.4. ^{19}F NMR (376 MHz, Acetone) δ -119.2 – -119.3 (m), -120.8 – -120.9 (m). HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{22}\text{H}_{19}\text{F}_2\text{O}_3$) requires m/z 369.1297, found m/z 369.1296; HPLC conditions: Daicel Chiralpak IF-3 column, n-hexane/2-propanol = 98.5/1.5, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (major) = 7.402min, t_R (minor) = 7.696min., 96% ee. $[\alpha]_D^{20} = 61.0700$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-(2-chlorophenyl)-5-((E)-2-chlorostyryl)-2,3-dihydrofuran-2-yl)acrylate (5ca):

Yellow oil, 33.2mg; 82.8% yield. ^1H NMR (500 MHz, Acetone) δ 7.82 (dd, $J = 7.7$, 1.6 Hz, 1H), 7.51 – 7.26 (m, 8H), 6.95 (d, $J = 16.0$ Hz, 1H), 6.32 (s, 1H), 5.95 (t, $J = 1.2$ Hz, 1H), 5.39 (d, $J = 5.3$ Hz, 1H), 5.30 (d, $J = 3.1$ Hz, 1H), 4.58 (dd, $J = 4.9$, 3.4 Hz, 1H), 3.69 (s, 3H). ^{13}C NMR (126 MHz, Acetone) δ 165.2, 155.3, 141.1,

140.3, 134.3, 133.1, 132.5, 129.9, 129.5, 129.2, 129.1, 128.4, 127.8, 127.4, 126.7, 126.0, 123.5, 119.5, 105.9, 85.8, 52.0, 51.3. HRMS: exact mass calculated for $[M+H]^+$ ($C_{22}H_{19}Cl_2O_3$) requires m/z 401.0706, found m/z 401.0699; HPLC conditions: Daicel Chiralpak AS-3 column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 6.848min, t_R (minor) = 7.608min., 96% ee. $[\alpha]_D^{20}$ = 69.4637(c = 1.00, CH_2Cl_2).

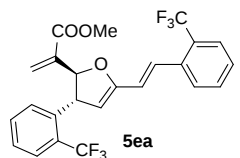
Methyl 2-((2S,3R)-3-(2-bromophenyl)-5-((E)-2-bromostyryl)-2,3-dihydrofuran-2-yl)acrylate (5da):



Yellow oil, 34.5mg; 70.4% yield. 1H NMR (500 MHz, Acetone) δ 7.82 (d, J = 7.9 Hz, 1H), 7.64 (dd, J = 26.1, 8.0 Hz, 2H), 7.52 – 7.36 (m, 4H), 7.32 – 7.19 (m, 2H), 6.92 (d, J = 16.0 Hz, 1H), 6.34 (s, 1H), 5.96 (s, 1H), 5.41 (d, J = 5.1 Hz, 1H), 5.32 (d, J = 3.0 Hz, 1H), 4.62 – 4.54 (m, 1H), 3.71 (s, 3H). ^{13}C NMR (126 MHz, Acetone) δ 165.2, 155.2, 142.9, 140.3, 136.0, 133.2, 132.6, 129.7, 129.1, 128.8, 128.7, 128.5, 128.0, 126.9,

123.8, 123.5, 123.1, 119.6, 106.1, 86.0, 54.8, 51.4. HRMS: exact mass calculated for $[M+H]^+$ ($C_{22}H_{19}Br_2O_3$) requires m/z 488.9695, found m/z 488.9700; HPLC conditions: Daicel Chiralpak IF-3 column, n-hexane/2-propanol = 98.5/1.5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 8.651min, t_R (minor) = 9.356min., 95% ee. $[\alpha]_D^{20}$ = 80.0000(c = 1.00, CH_2Cl_2).

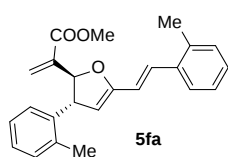
Methyl 2-((2S,3R)-3-(2-(trifluoromethyl)phenyl)-5-((E)-2-(trifluoromethyl)styryl)-2,3-dihydrofuran-2-yl)acrylate (5ea):



Yellow oil, 36.8mg; 78.5% yield. 1H NMR (500 MHz, Acetone) δ 7.94 (d, J = 7.9 Hz, 1H), 7.80 – 7.64 (m, 5H), 7.55 – 7.40 (m, 3H), 6.95 (d, J = 15.8 Hz, 1H), 6.32 (s, 1H), 5.90 (t, J = 1.3 Hz, 1H), 5.58 (d, J = 4.7 Hz, 1H), 5.33 (d, J = 3.1 Hz, 1H),

4.35 (s, 1H), 3.64 (s, 3H). Due to effect of the two kinds of $-CF_3$, C-F correlation lead to the complex of the spectra of the ^{13}C NMR. ^{13}C NMR (126 MHz, Acetone) δ 165.0, 154.5, 143.1, 140.0, 135.13 (q, J = 1.6 Hz), 133.3, 132.6, 128.2 (q, J = 254.5 Hz), 126.85 (q, J = 13.1 Hz), 126.6, 126.17 – 125.63 (m), 125.3 (q, J = 5.9 Hz), 123.6, 123.3, 120.7, 107.6, 86.3, 51.56 (q, J = 2.1 Hz), 51.2. ^{19}F NMR (376 MHz, Acetone) δ -58.7 (s), -59.7 (d, J = 1.3 Hz). HRMS: exact mass calculated for $[M+H]^+$ ($C_{24}H_{19}F_6O_5$) requires m/z 469.1233, found m/z 469.1234; HPLC conditions: Daicel Chiralpak AD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 6.742 min, t_R (minor) = 7.824 min., 95% ee. $[\alpha]_D^{20}$ = 222.9500(c = 1.00, CH_2Cl_2).

Methyl 2-((2S,3R)-5-((E)-2-methylstyryl)-3-(o-tolyl)-2,3-dihydrofuran-2-yl)acrylate (5fa):

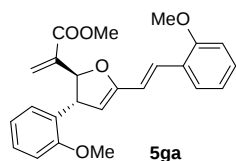


Yellow oil, 28.4mg; 78.8% yield. 1H NMR (400 MHz, Acetone) δ 7.64 (dd, J = 7.1, 2.4 Hz, 1H), 7.33 – 7.11 (m, 8H), 6.79 (d, J = 15.9 Hz, 1H), 6.30 (s, 1H), 5.95 (t, J = 1.3 Hz, 1H), 5.34 (d, J = 4.6 Hz, 1H), 5.22 (d, J = 3.2 Hz, 1H), 4.31 – 4.23 (m, 1H), 3.72 (s, 3H), 2.42 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (126 MHz, Acetone) δ 165.5,

154.9, 142.3, 140.6, 135.9, 135.3, 134.9, 130.5, 130.1, 127.9, 127.6, 127.2, 126.6, 126.5, 126.2, 125.1, 123.2, 117.9, 105.8, 86.0, 51.5, 51.2, 19.0, 18.7. HRMS: exact mass calculated for $[M+H]^+$ ($C_{24}H_{25}O_3$) requires m/z 361.1798, found m/z 361.1796; HPLC conditions: Daicel Chiralpak AD-H column,

n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 4.262 min, t_R (minor) = 5.3 min., 97% ee. $[\alpha]^{20}_D = 53.1600$ (c = 1.00, CH₂Cl₂).

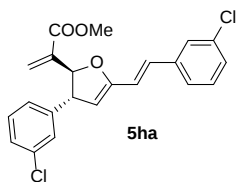
Methyl 2-((2S,3R)-3-(2-methoxyphenyl)-5-((E)-2-methoxystyryl)-2,3-dihydrofuran-2-yl)acrylate (5ga):



(5ga):

Colourless oil, 31.8mg; 81.0% yield. ¹H NMR (500 MHz, Acetone) δ 7.61 (dd, J = 7.7, 1.5 Hz, 1H), 7.35 – 7.21 (m, 4H), 7.04 – 6.89 (m, 5H), 6.27 (d, J = 0.4 Hz, 1H), 5.90 (t, J = 1.3 Hz, 1H), 5.27 (d, J = 5.6 Hz, 1H), 5.13 (d, J = 3.1 Hz, 1H), 4.49 (dd, J = 5.5, 3.1 Hz, 1H), 3.90 (s, 3H), 3.82 (s, 3H), 3.70 (s, 3H). ¹³C NMR (126 MHz, Acetone) δ 165.5, 157.2, 156.6, 155.6, 141.4, 132.0, 129.2, 127.8, 127.7, 126.6, 125.2, 124.9, 122.8, 120.8, 120.6, 117.2, 111.1, 110.5, 104.2, 85.7, 54.9, 54.9, 51.1, 48.4. HRMS: exact mass calculated for $[M+H]^+$ (C₂₄H₂₅O₅) requires m/z 393.1697, found m/z 393.1696; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 8.498 min, t_R (minor) = 13.540 min., 97% ee. $[\alpha]^{20}_D = 29.5700$ (c = 1.00, CH₂Cl₂).

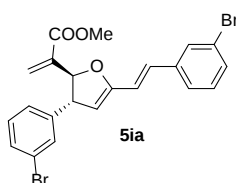
Methyl 2-((2S,3R)-3-(3-chlorophenyl)-5-((E)-3-chlorostyryl)-2,3-dihydrofuran-2-yl)acrylate (5ha):



Yellow oil, 34.0mg; 84.8% yield. ¹H NMR (400 MHz, Acetone) δ 7.66 (t, J = 1.8 Hz, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.46 – 7.27 (m, 6H), 7.14 – 6.95 (m, 2H), 6.31 (d, J = 0.9 Hz, 1H), 5.90 (t, J = 1.4 Hz, 1H), 5.32 (d, J = 3.2 Hz, 1H), 5.25 (dt, J = 4.1, 1.3 Hz, 1H), 4.06 (t, J = 3.7 Hz, 1H), 3.78 (s, 3H). ¹³C NMR (126 MHz, Acetone) δ

165.3, 155.4, 146.4, 139.9, 134.3, 130.4, 130.2, 129.3, 127.8, 127.5, 126.9, 126.7, 126.4, 126.1, 125.4, 123.2, 118.3, 105.2, 100.0, 86.1, 55.1, 51.4. HRMS: exact mass calculated for $[M+H]^+$ (C₂₂H₁₉Cl₂O₃) requires m/z 401.0706, found m/z 401.0706; HPLC conditions: Daicel Chiralpak AD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, λ = 280 nm, retention time: t_R (major) = 11.278 min, >99% ee. $[\alpha]^{20}_D = -4.8800$ (c = 1.00, CH₂Cl₂).

Methyl 2-((2S,3R)-3-(3-bromophenyl)-5-((E)-3-bromostyryl)-2,3-dihydrofuran-2-yl)acrylate (5ia):

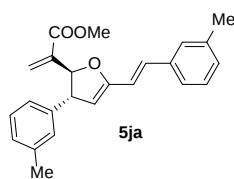


Yellow oil, 35.8mg; 73.2% yield. ¹H NMR (500 MHz, Acetone) δ 7.81 (t, J = 1.6 Hz, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.55 – 7.43 (m, 3H), 7.36 (dd, J = 10.5, 5.2 Hz, 3H), 7.09 – 6.98 (m, 2H), 6.30 (s, 1H), 5.90 (t, J = 1.4 Hz, 1H), 5.32 (d, J = 3.2 Hz, 1H), 5.28 – 5.20 (m, 1H), 4.05 (t, J = 3.6 Hz, 1H), 3.78 (s, 3H). ¹³C NMR (126

MHz, Acetone) δ 165.3, 155.4, 146.6, 139.9, 139.1, 130.8, 130.6, 130.5, 130.5, 129.9, 129.4, 129.2, 126.5, 125.7, 123.4, 122.5, 122.1, 118.3, 105.2, 86.1, 55.1, 51.3. HRMS: exact mass calculated for $[M+H]^+$ (C₂₂H₁₉Br₂O₃) requires m/z 488.9695, found m/z 488.9700; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 6.702 min, t_R (major) = 7.230 min, 97% ee. $[\alpha]^{20}_D = 56.4500$ (c = 1.00, CH₂Cl₂).

Methyl 2-((2S,3R)-5-((E)-3-methylstyryl)-3-(m-tolyl)-2,3-dihydrofuran-2-yl)acrylate (5ja):

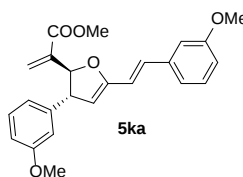
Yellow oil, 28.8mg; 79.9% yield. ¹H NMR (400 MHz, Acetone) δ 7.42 – 7.01 (m, 9H), 6.90 (d, J = 16.1 Hz,



1H), 6.28 (t, $J = 1.1$ Hz, 1H), 5.88 (t, $J = 1.5$ Hz, 1H), 5.25 – 5.18 (m, 2H), 3.96 (t, $J = 3.7$ Hz, 1H), 3.76 (s, 3H), 2.35 (d, $J = 7.3$ Hz, 6H). ^{13}C NMR (101 MHz, Acetone) δ 165.4, 155.2, 144.0, 140.4, 138.2, 137.9, 136.6, 130.6, 128.8, 128.6, 128.4, 128.1, 127.5, 127.4, 124.6, 124.0, 123.0, 116.7, 104.8, 86.3, 55.6, 51.2, 20.6,

20.5. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+(\text{C}_{24}\text{H}_{25}\text{O}_3)$ requires m/z 361.1798, found m/z 361.1792; HPLC conditions: Daicel Chiralpak IJ column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: $t_R(\text{major}) = 7.953$ min, $t_R(\text{minor}) = 10.507$ min, 98% ee. $[\alpha]_D^{20} = 95.9247$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-(3-methoxyphenyl)-5-((E)-3-methoxystyryl)-2,3-dihydrofuran-2-yl)acrylate

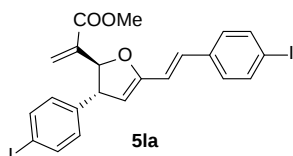


(5ka):

Yellow oil, 30.5mg; 77.7% yield. ^1H NMR (400 MHz, Acetone) δ 7.29 (dt, $J = 9.2$, 8.2 Hz, 2H), 7.17 (dd, $J = 4.9$, 3.1 Hz, 2H), 7.04 (d, $J = 16.1$ Hz, 1H), 6.99 – 6.81 (m, 5H), 6.29 (t, $J = 1.0$ Hz, 1H), 5.88 (t, $J = 1.4$ Hz, 1H), 5.28 – 5.19 (m, 2H),

4.05 – 3.95 (m, 1H), 3.85 (s, 3H), 3.81 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (126 MHz, Acetone) δ 165.4, 160.2, 160.0, 155.3, 145.5, 140.3, 138.1, 130.5, 129.7, 129.5, 123.1, 119.6, 119.3, 117.1, 114.1, 113.3, 112.0, 111.6, 104.8, 86.2, 55.5, 54.6, 54.5, 51.2. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+(\text{C}_{24}\text{H}_{25}\text{O}_5)$ requires m/z 393.1697, found m/z 393.1694; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 280$ nm, retention time: $t_R(\text{minor}) = 8.884$ min, $t_R(\text{major}) = 15.847$ min, 97% ee. $[\alpha]_D^{20} = 133.3302$ ($c = 1.00$, CH_2Cl_2).

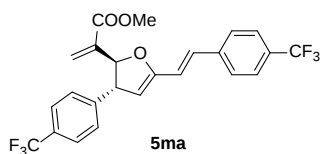
Methyl 2-((2S,3R)-3-(4-iodophenyl)-5-((E)-4-iodostyryl)-2,3-dihydrofuran-2-yl)acrylate (5la):



Yellow oil, 42.3mg; 72.4% yield. ^1H NMR (400 MHz, Acetone) δ 7.83 – 7.70 (m, 4H), 7.46 – 7.37 (m, 2H), 7.21 – 7.12 (m, 2H), 6.98 (t, $J = 12.9$ Hz, 2H), 6.29 (t, $J = 1.1$ Hz, 1H), 5.88 (t, $J = 1.4$ Hz, 1H), 5.27 (d, $J = 3.2$ Hz, 1H), 5.20 (dt, $J = 4.2$, 1.3 Hz, 1H), 4.04 – 3.95 (m, 1H), 3.77 (d, $J = 4.1$ Hz, 3H). ^{13}C

NMR (126 MHz, Acetone) δ 165.3, 155.4, 143.9, 140.0, 137.9, 137.6, 136.4, 129.9, 129.6, 128.7, 123.2, 117.7, 105.1, 93.0, 91.7, 86.1, 55.1, 51.3. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+(\text{C}_{22}\text{H}_{19}\text{I}_2\text{O}_3)$ requires m/z 584.9418, found m/z 584.9412; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: $t_R(\text{major}) = 6.291$ min, $t_R(\text{minor}) = 7.158$ min, 97% ee. $[\alpha]_D^{20} = 16.9163$ ($c = 1.00$, CH_2Cl_2).

Methyl 2-((2S,3R)-3-(4-(trifluoromethyl)phenyl)-5-((E)-4-(trifluoromethyl)styryl)-2,3-dihydrofuran-2-yl)acrylate (5ma):

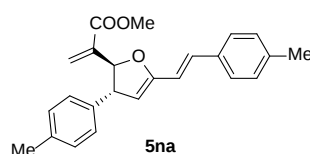


White oil, 38.2mg; 81.5% yield. ^1H NMR (500 MHz, Acetone) δ 7.82 (d, $J = 8.1$ Hz, 2H), 7.78 – 7.66 (m, 4H), 7.58 (d, $J = 8.0$ Hz, 2H), 7.23 – 7.07 (m, 2H), 6.32 (t, $J = 1.2$ Hz, 1H), 5.93 (t, $J = 1.4$ Hz, 1H), 5.39 (d, $J = 3.2$ Hz, 1H), 5.29 (d, $J = 4.3$ Hz, 1H), 4.17 (s, 1H), 3.77 (s, 3H). Due to effect of the two kinds of $-\text{CF}_3$, C-F

correlation lead to the complex of the spectra of the ^{13}C NMR. ^{13}C NMR (126 MHz, Acetone) δ 165.3,

155.5, 148.4, 140.6, 139.8, 129.3, 128.9 (q, $J = 30.2$ Hz), 128.3, 127.3, 126.6, 125.7, 125.6 (q, $J = 3.8$ Hz), 125.4 (q, $J = 3.8$ Hz), 123.4, 119.4, 105.9, 86.1, 64.4, 55.4, 51.3. ^{19}F NMR (471 MHz, Acetone) δ -62.8 (s), -63.0 (s). HRMS: exact mass calculated for $[\text{M}+\text{H}]^+(\text{C}_{24}\text{H}_{19}\text{F}_6\text{O}_3)$ requires m/z 469.1233, found m/z 469.1234; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 97/3, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: $t_{\text{R}}(\text{minor}) = 4.648$ min, $t_{\text{R}}(\text{major}) = 5.128$ min, 99% ee. $[\alpha]_{\text{D}}^{20} = 12.4200(c = 1.00, \text{CH}_2\text{Cl}_2)$.

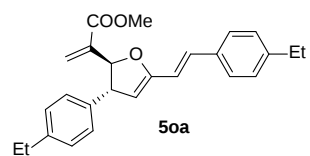
Methyl 2-((2S,3R)-5-((E)-4-methylstyryl)-3-(p-tolyl)-2,3-dihydrofuran-2-yl)acrylate (5na):



Yellow oil, 25.9mg; 72.0% yield. ^1H NMR (500 MHz, Acetone) δ 7.49 – 7.39 (m, 2H), 7.21 – 7.17 (m, 4H), 7.15 (d, $J = 7.9$ Hz, 2H), 7.02 (d, $J = 16.1$ Hz, 1H), 6.83 (d, $J = 16.1$ Hz, 1H), 6.25 (t, $J = 1.2$ Hz, 1H), 5.85 (t, $J = 1.5$ Hz, 1H), 5.19 – 5.15 (m, 2H), 3.94 (t, $J = 3.8$ Hz, 1H), 3.74 (s, 3H), 2.33 (s, 3H), 2.31 (s, 3H).

^{13}C NMR (126 MHz, Acetone) δ 165.4, 155.2, 141.1, 140.4, 137.9, 136.2, 133.9, 130.4, 129.4, 129.1, 127.4, 126.7, 122.9, 115.9, 104.5, 86.3, 55.2, 51.2, 20.4, 20.2. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+(\text{C}_{24}\text{H}_{25}\text{O}_3)$ requires m/z 361.1798, found m/z 361.1796; HPLC conditions: Daicel Chiralpak AD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, $\lambda = 280$ nm, retention time: $t_{\text{R}}(\text{major}) = 10.245$ min, $t_{\text{R}}(\text{minor}) = 15.318$ min, 97% ee. $[\alpha]_{\text{D}}^{20} = 26.1300(c = 1.00, \text{CH}_2\text{Cl}_2)$.

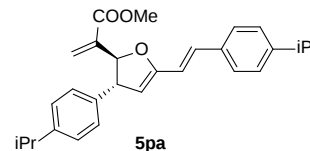
Methyl 2-((2S,3R)-3-(4-ethylphenyl)-5-((E)-4-ethylstyryl)-2,3-dihydrofuran-2-yl)acrylate (5oa):



Yellow oil, 34.3mg; 88.4% yield. ^1H NMR (400 MHz, Acetone) δ 7.51 (d, $J = 8.1$ Hz, 2H), 7.29 – 7.14 (m, 6H), 7.04 (d, $J = 16.1$ Hz, 1H), 6.86 (d, $J = 16.1$ Hz, 1H), 6.27 (t, $J = 1.1$ Hz, 1H), 5.88 (t, $J = 1.5$ Hz, 1H), 5.24 – 5.16 (m, 2H), 3.96 (t, $J = 3.7$ Hz, 1H), 3.76 (s, 3H), 2.71 – 2.58 (m, 4H), 1.23 (td, $J = 7.6$, 3.7 Hz, 6H).

^{13}C NMR (126 MHz, Acetone) δ 165.4, 155.2, 144.4, 142.7, 141.3, 140.4, 134.2, 130.4, 128.2, 127.9, 127.4, 126.8, 122.9, 116.0, 104.5, 86.3, 55.2, 51.2, 28.3, 28.2, 15.3, 15.1. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+(\text{C}_{26}\text{H}_{29}\text{O}_3)$ requires m/z 389.2111, found m/z 389.2112; HPLC conditions: Daicel Chiralpak AD-H column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, $\lambda = 280$ nm, retention time: $t_{\text{R}}(\text{minor}) = 9.315$ min, $t_{\text{R}}(\text{major}) = 15.500$ min, 97% ee. $[\alpha]_{\text{D}}^{20} = 44.6400(c = 1.00, \text{CH}_2\text{Cl}_2)$.

Methyl 2-((2S,3R)-3-(4-isopropylphenyl)-5-((E)-4-isopropylstyryl)-2,3-dihydrofuran-2-yl)acrylate (5pa):

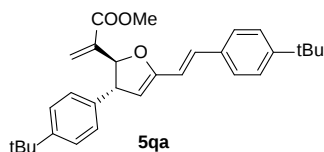


Yellow oil, 31.9mg; 76.8% yield. ^1H NMR (400 MHz, Acetone) δ 7.52 (d, $J = 8.2$ Hz, 2H), 7.32 – 7.21 (m, 6H), 7.05 (d, $J = 16.1$ Hz, 1H), 6.86 (d, $J = 16.1$ Hz, 1H), 6.27 (s, 1H), 5.88 (t, $J = 1.4$ Hz, 1H), 5.21 (dd, $J = 7.0$, 3.7 Hz, 2H), 3.96 (t, $J = 3.7$ Hz, 1H), 3.76 (s, 3H), 2.99 – 2.88 (m, 2H), 1.25 (dd, $J = 6.9$, 3.9 Hz, 12H).

^{13}C NMR (126 MHz, Acetone) δ 165.5, 155.2, 149.0, 147.3, 141.4, 140.4, 134.4, 130.4, 127.4, 126.8, 126.7, 126.4, 122.9, 116.0, 104.5, 86.2, 55.2, 51.2, 33.8, 33.6, 23.5, 23.3. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+(\text{C}_{28}\text{H}_{33}\text{O}_3)$ requires m/z 417.2424, found m/z 417.2422; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 98/2, flow rate = 1.0 mL/min, $\lambda = 280$ nm, retention time: $t_{\text{R}}(\text{minor})$

= 4.440 min, t_R (major) = 4.697 min, 97% ee. $[\alpha]_D^{20} = 52.3102$ (c = 1.00, CH₂Cl₂).

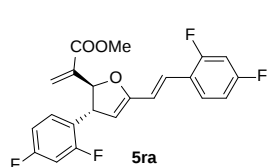
Methyl 2-((2S,3R)-3-(4-(tert-butyl)phenyl)-5-((E)-4-(tert-butyl)styryl)-2,3-dihydrofuran-2-yl)acrylate



(5qa):

Yellow oil, 32.2mg; 72.5% yield. ¹H NMR (400 MHz, Acetone) δ 7.52 (d, J = 8.4 Hz, 2H), 7.48 – 7.38 (m, 4H), 7.29 – 7.21 (m, 2H), 7.05 (d, J = 16.1 Hz, 1H), 6.87 (d, J = 16.1 Hz, 1H), 6.28 (s, 1H), 5.88 (t, J = 1.4 Hz, 1H), 5.21 (dd, J = 8.5, 3.7 Hz, 2H), 3.97 (t, J = 3.6 Hz, 1H), 3.77 (d, J = 4.1 Hz, 3H), 1.34 (s, 9H), 1.33 (s, 9H). ¹³C NMR (126 MHz, Acetone) δ 165.5, 155.2, 151.1, 149.5, 141.0, 140.4, 133.9, 130.3, 127.1, 126.6, 125.6, 125.3, 122.9, 116.1, 104.5, 86.2, 55.1, 51.2, 34.3, 34.1, 30.8, 30.6. HRMS: exact mass calculated for $[M+H]^+$ (C₃₀H₃₇O₃) requires m/z 445.2737, found m/z 445.2736; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 98/2, flow rate = 1.0 mL/min, λ = 280 nm, retention time: t_R (minor) = 4.292 min, t_R (major) = 4.716 min, 98% ee. $[\alpha]_D^{20} = 54.6413$ (c = 1.00, CH₂Cl₂).

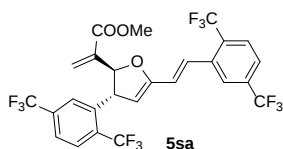
Methyl 2-((2S,3R)-3-(2,4-difluorophenyl)-5-((E)-2,4-difluorostyryl)-2,3-dihydrofuran-2-yl)acrylate



(5ra):

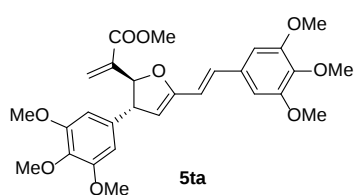
Yellow oil, 32.5mg; 80.4% yield. ¹H NMR (400 MHz, Acetone) δ 7.80 (td, J = 8.9, 6.5 Hz, 1H), 7.42 (td, J = 8.6, 6.5 Hz, 1H), 7.19 – 6.86 (m, 6H), 6.31 (t, J = 1.0 Hz, 1H), 5.93 (t, J = 1.3 Hz, 1H), 5.30 (d, J = 5.3 Hz, 1H), 5.25 (d, J = 3.1 Hz, 1H), 4.33 (dd, J = 5.1, 3.2 Hz, 1H), 3.72 (s, 3H). Due to effect of the four kinds of -F, C-F correlation lead to the complex of the spectra of the ¹³C NMR, which means it is very hard to assign the right peaks. ¹⁹F NMR (376 MHz, Acetone) δ -111.19 – -111.44 (m), -113.72 – -113.88 (m), -114.70 – -114.85 (m), -116.28 (dd, J = 17.4, 8.4 Hz). HRMS: exact mass calculated for $[M+H]^+$ (C₂₂H₁₇F₄O₃) requires m/z 405.1108, found m/z 405.1109; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 4.660 min, t_R (minor) = 4.920 min, 96% ee. $[\alpha]_D^{20} = 14.7400$ (c = 1.00, CH₂Cl₂).

Methyl 2-((2S,3R)-3-(2,6-bis(trifluoromethyl)phenyl)-5-((E)-2,6-bis(trifluoromethyl)styryl)-2,3-dihydrofuran-2-yl)acrylate (5sa):



White oil, 48.2mg; 79.8% yield. ¹H NMR (400 MHz, Acetone) δ 8.29 (s, 2H), 8.07 – 7.89 (m, 4H), 7.34 (d, J = 4.9 Hz, 2H), 6.36 (s, 1H), 5.98 (s, 1H), 5.53 (d, J = 3.2 Hz, 1H), 5.36 (d, J = 4.2 Hz, 1H), 4.41 (t, J = 3.7 Hz, 1H), 3.78 (s, 3H). Due to effect of -CF₃, C-F correlation lead to the complex of the spectra of the ¹³C NMR. Many peaks split to small peaks, which means it is very hard to assign the right peaks. ¹⁹F NMR (376 MHz, Acetone) δ -63.2 (s), -63.5 (s). HRMS: exact mass calculated for $[M-H]^-$ (C₂₆H₁₅F₁₂O₃) requires m/z 603.0835, found m/z 603.0841; HPLC conditions: Daicel Chiralpak IJ column, n-hexane/2-propanol = 99/1, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (major) = 4.231 min, t_R (minor) = 5.350 min, 93% ee. $[\alpha]_D^{20} = 7.2392$ (c = 1.00, CH₂Cl₂).

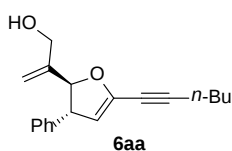
Methyl 2-((2S,3R)-3-(3,4,5-trimethoxyphenyl)-5-((E)-3,4,5-trimethoxystyryl)-2,3-dihydrofuran-2-yl)acrylate (5ta):



acrylate (5ta):

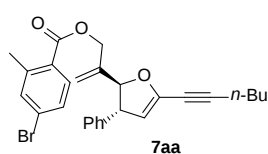
Yellow oil, 37.8mg; 73.8% yield. ^1H NMR (500 MHz, Acetone) δ 7.04 – 6.83 (m, 4H), 6.65 (s, 2H), 6.29 (s, 1H), 5.87 (t, J = 1.4 Hz, 1H), 5.23 (d, J = 4.5 Hz, 1H), 5.18 (d, J = 3.1 Hz, 1H), 3.89 (s, 6H), 3.83 (s, 6H), 3.79 (s, 3H), 3.76 (s, 3H), 3.73 (s, 3H). ^{13}C NMR (126 MHz, Acetone) δ 165.5, 155.4, 153.7, 153.5, 140.4, 139.5, 138.7, 137.3, 132.2, 130.8, 123.2, 116.1, 104.8, 104.3, 104.0, 86.2, 59.7, 59.7, 59.6, 55.7, 55.5, 51.2. HRMS: exact mass calculated for $[\text{M}-\text{H}]^-$ ($\text{C}_{28}\text{H}_{33}\text{O}_9$) requires m/z 513.2119, found m/z 513.2123; HPLC conditions: Daicel Chiralpak IF-3 column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{R} (minor) = 44.707 min, t_{R} (major) = 48.754 min, 97% ee. $[\alpha]_{\text{D}}^{20}$ = 15.9230 (c = 1.00, CH_2Cl_2).

2-((2S,3R)-5-(hex-1-yn-1-yl)-3-phenyl-2,3-dihydrofuran-2-yl)prop-2-en-1-ol (6aa):



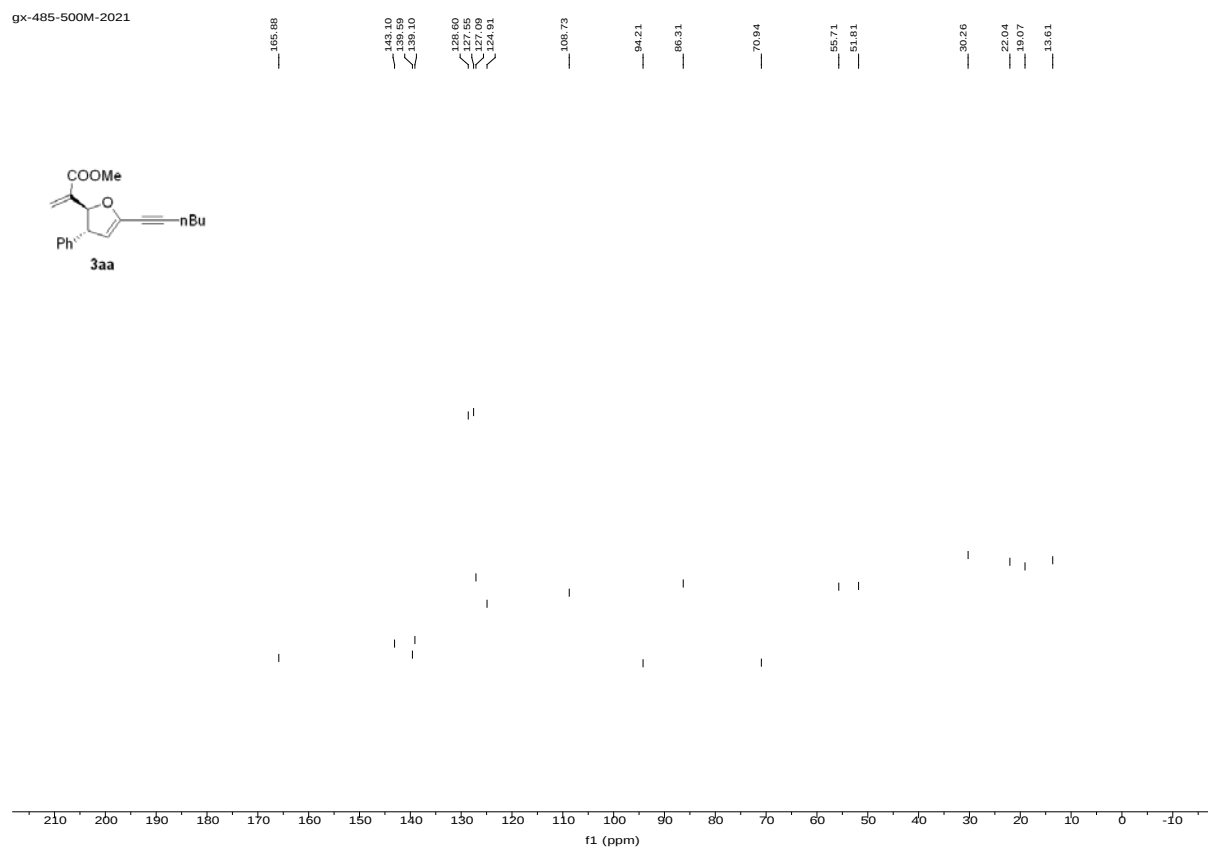
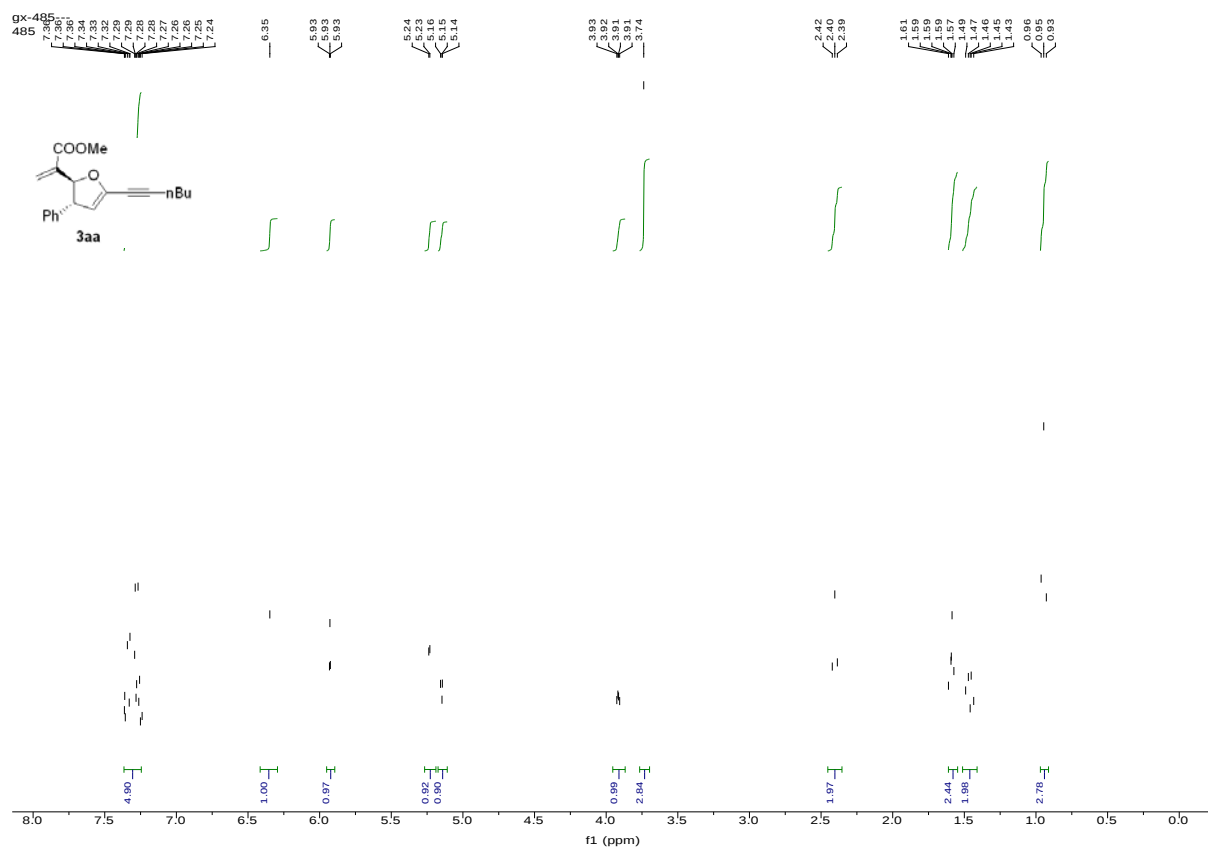
Light-green oil, 24.4mg; 86.3% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.35 (dd, J = 9.3, 5.1 Hz, 2H), 7.28 (ddd, J = 11.4, 5.9, 2.8 Hz, 3H), 5.28 (d, J = 2.7 Hz, 1H), 5.25 (s, 1H), 5.13 (s, 1H), 4.90 (d, J = 8.0 Hz, 1H), 4.31 (dd, J = 29.2, 13.9 Hz, 2H), 4.14 (dd, J = 8.0, 2.6 Hz, 1H), 2.41 (t, J = 7.1 Hz, 2H), 1.85 (s, 1H), 1.59 (tt, J = 7.2, 5.8 Hz, 2H), 1.52 – 1.38 (m, 2H), 0.96 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 146.8, 142.8, 139.9, 128.9, 128.8, 127.7, 127.2, 112.7, 109.3, 94.2, 91.0, 62.6, 54.7, 30.3, 22.0, 19.0, 13.6. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{26}\text{H}_{21}\text{O}_3$) requires m/z 283.1693, found m/z 283.1693; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{R} (minor) = 6.421 min, t_{R} (major) = 7.483 min, 94% ee. $[\alpha]_{\text{D}}^{20}$ = 14.6932 (c = 1.00, CH_2Cl_2).

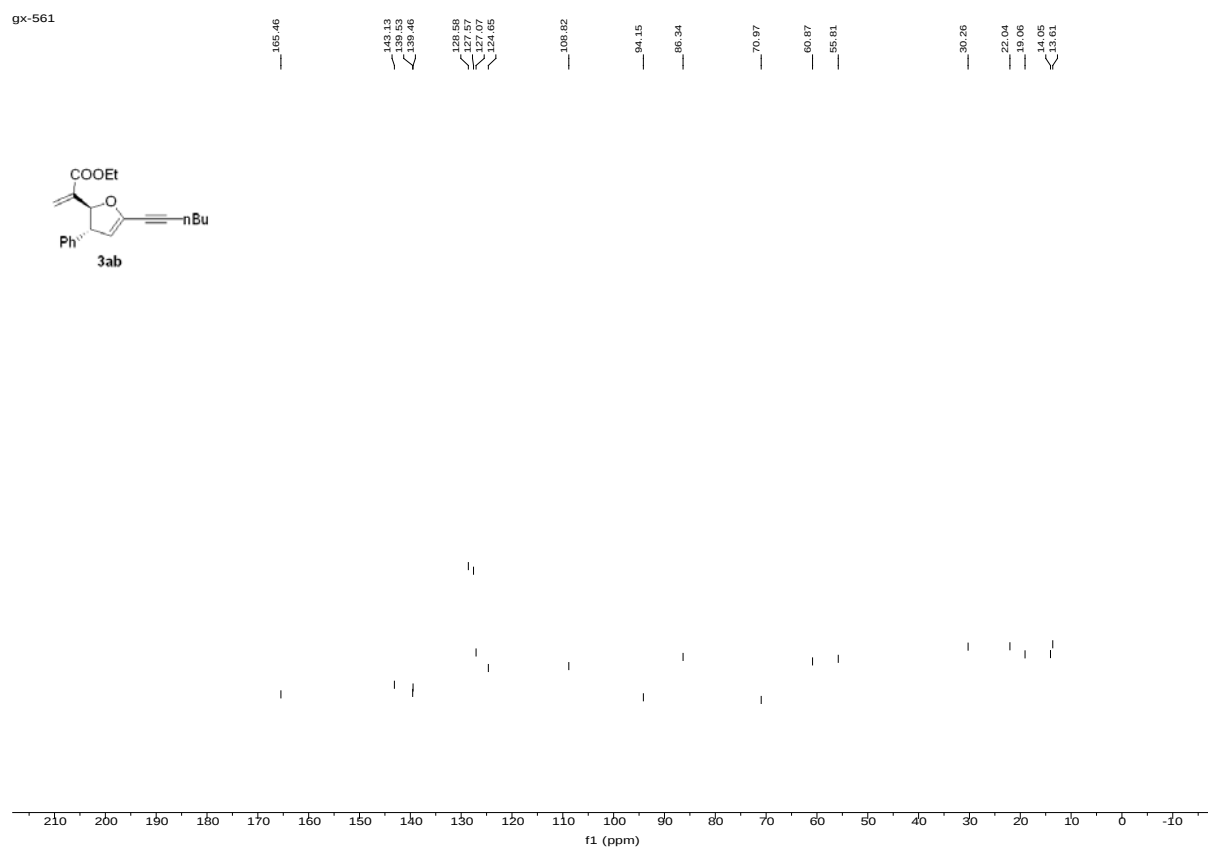
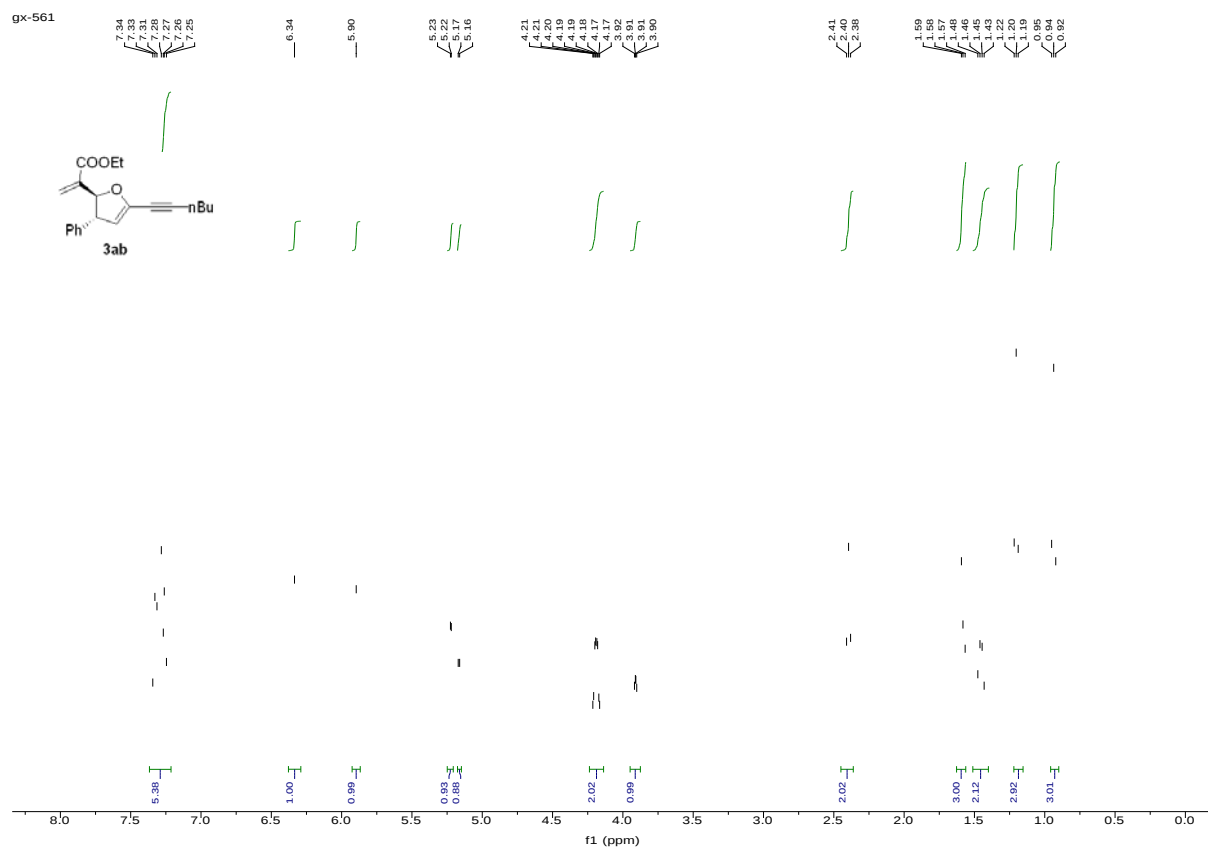
2-((2S,3R)-5-(hex-1-yn-1-yl)-3-phenyl-2,3-dihydrofuran-2-yl)allyl 4-bromo-2-methylbenzoate (7aa):

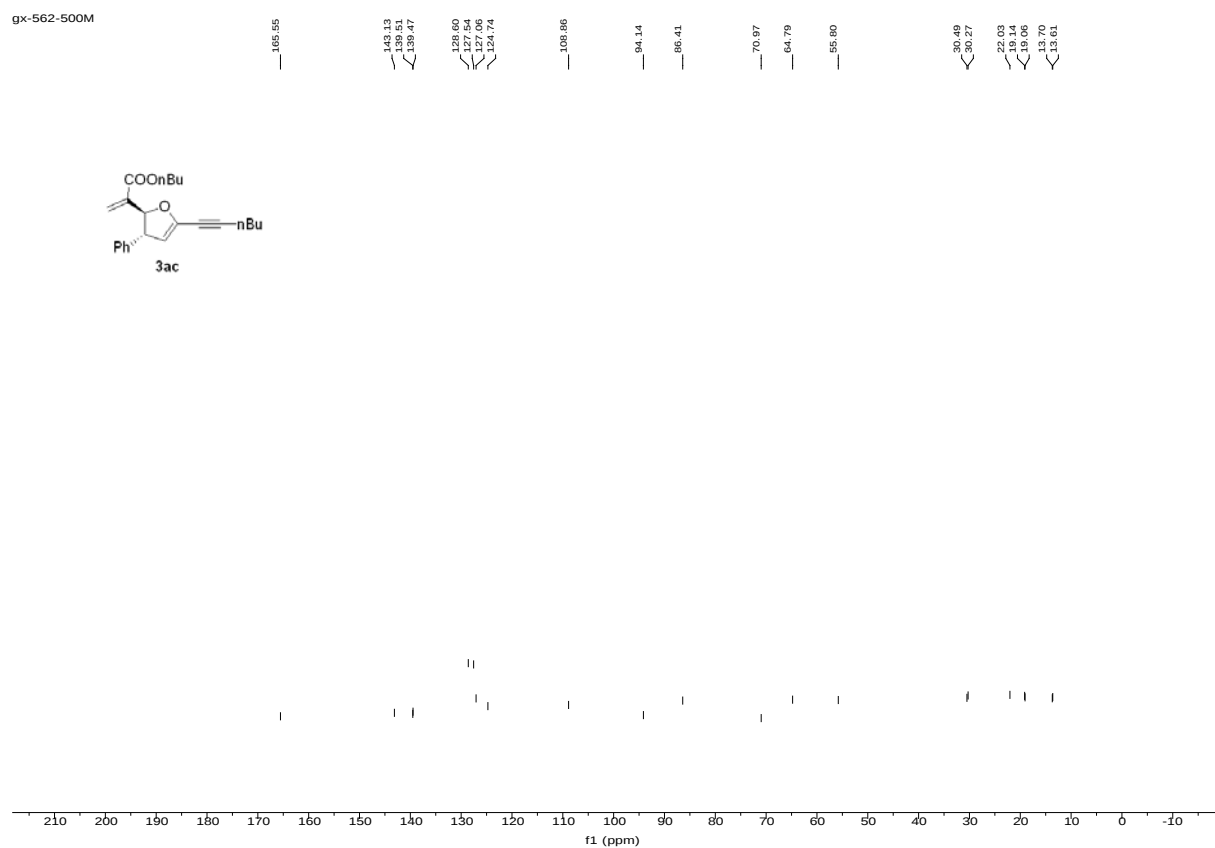
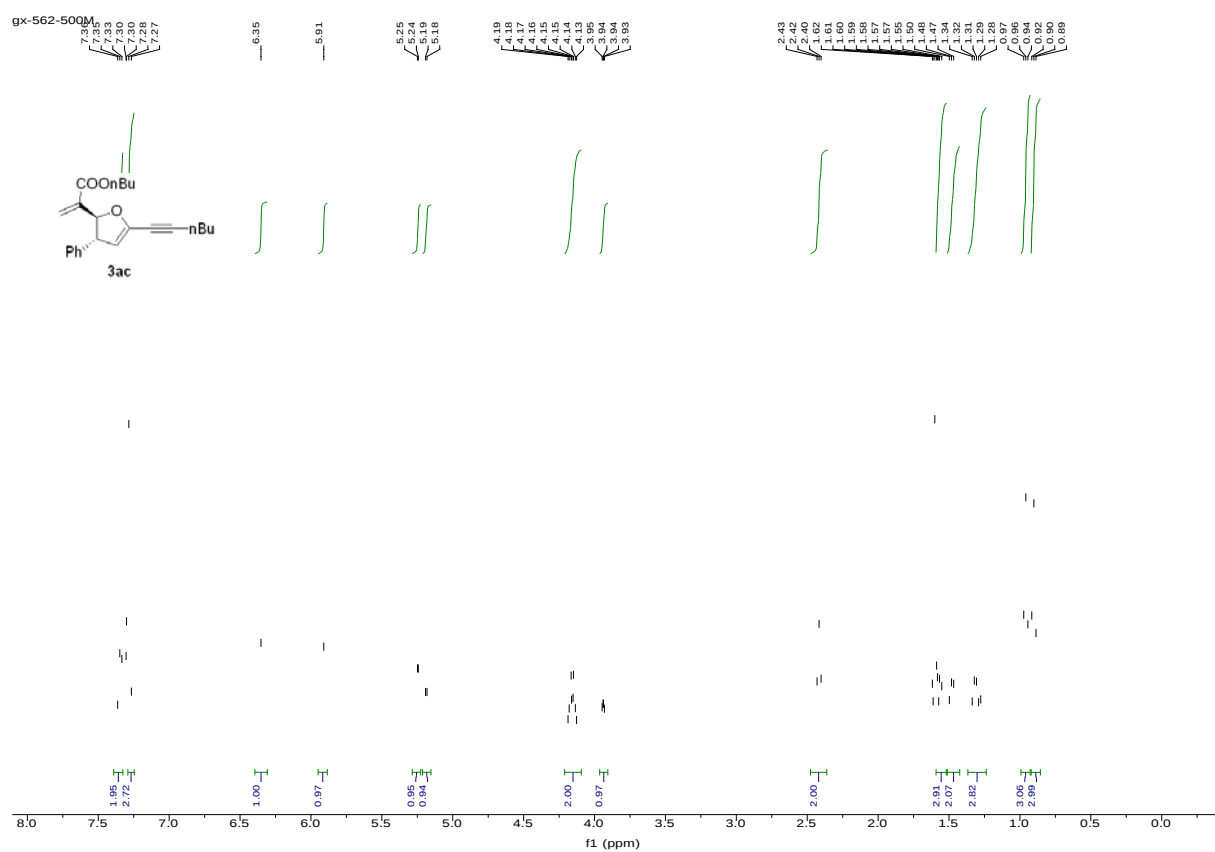


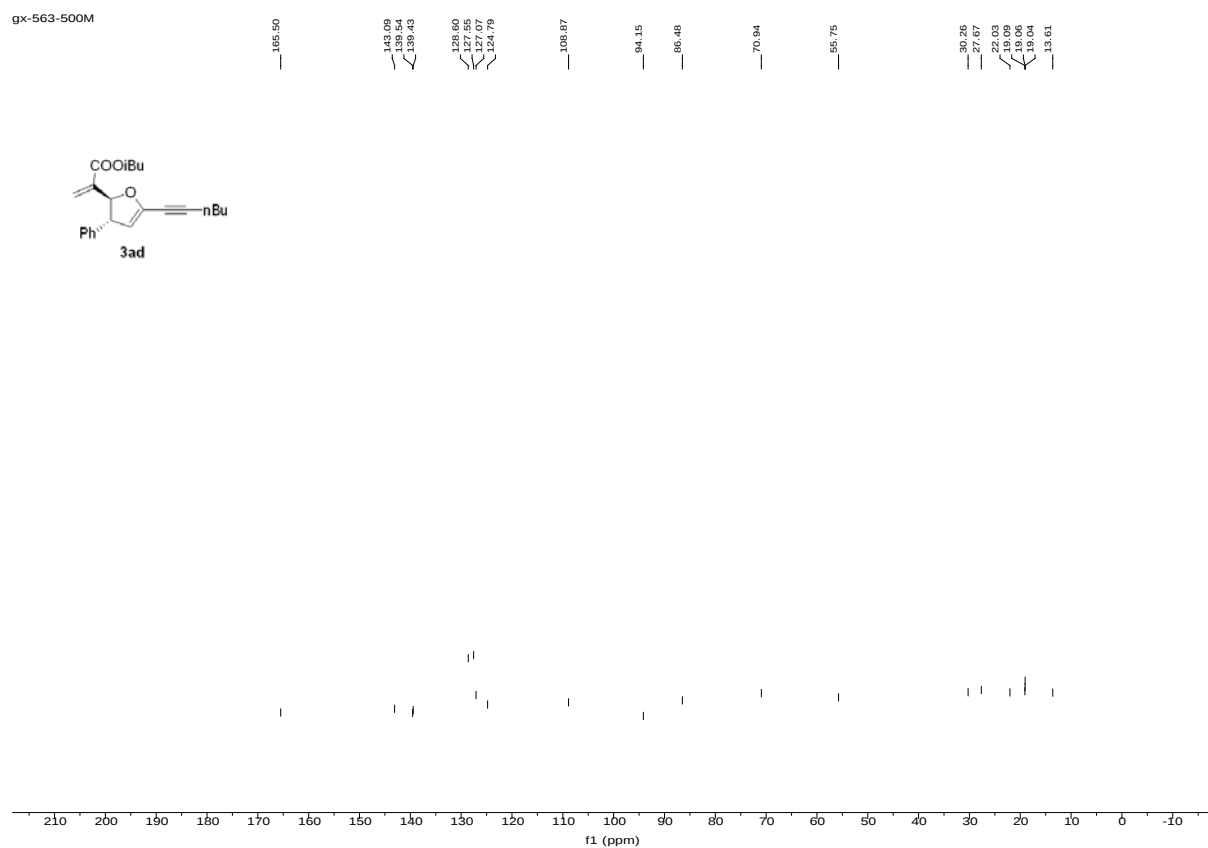
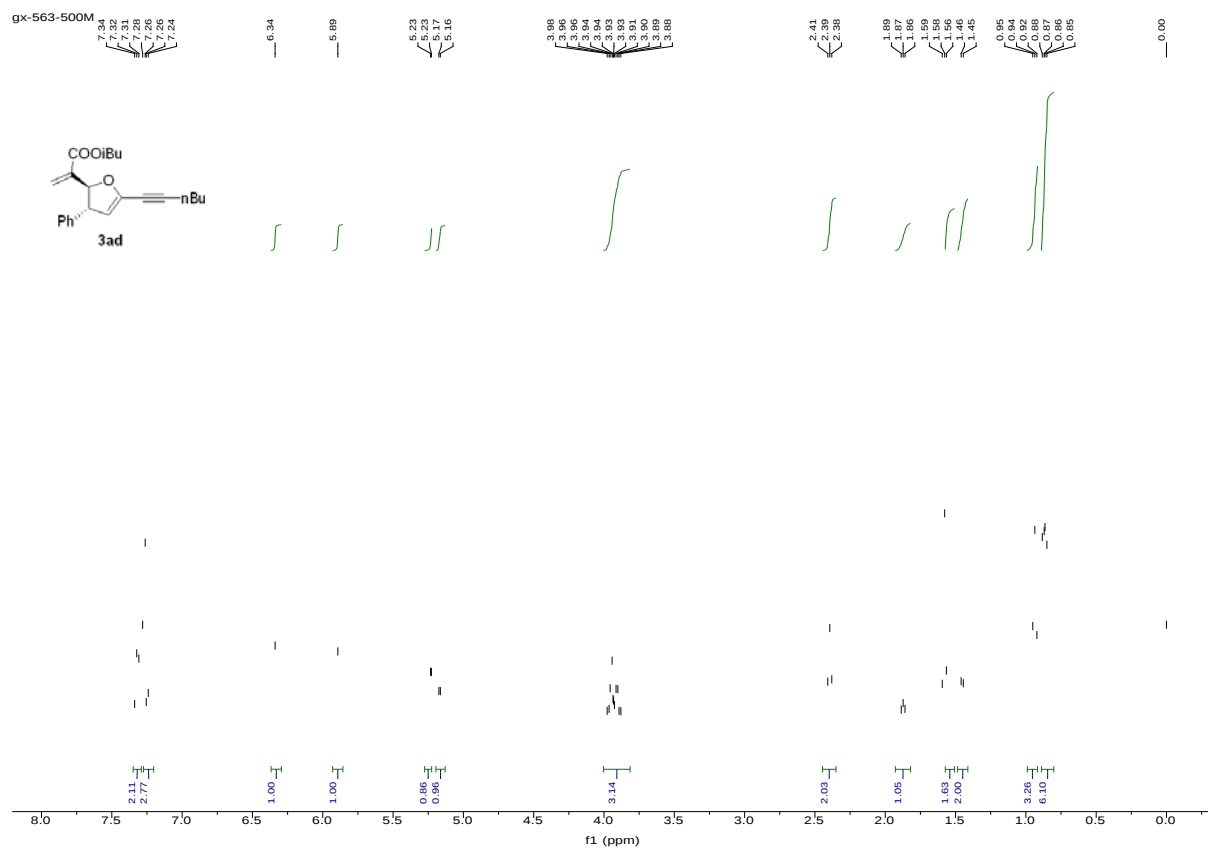
Yellow oil, 38.9mg; 81.3% yield. ^1H NMR (500 MHz, Acetone) δ 7.77 (d, J = 8.4 Hz, 1H), 7.54 (d, J = 1.4 Hz, 1H), 7.47 (dd, J = 8.4, 1.8 Hz, 1H), 7.33 (dd, J = 10.2, 4.6 Hz, 2H), 7.29 – 7.21 (m, 3H), 5.34 (s, 1H), 5.30 – 5.26 (m, 2H), 4.96 (dd, J = 14.1, 9.0 Hz, 3H), 4.27 (dd, J = 7.5, 2.7 Hz, 1H), 2.56 (s, 3H), 2.40 (t, J = 7.0 Hz, 2H), 1.57 – 1.50 (m, 2H), 1.49 – 1.39 (m, 2H), 0.93 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, Acetone) δ 165.7, 143.2, 142.9, 142.6, 140.0, 134.3, 132.2, 129.0, 128.76, 128.6, 127.5, 127.1, 126.2, 113.8, 109.1, 93.5, 90.0, 71.2, 63.5, 54.2, 30.2, 21.7, 20.6, 18.3, 13.0. HRMS: exact mass calculated for $[\text{M}+\text{H}]^+$ ($\text{C}_{27}\text{H}_{28}\text{BrO}_3$) requires m/z 479.1216, found m/z 479.1211; HPLC conditions: Daicel Chiralpak OD-H column, n-hexane/2-propanol = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{R} (minor) = 4.524 min, t_{R} (major) = 6.696 min, 91% ee. $[\alpha]_{\text{D}}^{20}$ = 65.8927 (c = 1.00, CH_2Cl_2).

C: Copies of NMR Analysis

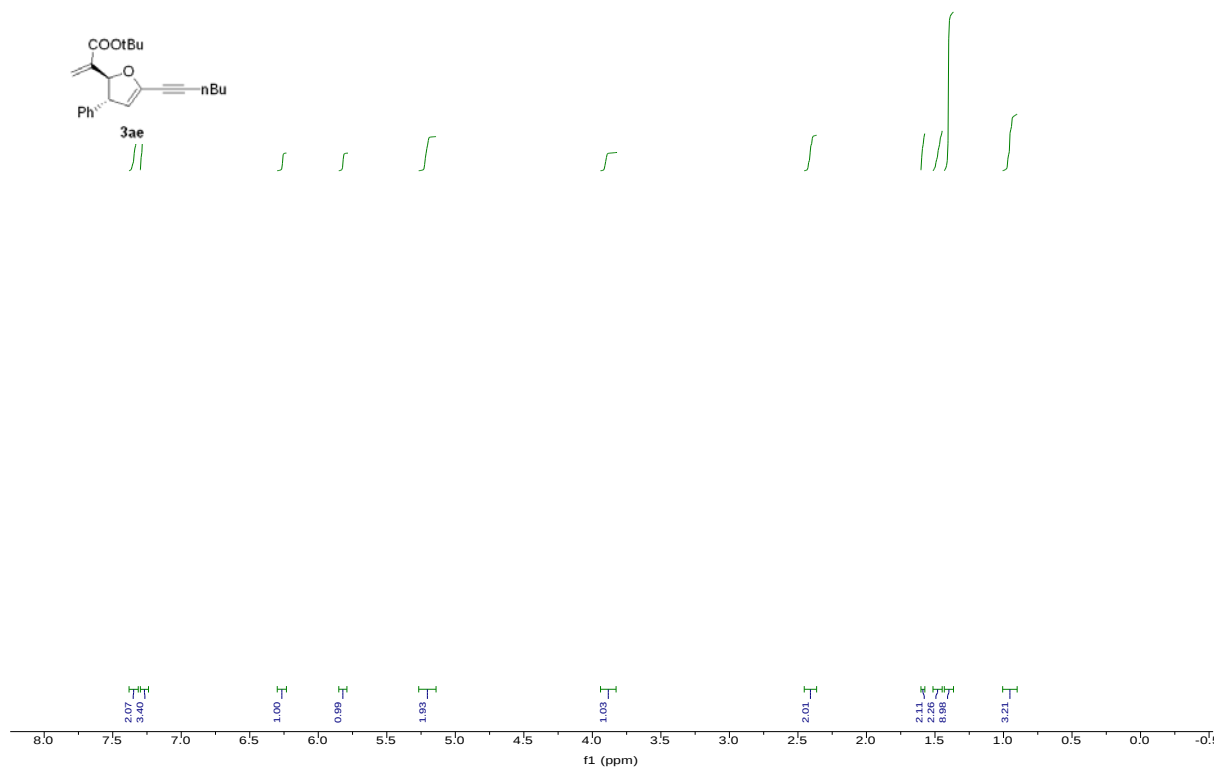




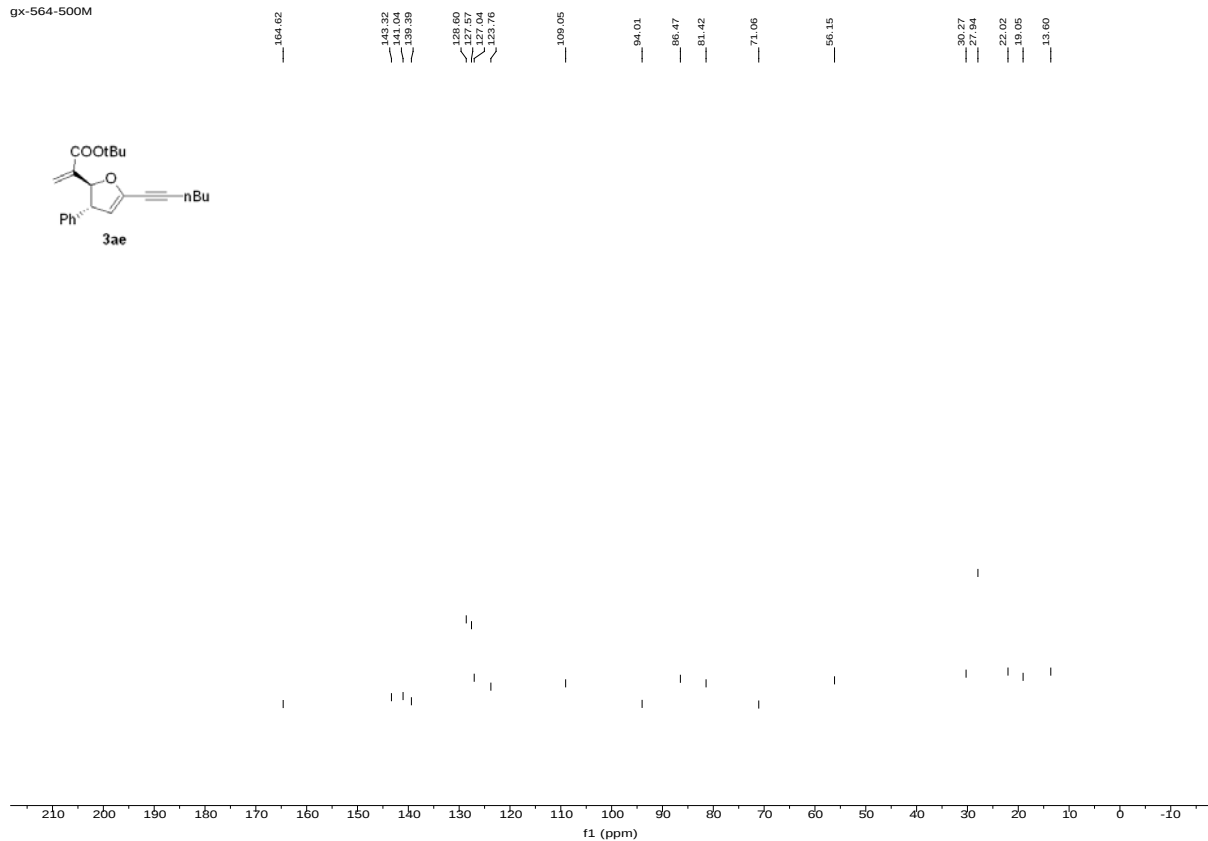


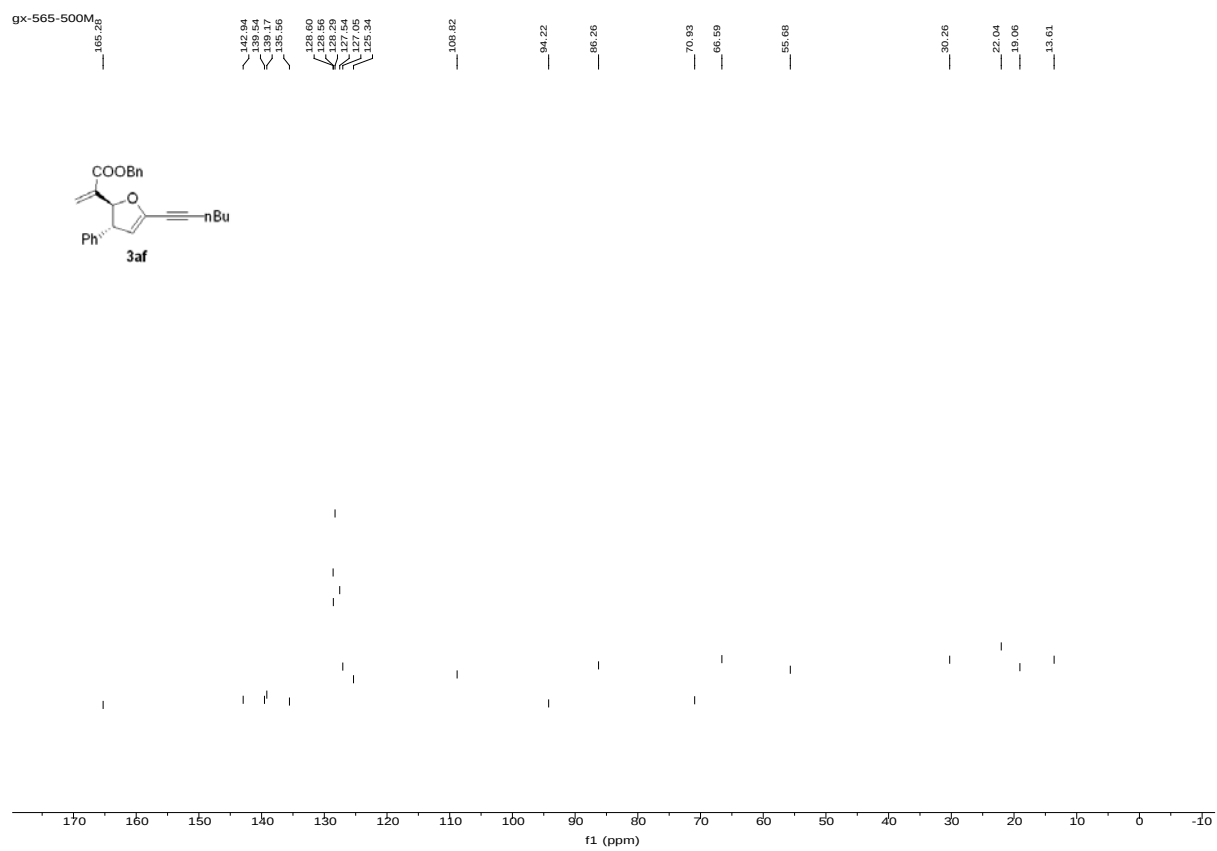
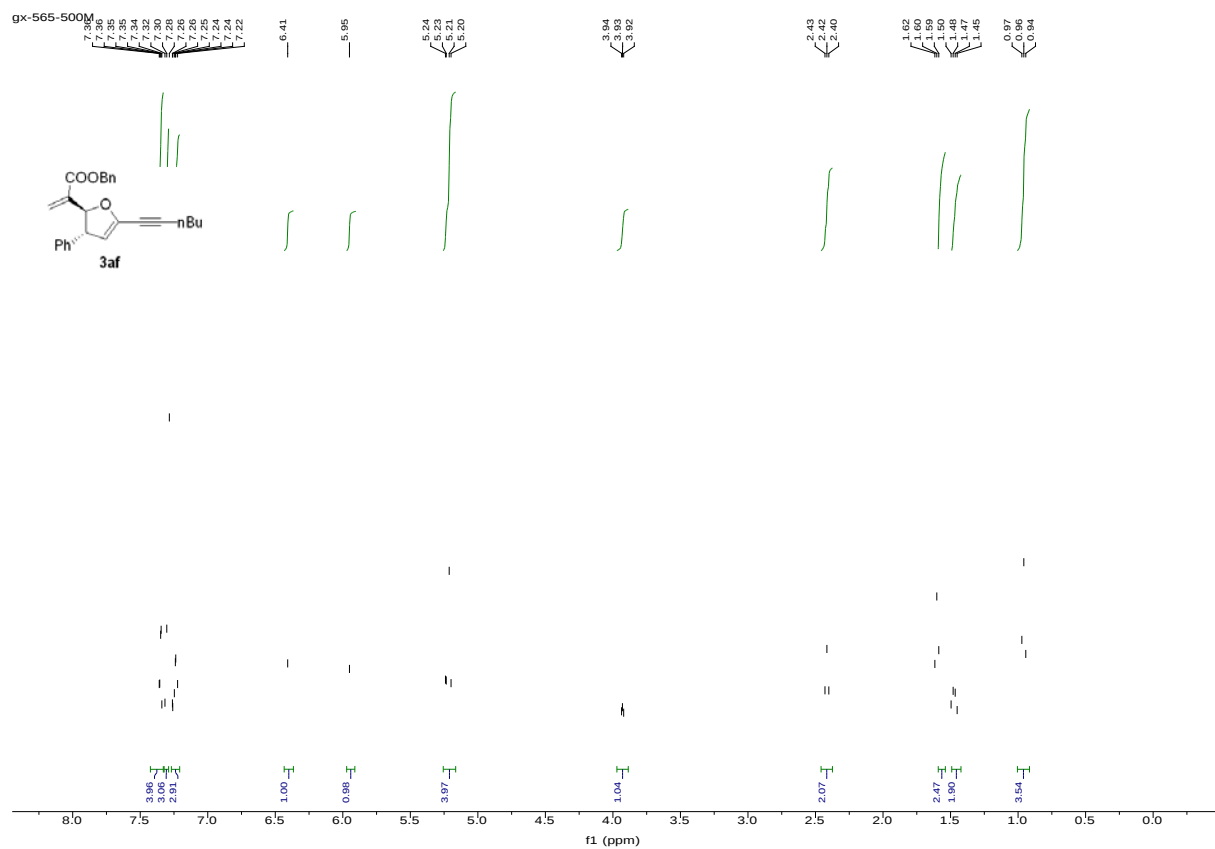


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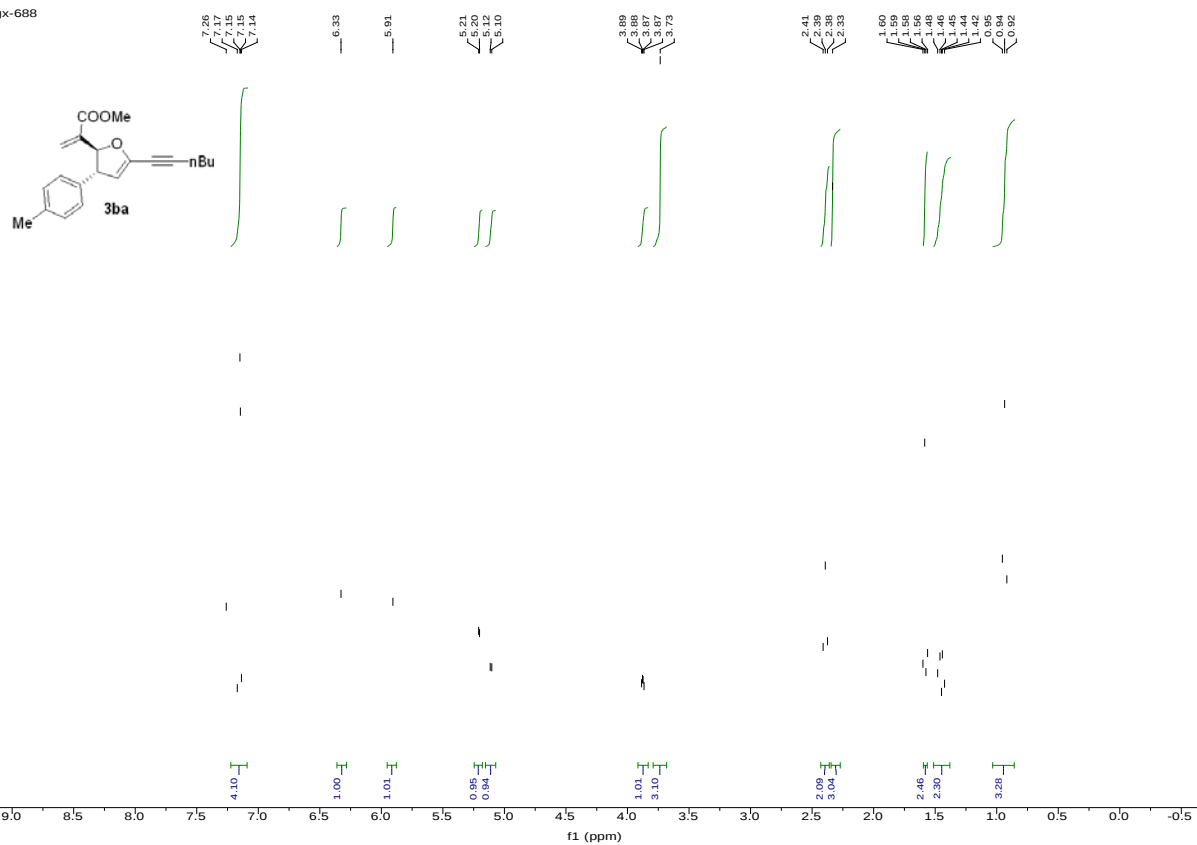


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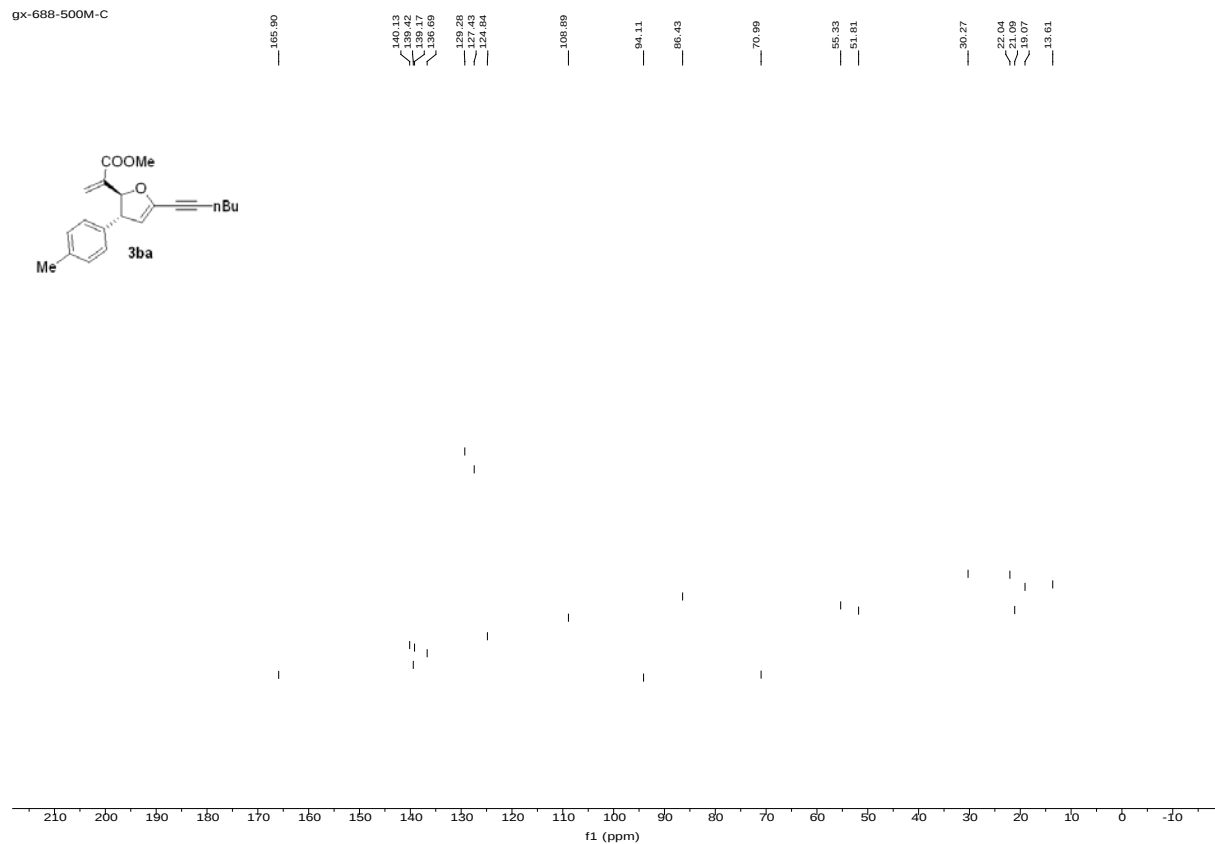




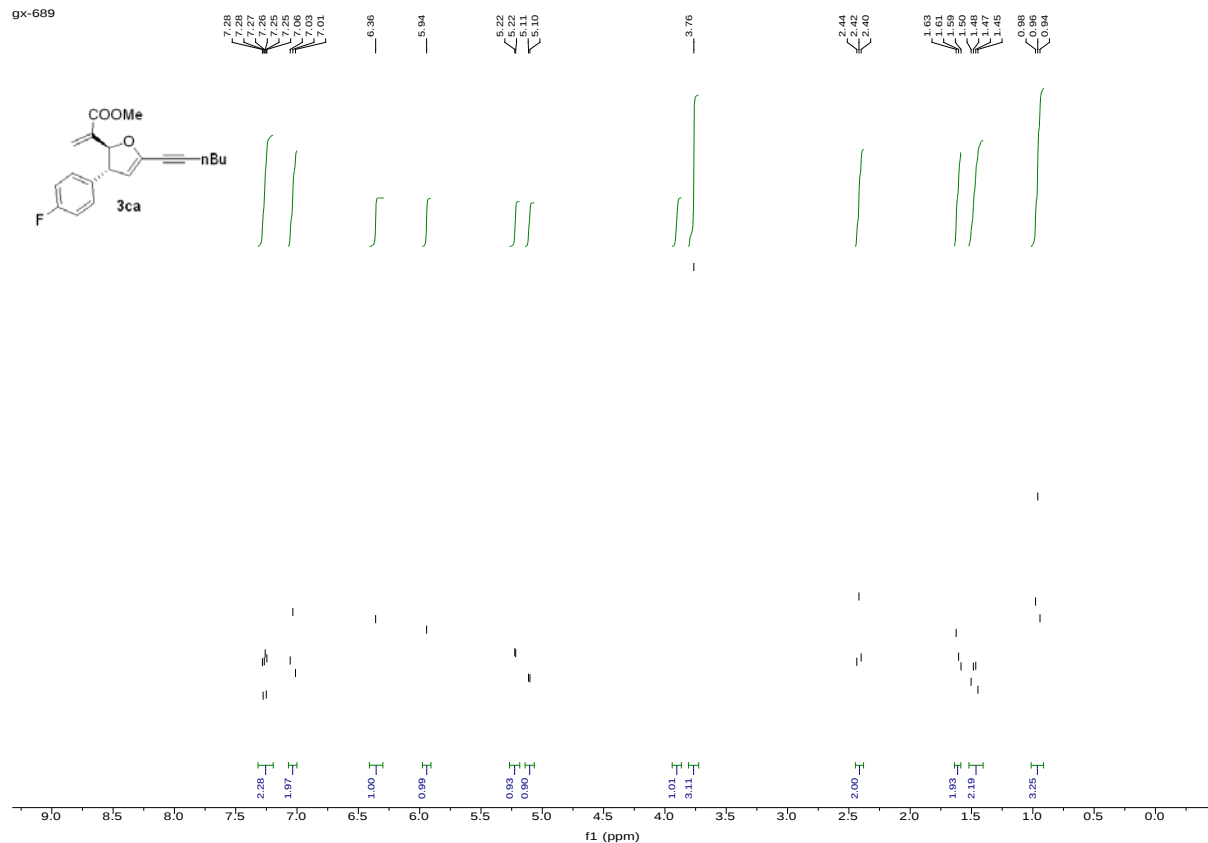
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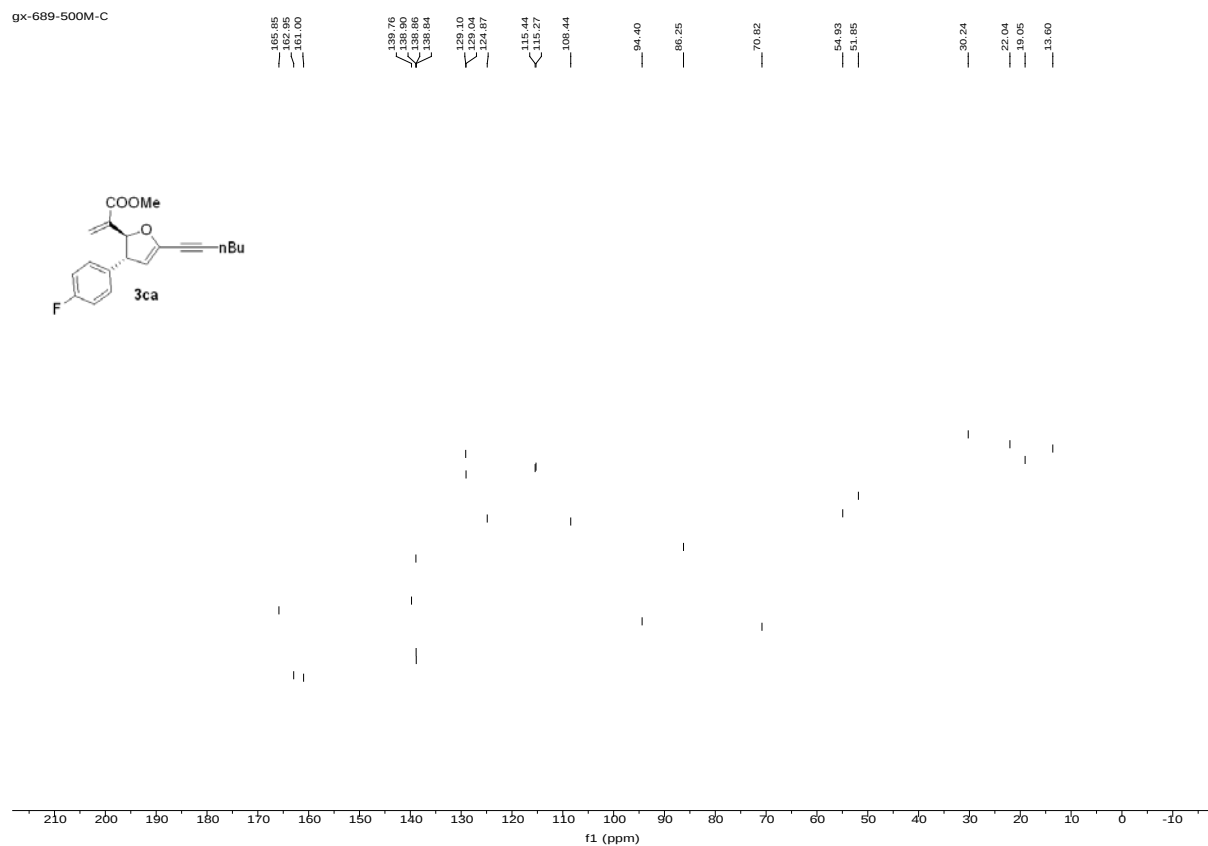
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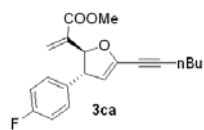
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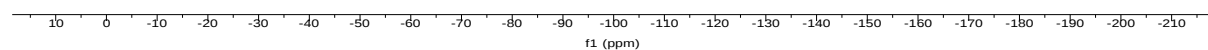
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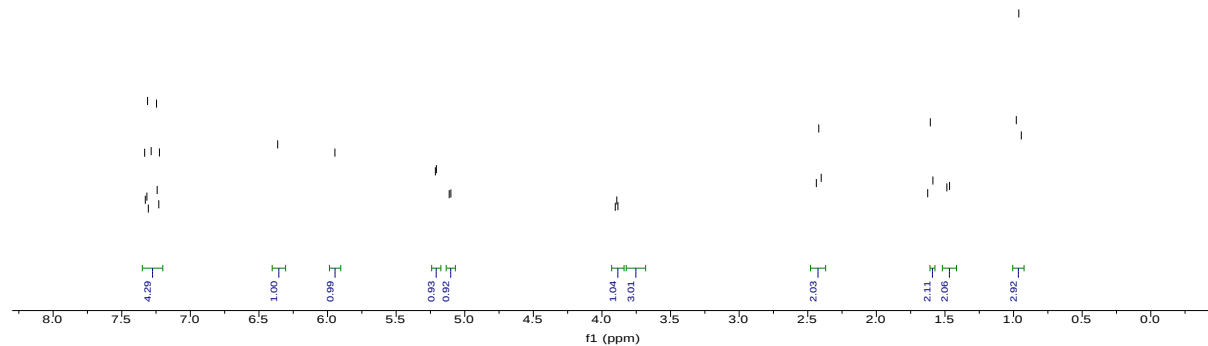
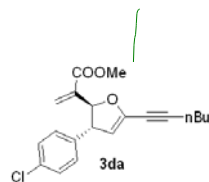
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697F



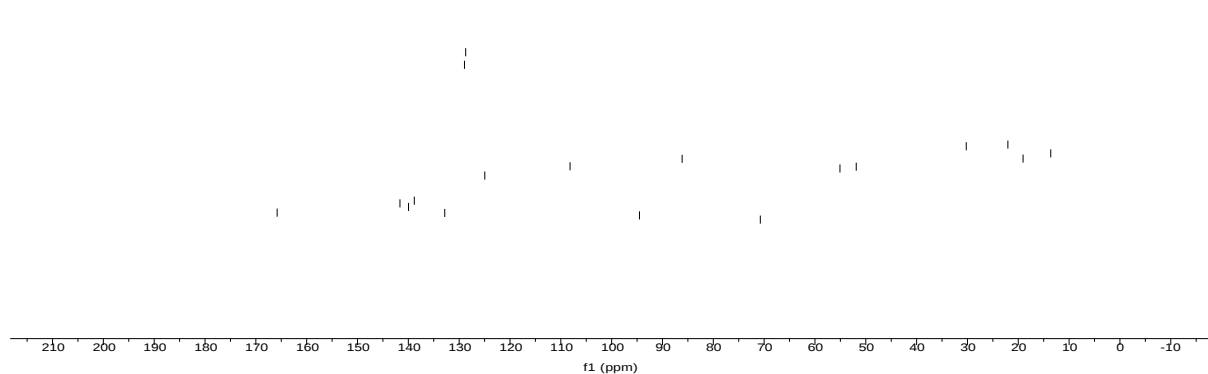
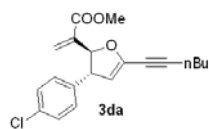
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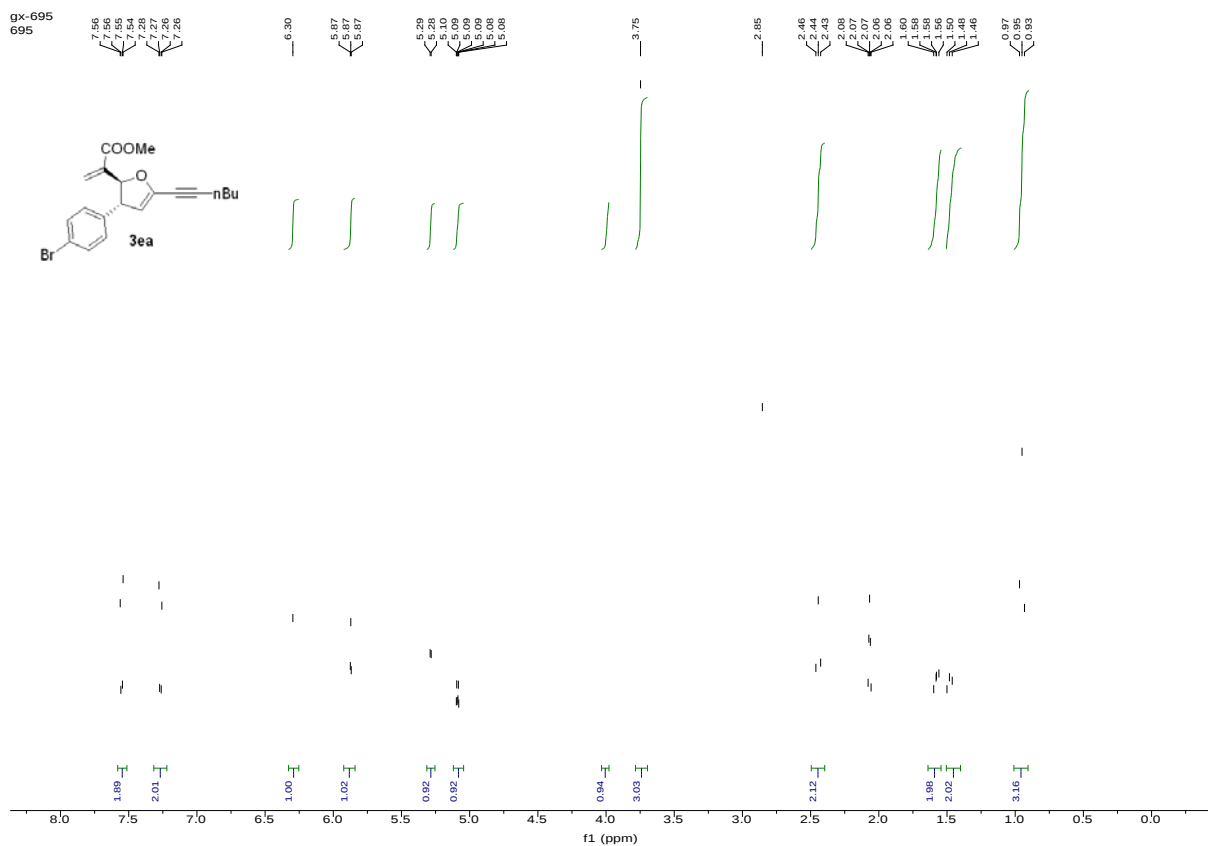
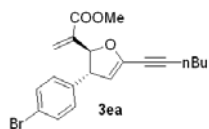
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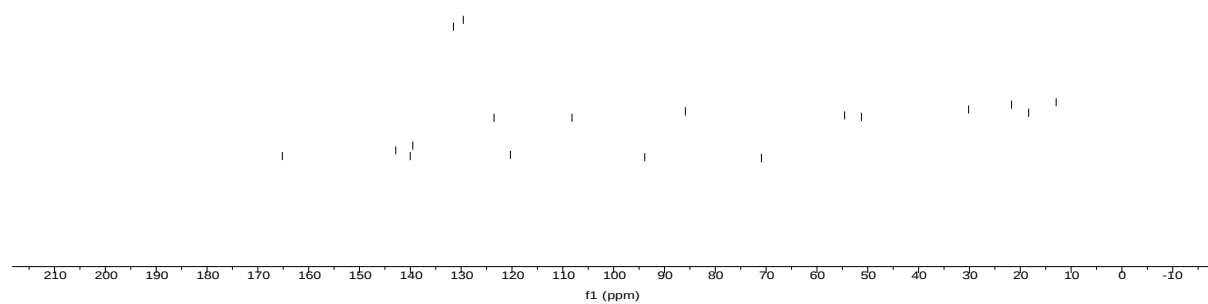
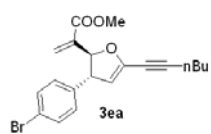
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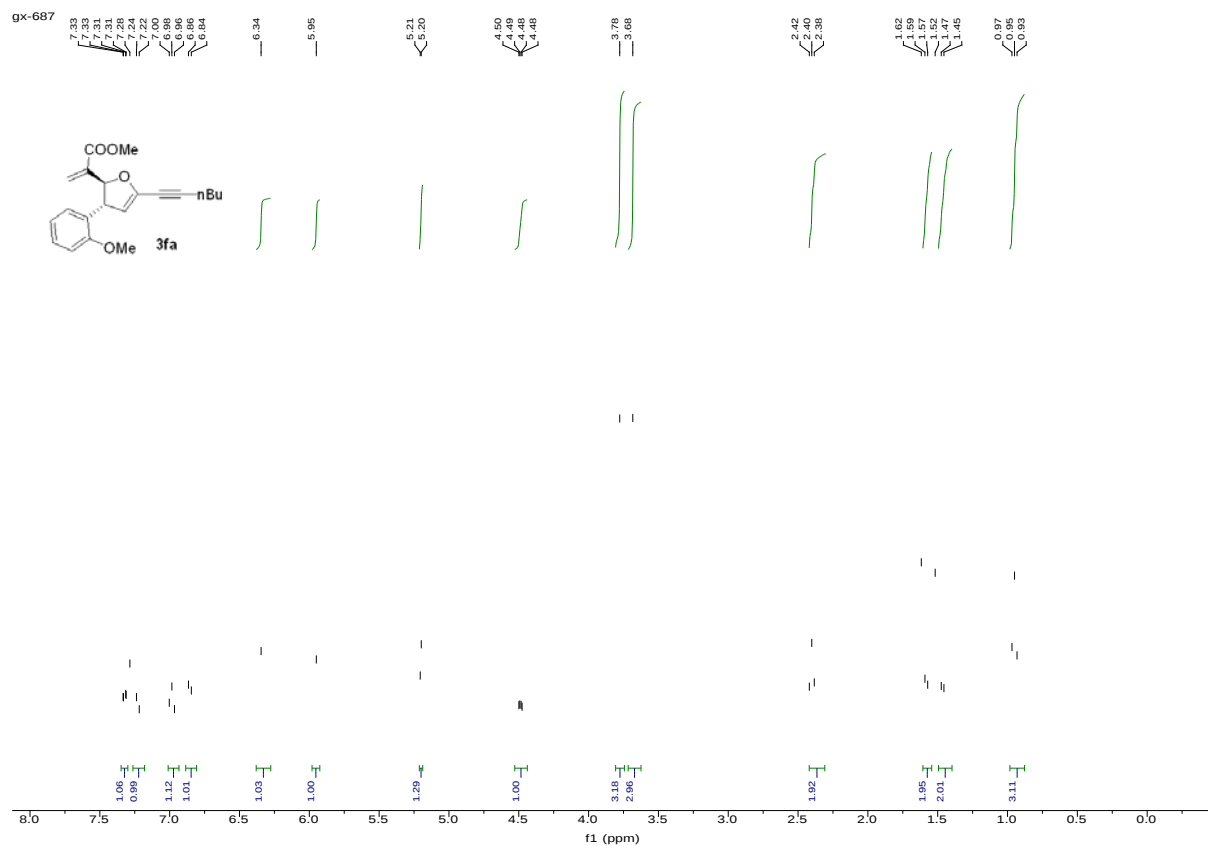
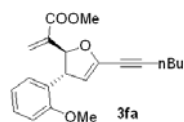
gx-695
695



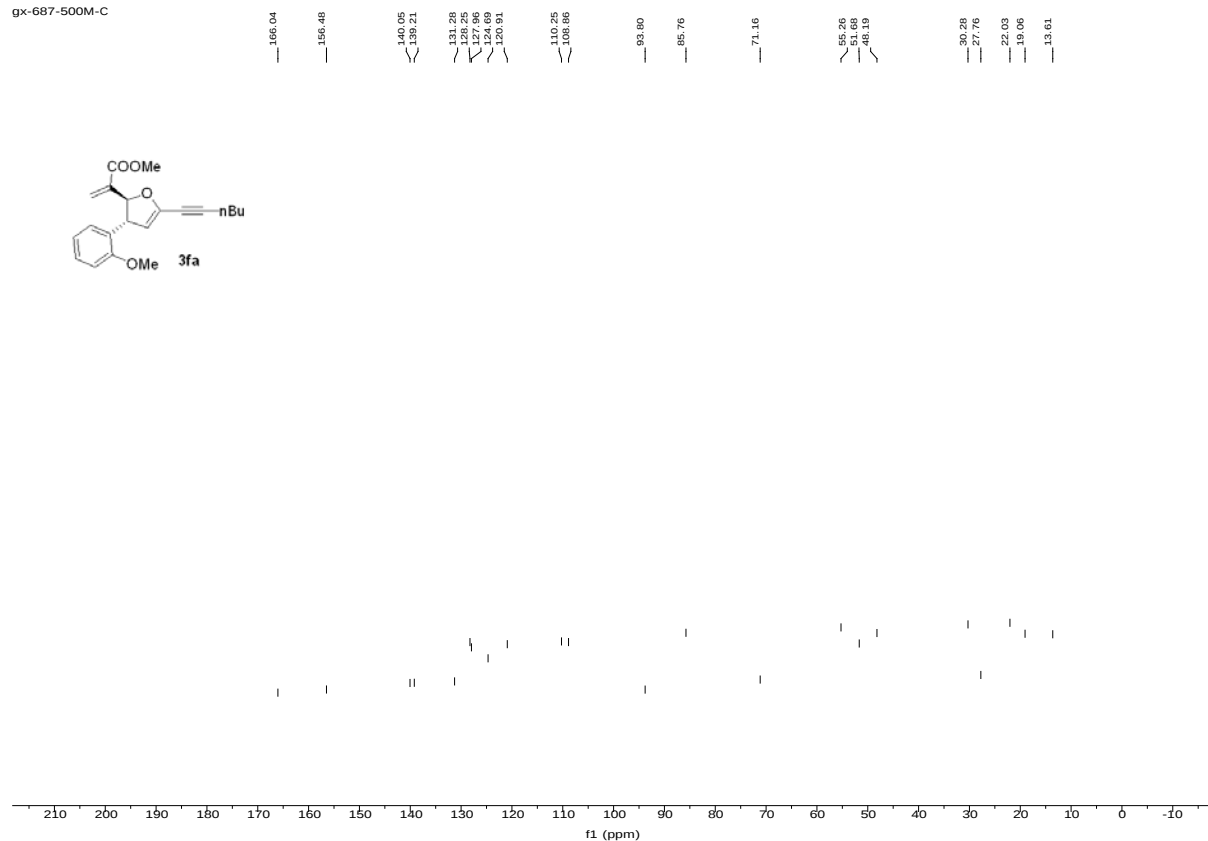
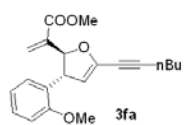
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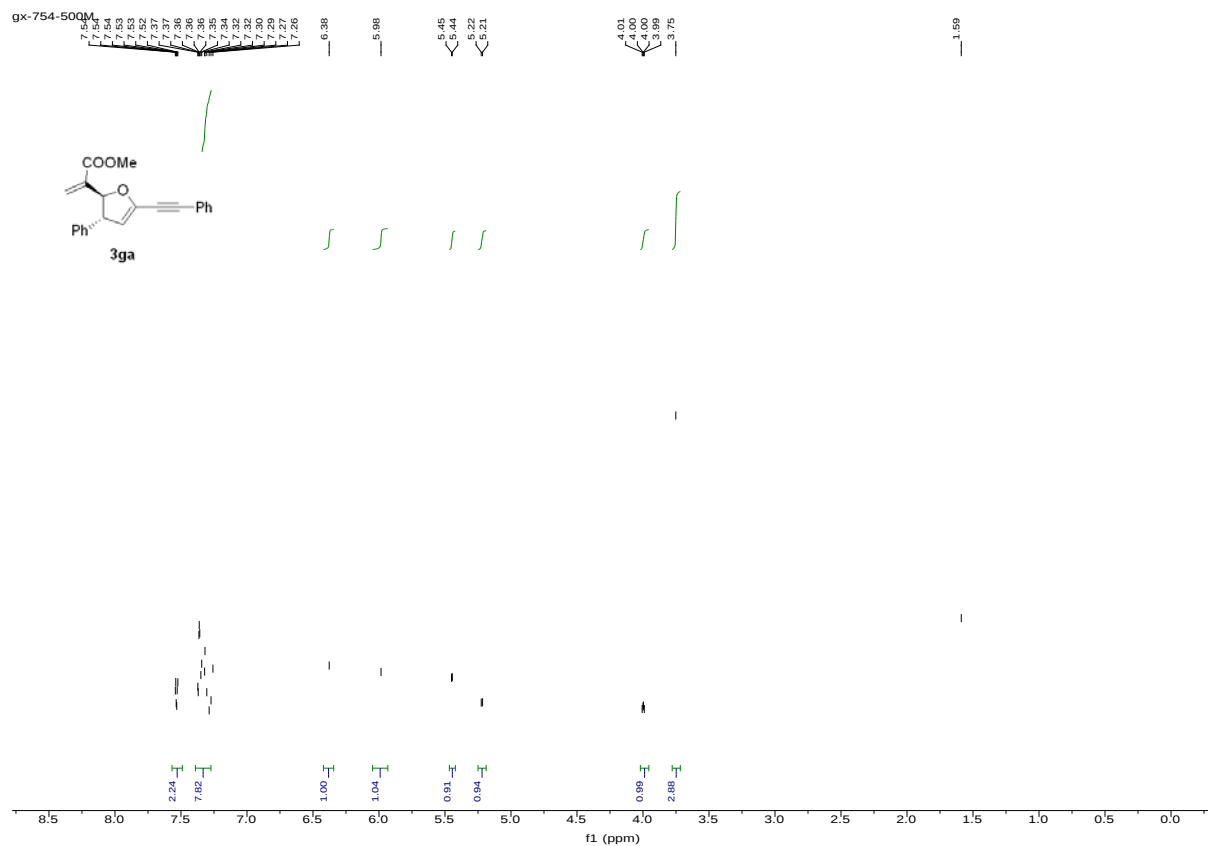
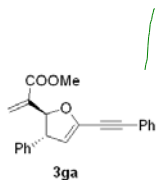
gx-687



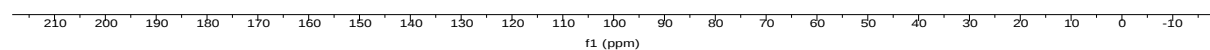
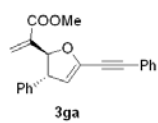
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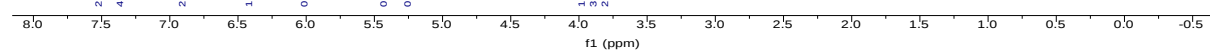
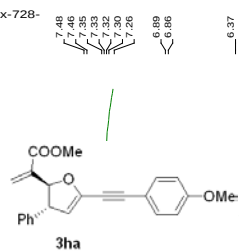
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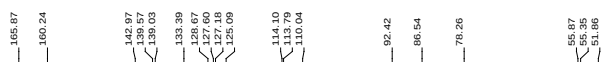
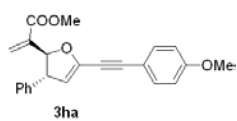
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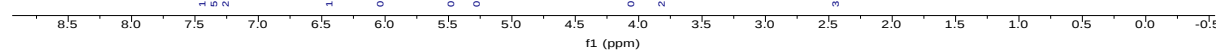
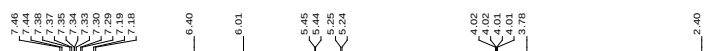
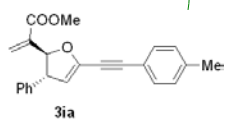
gx-728-



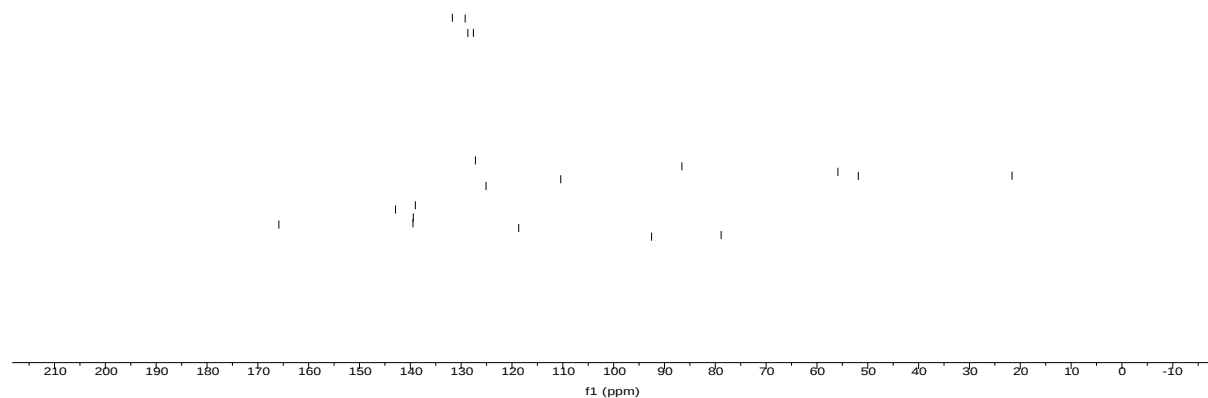
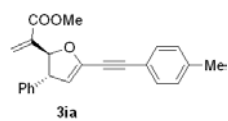
gx-728-500M-C



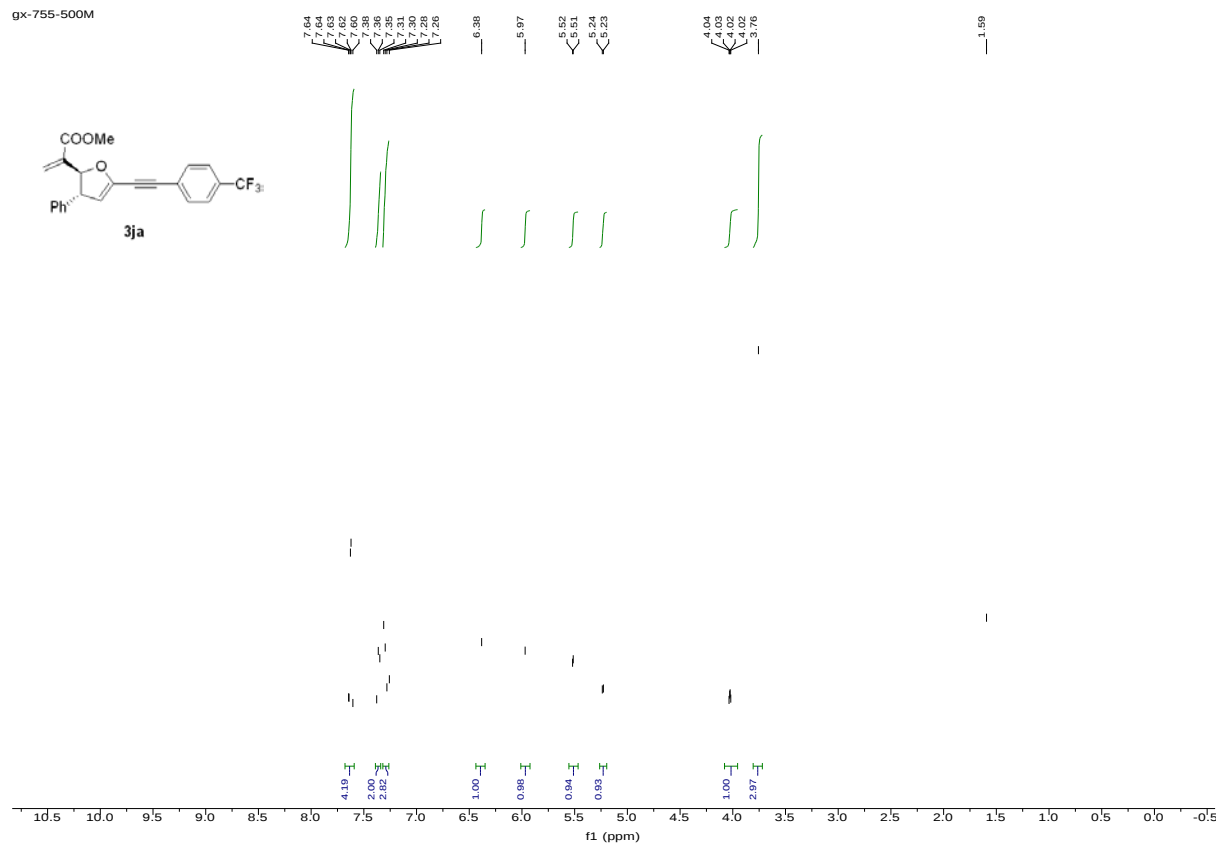
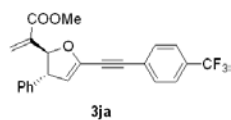
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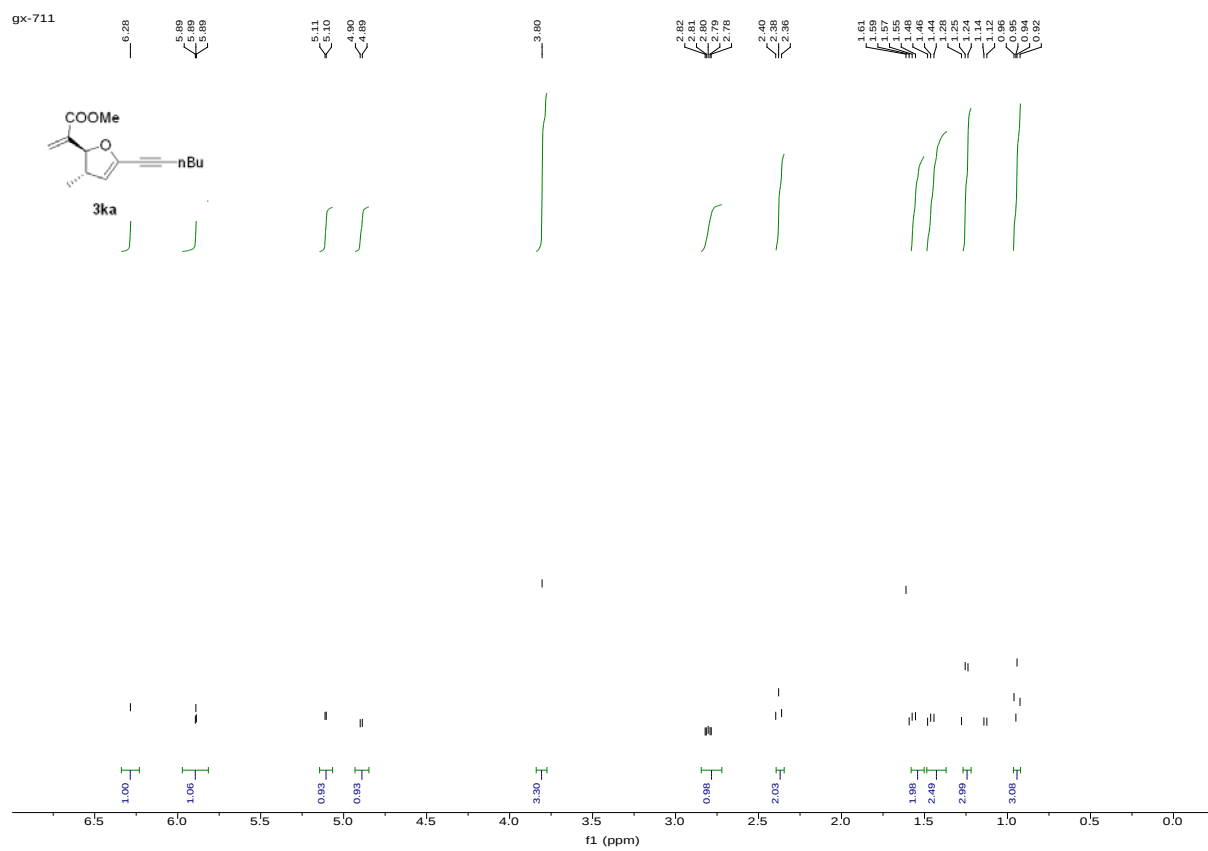
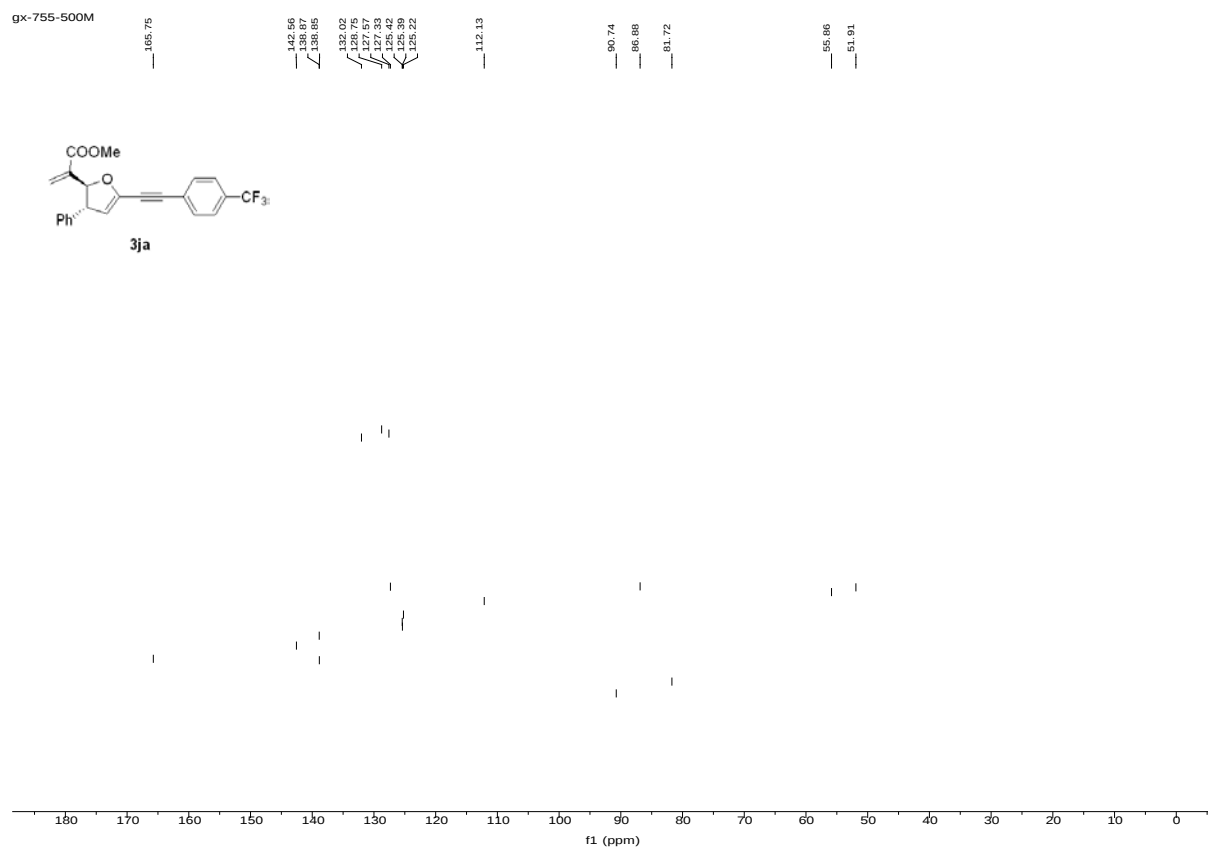


gx-780-500M

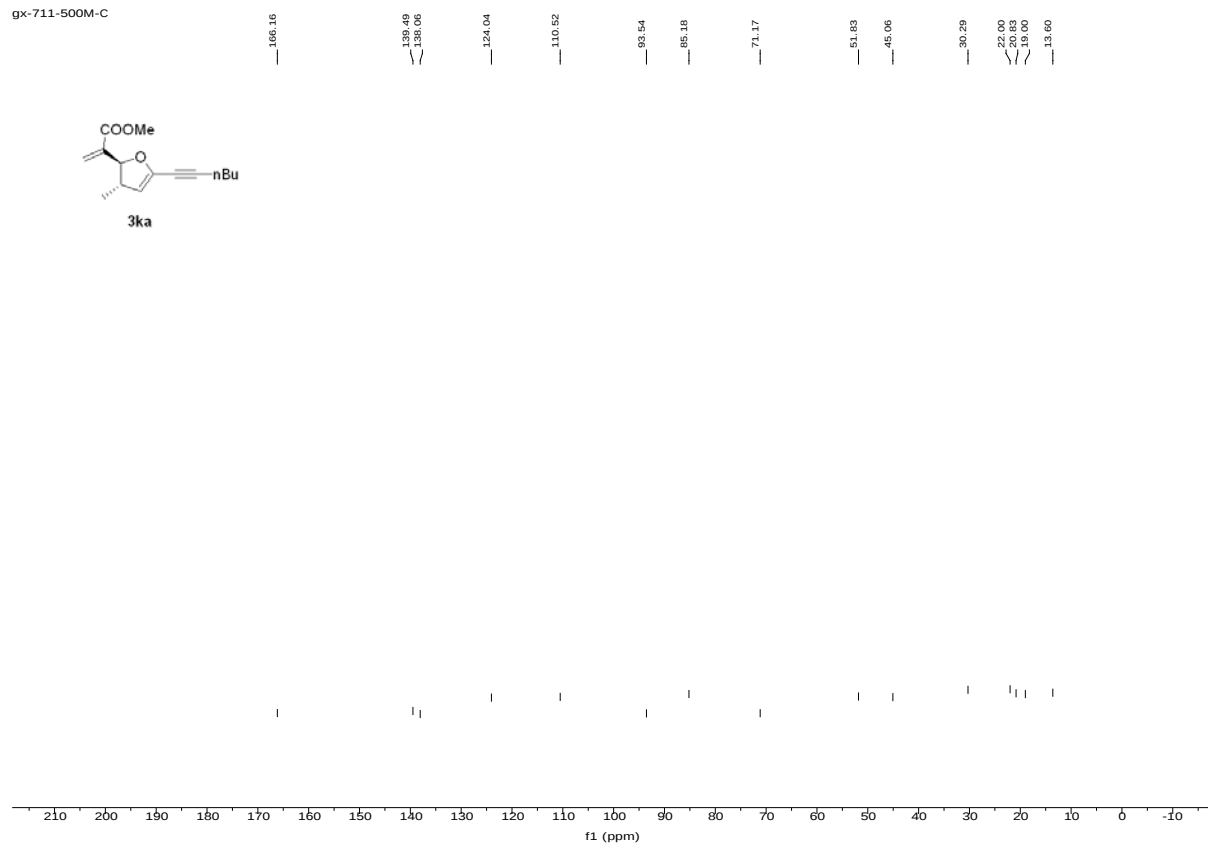


gx-755-500M

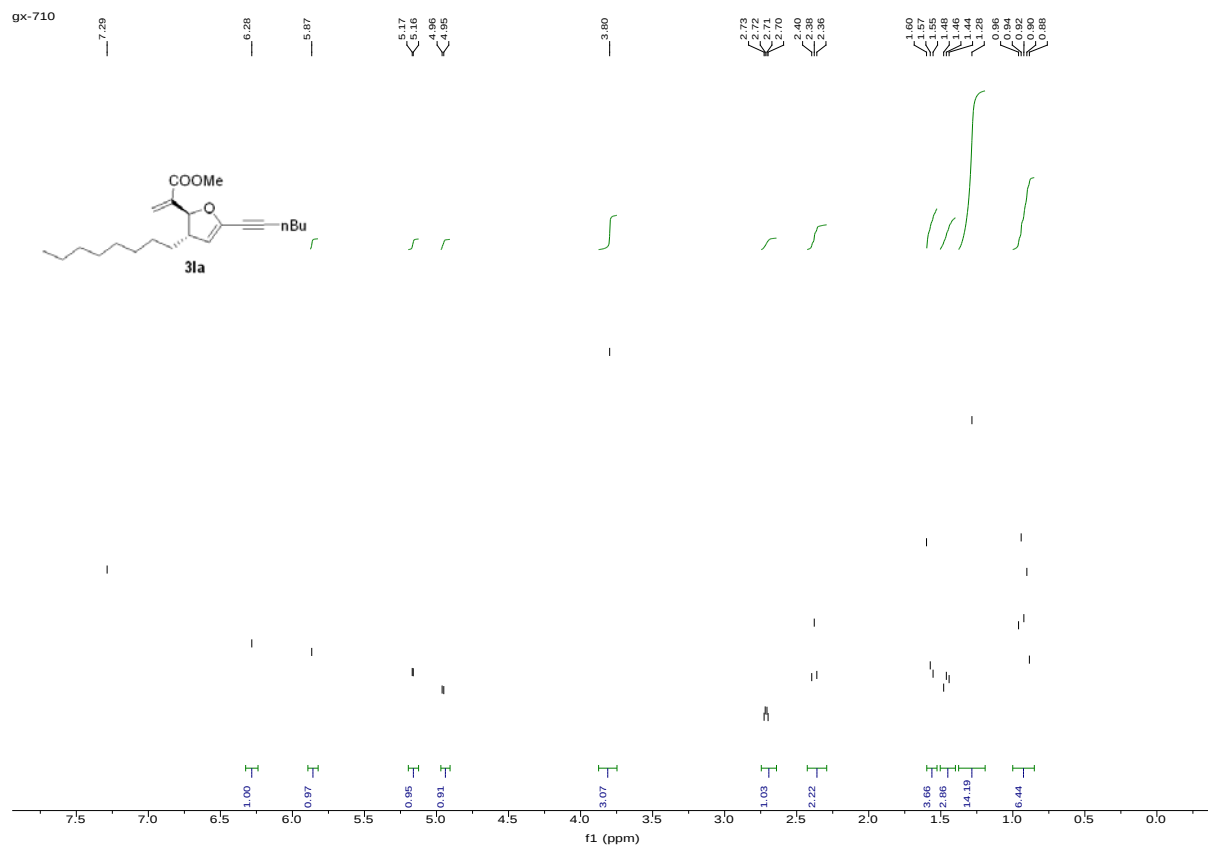




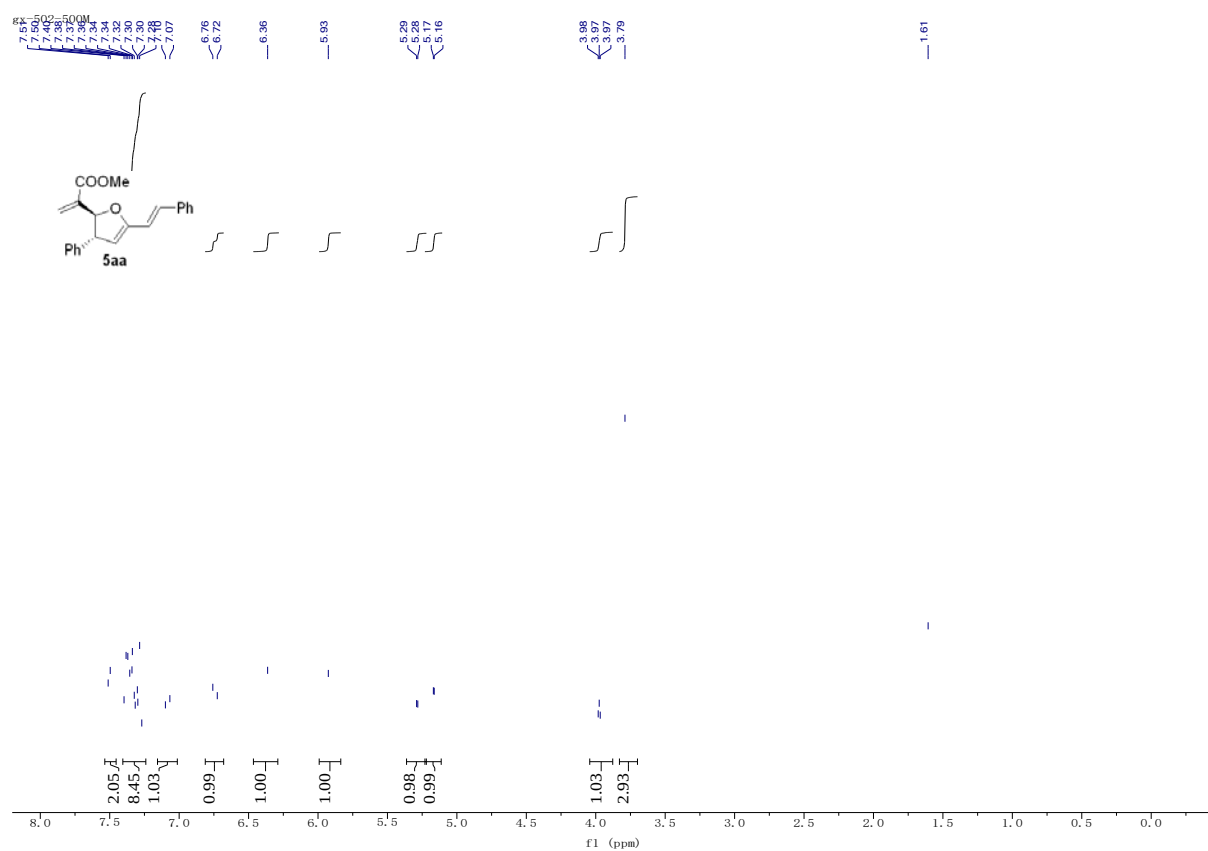
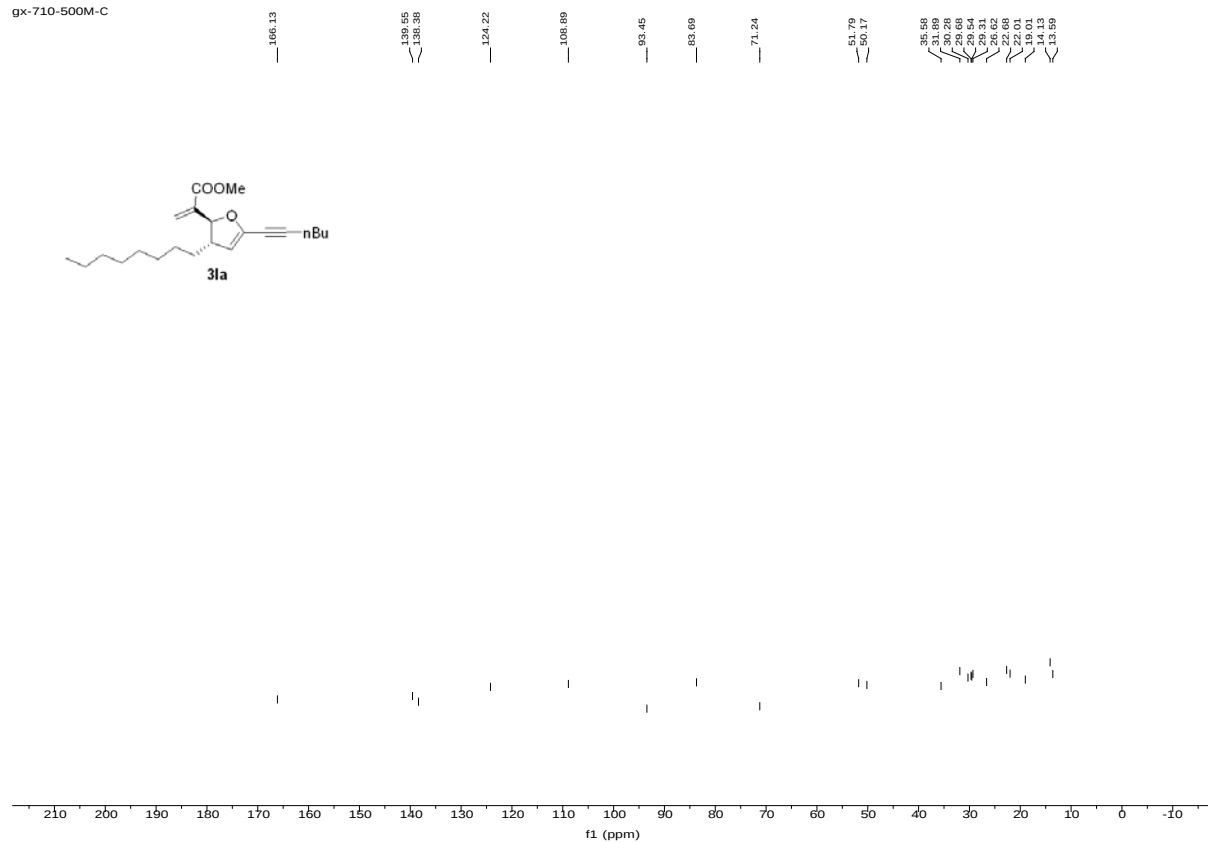
gx-711-500M-C



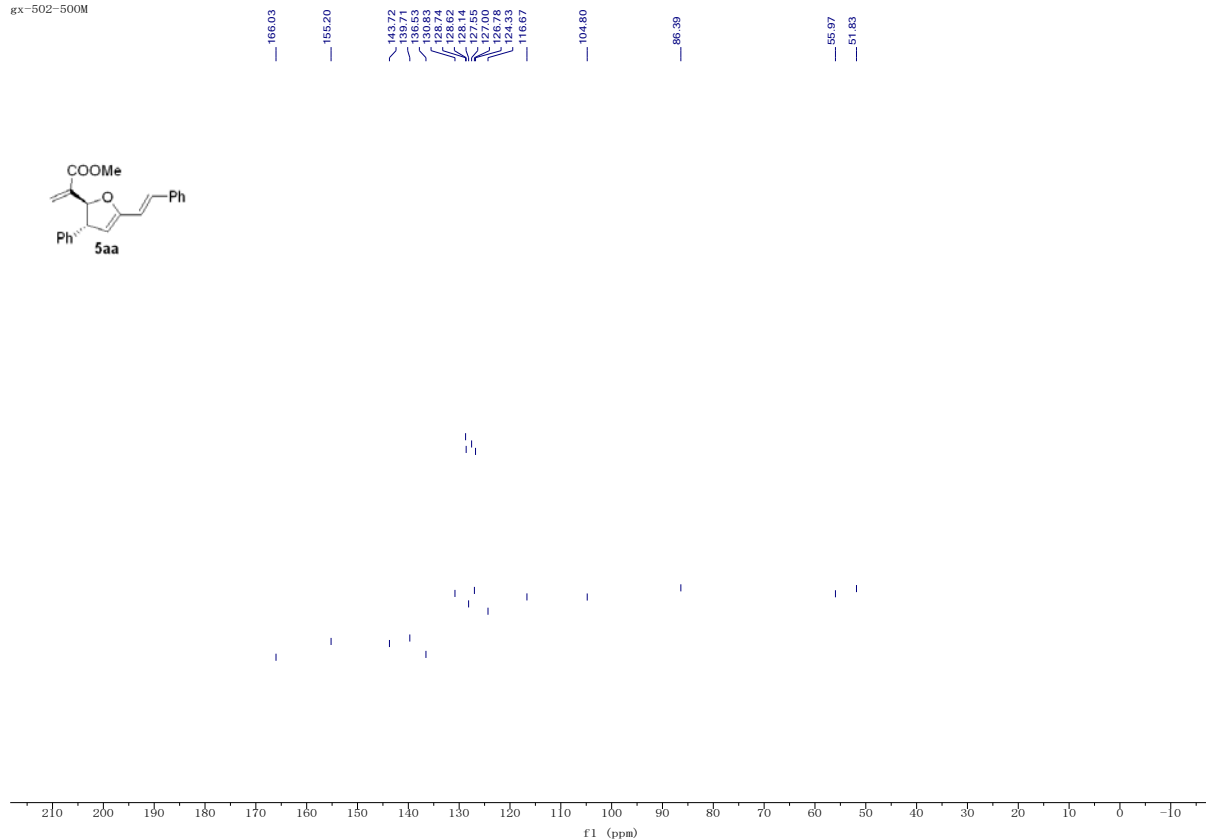
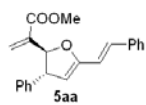
gx-710



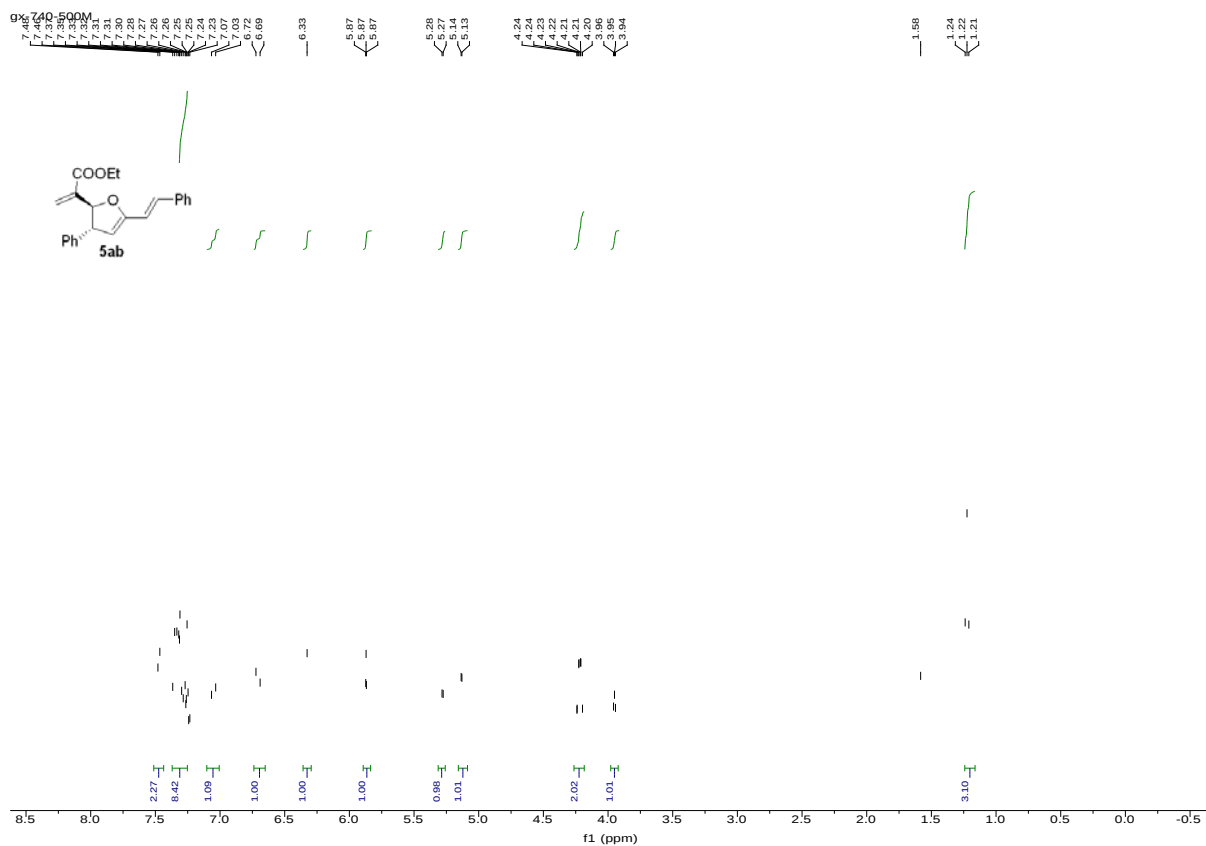
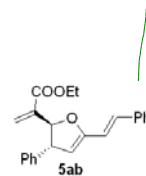
gx-710-500M-C



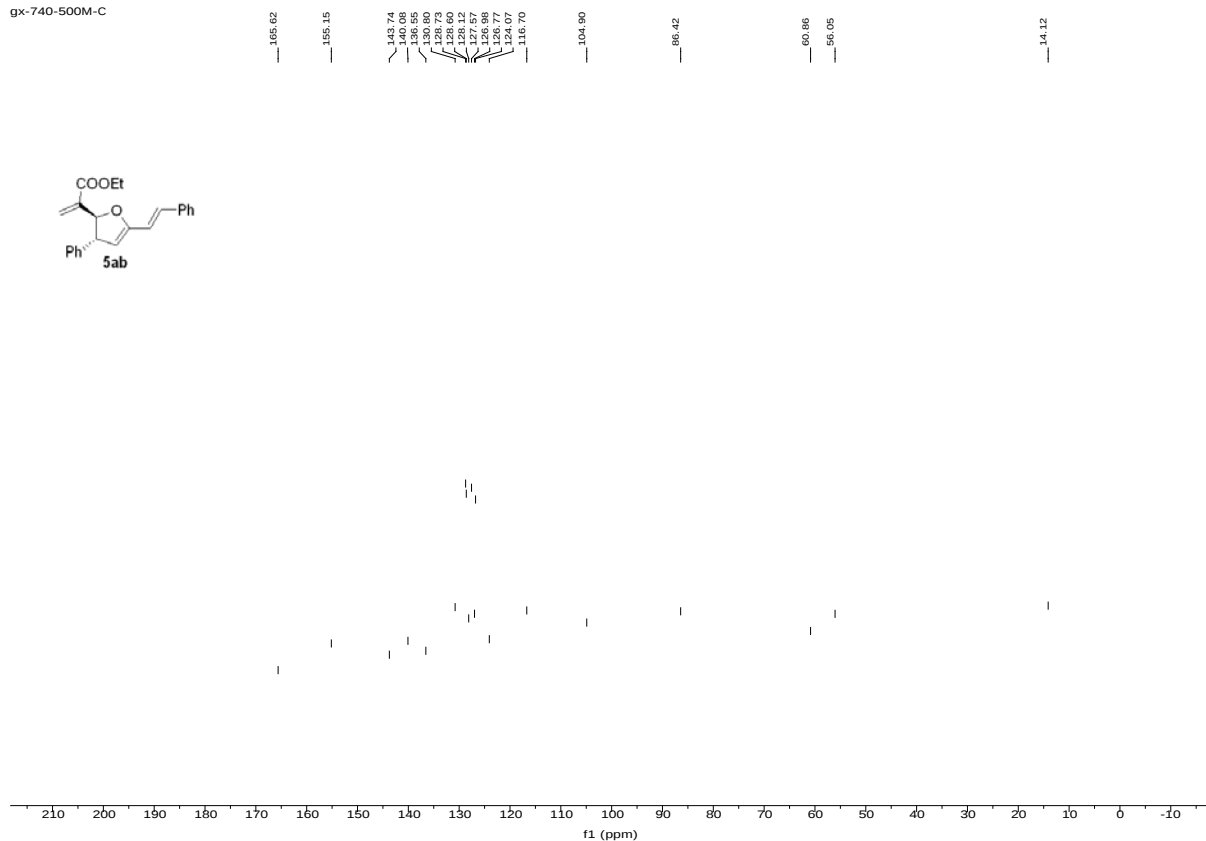
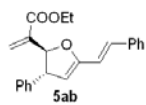
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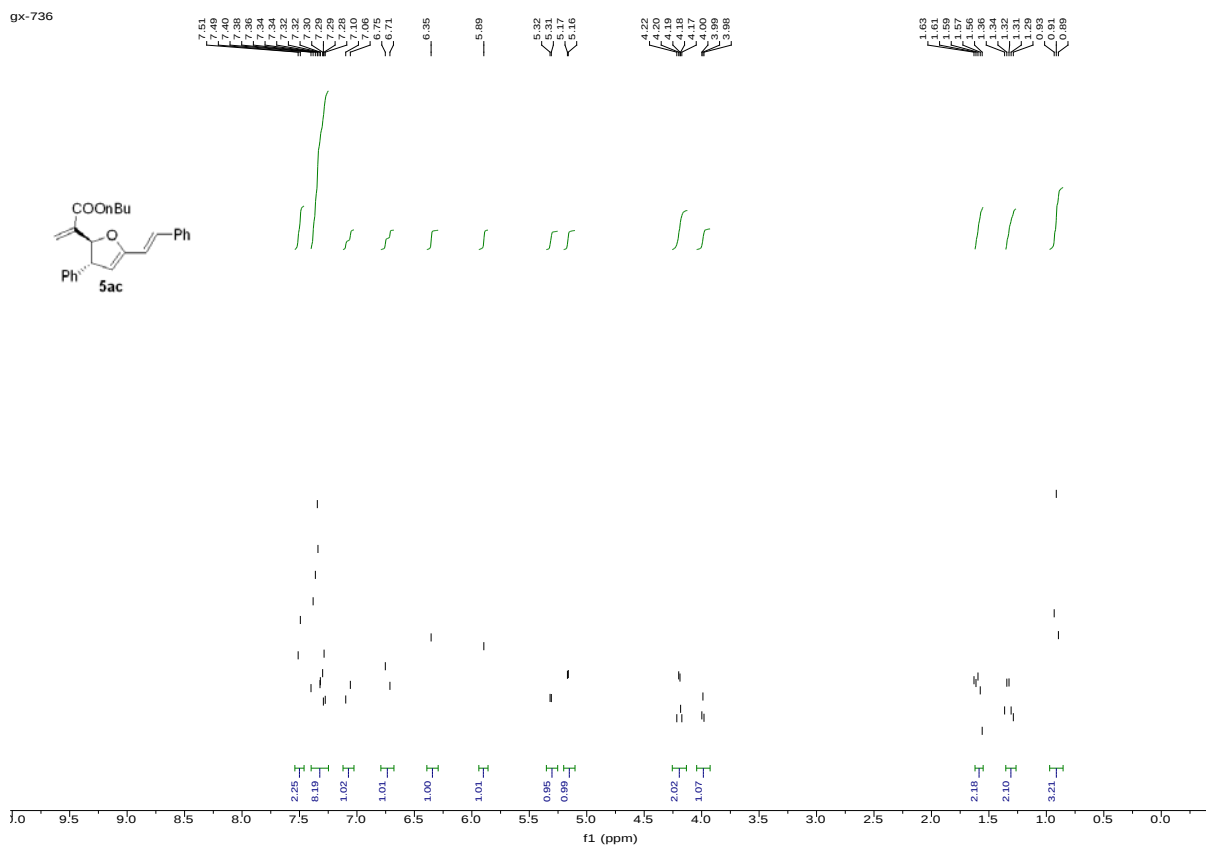
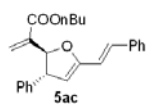
gx-740-500M



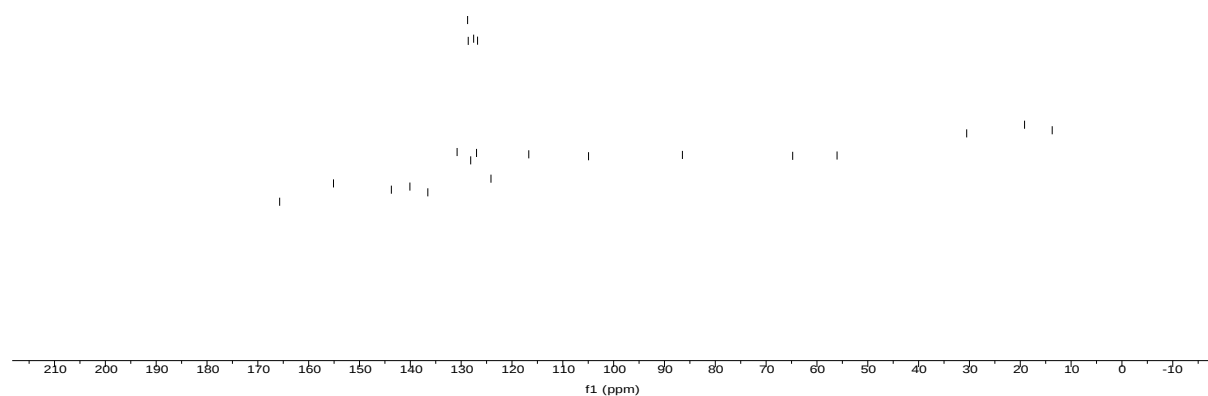
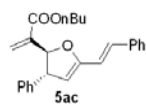
gx-740-500M-C



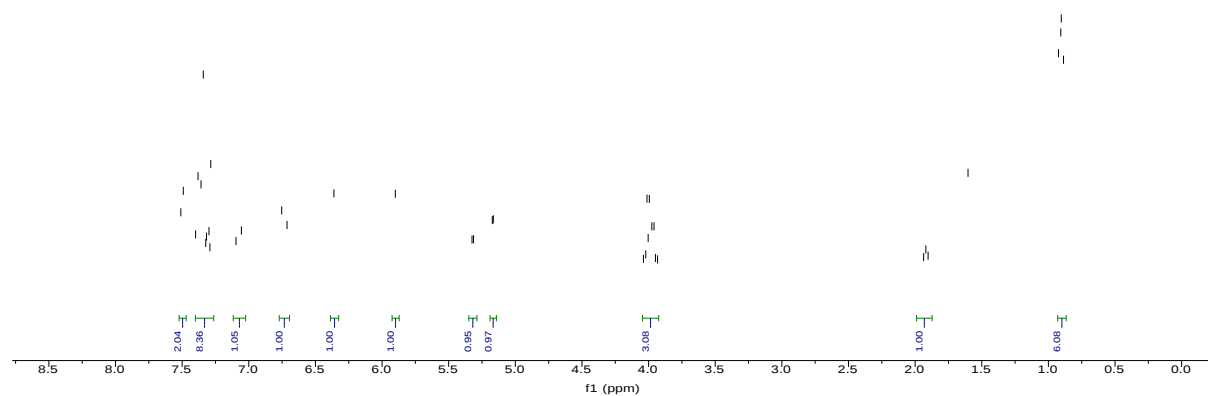
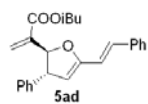
gx-736



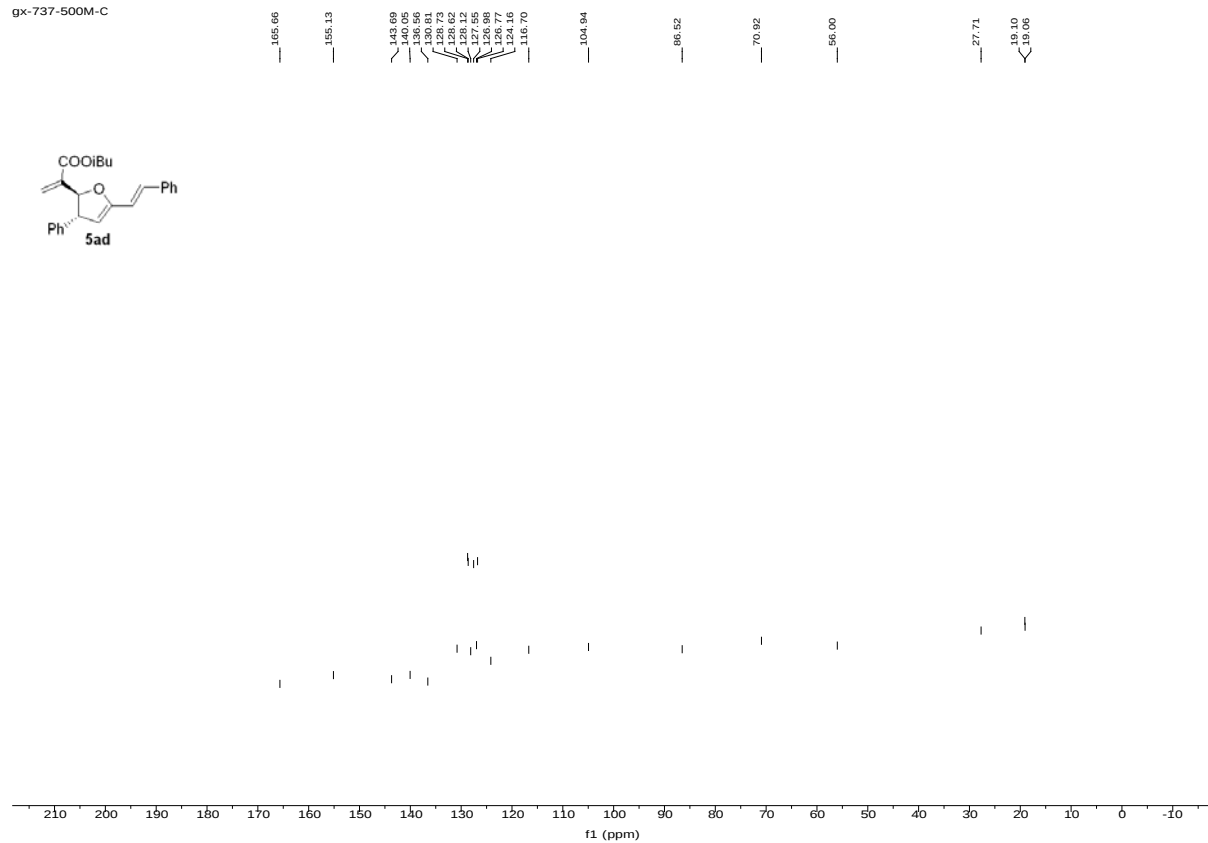
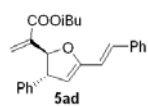
gx-736-500M-C



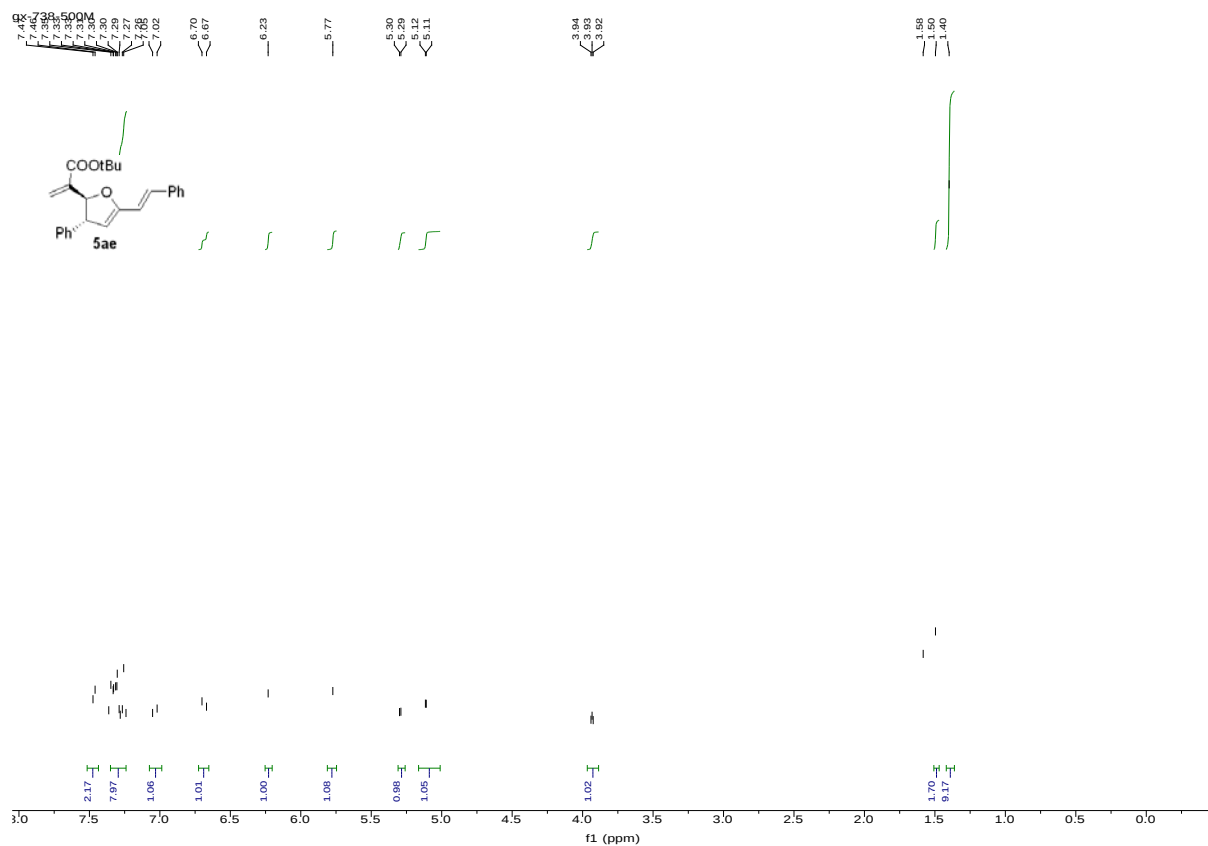
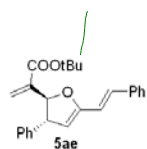
gx-737



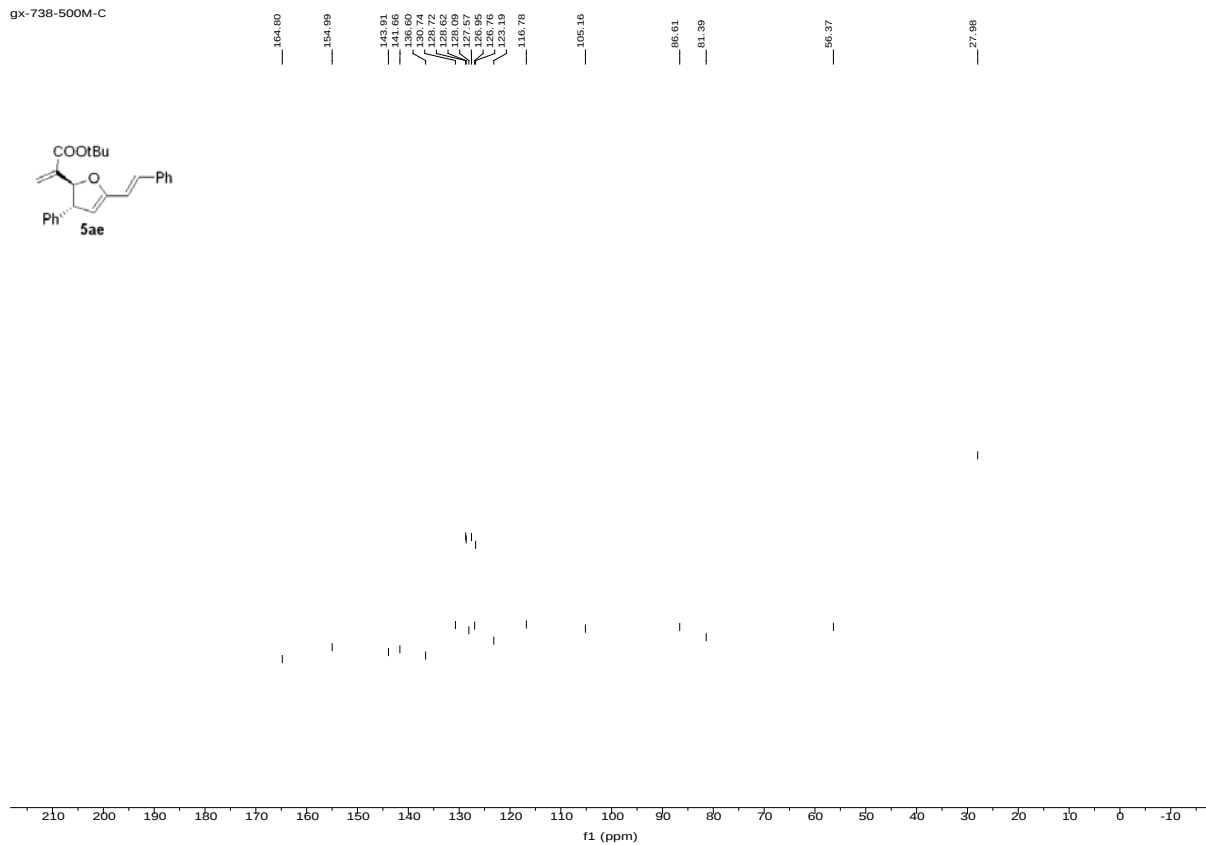
gx-737-500M-C



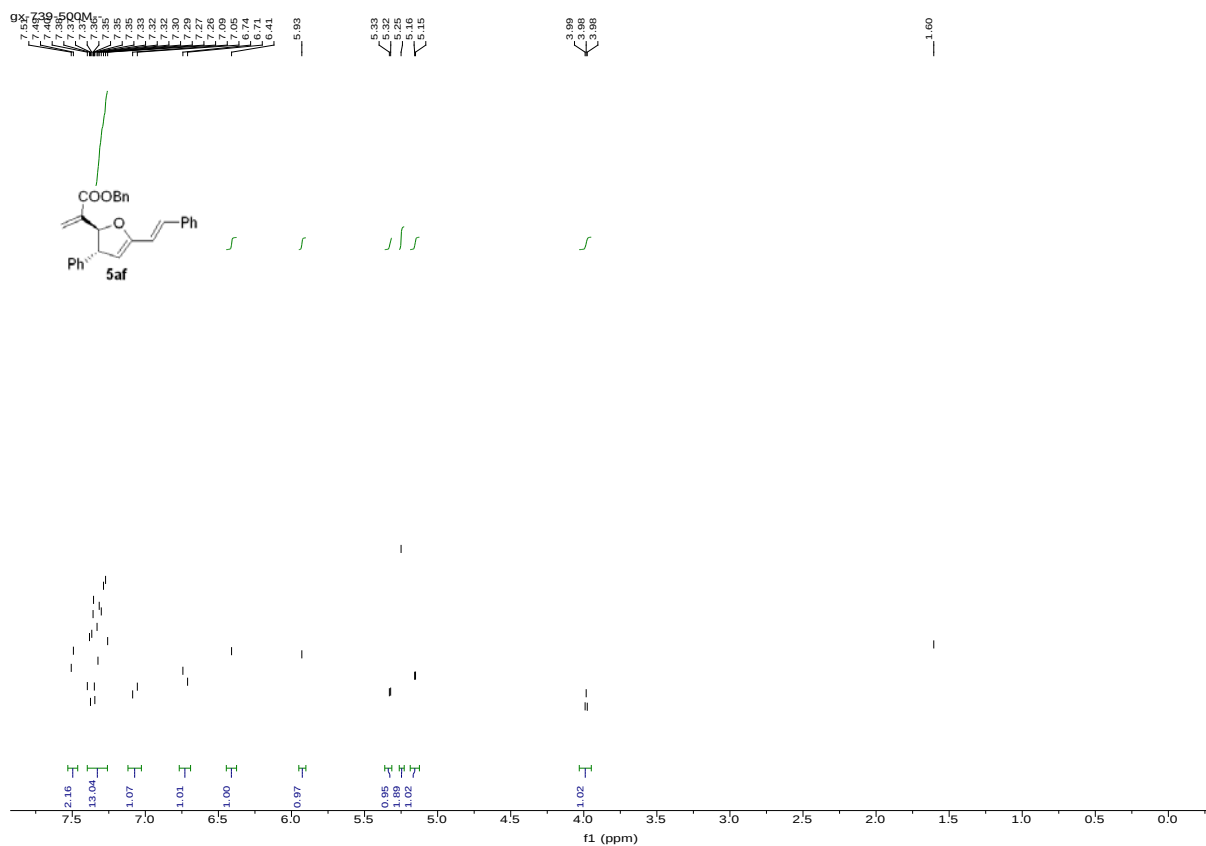
gx-738-500M



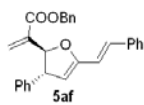
Chemical structure of 5ae: CC(C)(C)OC(=O)[C@H]1C=C(C=Cc2ccccc2)O[C@@H]1c3ccccc3



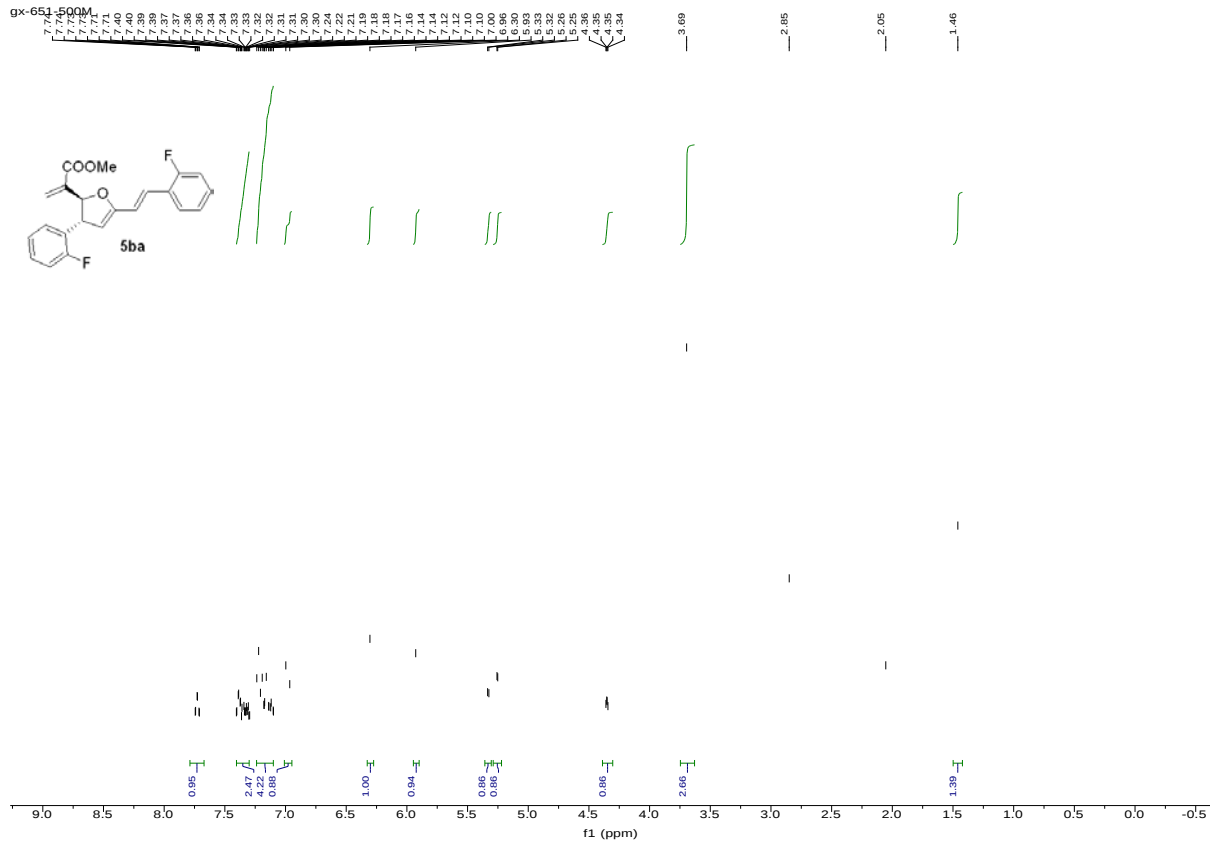
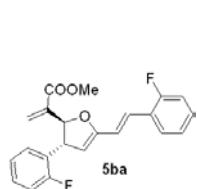

5af



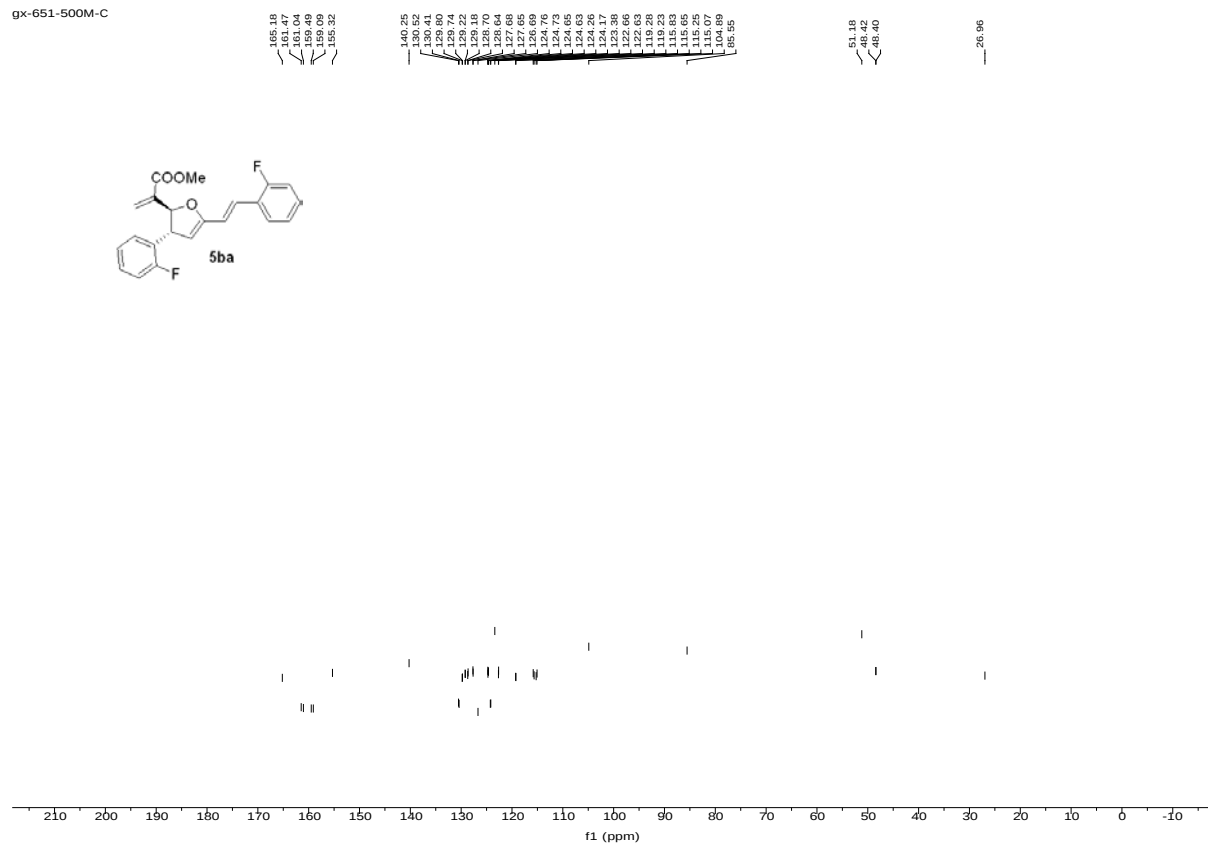
gx-739-500M-C



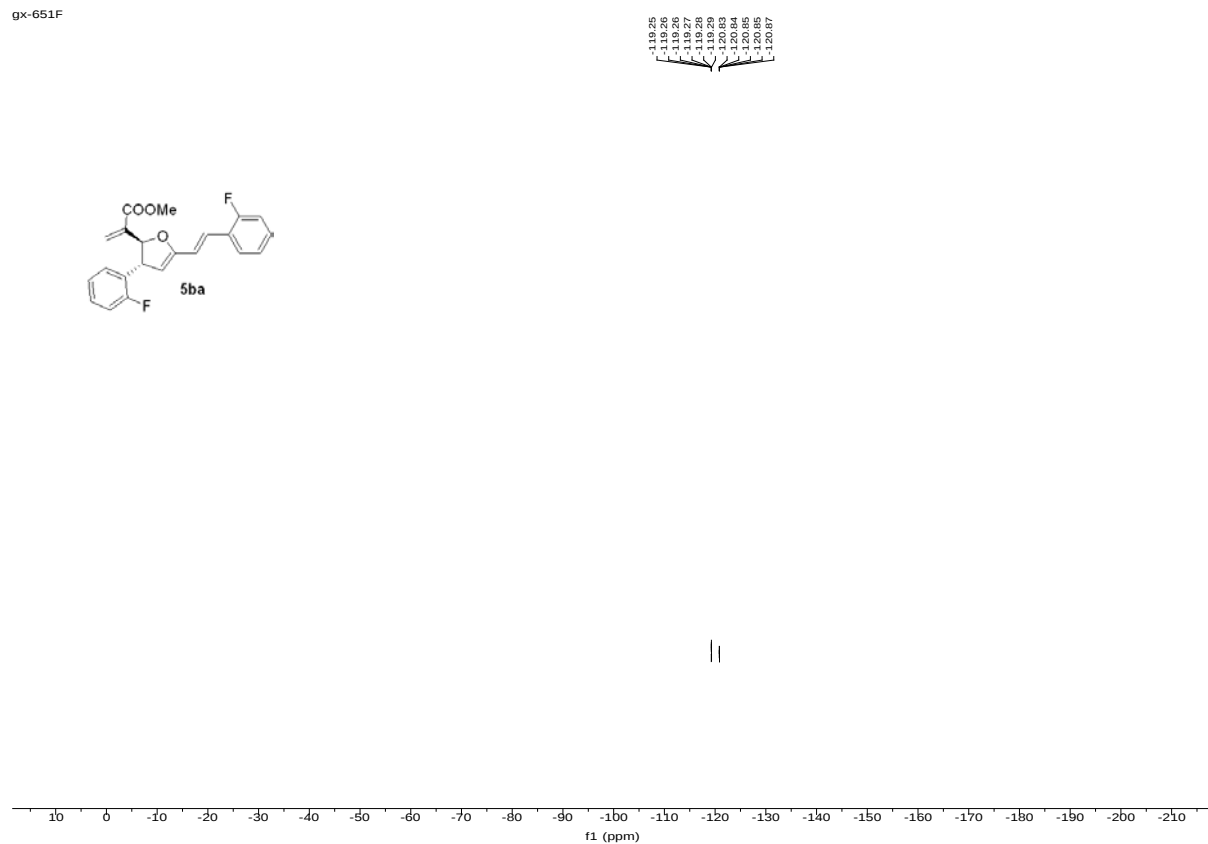
gx-651-500M

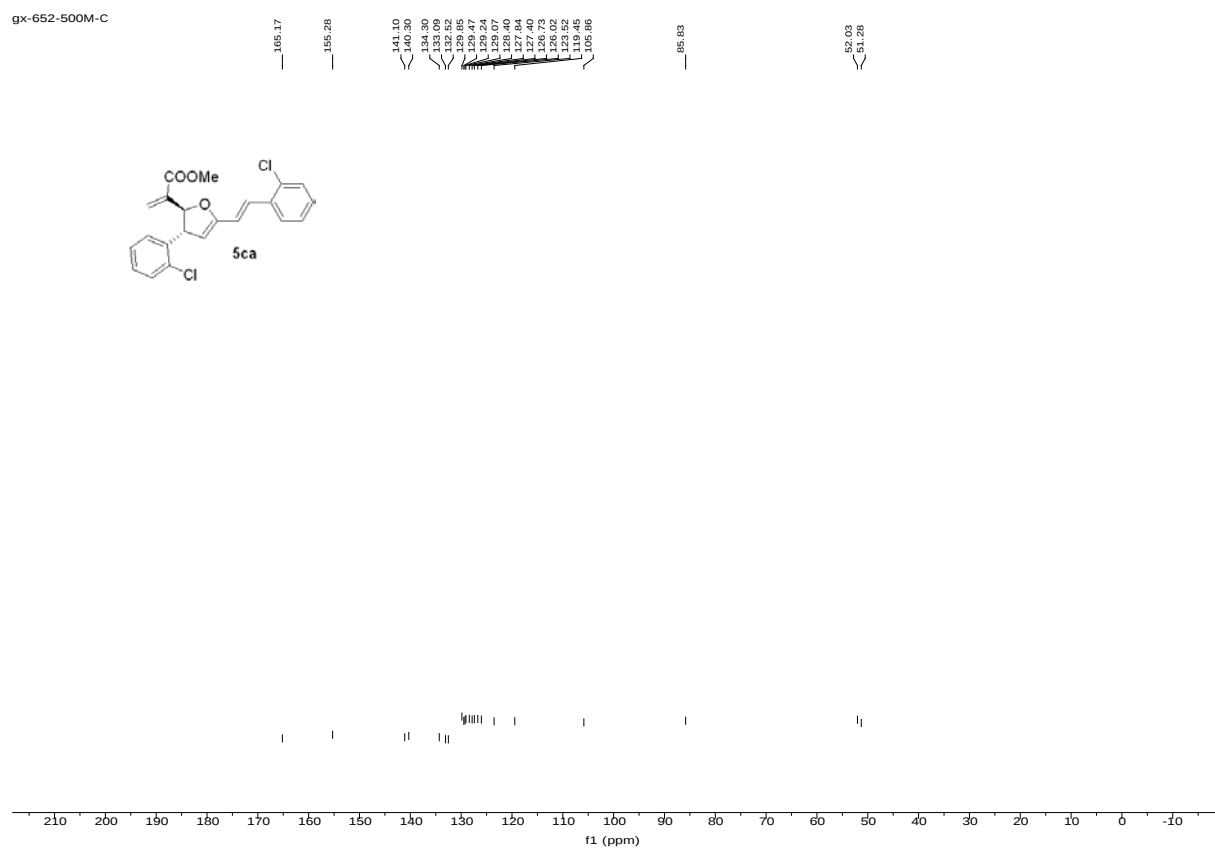
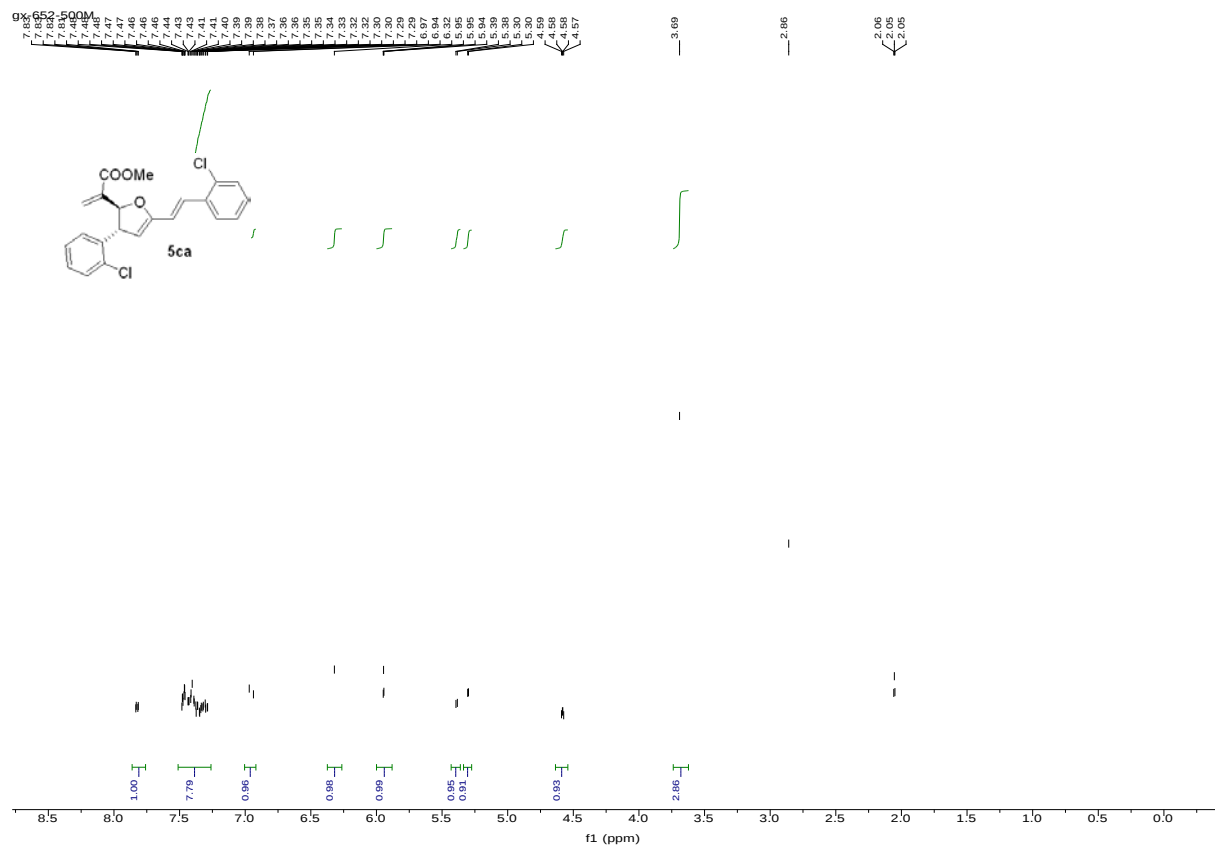


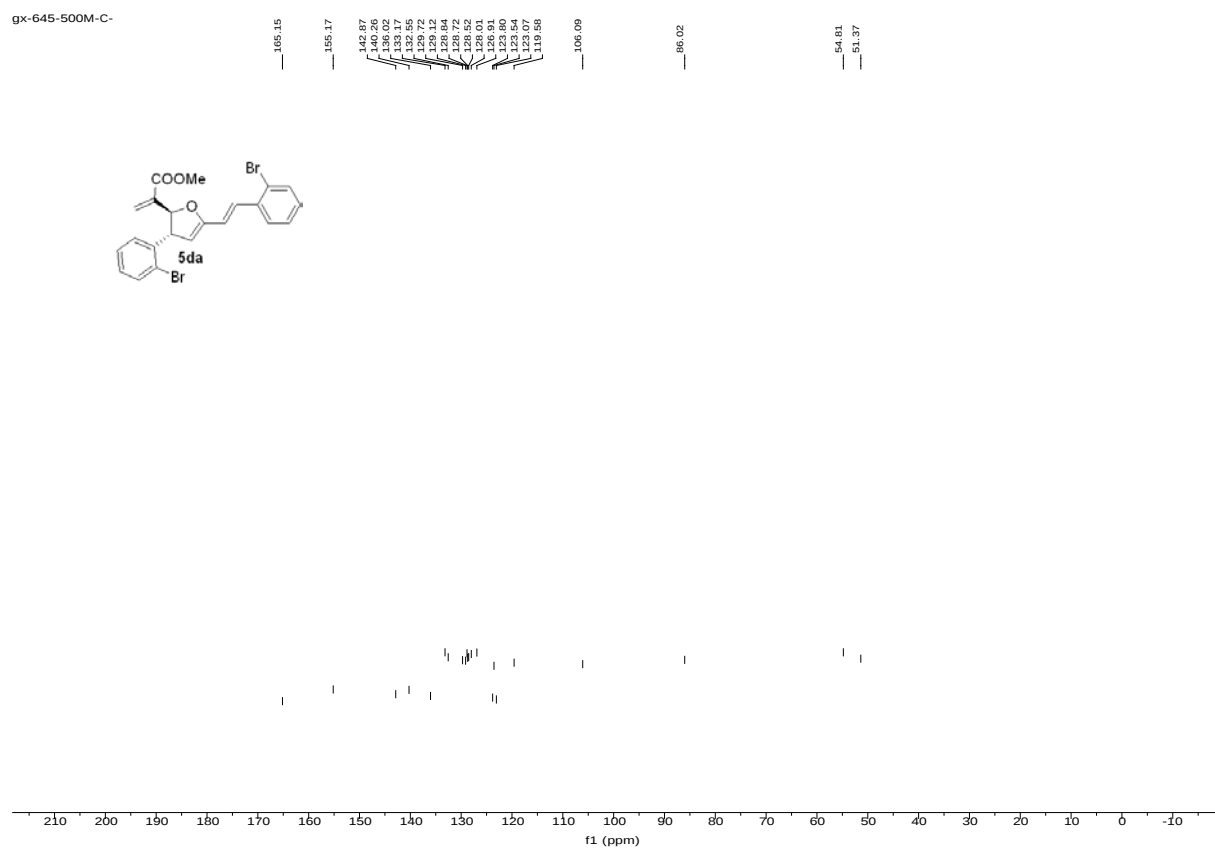
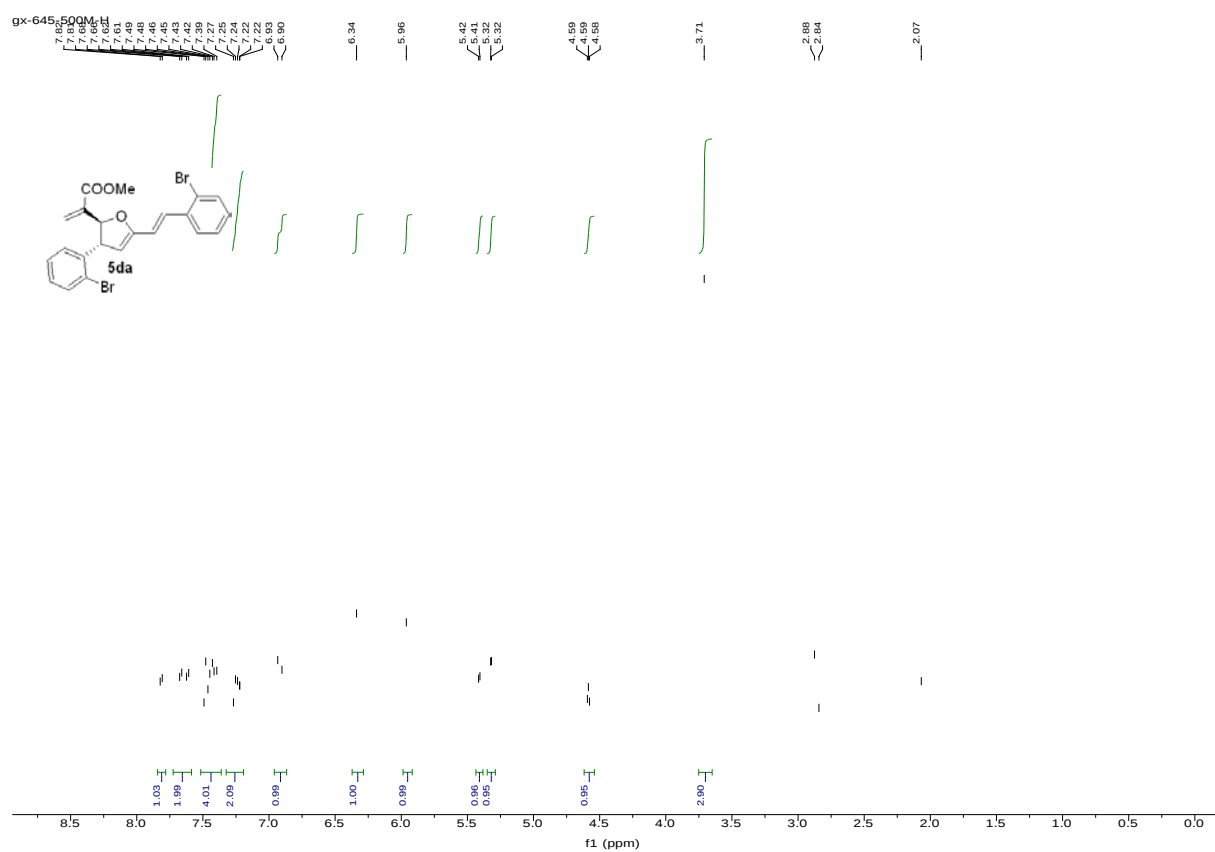
gx-651-500M-C



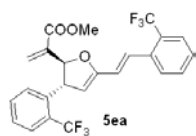
gx-651F



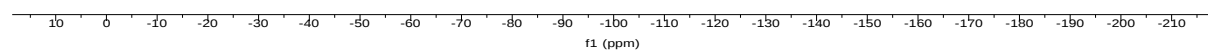




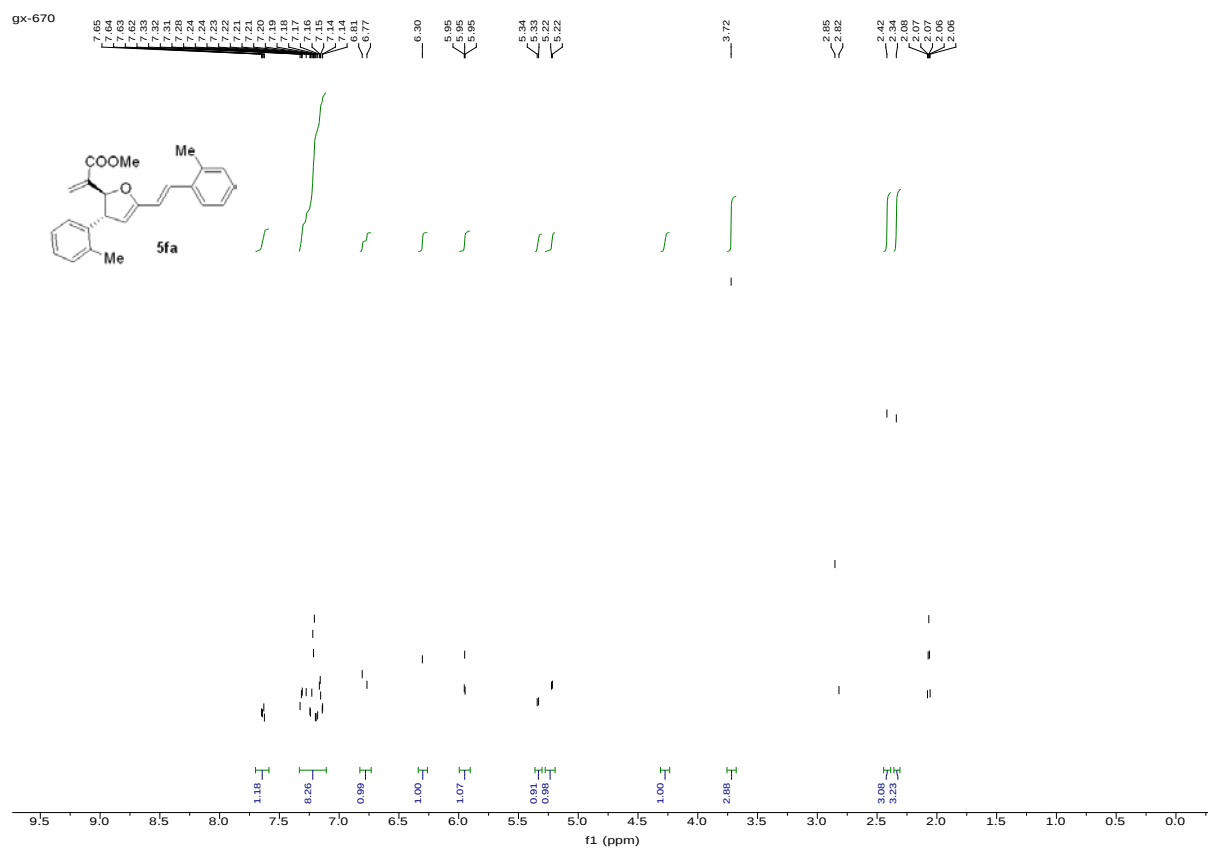
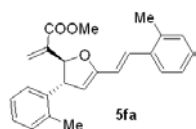
gx-650F



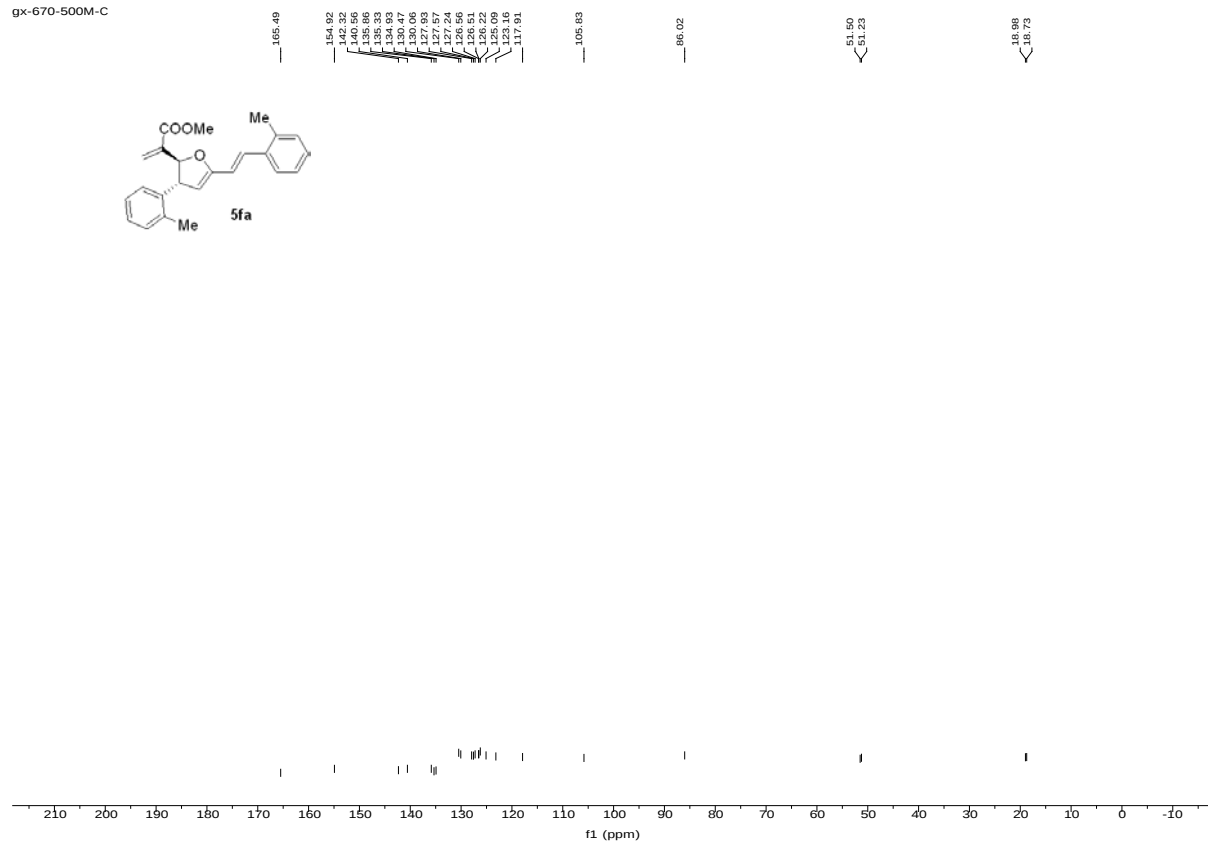
58.69
58.69



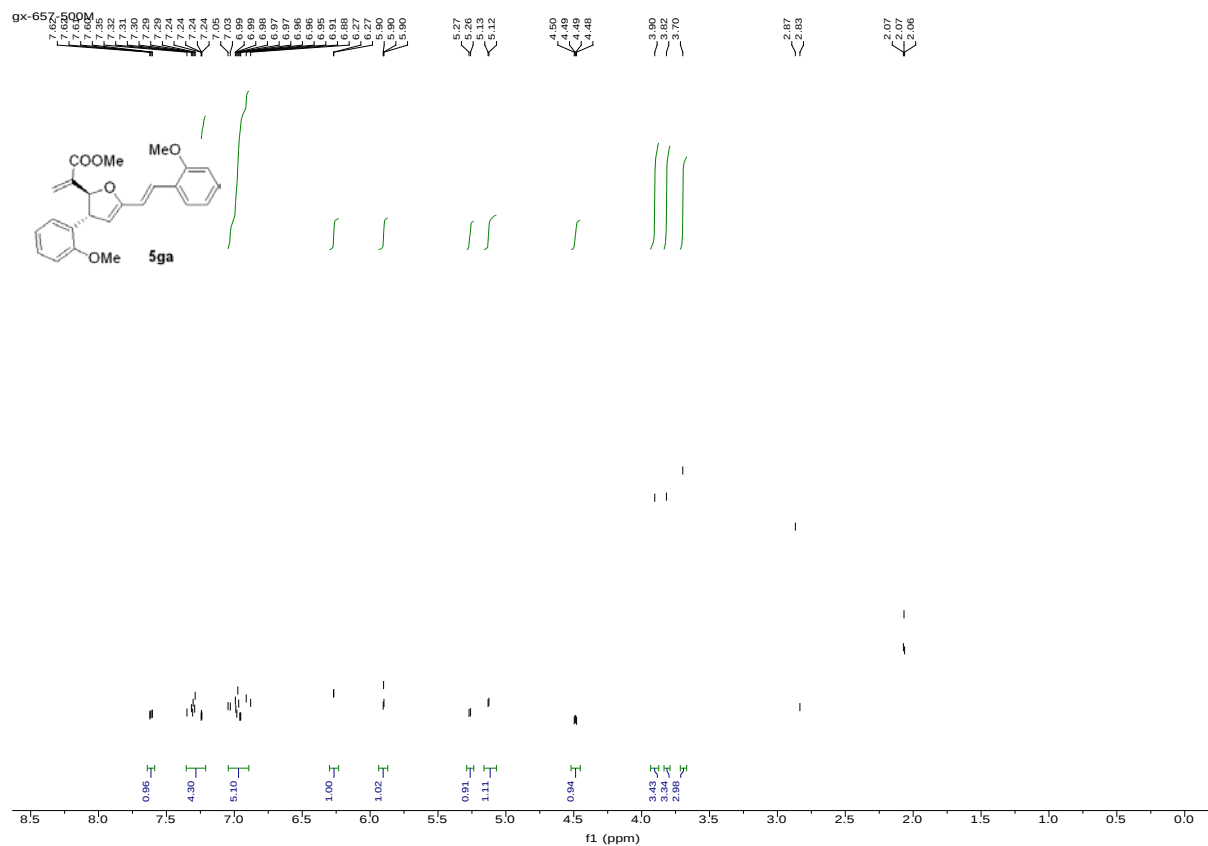
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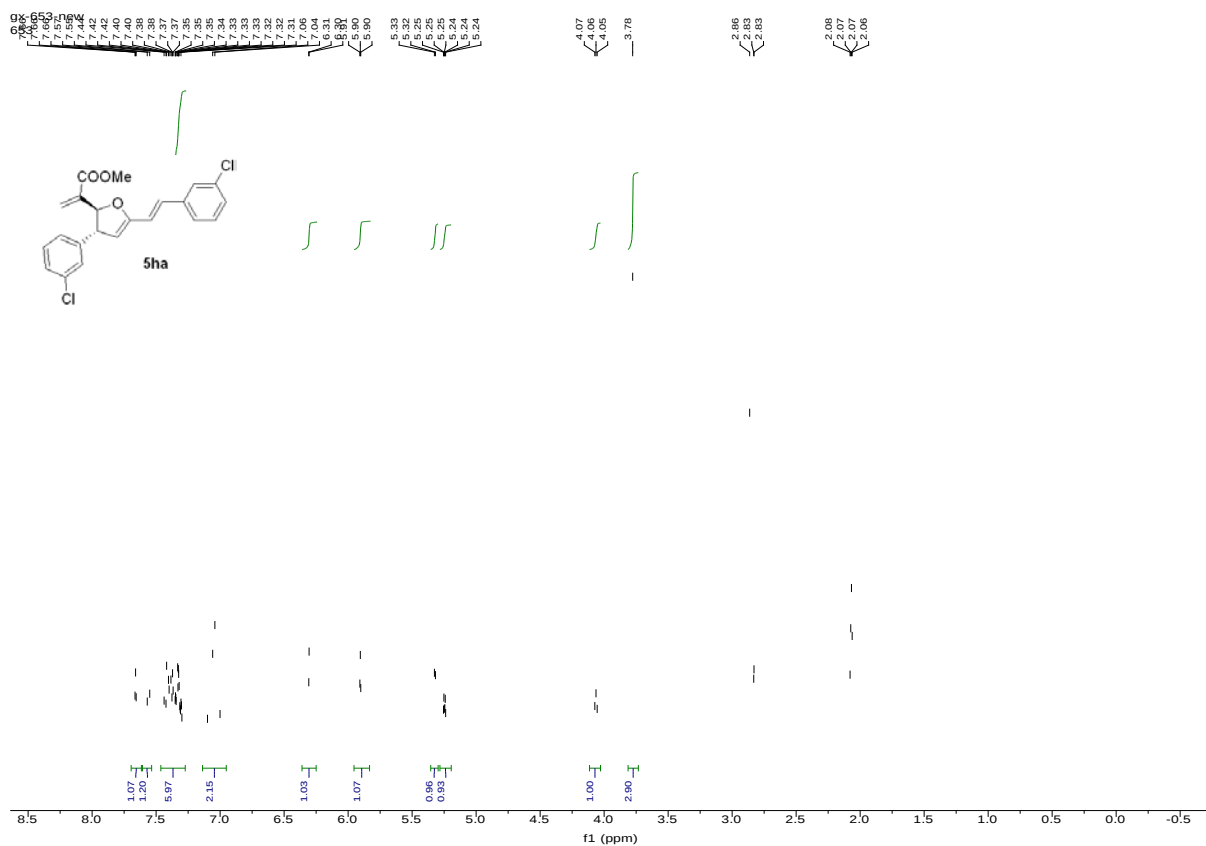
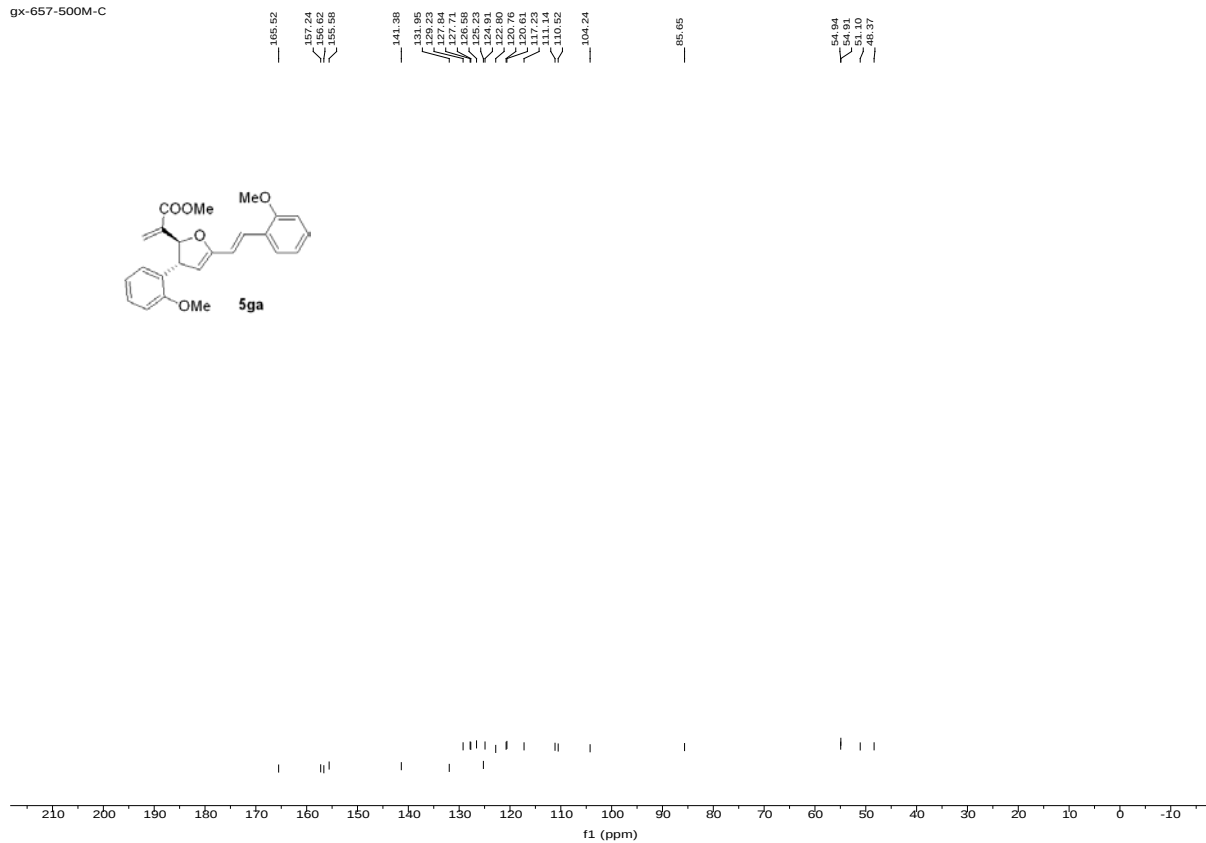
gx-670-500M-C



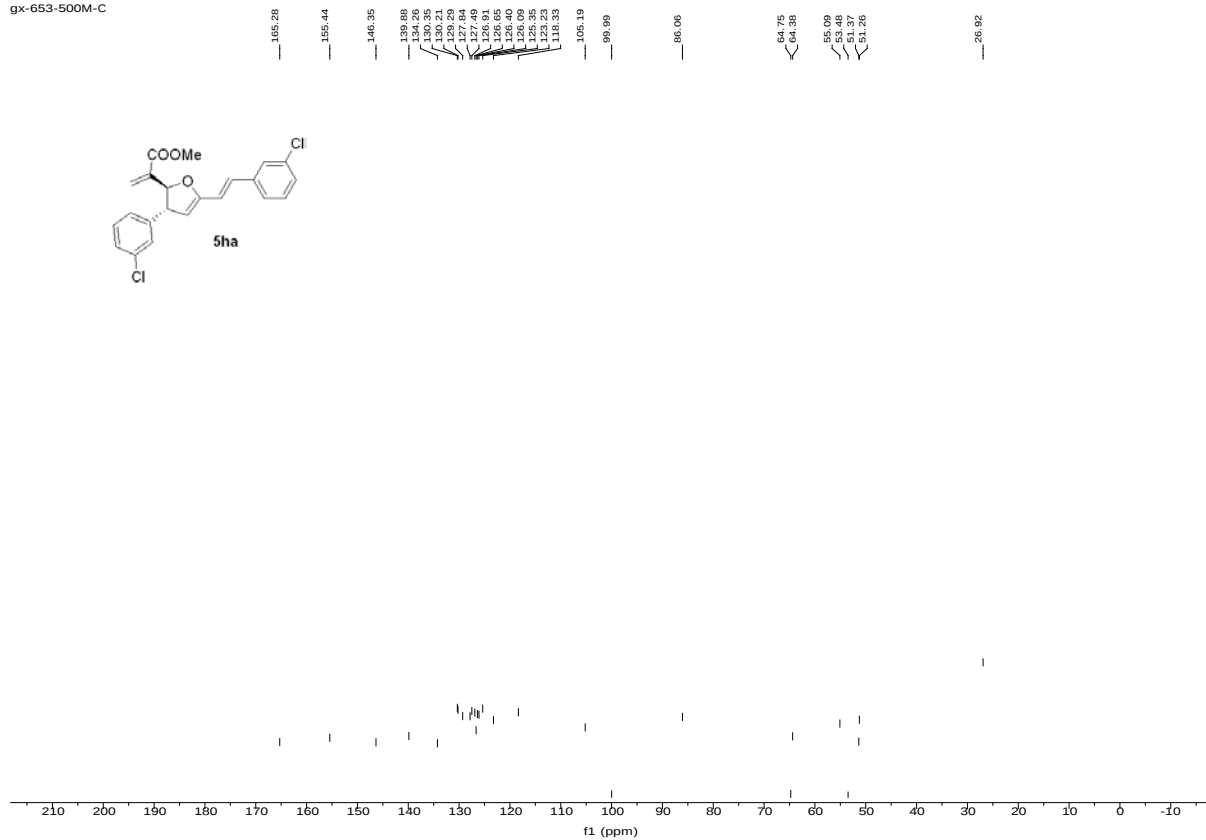
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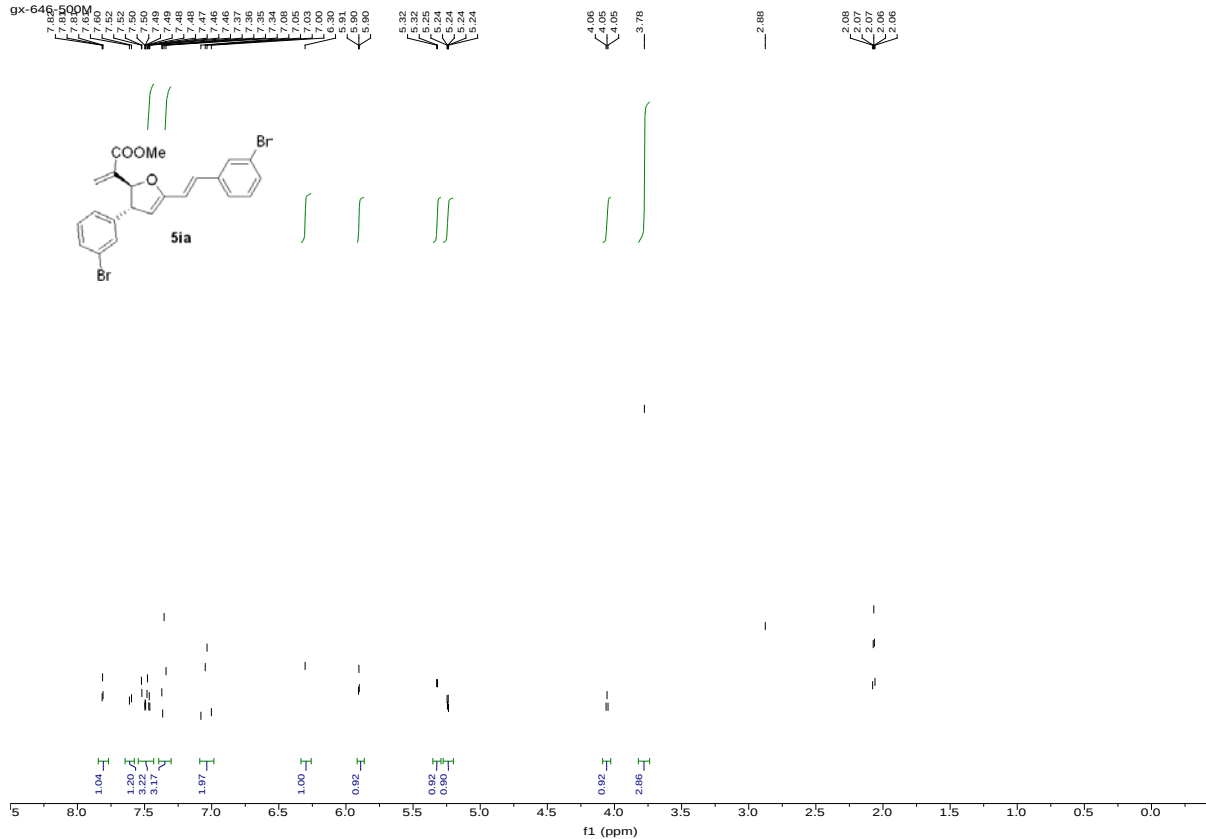
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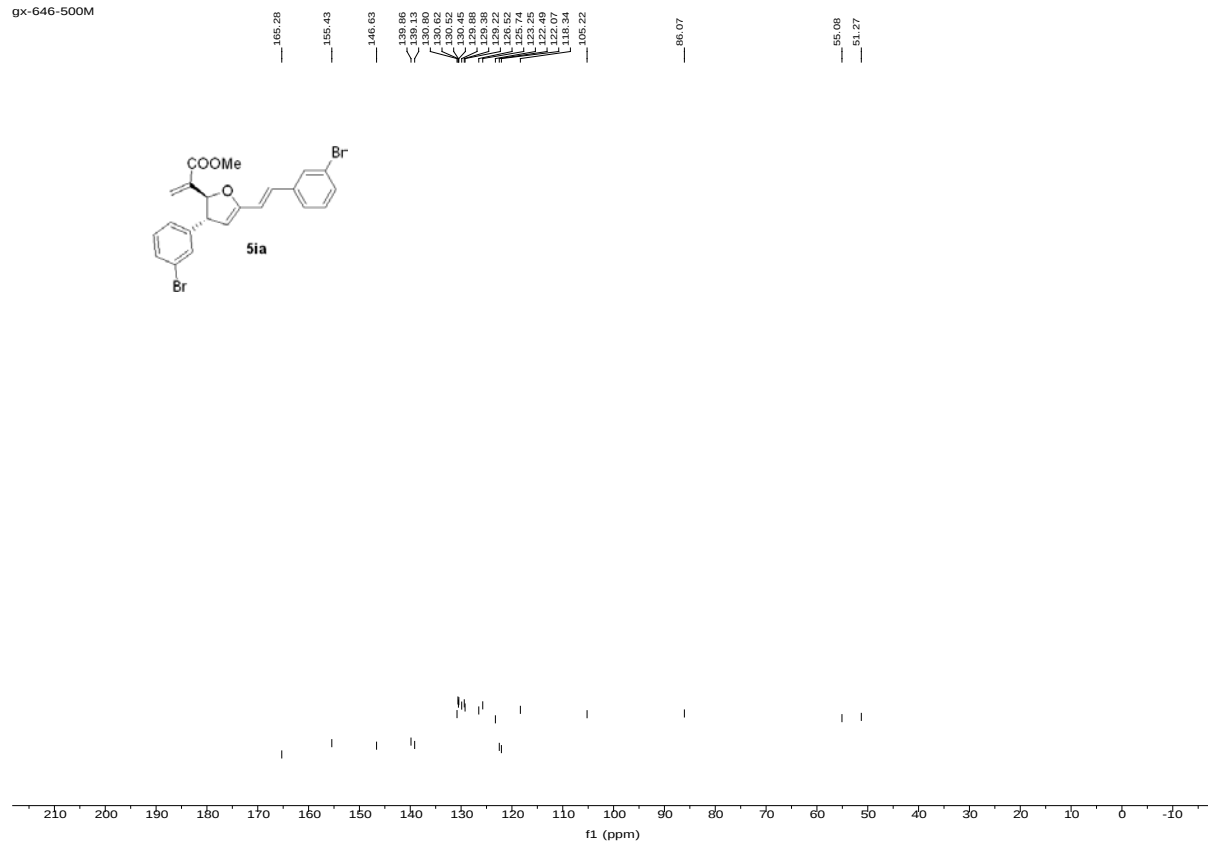
gx-653-500M-C



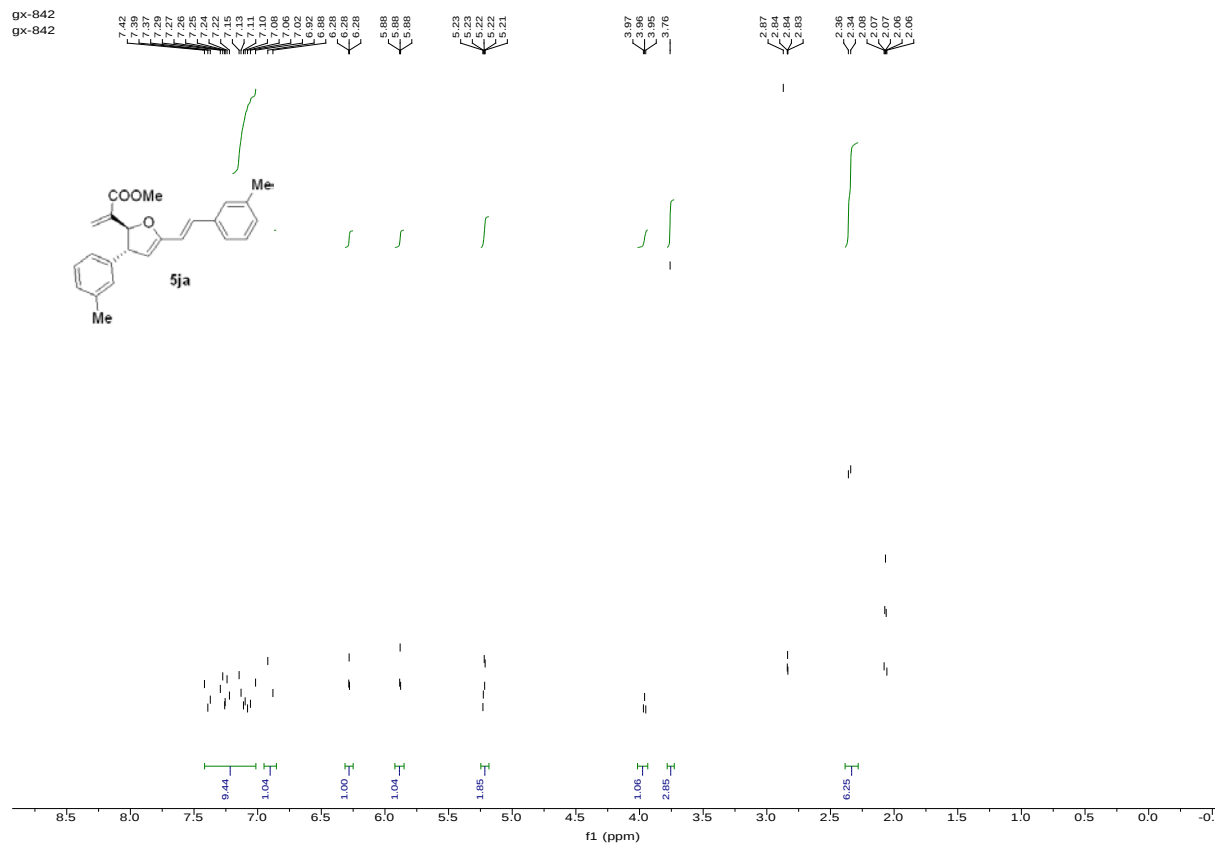
gx-646-500M

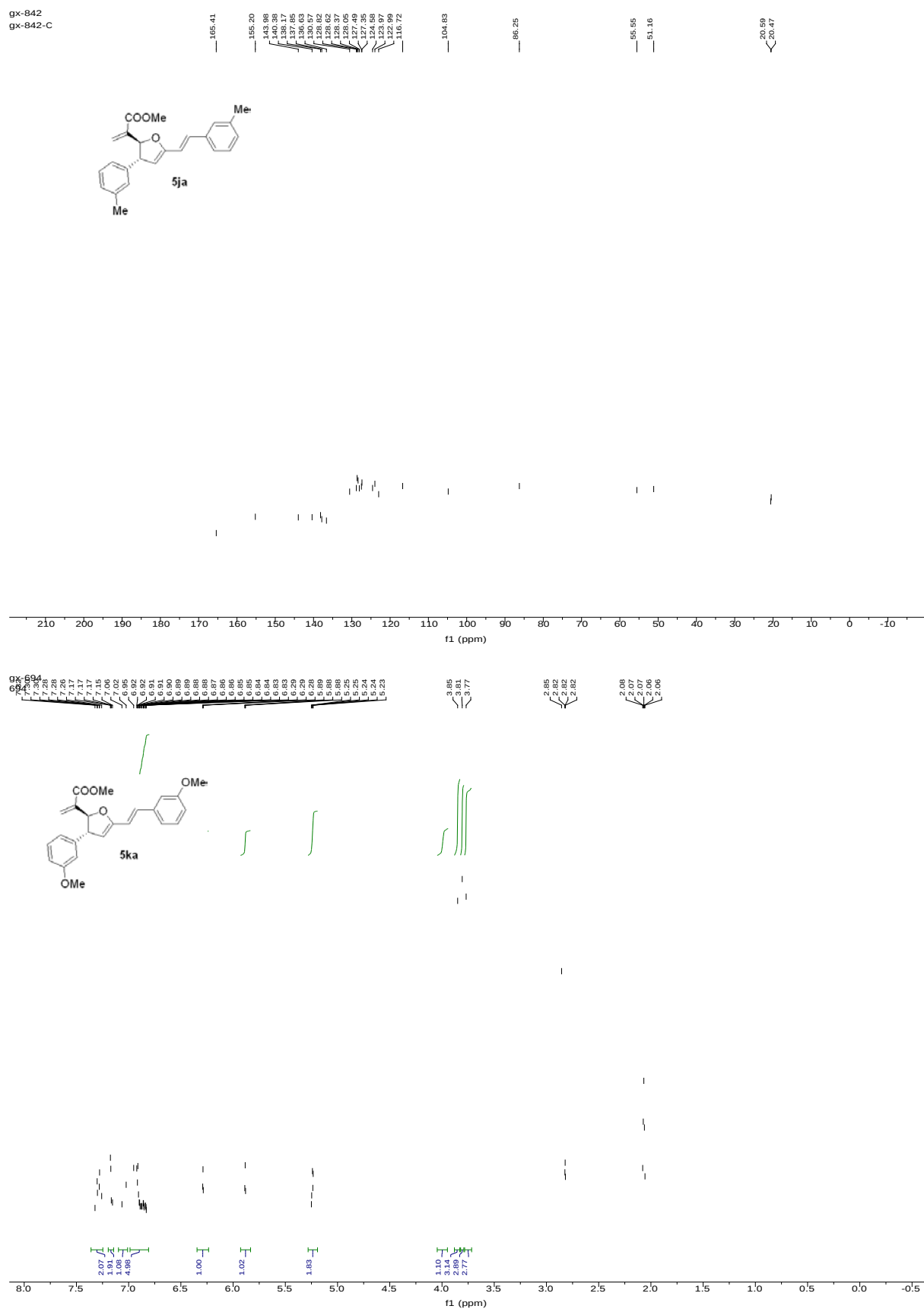


gx-646-500M

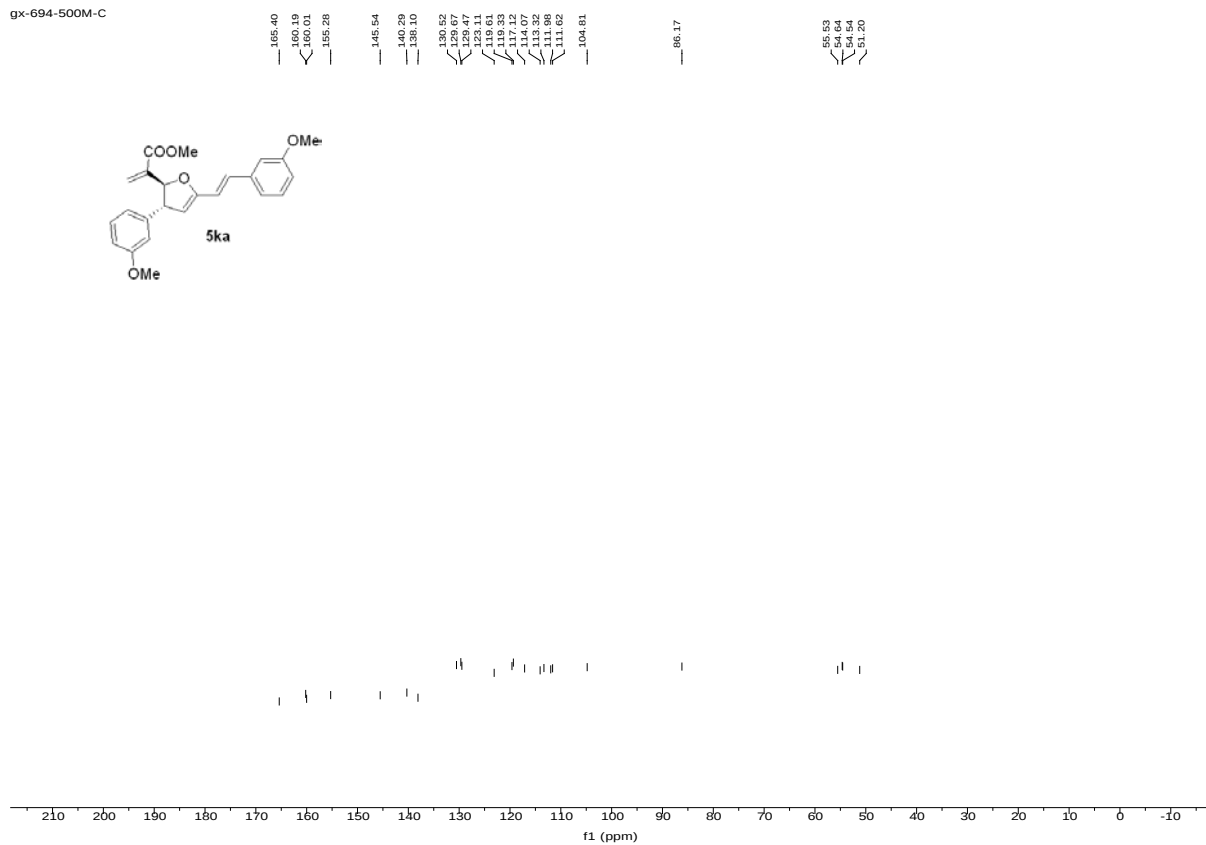


gx-842
gx-842

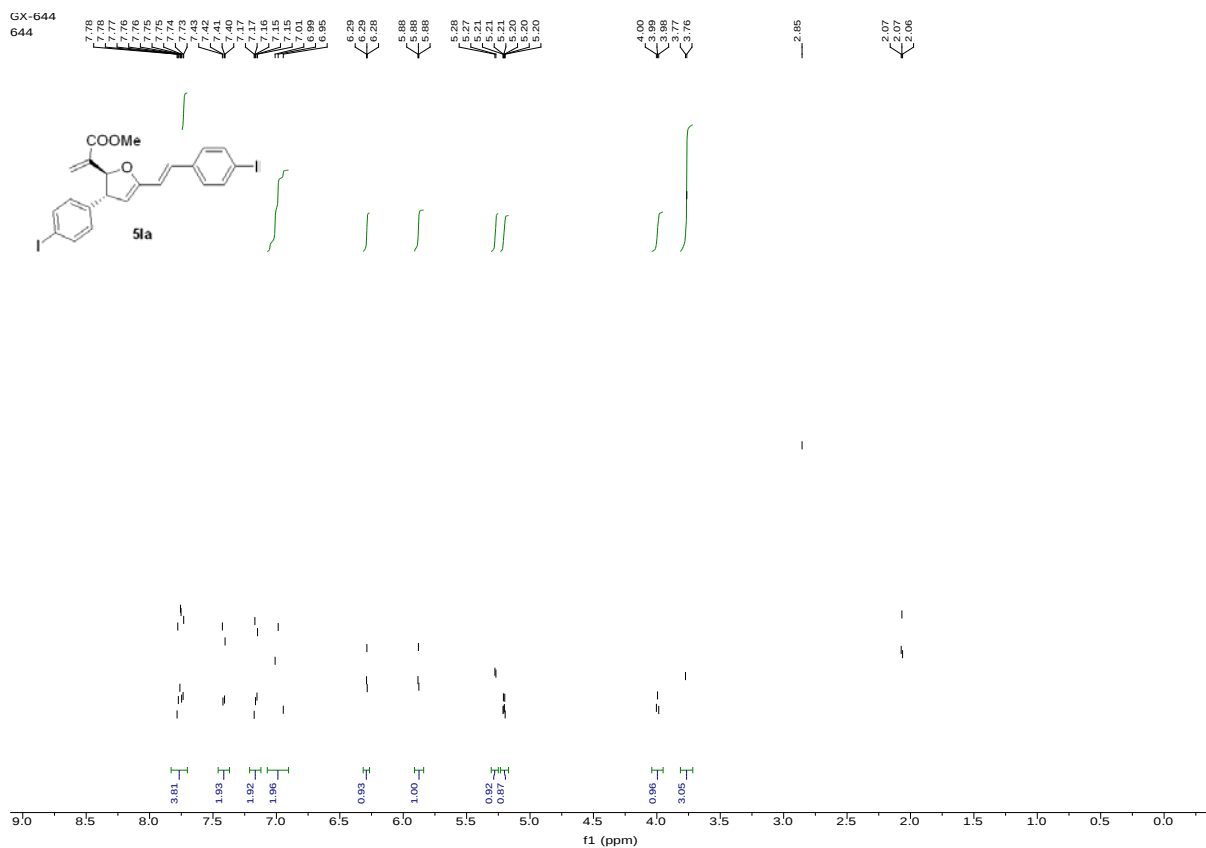




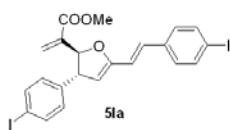
gx-694-500M-C



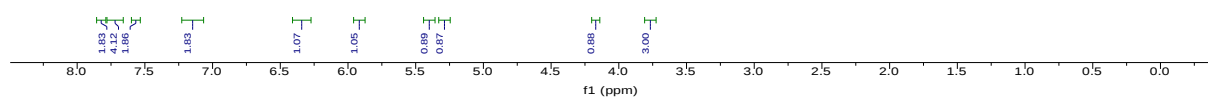
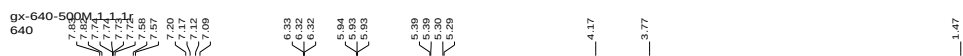
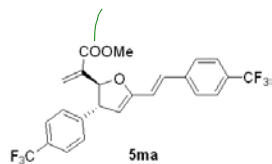
GX-644
644



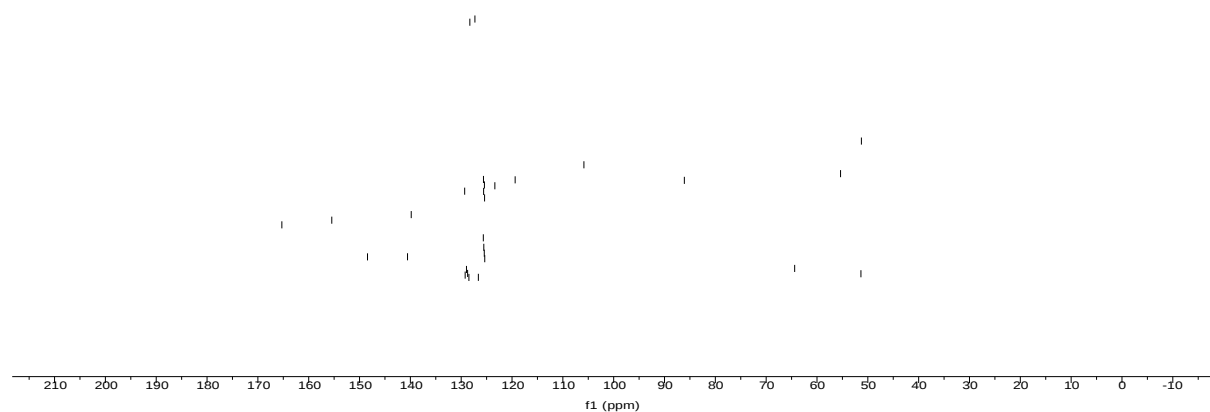
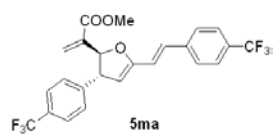
gx-644-C-500M



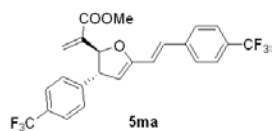
gx-640-500M-1-1-1r
640



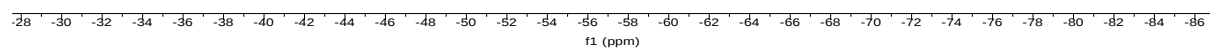
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640C

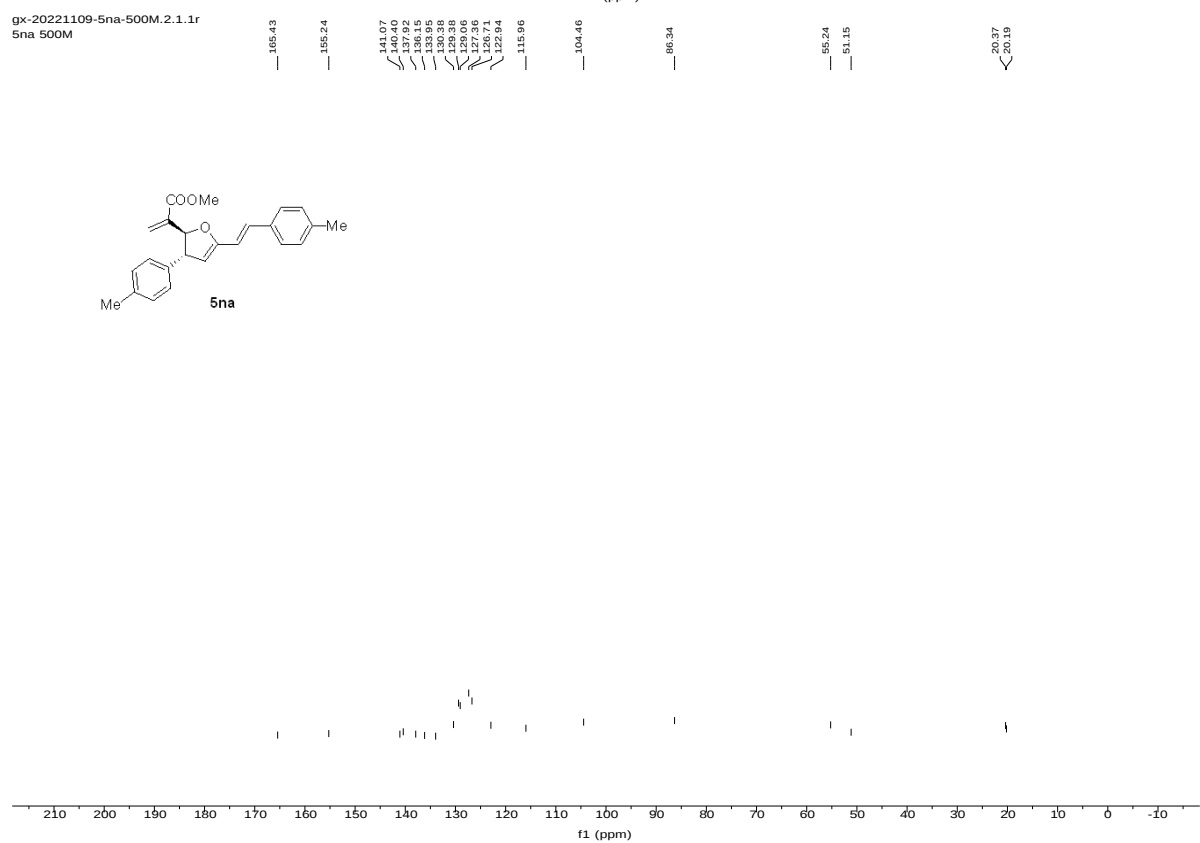
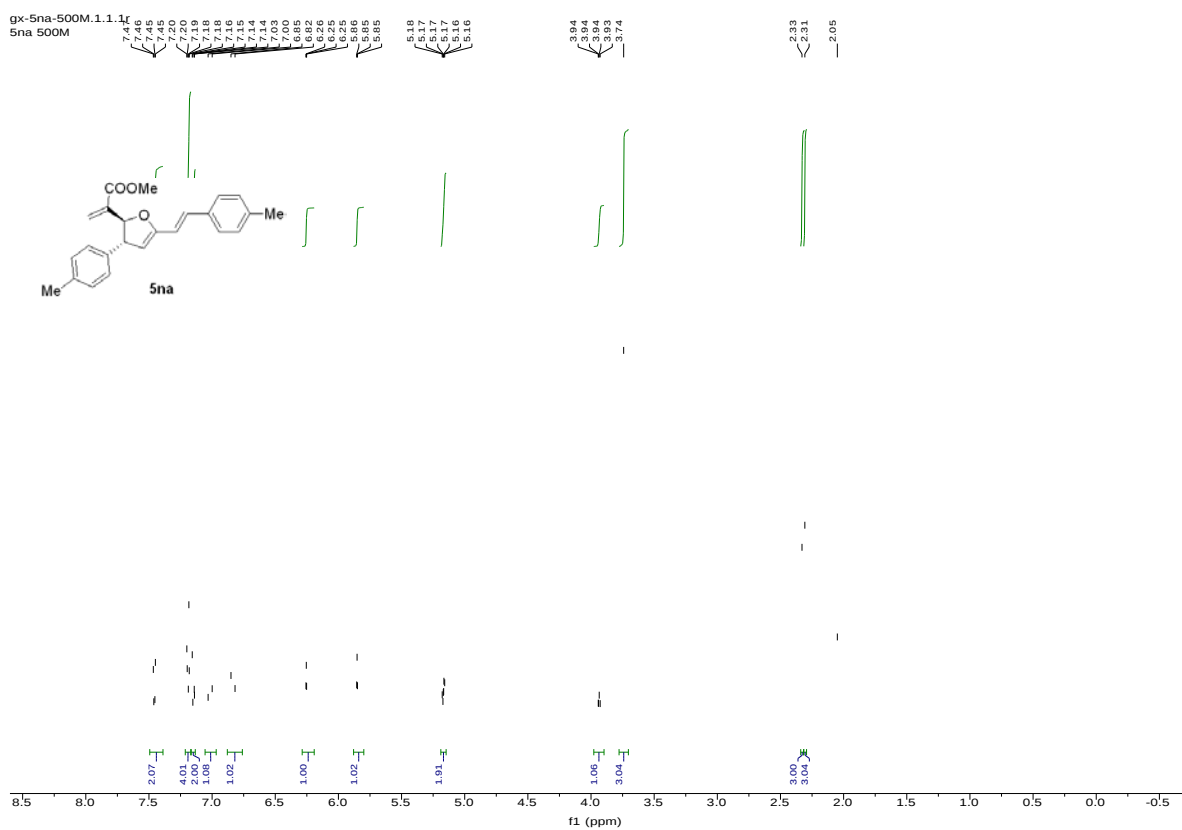


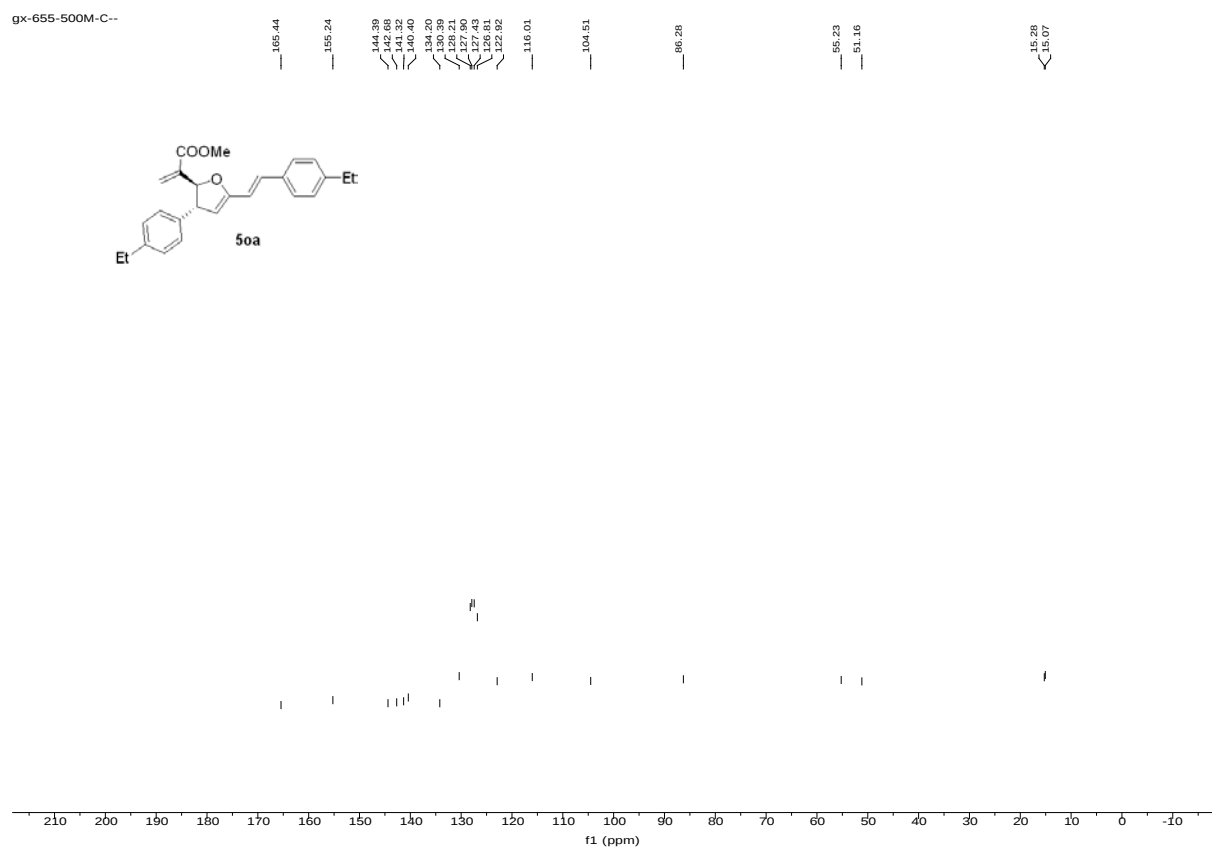
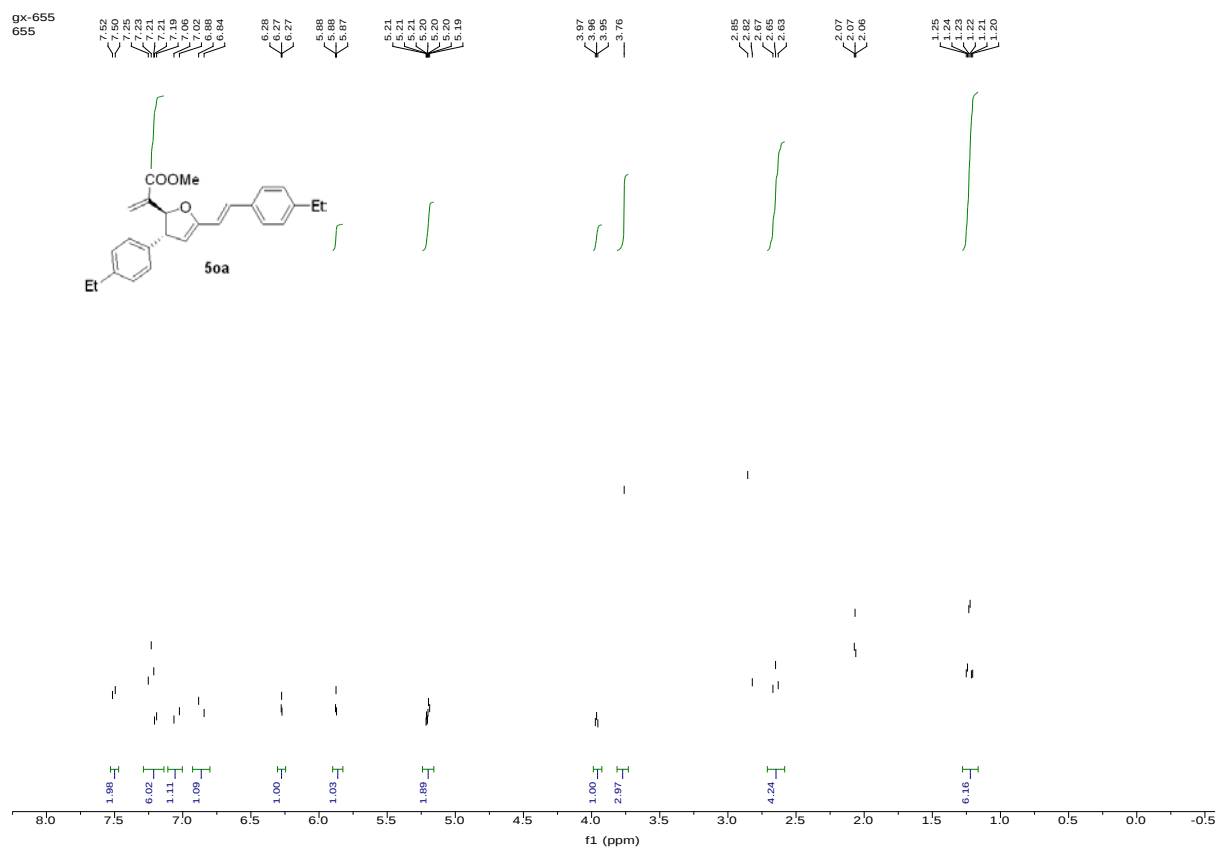
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640F

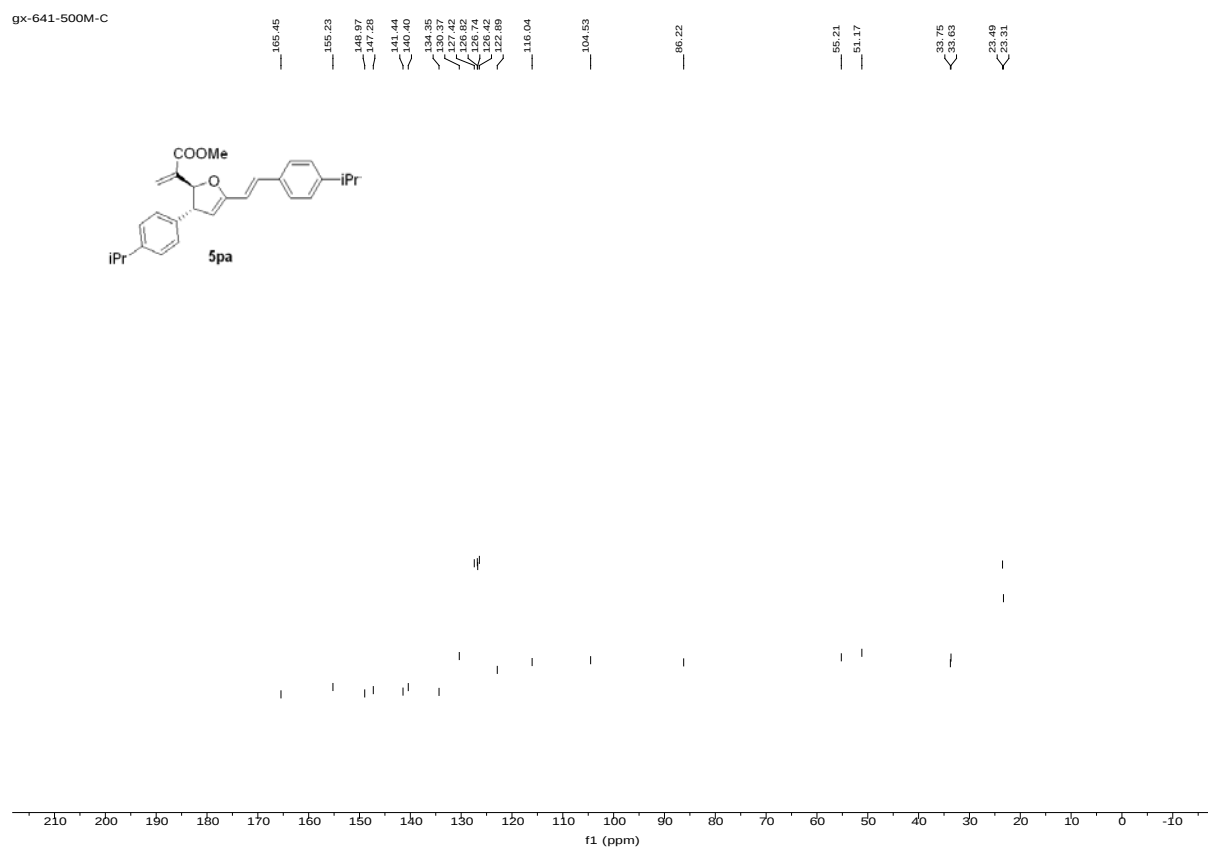
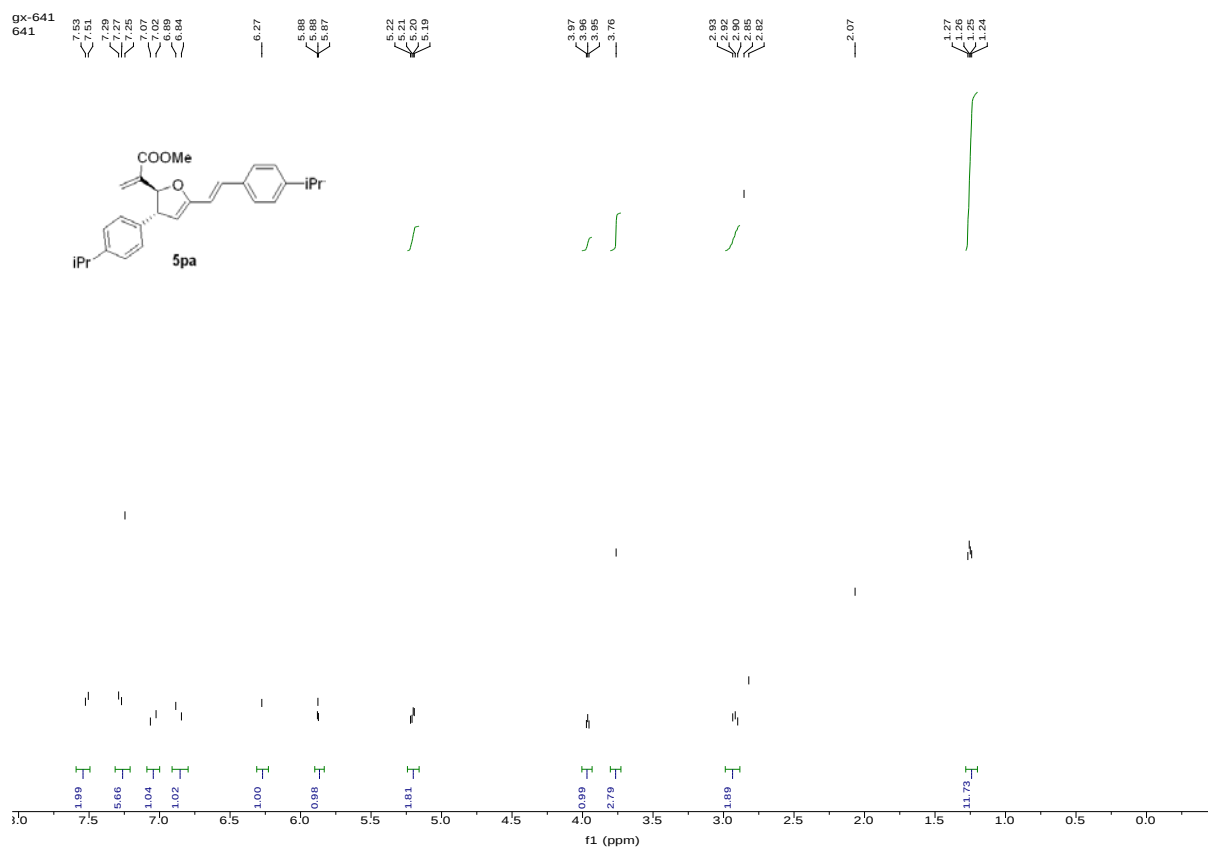


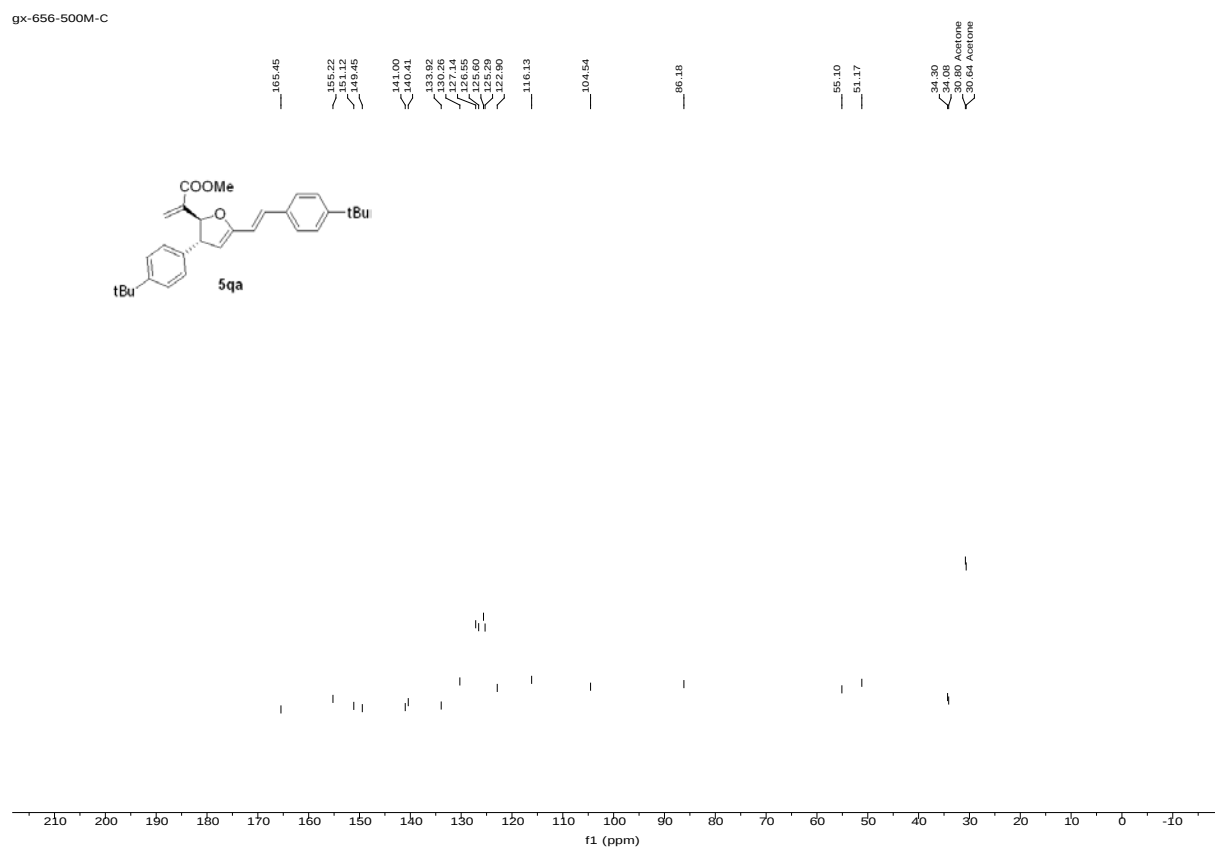
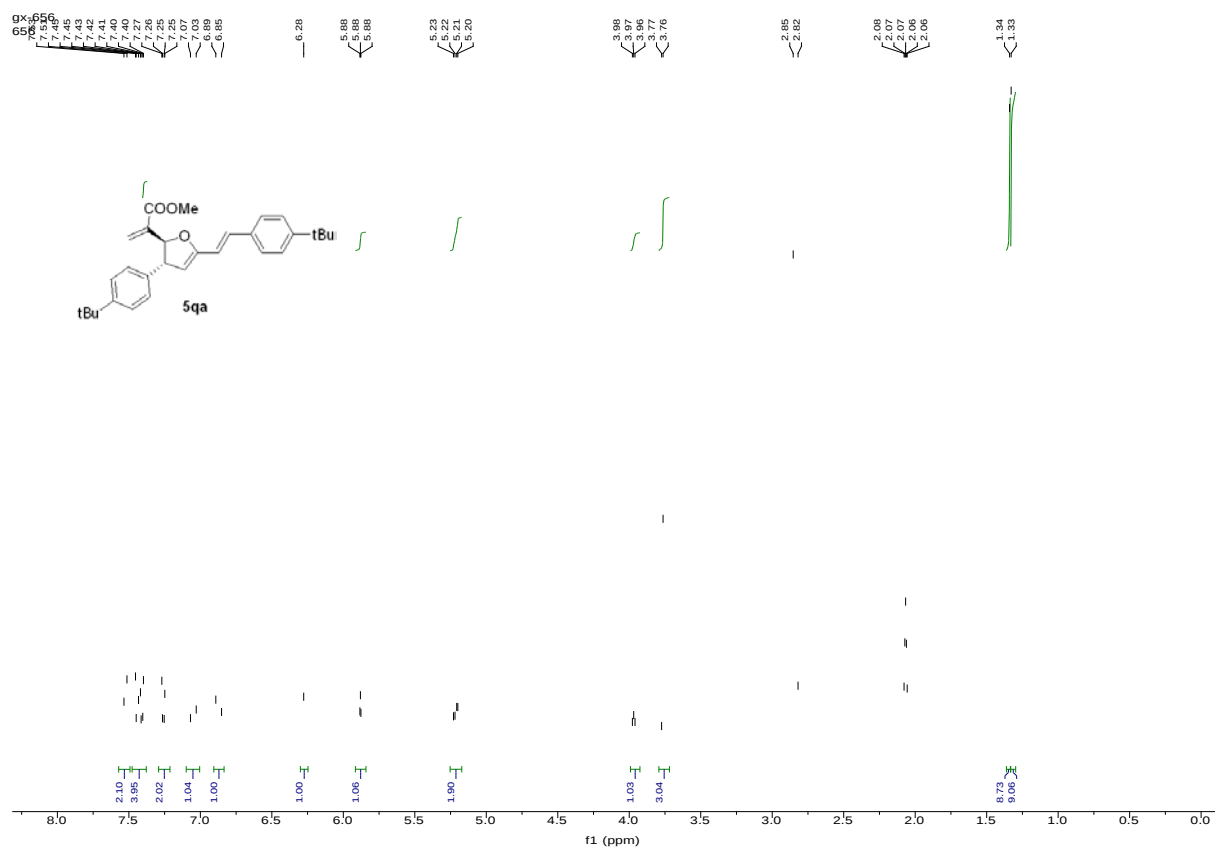
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43.00

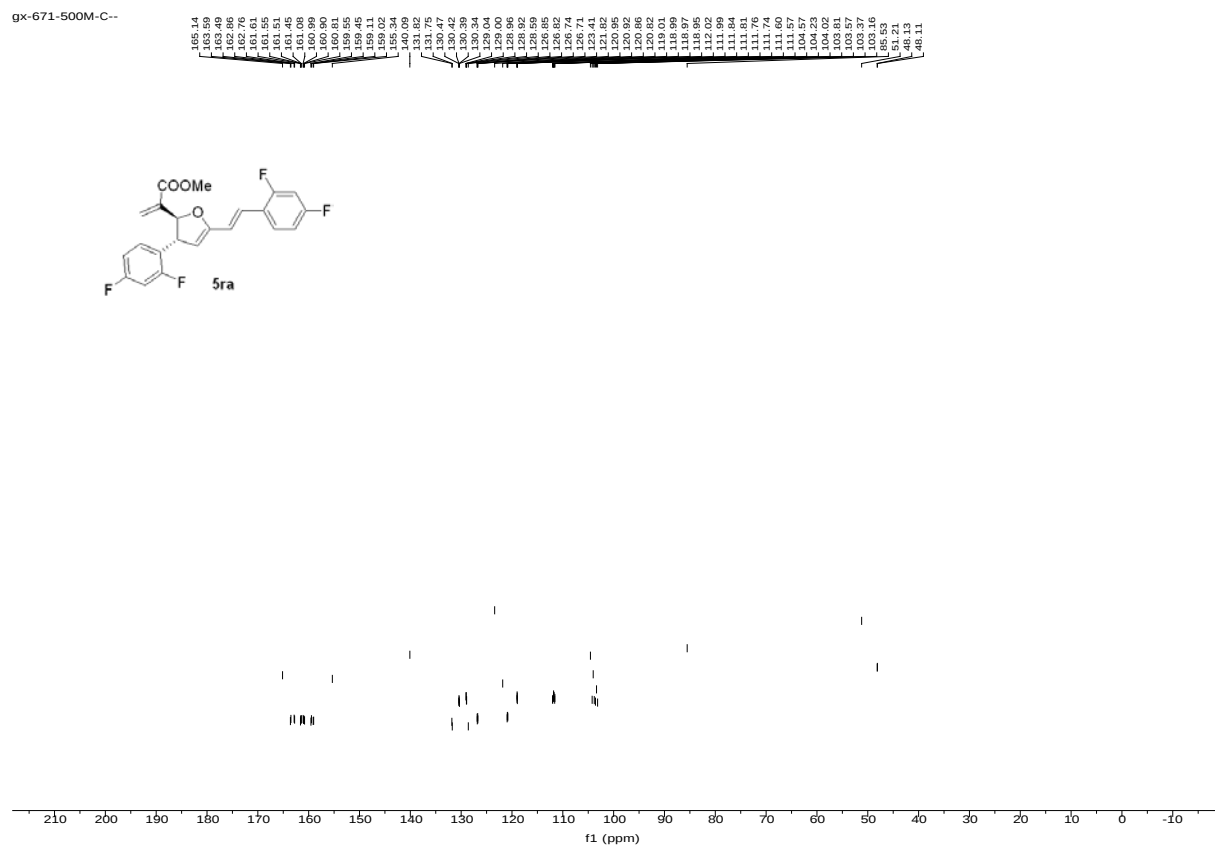
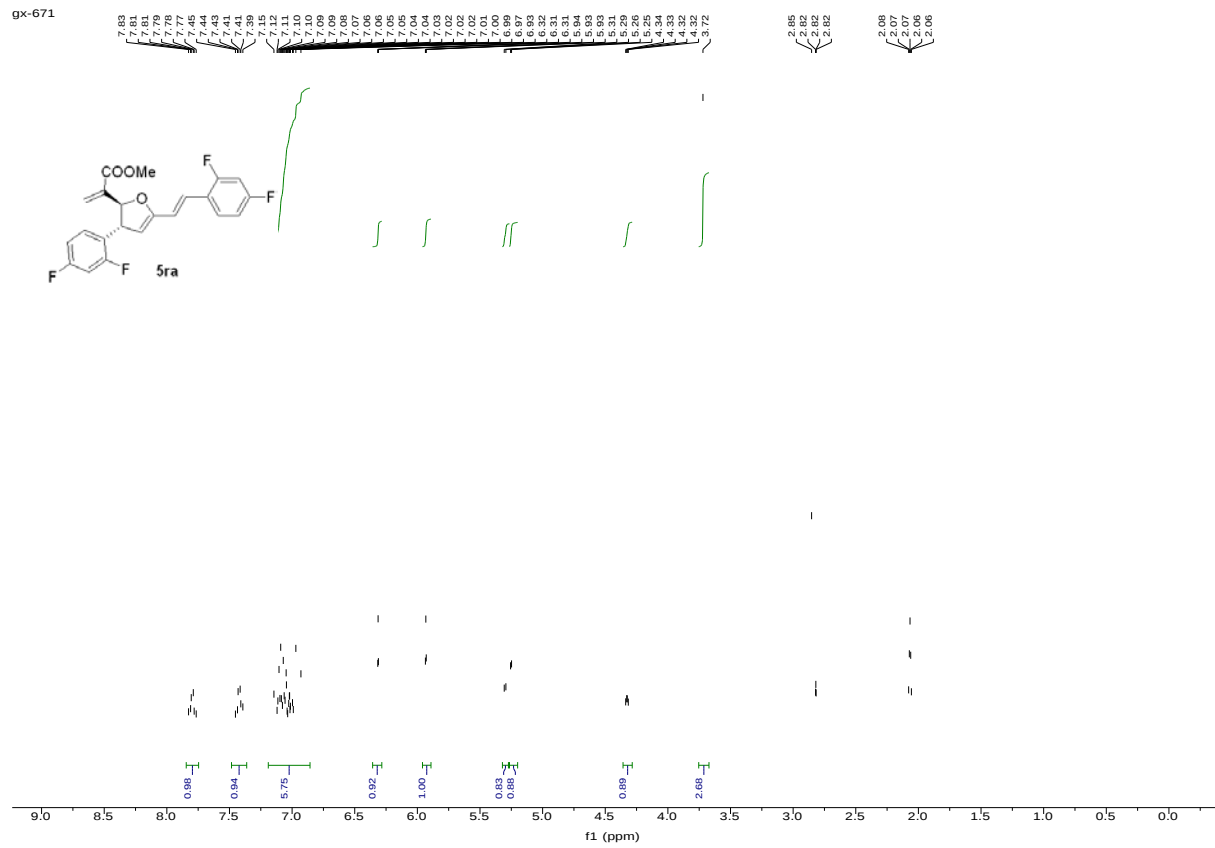




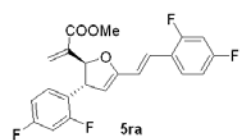




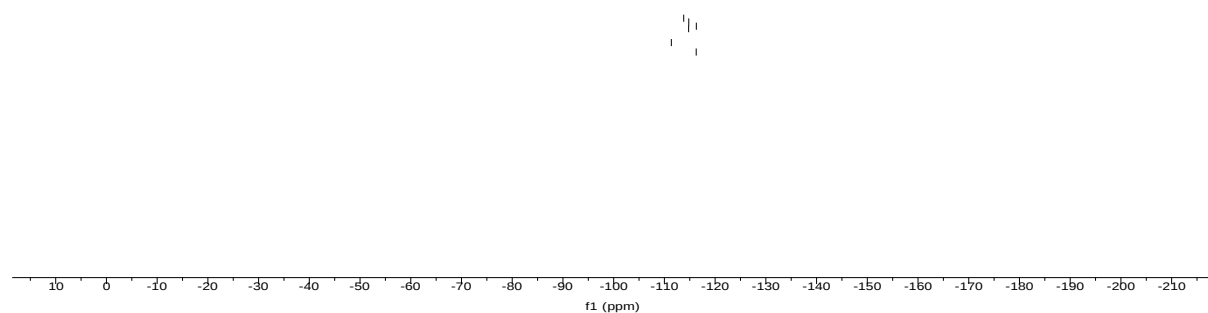




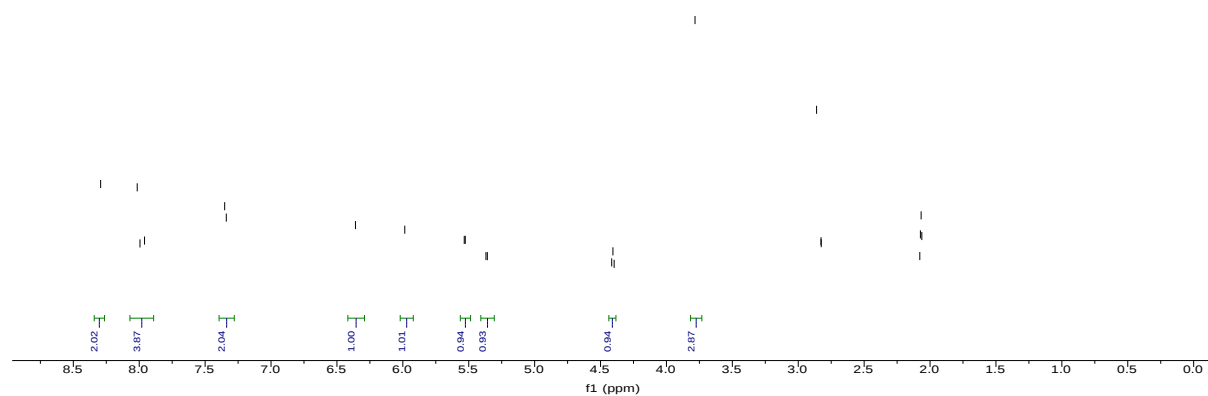
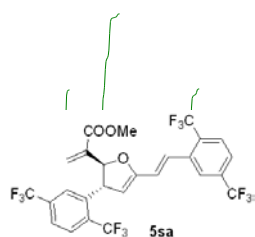
gx-671F.1.1.1r



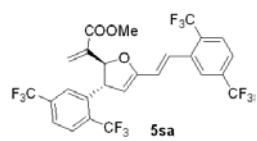
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-111.37
-114.78
-114.81
-116.27
-116.28



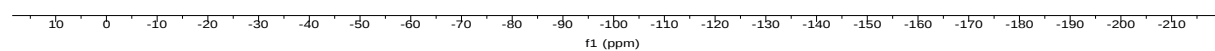
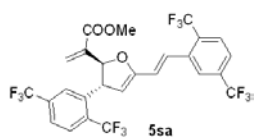
gx-693
693



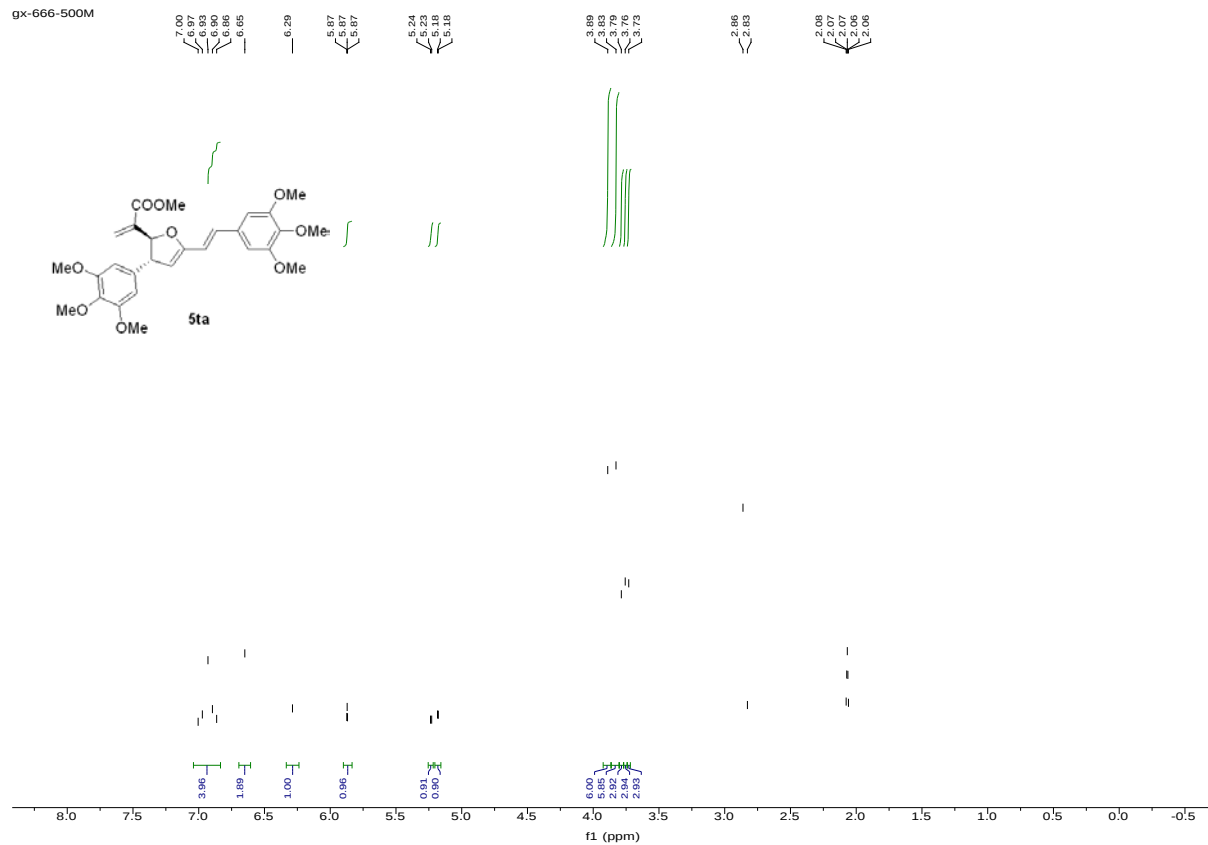
gx-693-500M-C



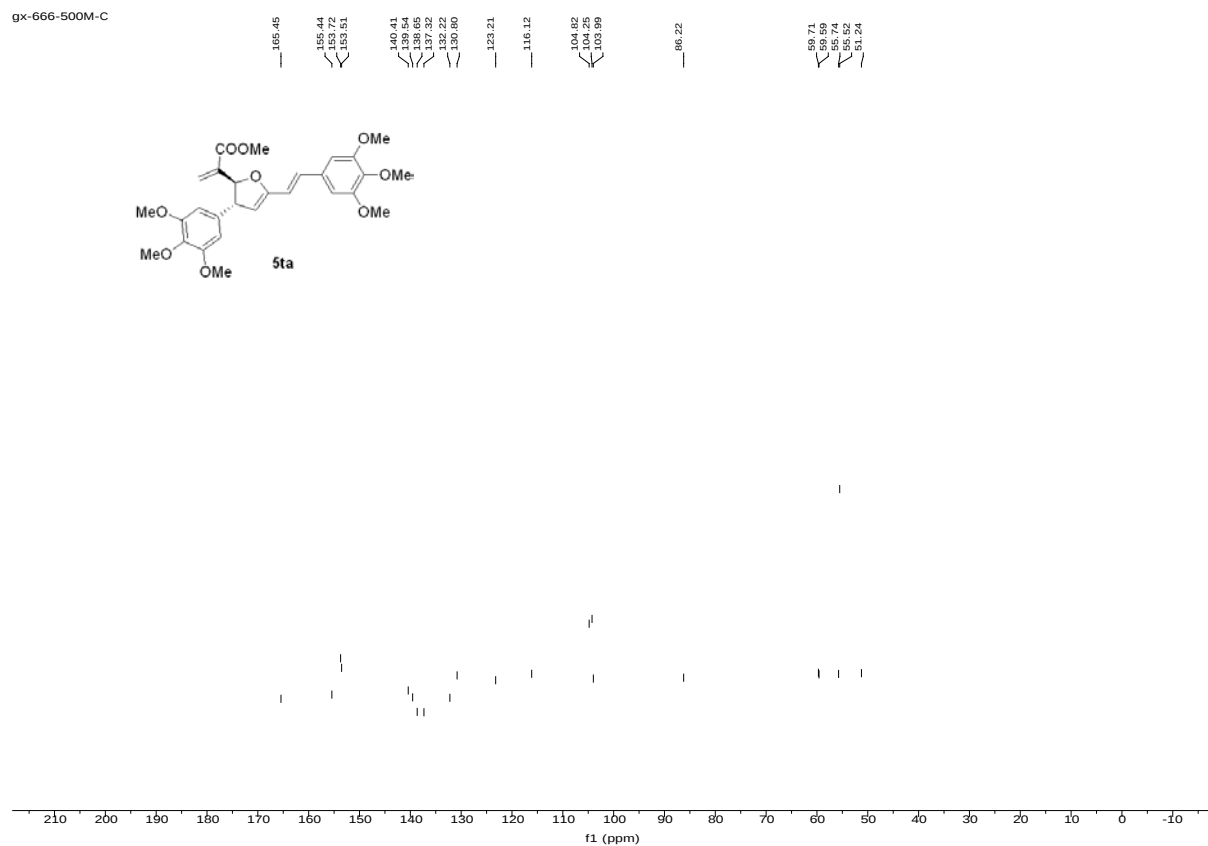
gx-693F

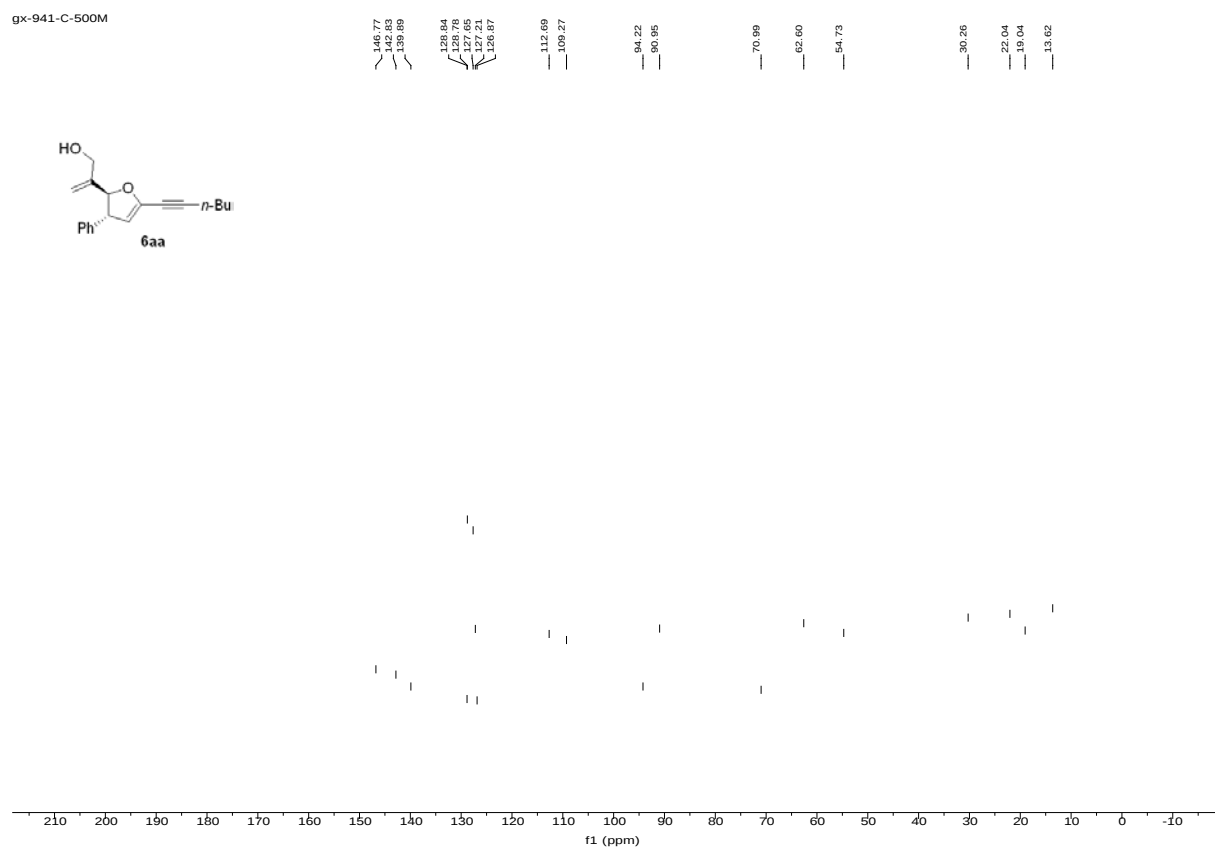
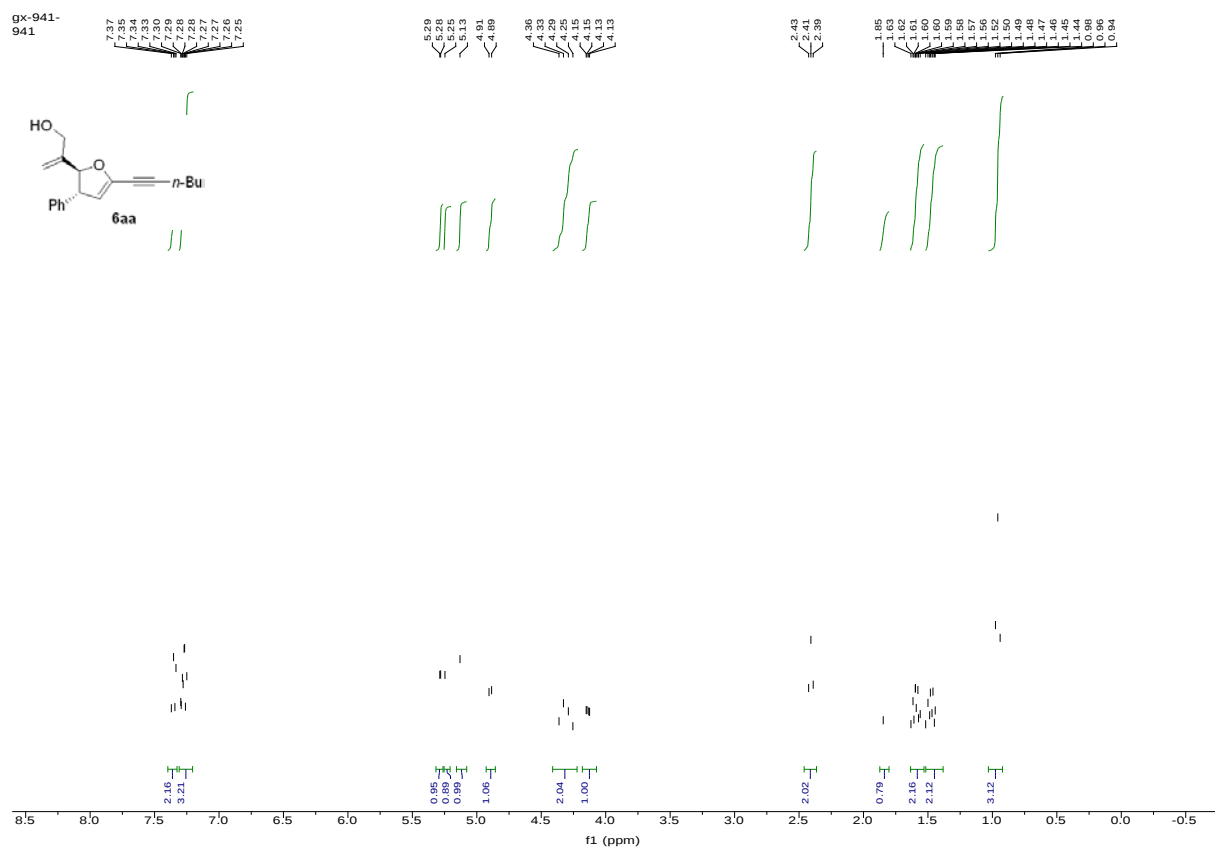


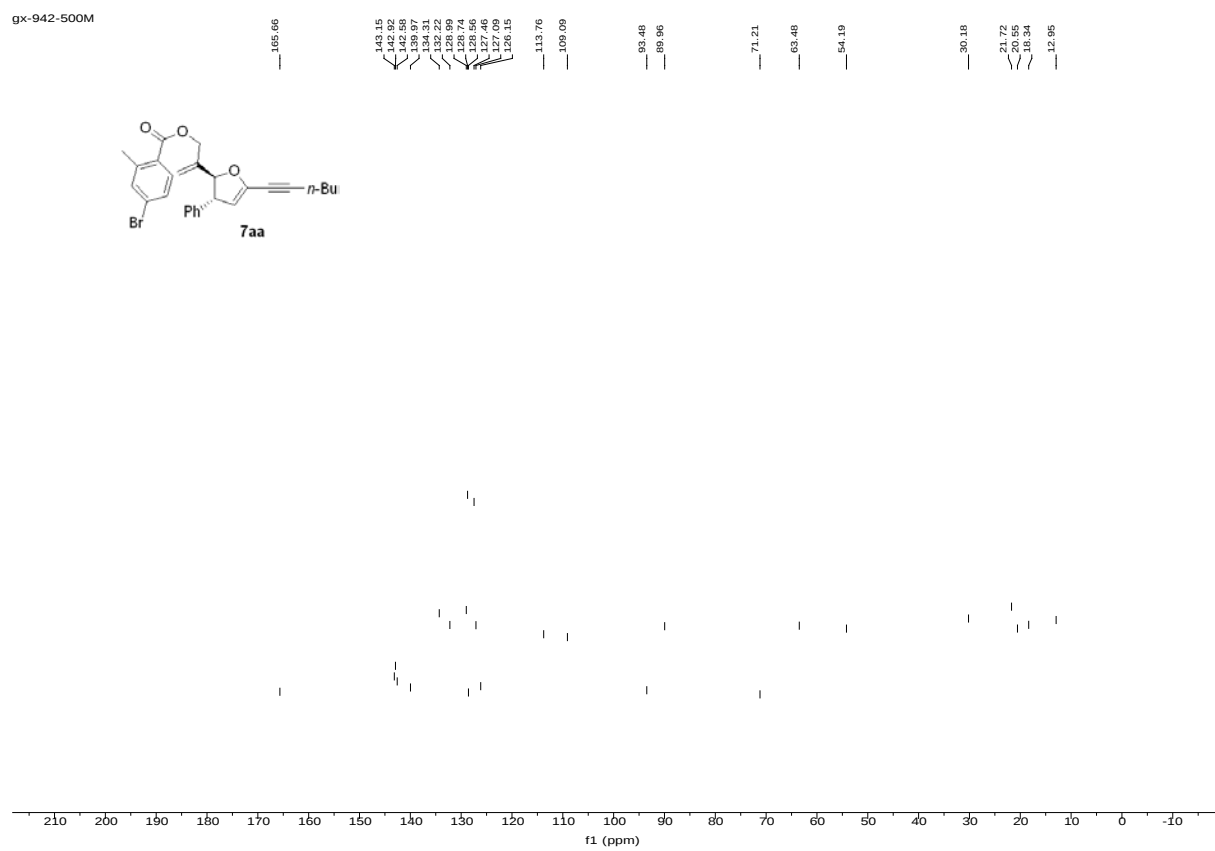
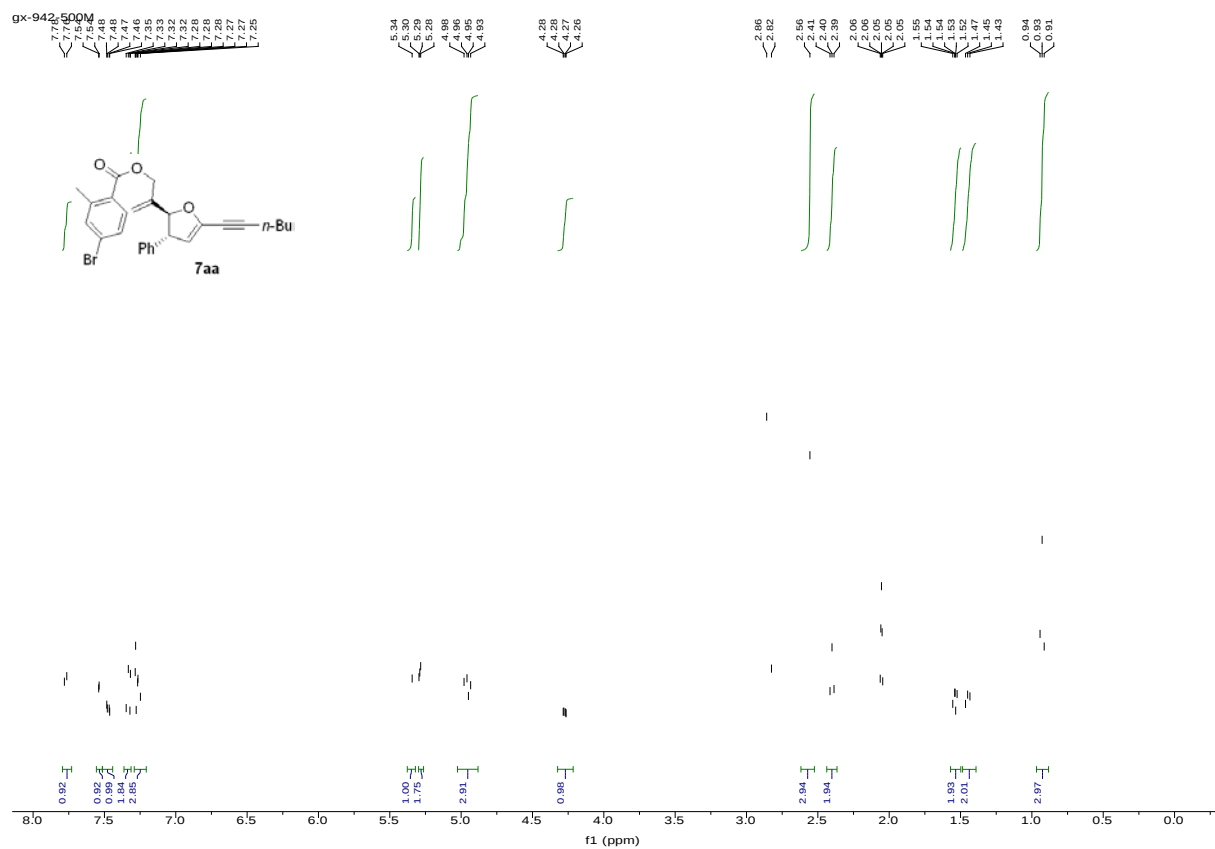
gx-666-500M



gx-666-500M-C

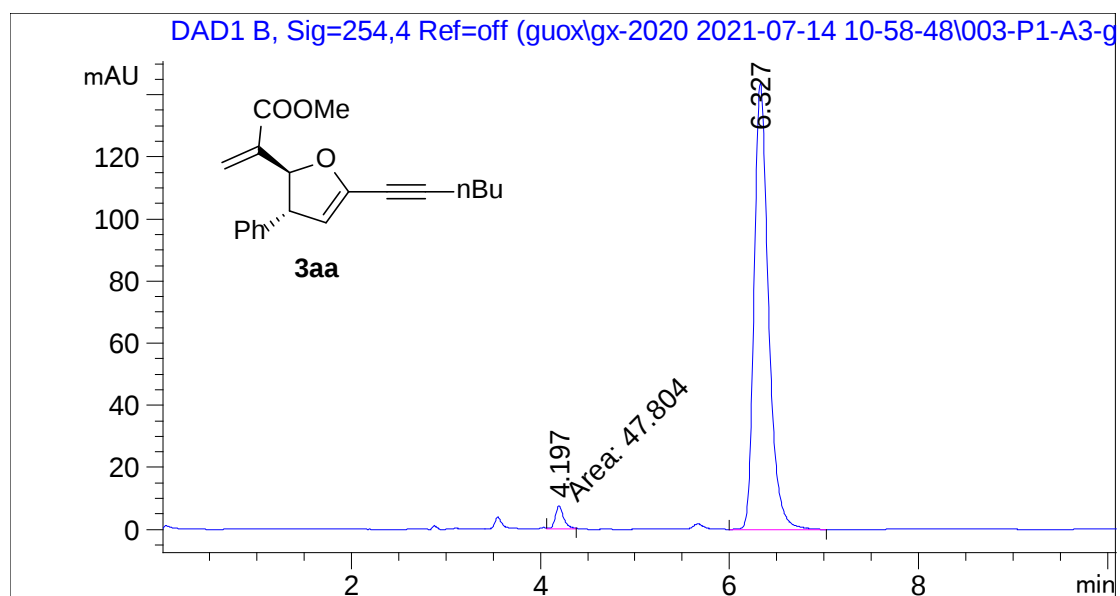
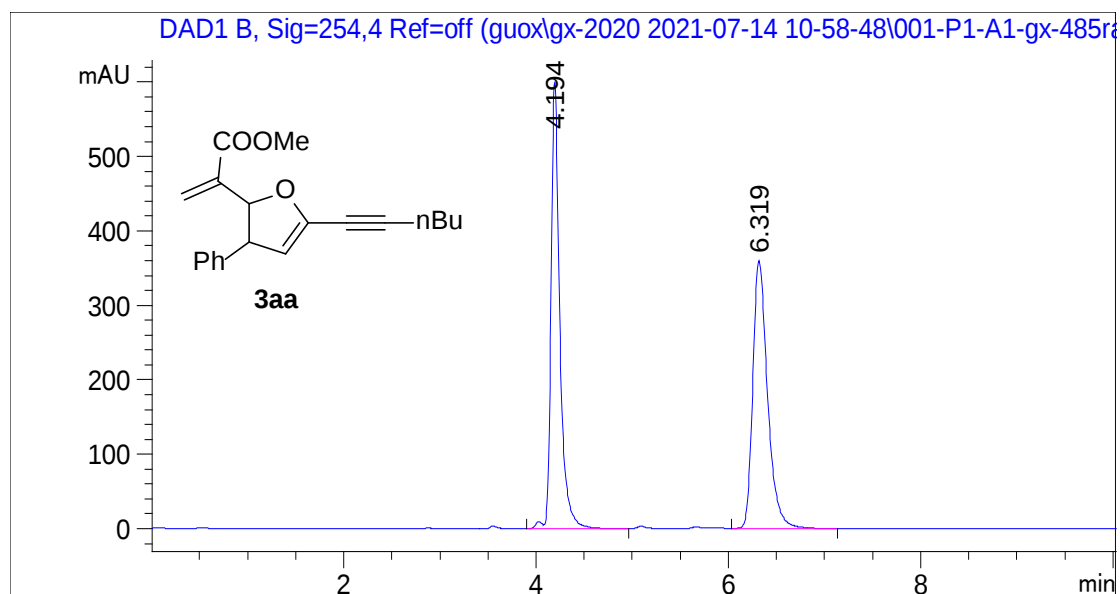




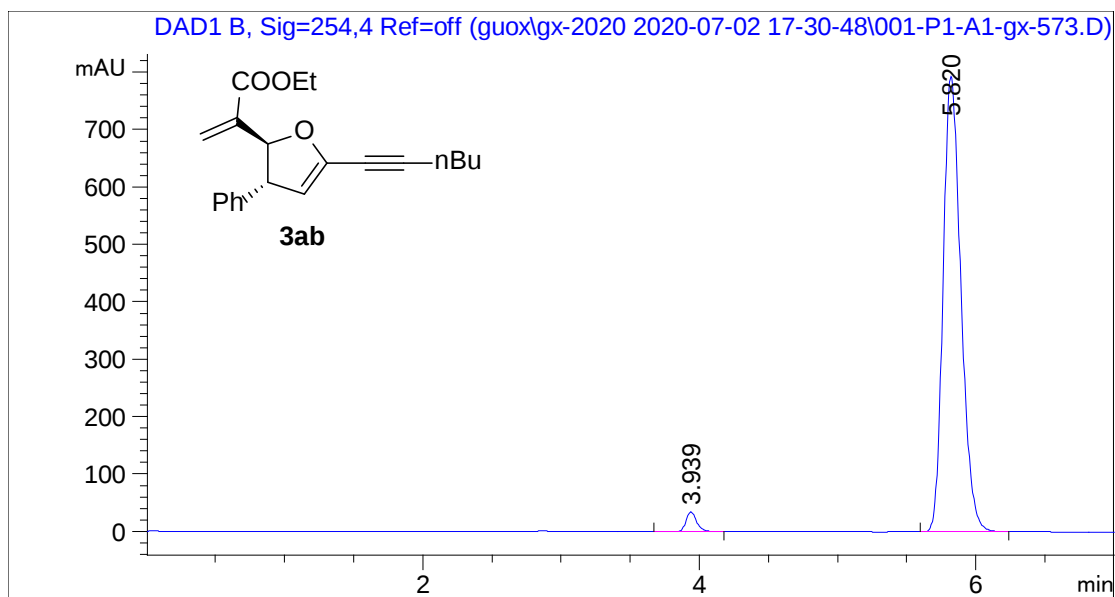
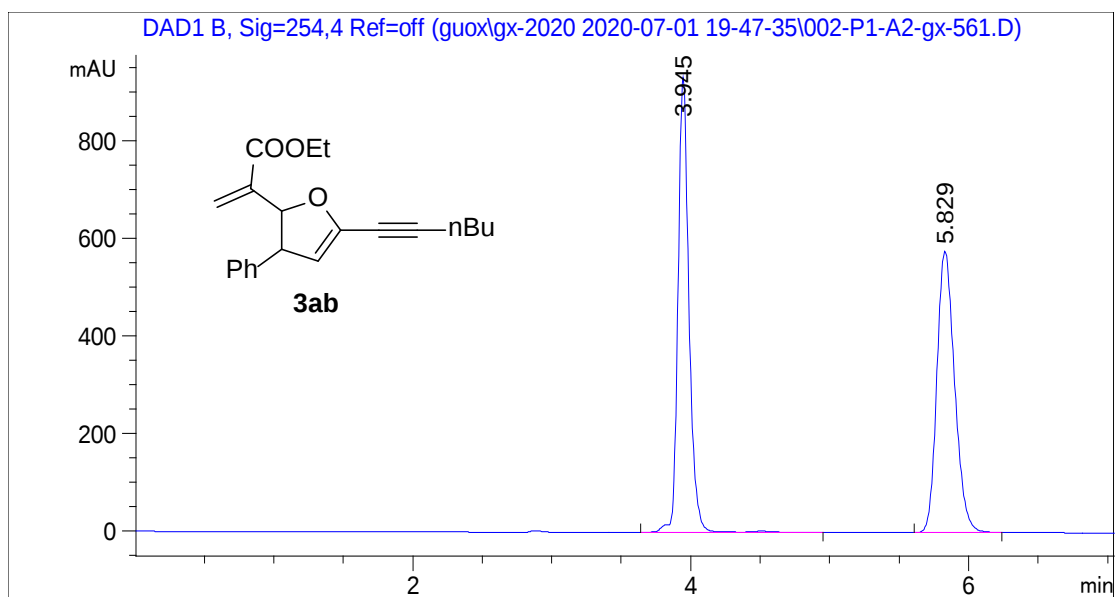


D: HPLC Analysis

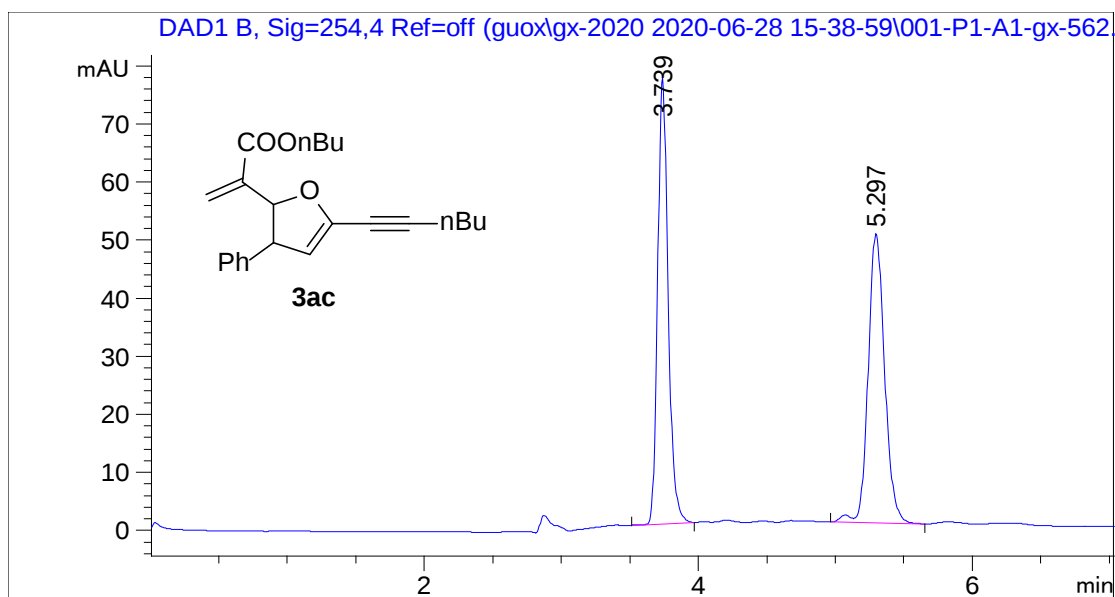
3aa: OD-H, 90/10, 1.0 ml/min, 254 nm



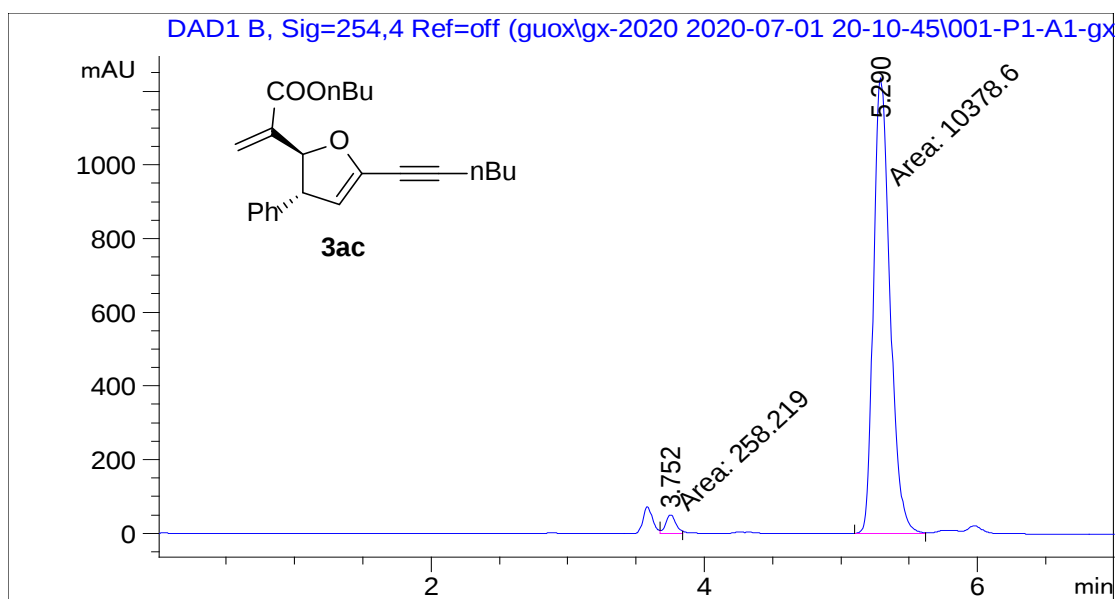
3ab: OD-H, 90/10, 1.0 ml/min, 254 nm



3ac: OD-H, 90/10, 1.0 ml/min, 254 nm

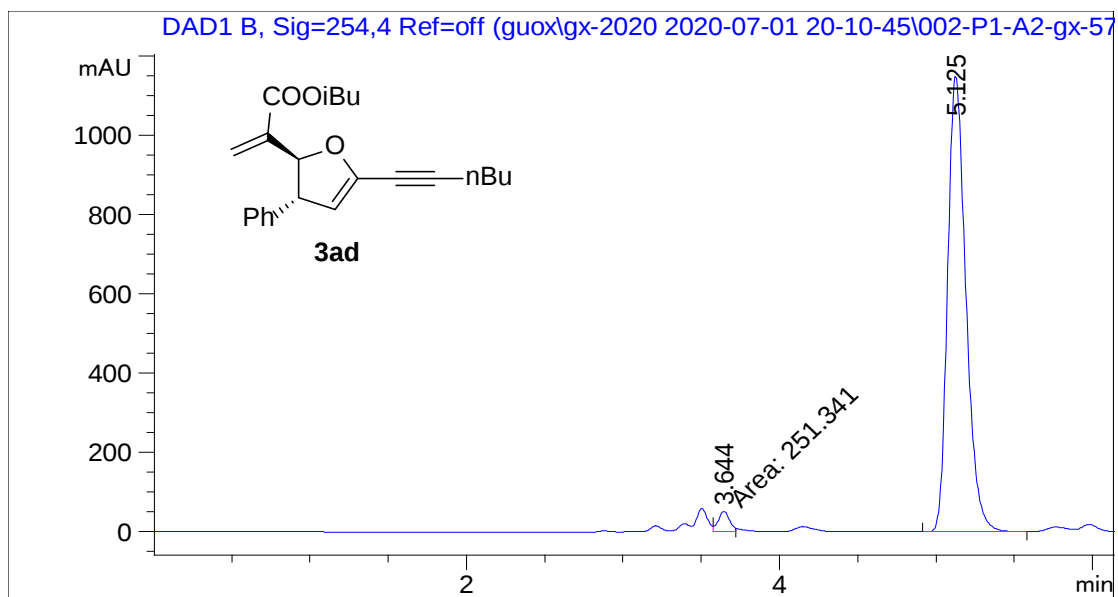
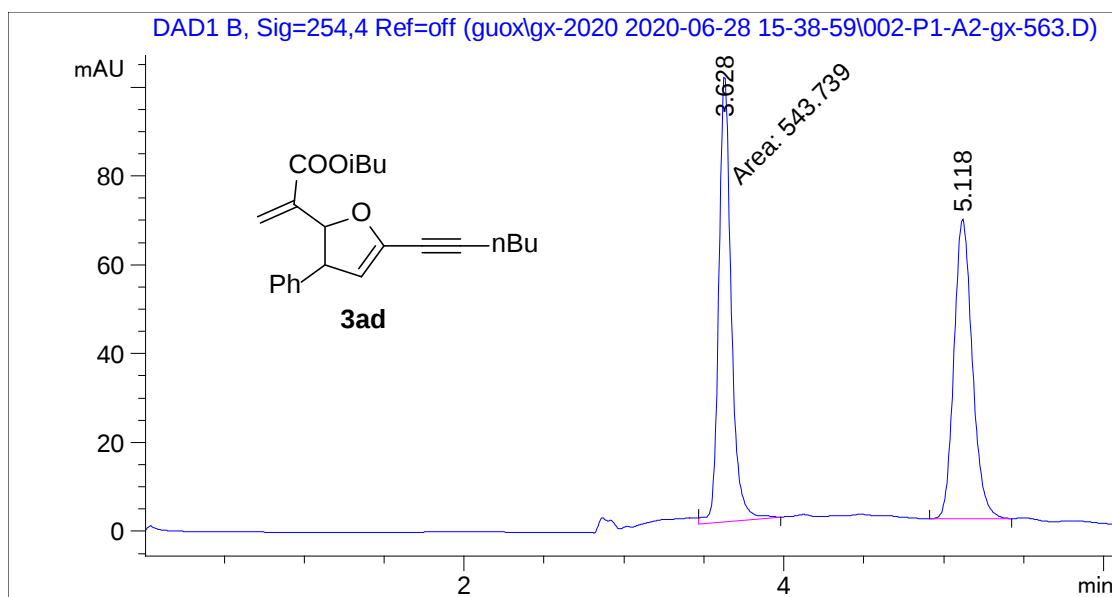


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	3.739	BB	409.4	76.9	0.0821	49.574	0.792
2	5.297	VBR	416.4	49.8	0.1281	50.426	0.897

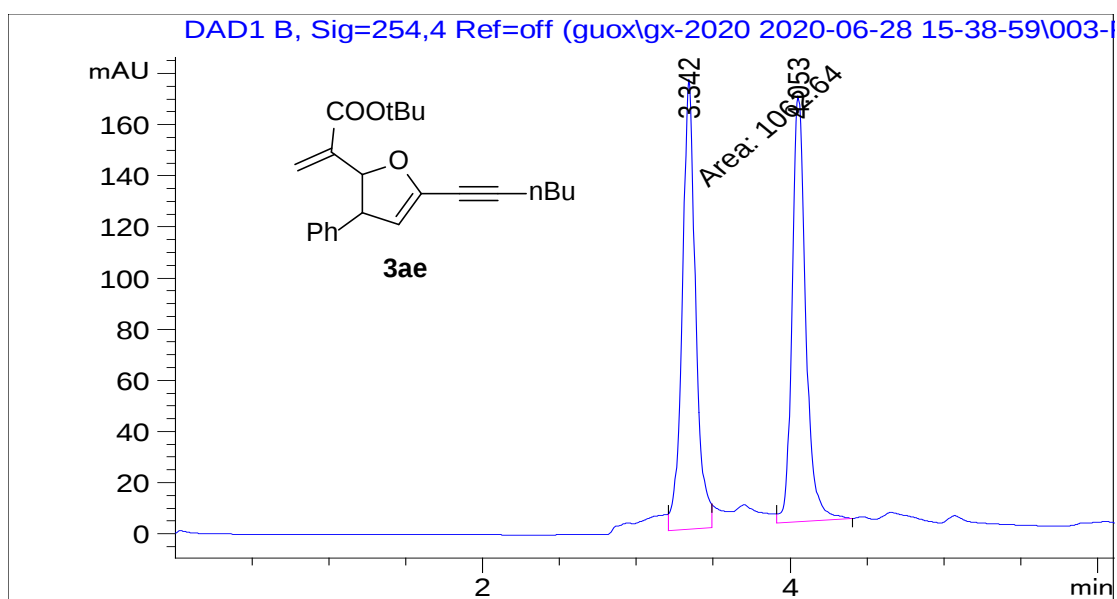


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	3.752	MF	258.2	50.6	0.085	2.428	0.864
2	5.29	MF	10378.6	1236.1	0.1399	97.572	0.721

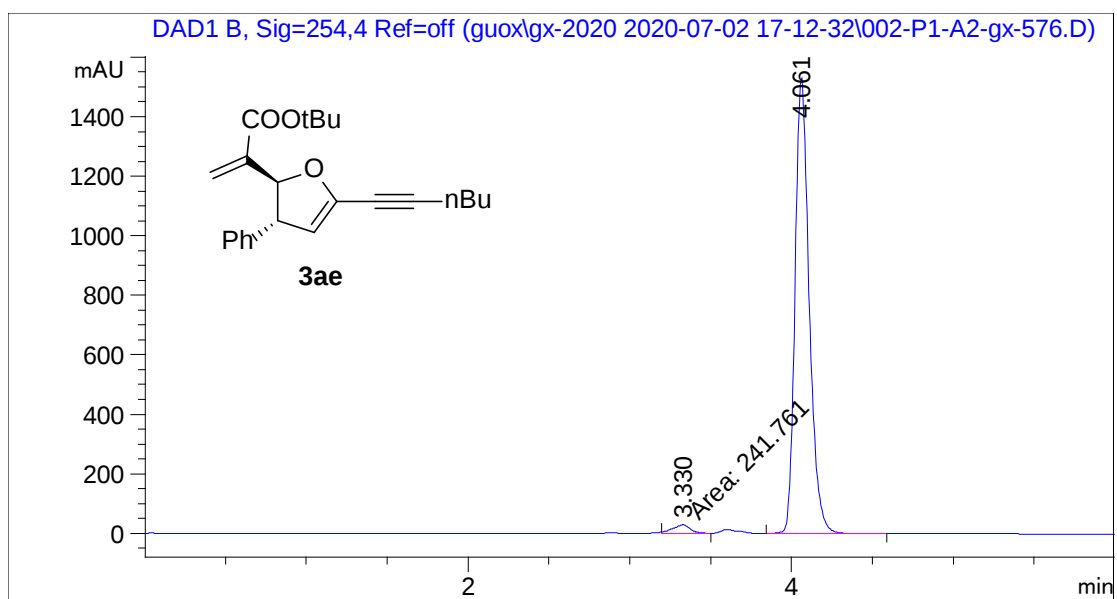
3ad: OD-H, 90/10, 1.0 ml/min, 254 nm



3ae: OD-H, 90/10, 1.0 ml/min, 254 nm

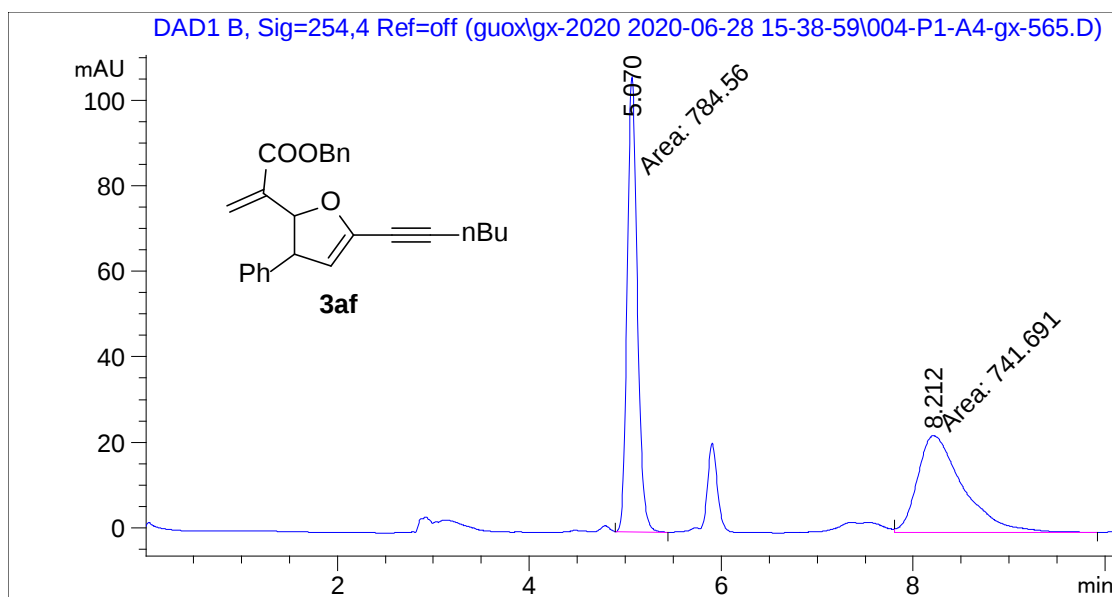


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	3.342	MF	1062.6	176.1	0.1006	50.716	0.929
2	4.053	VB	1032.6	166.2	0.0945	49.284	0.774

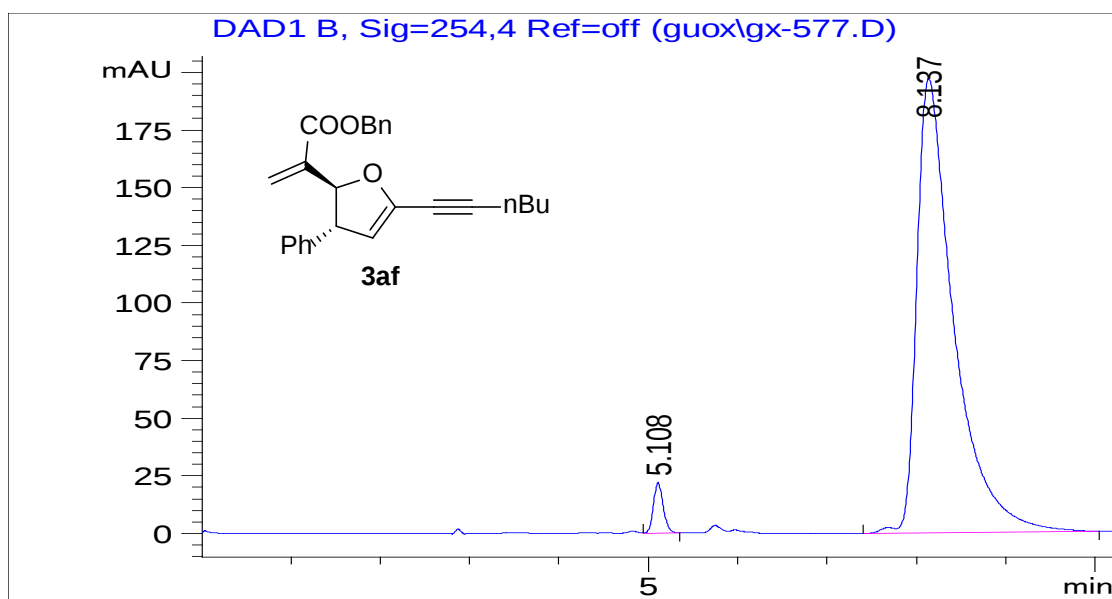


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	3.33	FM	241.8	30.4	0.1327	2.526	1.295
2	4.061	BB	9327.7	1528.8	0.0932	97.474	0.738

3af: OD-H, 90/10, 1.0 ml/min, 254 nm

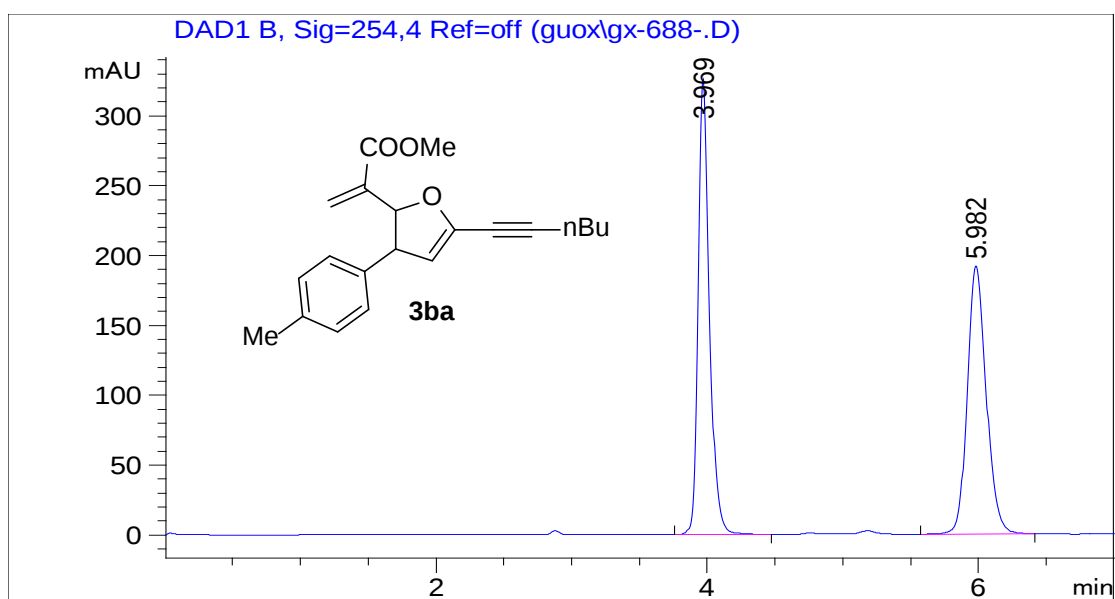


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	5.07	FM	784.6	106.4	0.1229	51.404	0.84
2	8.212	FM	741.7	22.6	0.5469	48.596	0.532

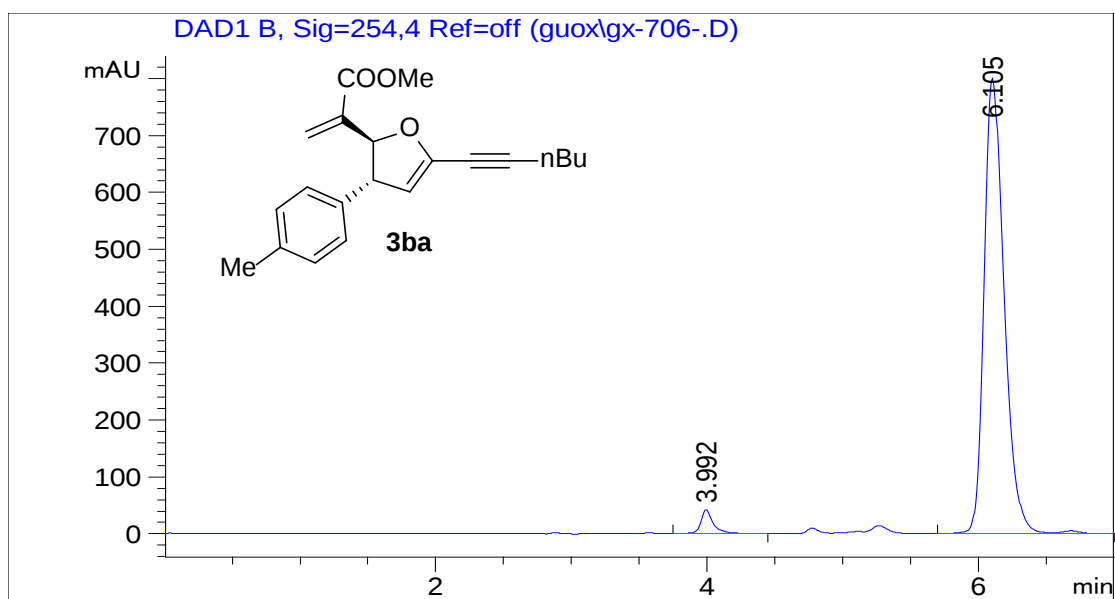


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	5.108	VB	166.7	21.8	0.1171	2.855	0.825
2	8.137	VB R	5672	197	0.4163	97.145	0.435

3ba: OD-H, 90/10, 1.0 ml/min, 254 nm

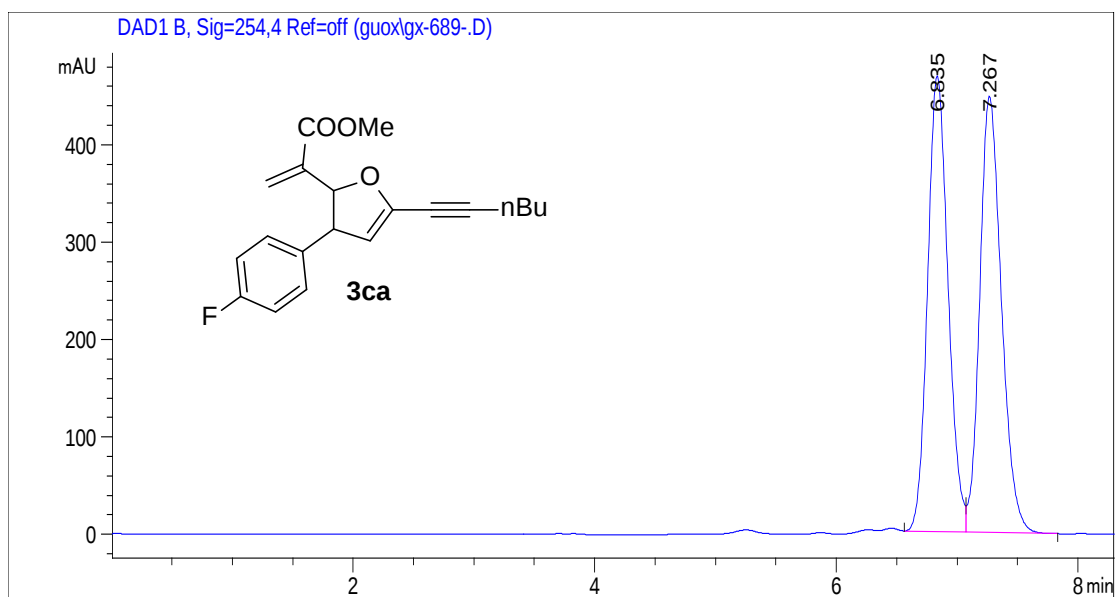


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	3.969	BB	1906.2	326.1	0.0882	50.489	0.721
2	5.982	BB	1869.3	191.7	0.1498	49.511	0.811

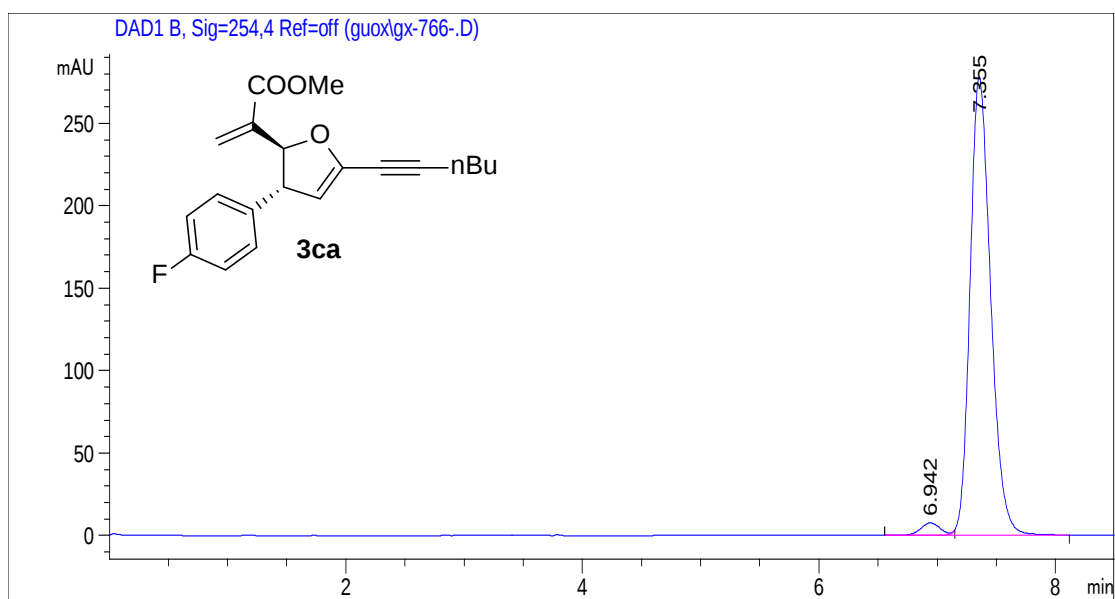


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	3.992	BB	269.1	41.7	0.0952	3.162	0.675
2	6.105	BV R	8241.3	799.3	0.1575	96.838	0.701

3ca: OD-H, 99/1, 1.0 ml/min, 254 nm

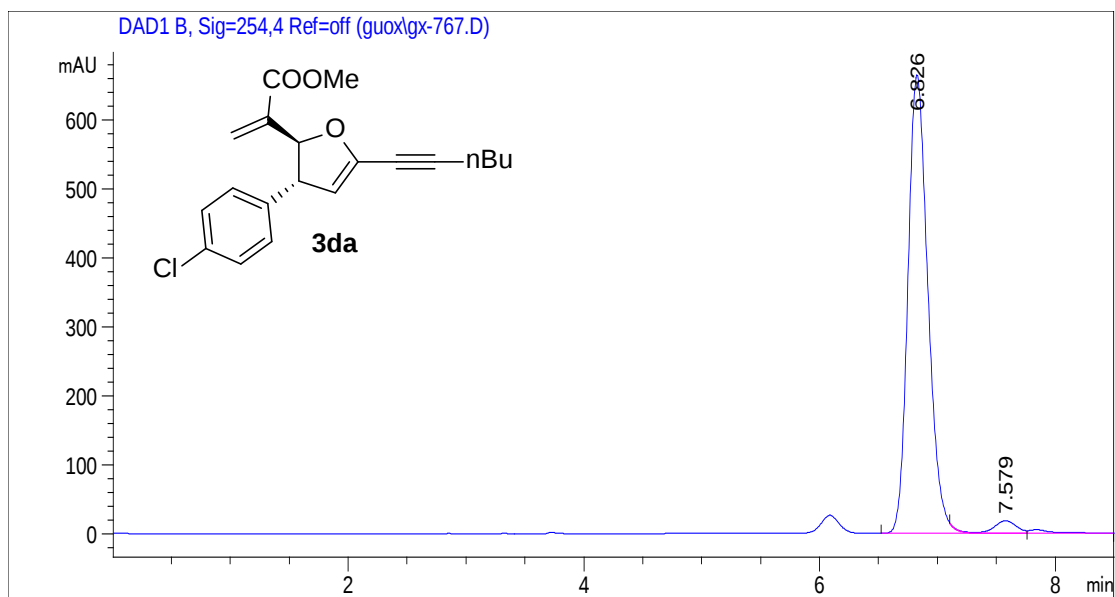
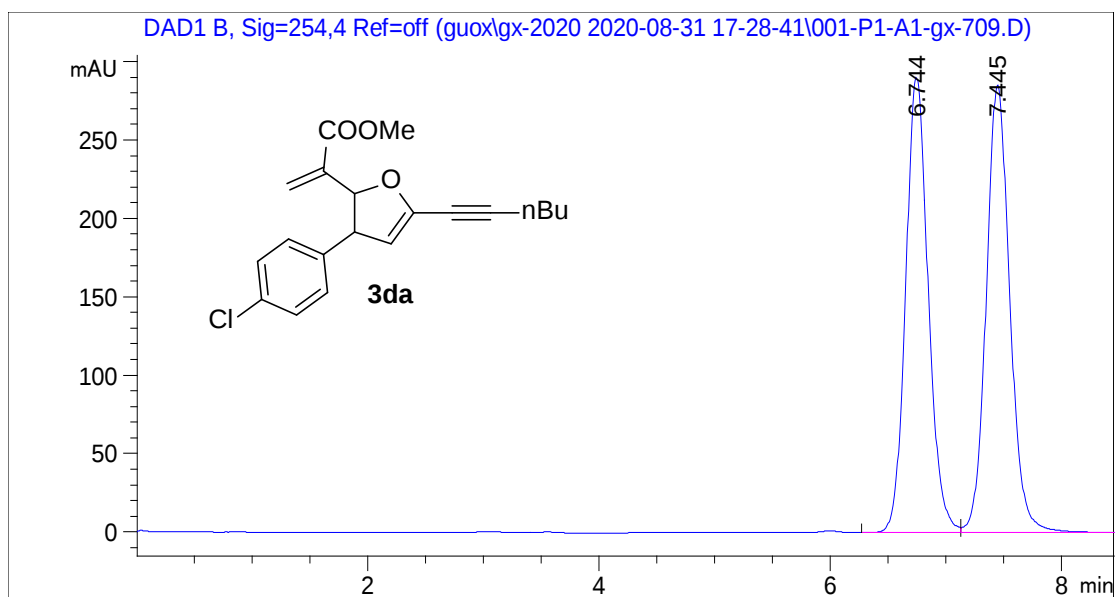


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.835	BV	5495.9	468.2	0.181	49.633	0.84
2	7.267	VB	5577.3	447.8	0.1913	50.367	0.76

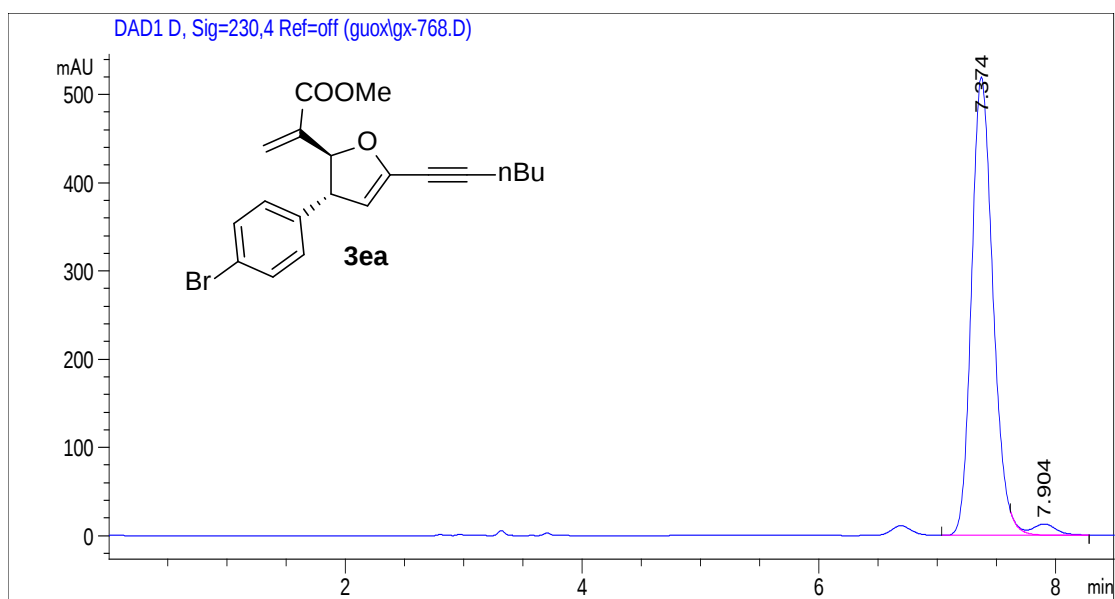
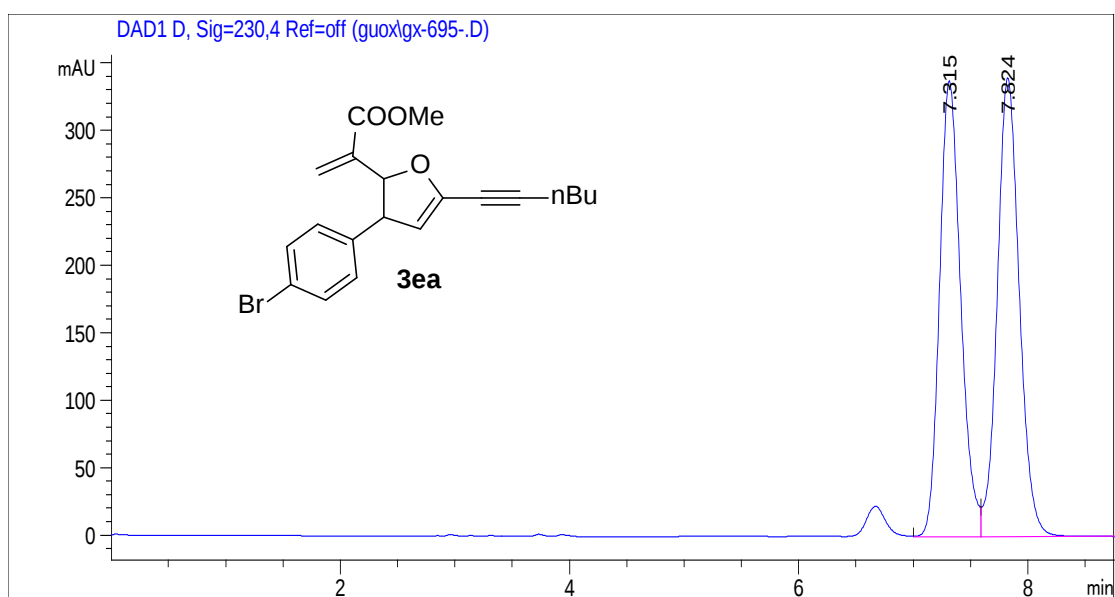


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.942	BVE	84.7	7.5	0.1733	2.458	1.009
2	7.355	VBR	3359.7	277.9	0.185	97.542	0.857

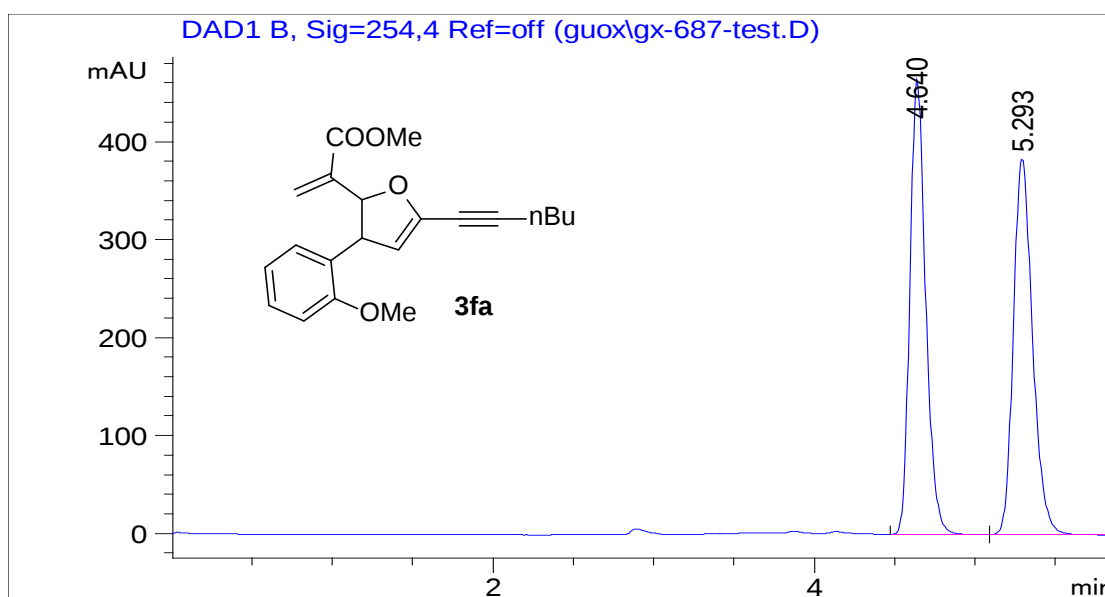
3da: OD-H, 99/1, 1.0 ml/min, 254 nm



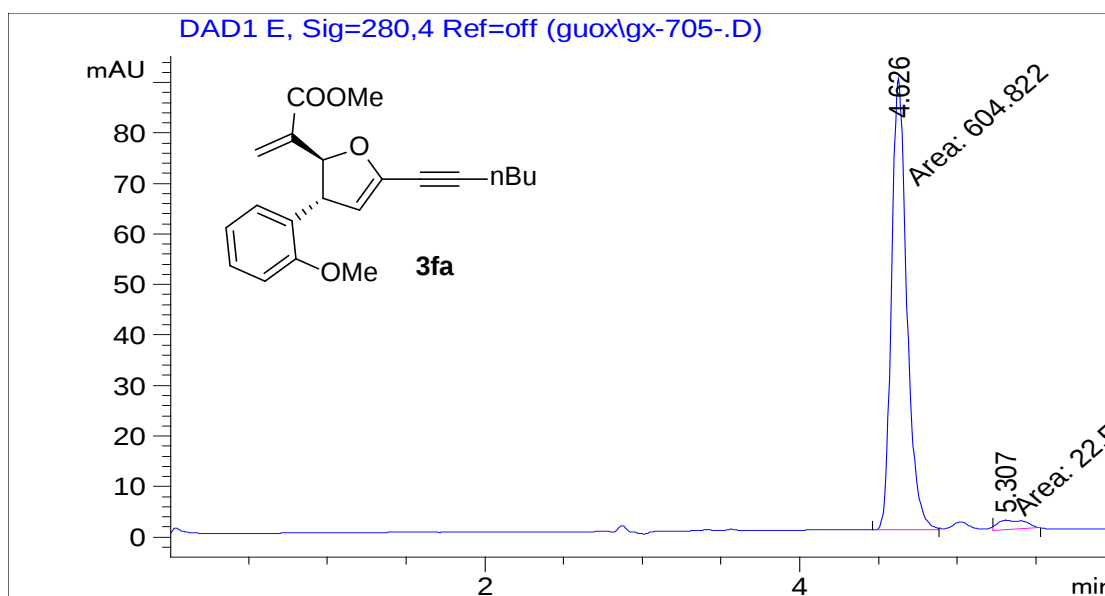
3ea: OD-H, 99/1, 1.0 ml/min, 230 nm



3fa: OD-H, 90/10, 1.0 ml/min, 254 nm

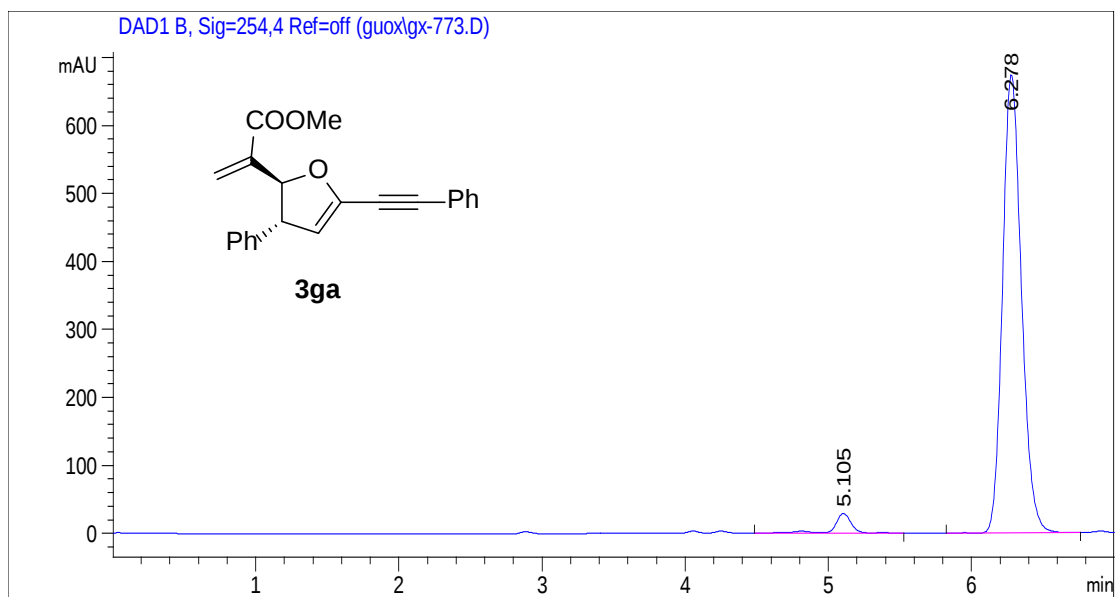
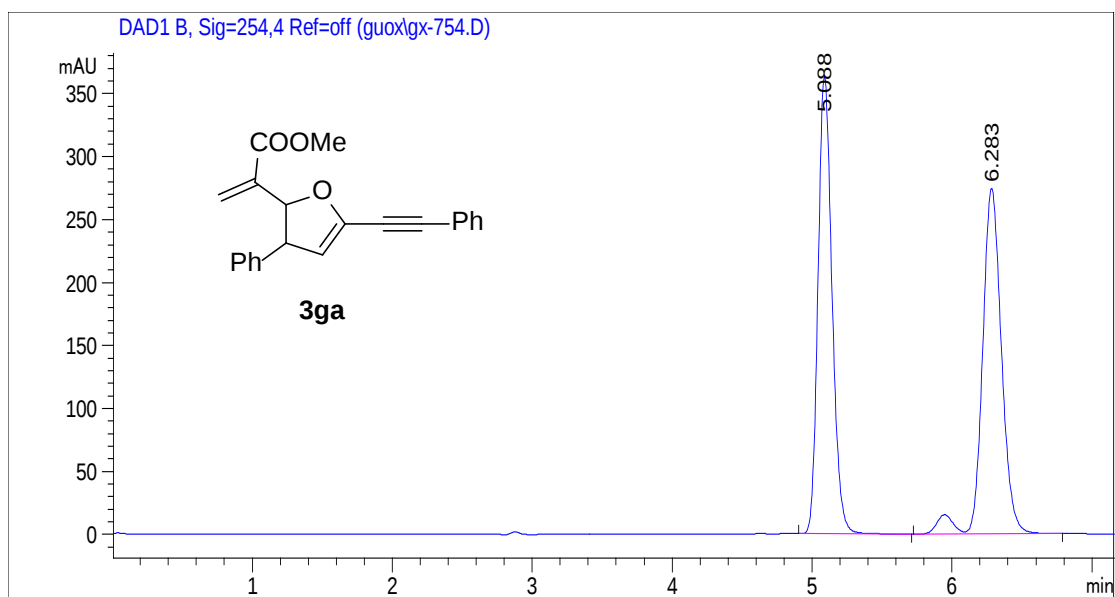


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.64	BB	3169.7	464.6	0.1056	49.915	0.766
2	5.293	BB	3180.5	383.5	0.1267	50.085	0.761

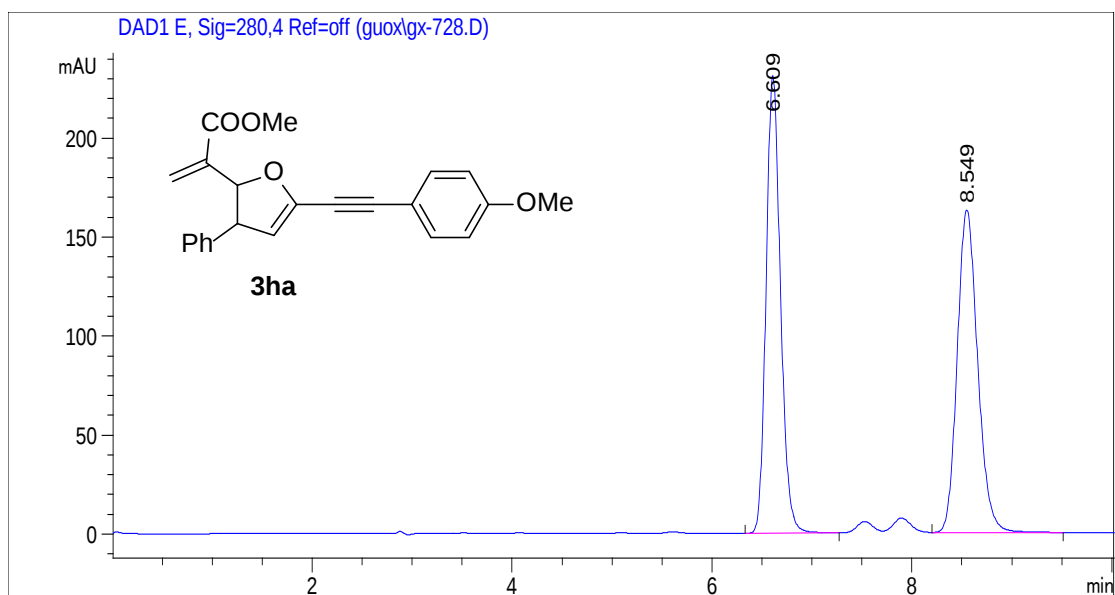


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.626	MF	604.8	89.5	0.1127	96.408	0.773
2	5.307	MM	22.5	1.9	0.1942	3.592	0.452

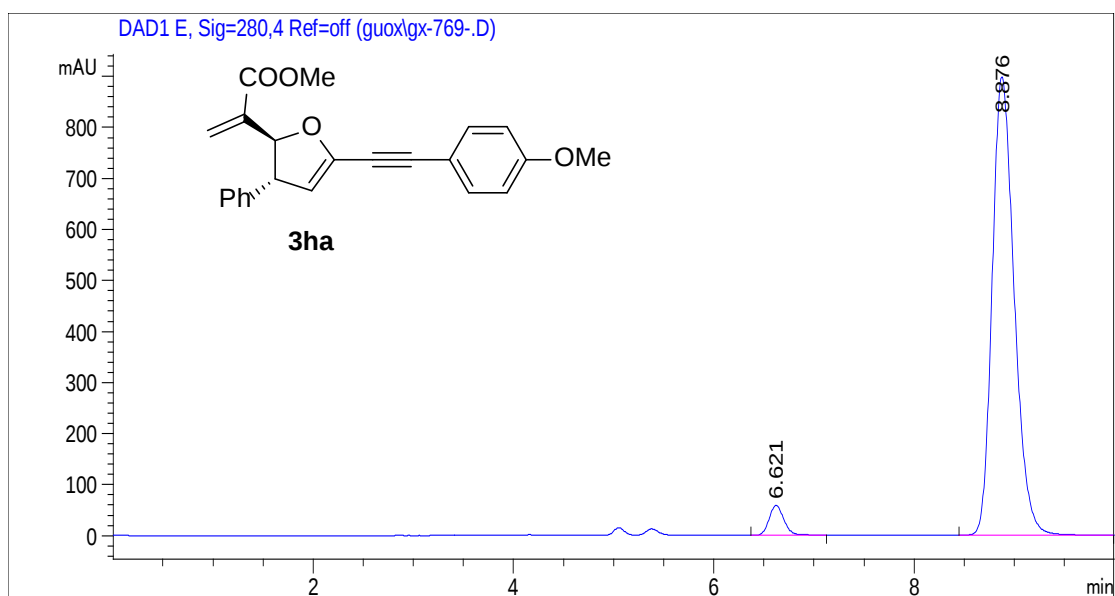
3ga: OD-H, 90/10, 1.0 ml/min, 254 nm



3ha: OD-H, 90/10, 1.0 ml/min, 254 nm

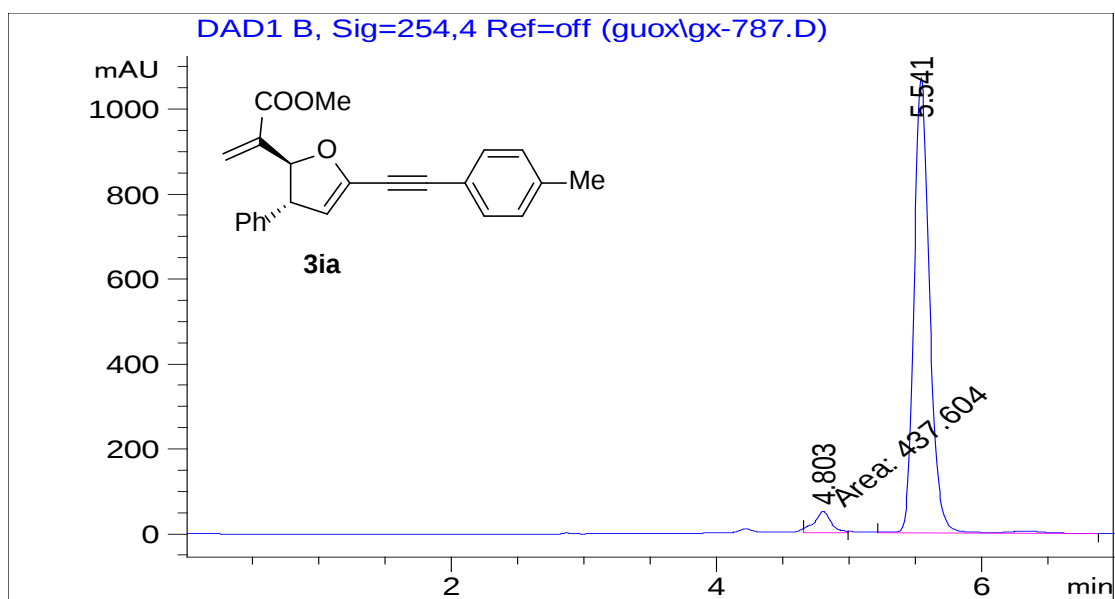
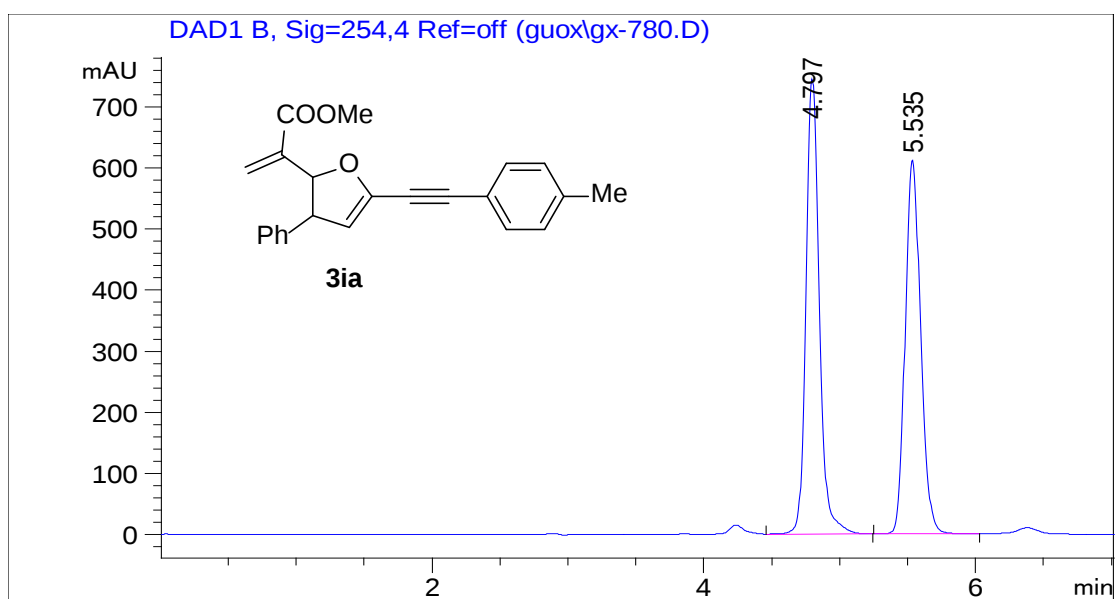


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.609	BB	2313.1	231.2	0.1527	49.921	0.816
2	8.549	VB	2320.5	163.1	0.218	50.079	0.814

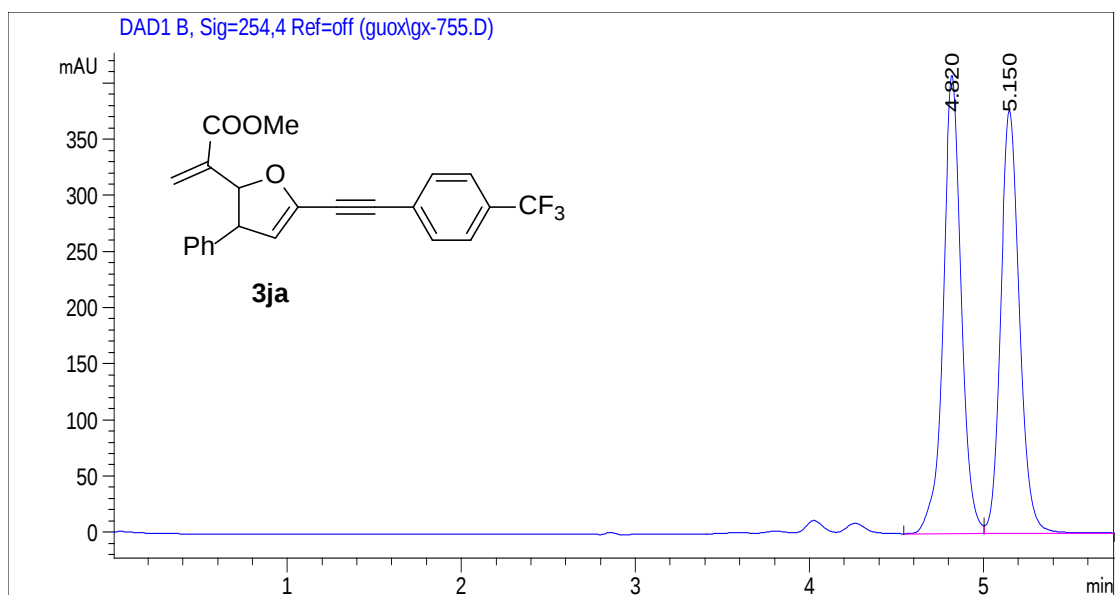


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.621	BB	603.9	59	0.1574	4.236	0.823
2	8.876	BBA	13651.5	897.7	0.2334	95.764	0.744

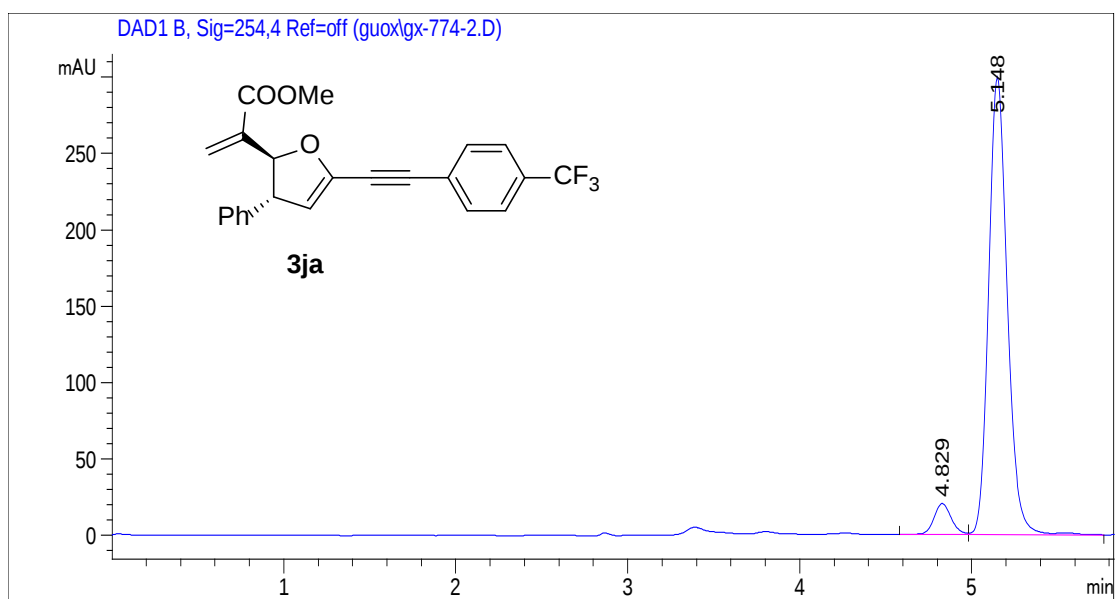
3ia: OD-H, 90/10, 1.0 ml/min, 254 nm



3ja: OD-H, 90/10, 1.0 ml/min, 254 nm

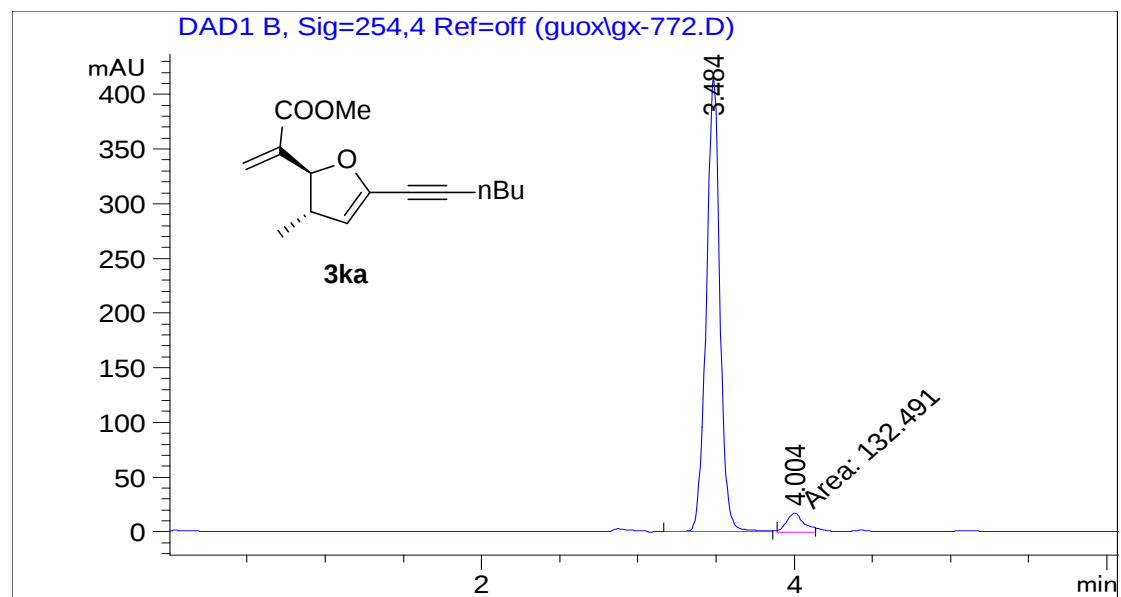
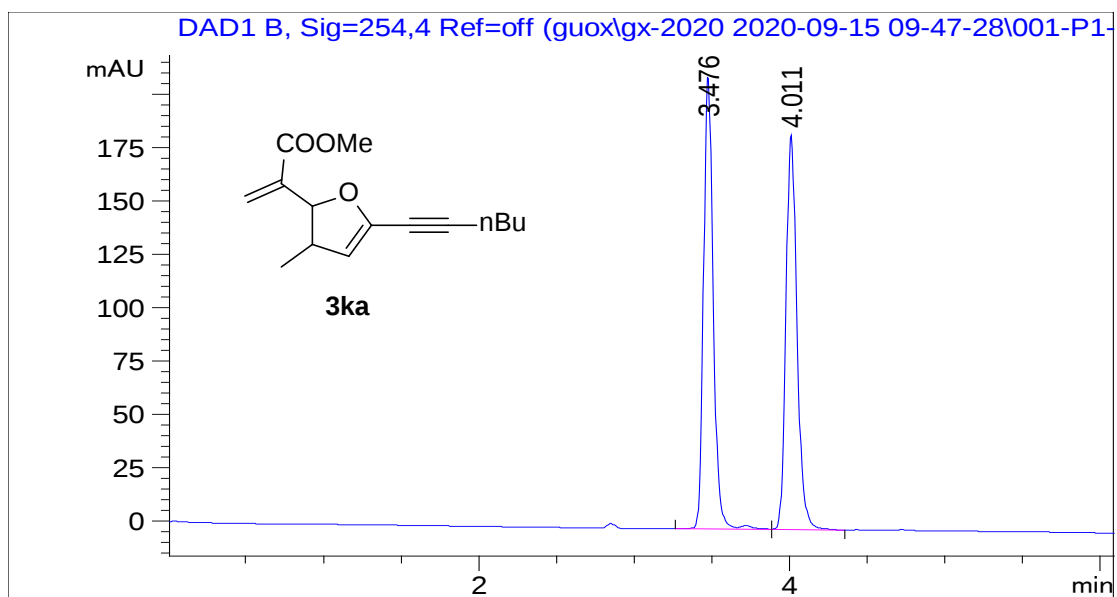


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.82	BV	2961.4	408.7	0.1085	51.101	0.948
2	5.15	VBA	2833.7	377.3	0.1136	48.899	0.835

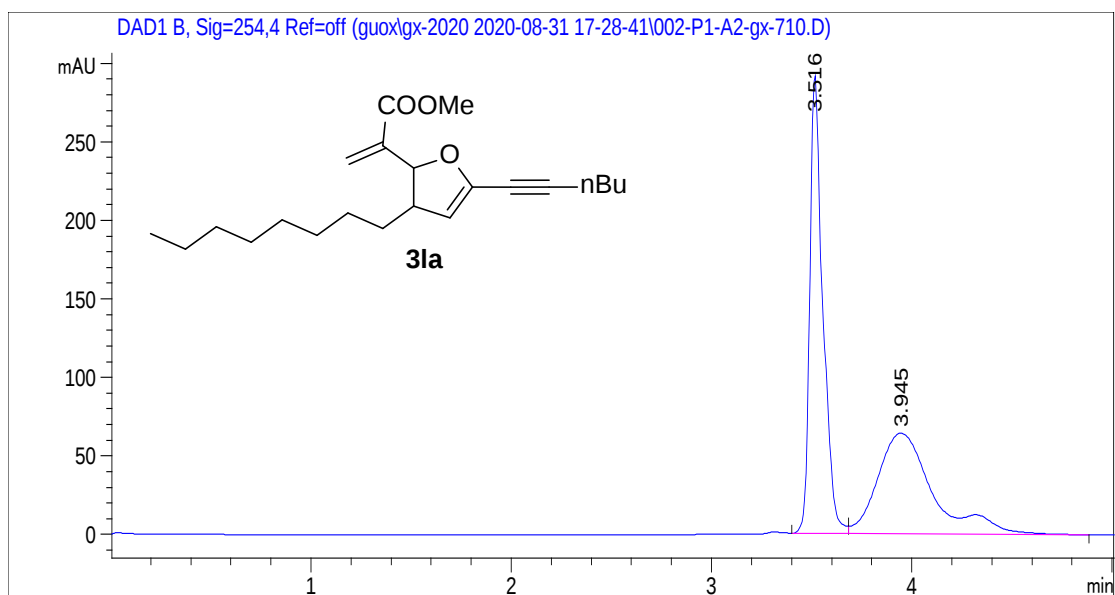


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.829	BV	142.3	20.4	0.1072	5.942	0.869
2	5.148	VVR	2252.1	299.5	0.1154	94.058	0.816

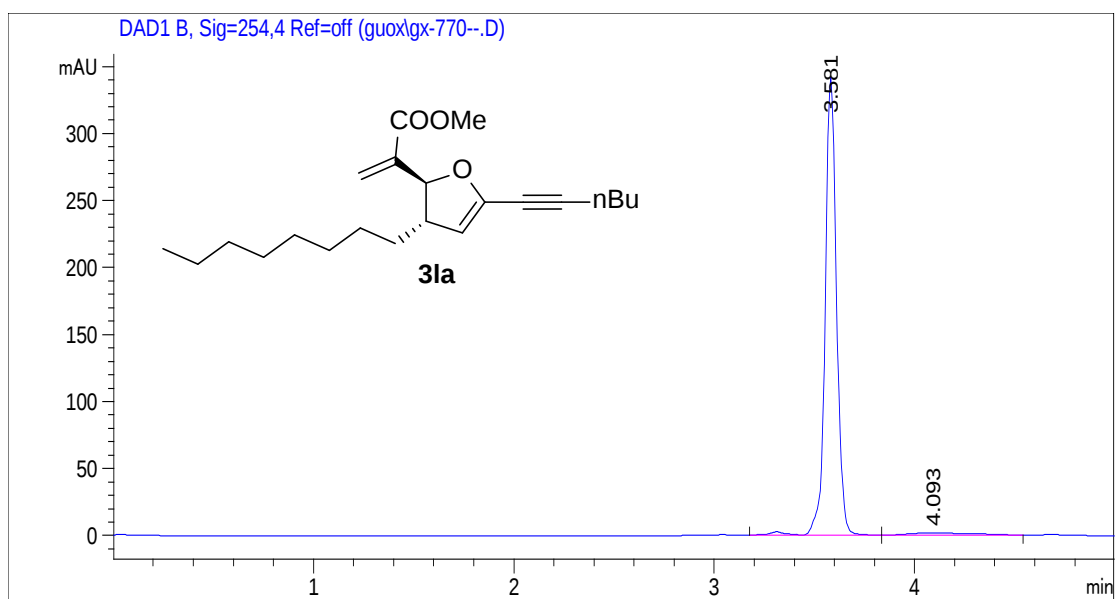
3ka: OD-H, 90/10, 1.0 ml/min, 254 nm



3la: OD-H, 99/1, 1.0 ml/min, 254 nm

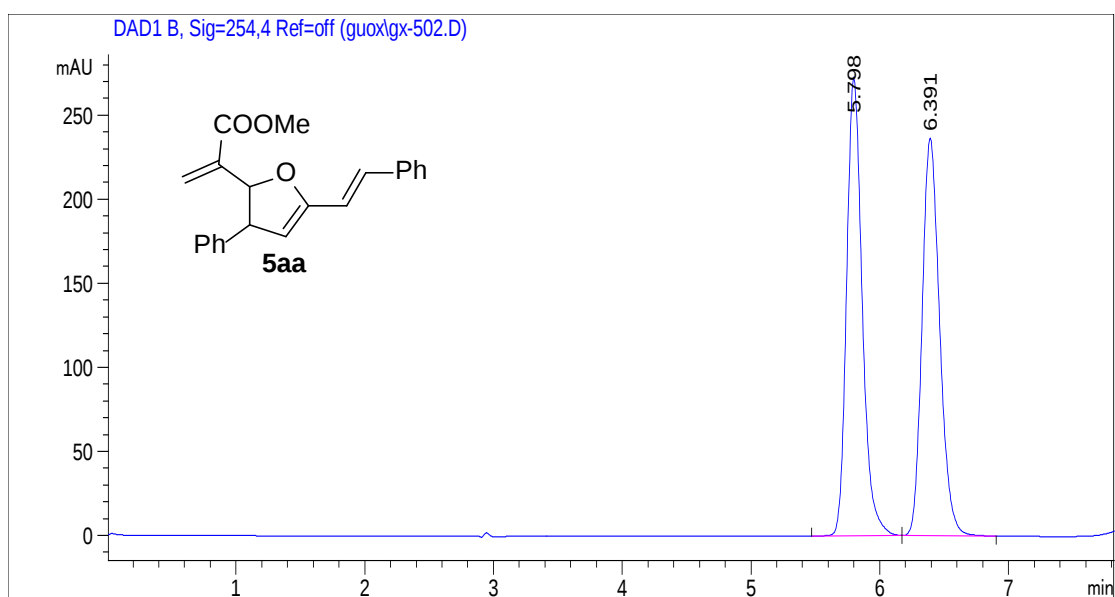


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	3.516	BV	1322.7	292.4	0.0648	51.785	0.576
2	3.945	VV R	1231.5	64.2	0.2701	48.215	0.803

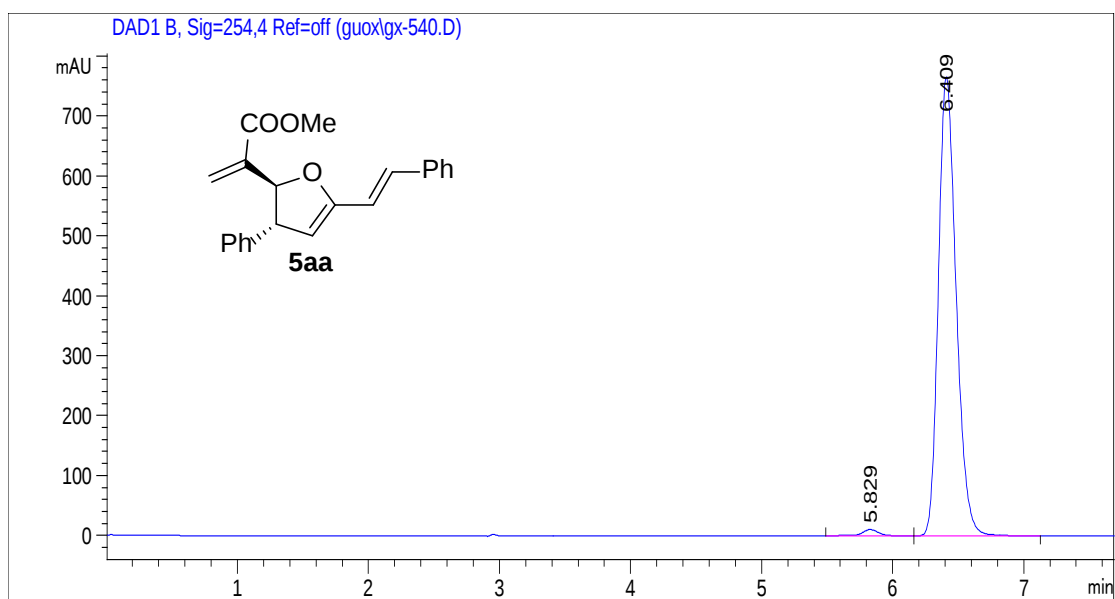


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	3.581	VB R	1346.6	342	0.0595	97.351	0.941
2	4.093	BB	36.6	1.7	0.3042	2.649	0.57

5aa: OD-H, 95/5, 1.0 ml/min, 254 nm

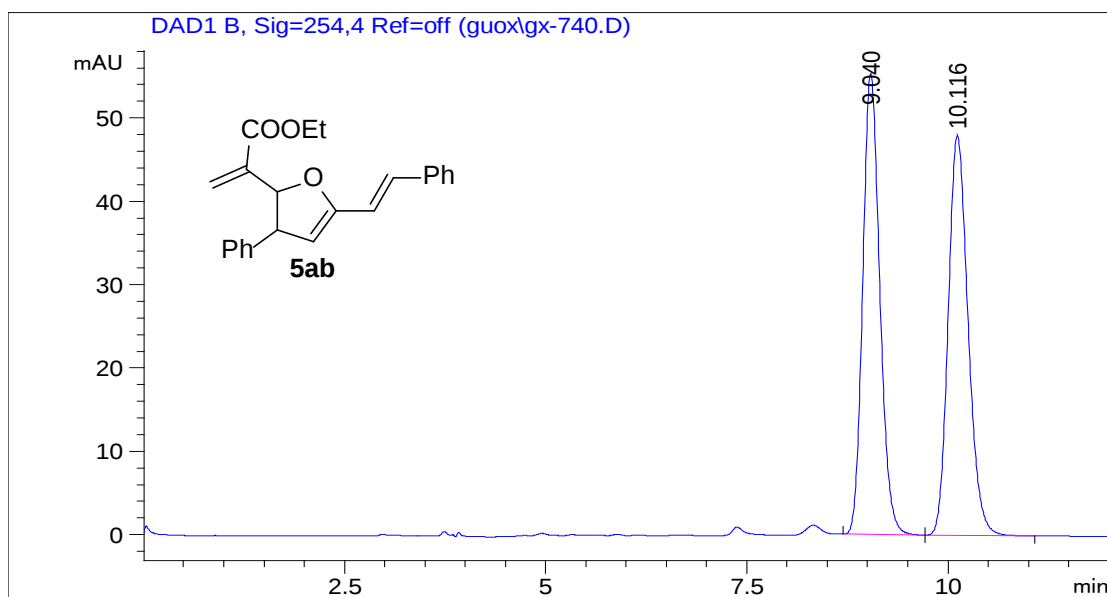


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	5.798	BB	2288.8	272.8	0.1279	50.496	0.783
2	6.391	BB	2243.9	236.7	0.1466	49.504	0.789

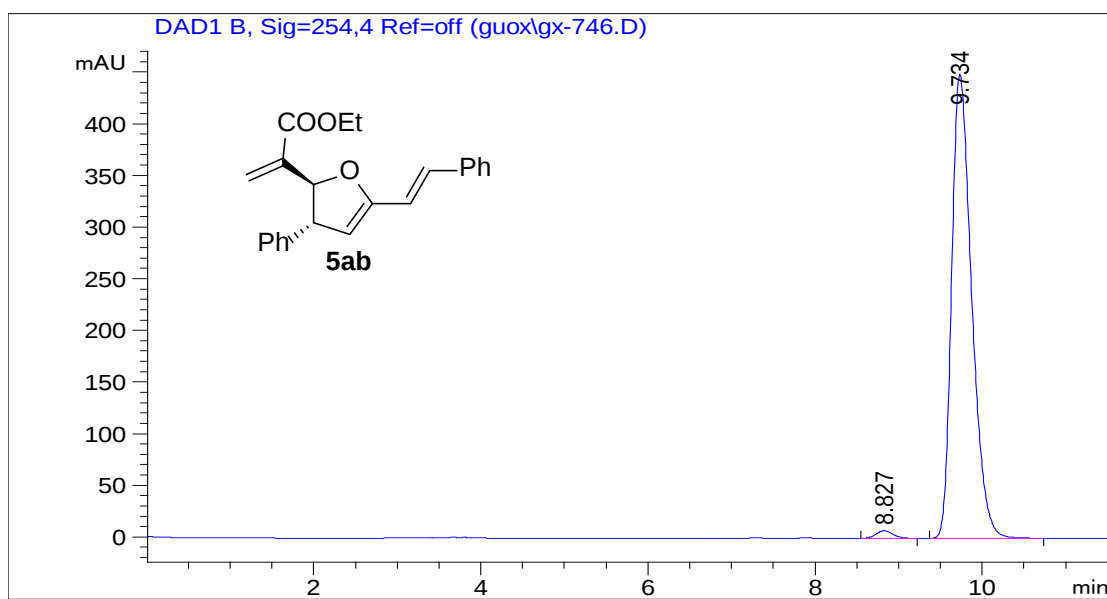


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	5.829	VB R	99.3	10.6	0.131	1.354	1.313
2	6.409	BB	7231.5	766.6	0.1441	98.646	0.75

5ab: OD-H, 99/1, 1.0 ml/min, 254 nm

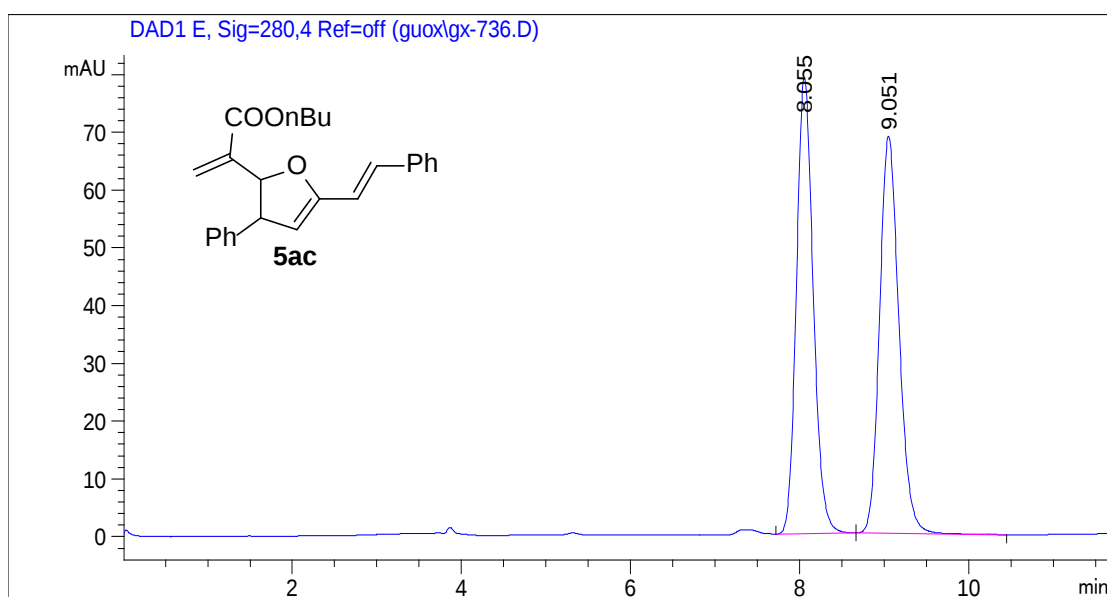


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	9.04	BB	817.3	55.3	0.2284	49.884	0.824
2	10.116	BB	821.1	48	0.2636	50.116	0.8

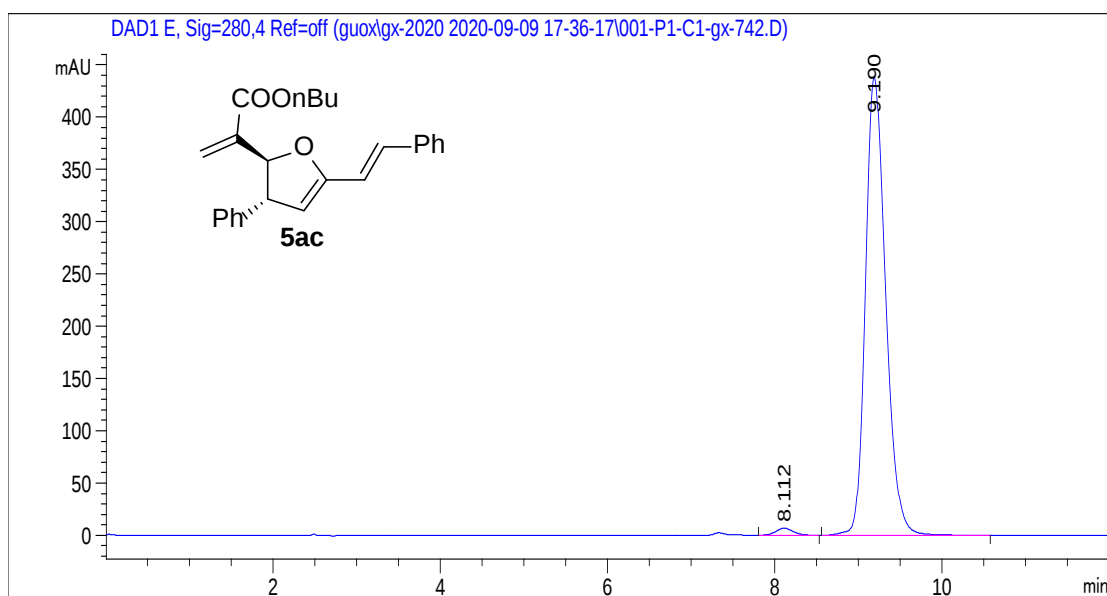


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	8.827	BB	100.2	7.3	0.2148	1.325	0.86
2	9.734	BB	7462.9	449.2	0.2538	98.675	0.651

5ac: OD-H, 99/1, 1.0 ml/min, 280 nm

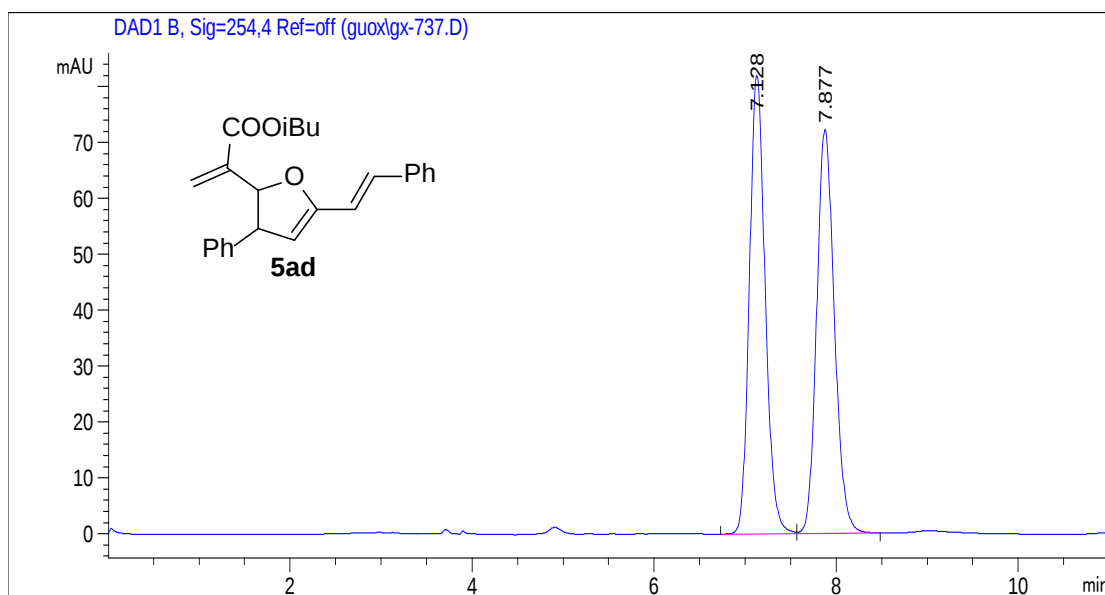


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	8.055	BB	1089.4	78.9	0.2131	49.888	0.832
2	9.051	BB	1094.2	68.8	0.2456	50.112	0.807

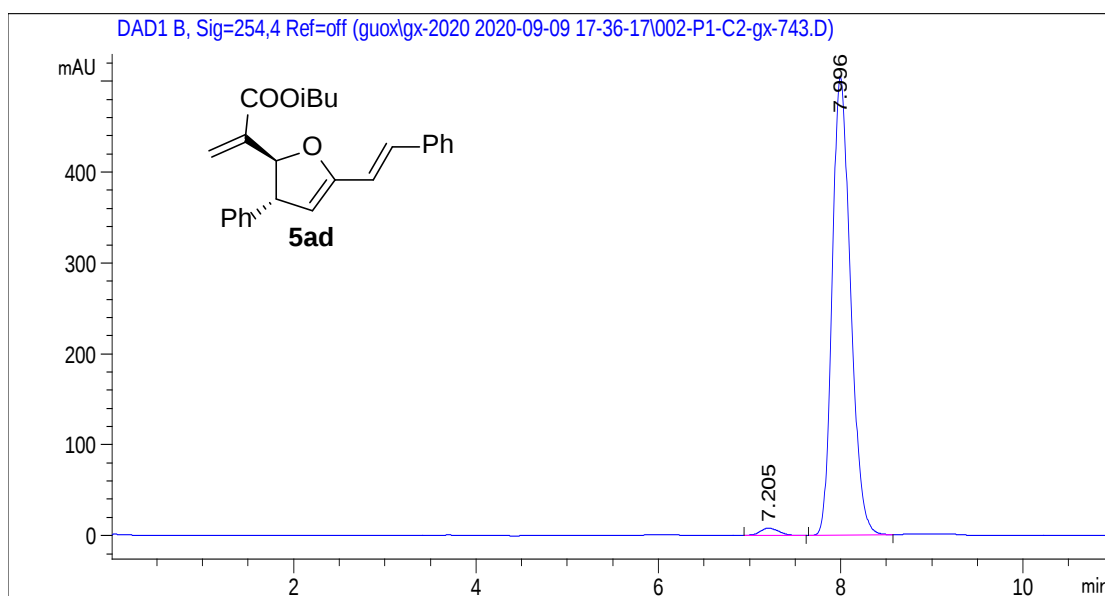


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	8.112	BB	95.6	6.7	0.2214	1.283	0.875
2	9.19	BB	7357.5	438.3	0.2598	98.717	0.747

5ad: OD-H, 99/1, 1.0 ml/min, 254 nm

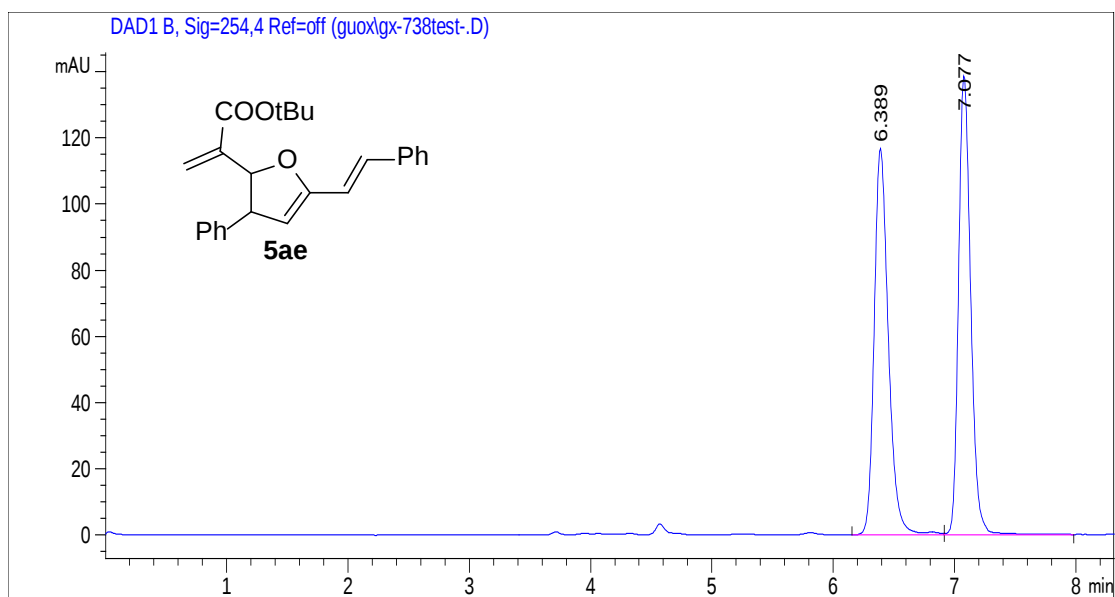


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.128	BV	989.7	82	0.1849	50.324	0.838
2	7.877	VB	976.9	72.2	0.2078	49.676	0.828

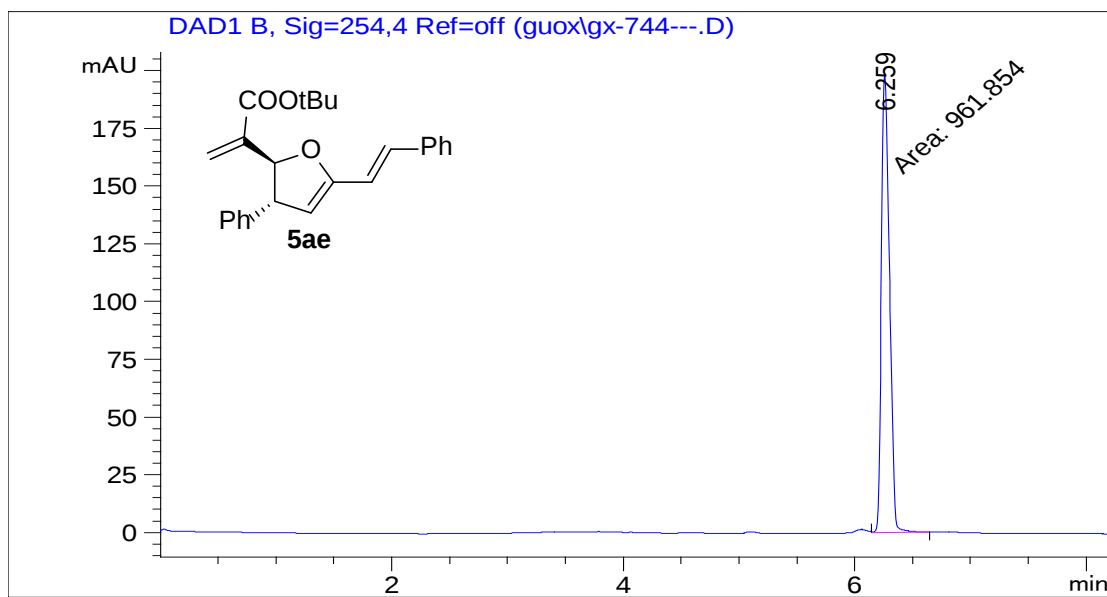


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.205	BB	109.2	7.9	0.2275	1.527	0.715
2	7.996	BB	7044.2	504.4	0.2169	98.473	0.748

5ae: IB, 99.5/0.5, 1.0 ml/min, 254 nm

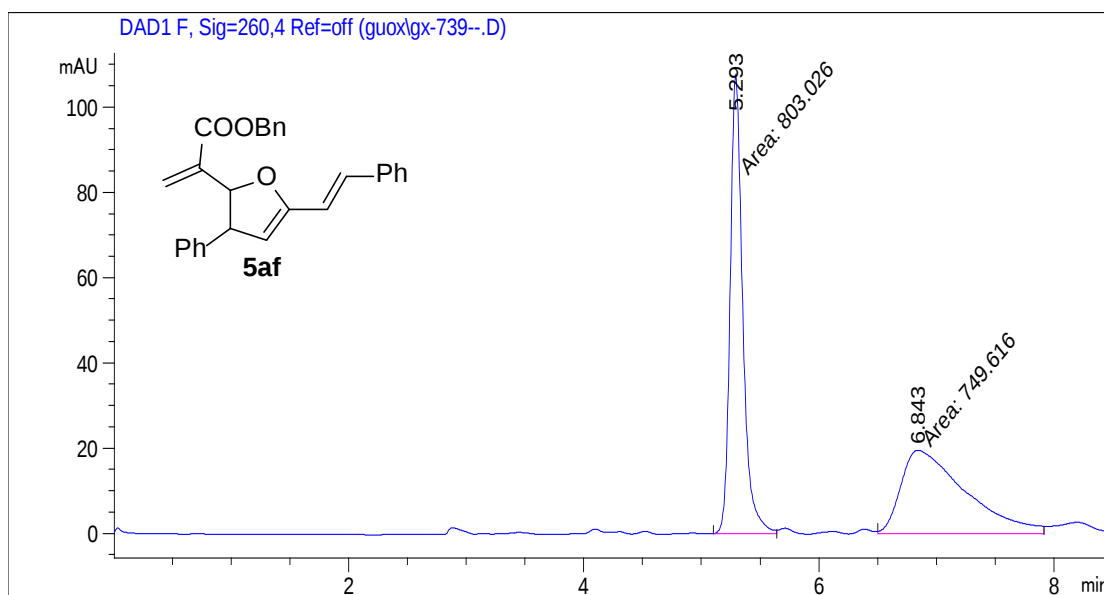


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.389	BVR	946.1	116.8	0.1245	49.565	0.722
2	7.077	VB	962.7	138.8	0.1069	50.435	0.749

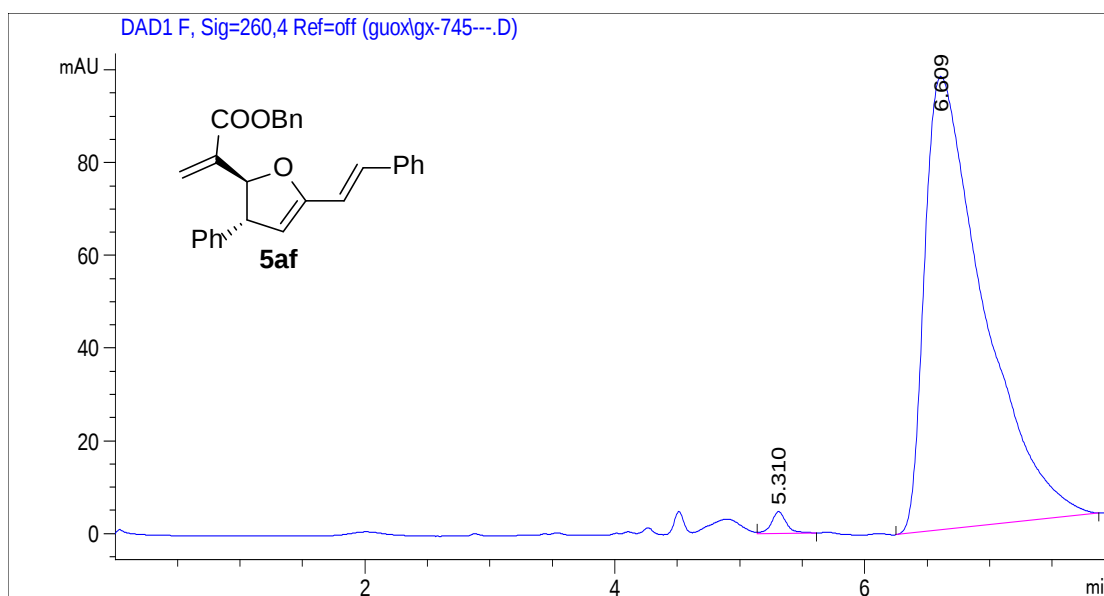


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.259	FM	961.9	198.8	0.0806	100.000	0.665

5af: IB, 80/20, 1.0 ml/min, 260 nm

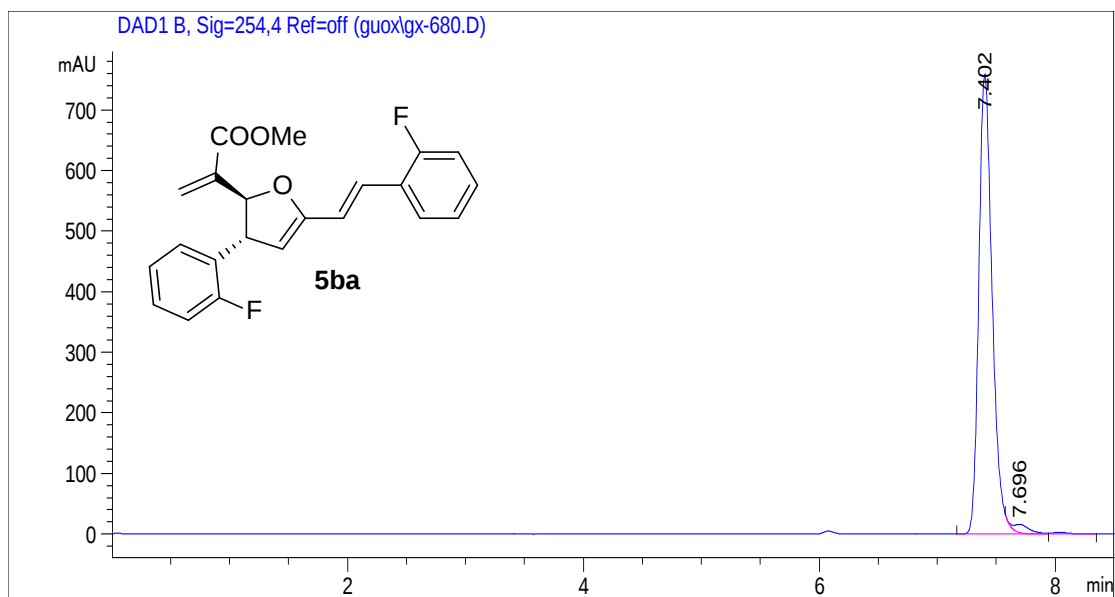
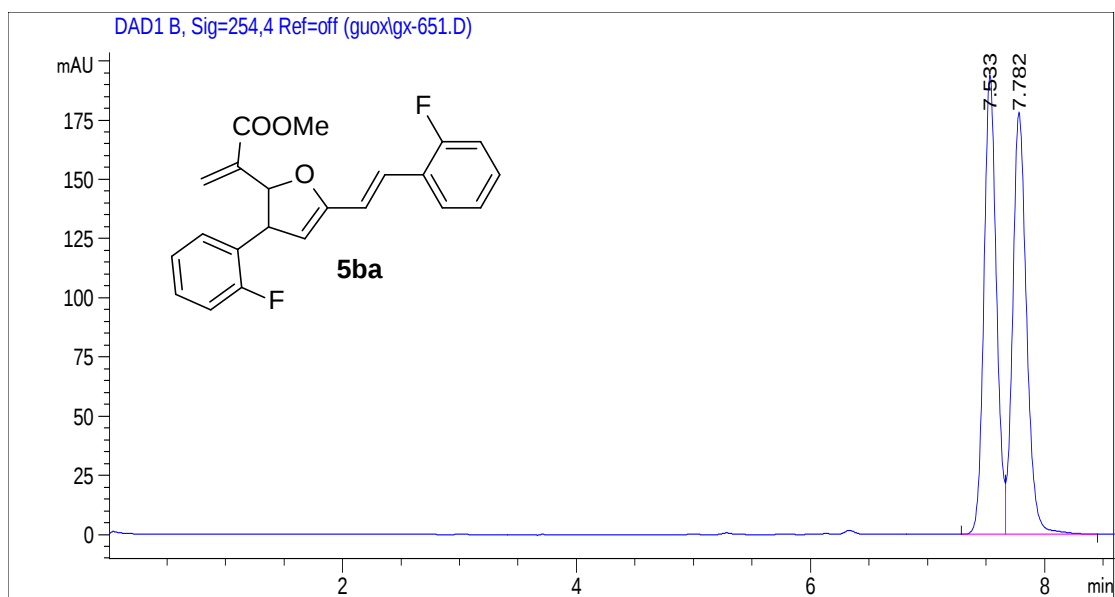


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	5.293	MM	803	107.5	0.1244	51.720	0.742
2	6.843	MM	749.6	19.6	0.6384	48.280	0.354

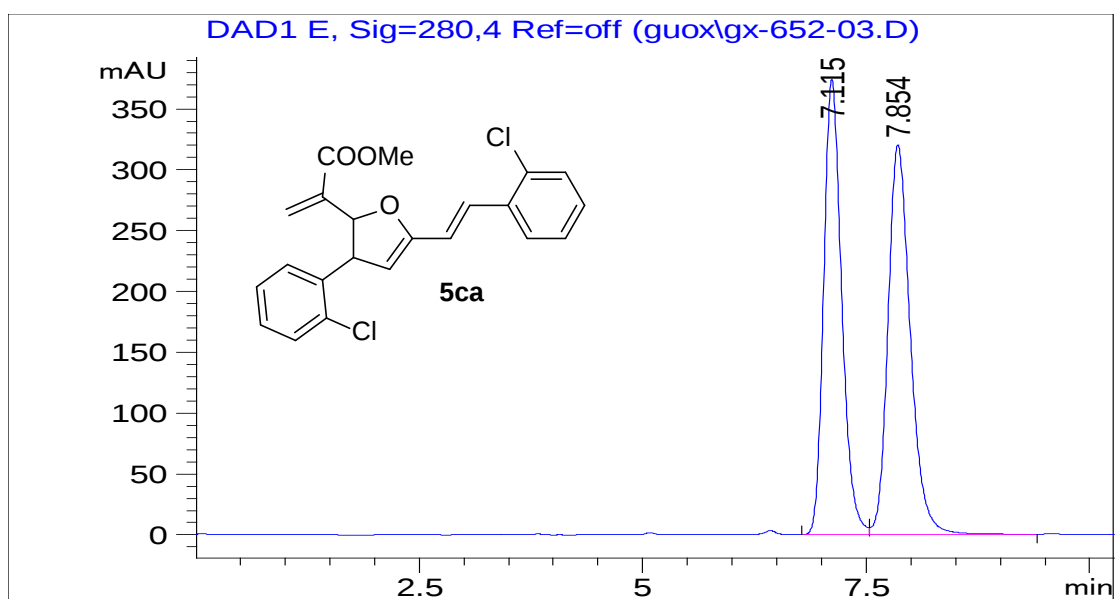


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	5.31	VB	38.6	4.7	0.1244	1.193	0.877
2	6.609	BB	3196.8	97.8	0.4854	98.807	0.348

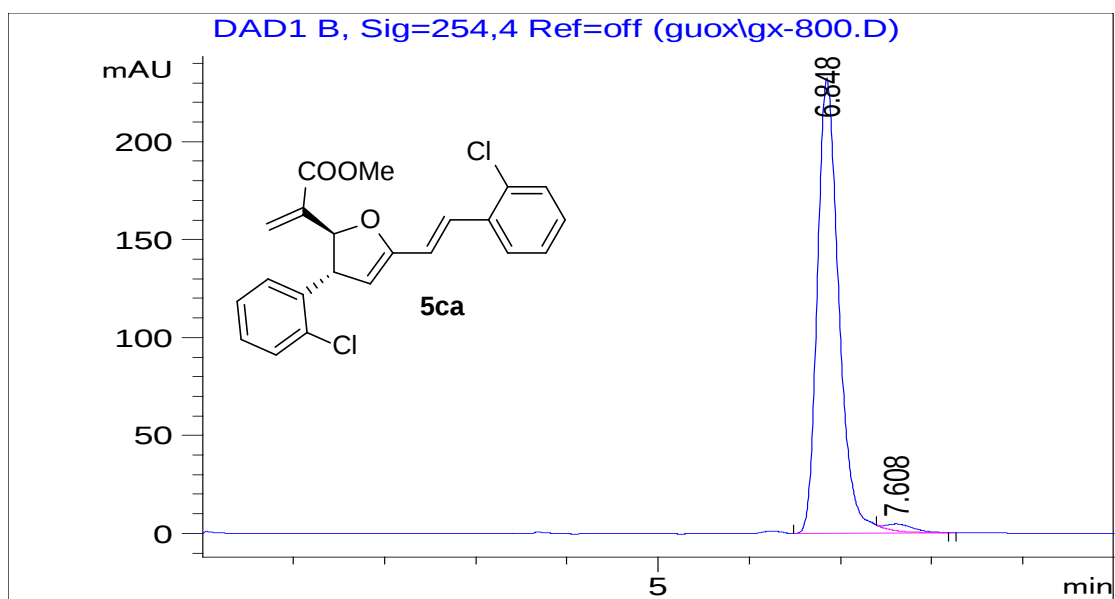
5ba: IF-3, 98.5/1.5, 1.0 ml/min, 254 nm



5ca: AS-3, 99/1, 1.0 ml/min, 254 nm

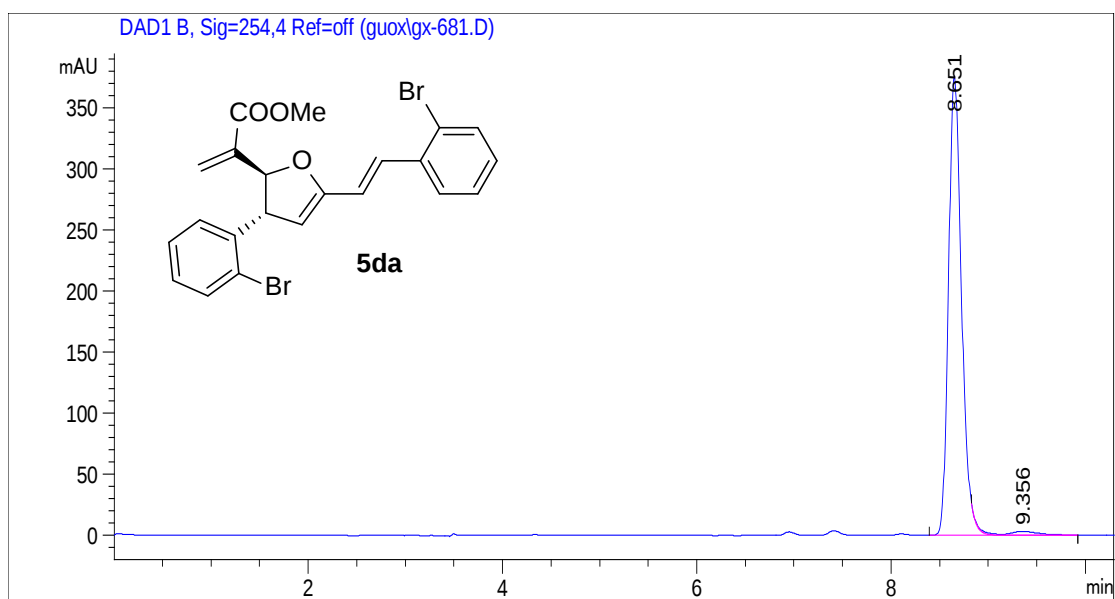
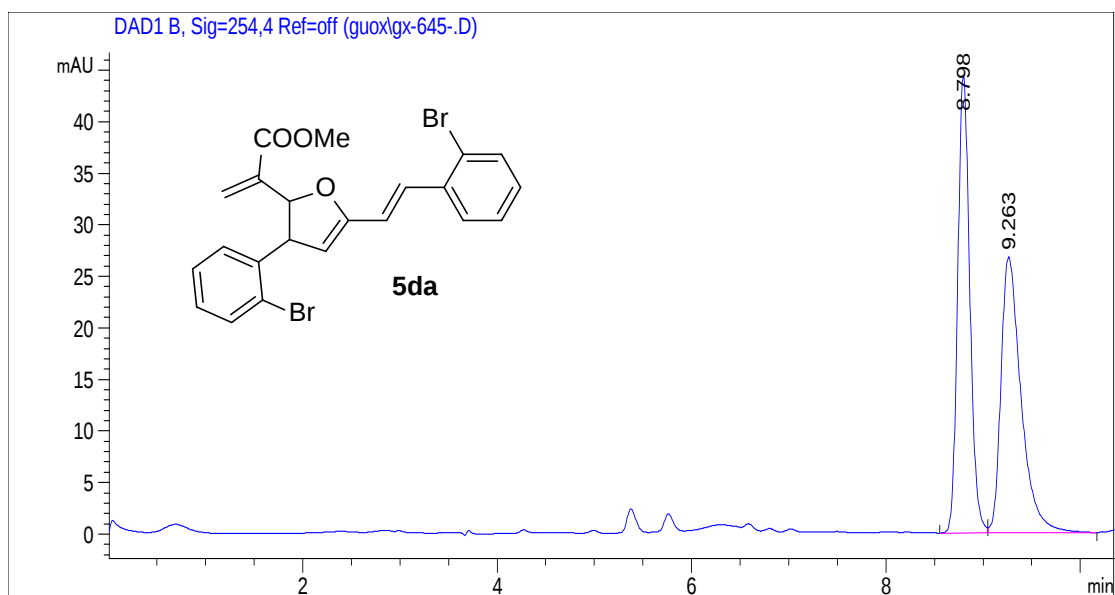


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	7.115	BV	5242.3	373.8	0.2156	48.494	0.768
2	7.854	VB	5567.8	320.2	0.2668	51.506	0.738

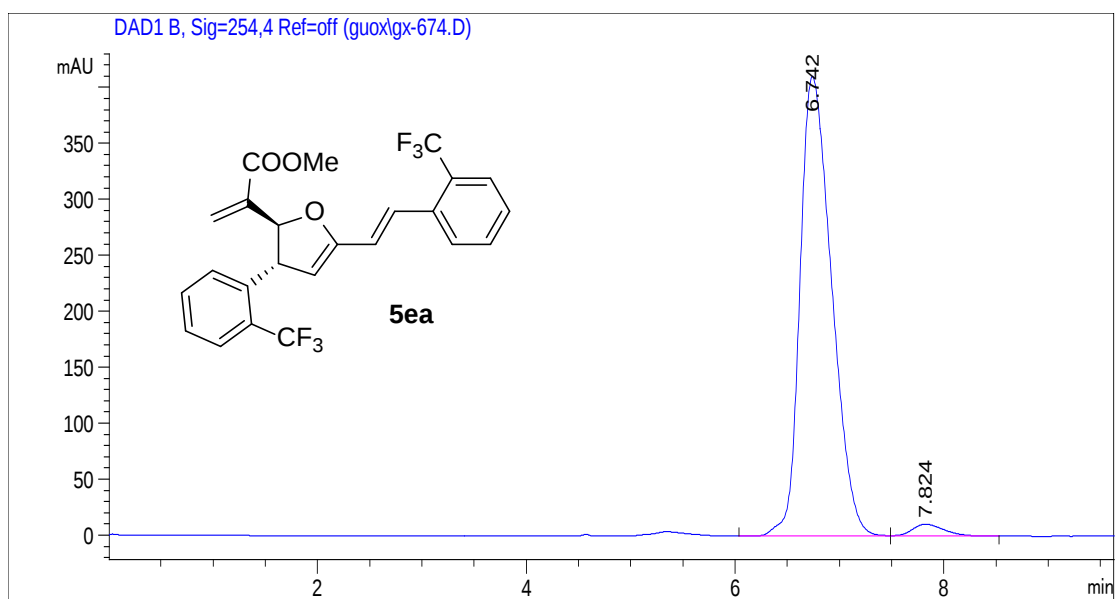
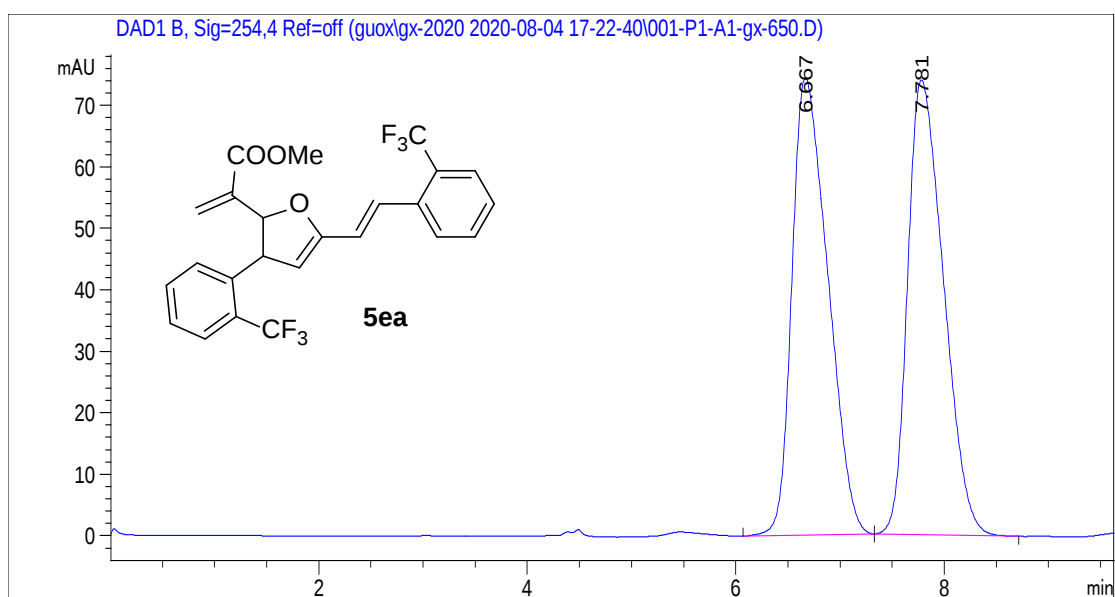


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.848	BVR	3832.9	232	0.2507	98.173	0.7
2	7.608	VBE	71.3	3.4	0.3133	1.827	0.454

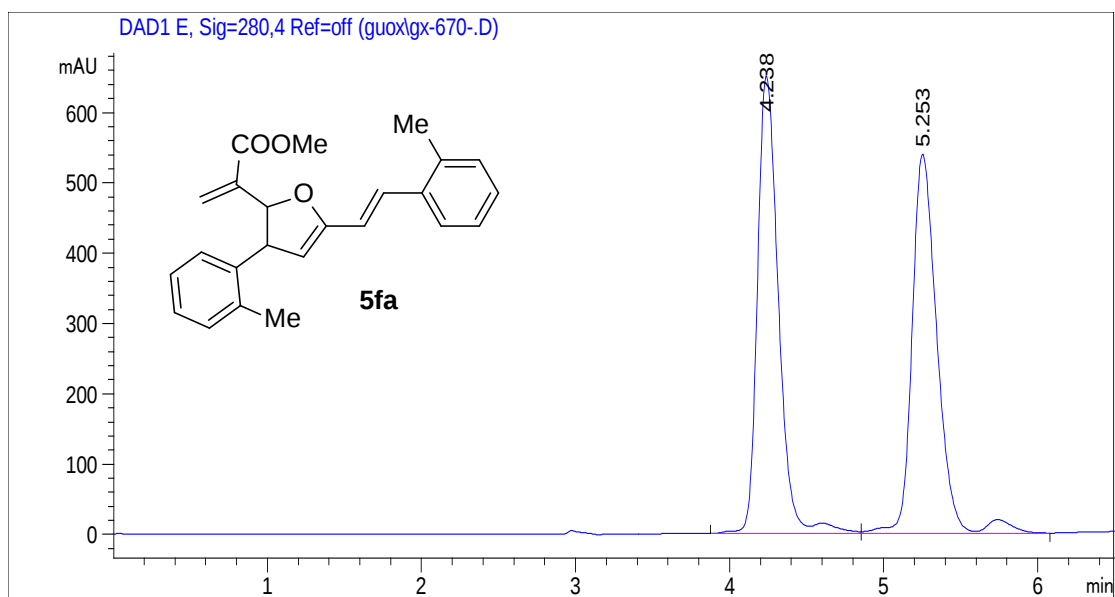
5da: IF-3, 98.5/1.5, 1.0 ml/min, 254 nm



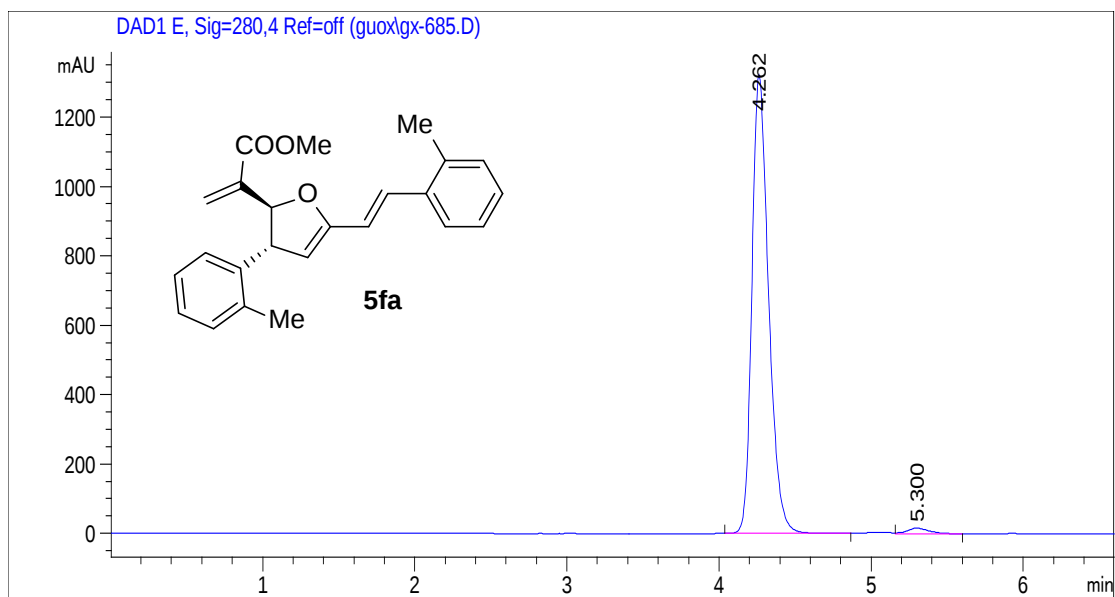
5ea: AD-H, 99/1, 1.0 ml/min, 254 nm



5fa: AD-H, 95/5, 1.0 ml/min, 254 nm

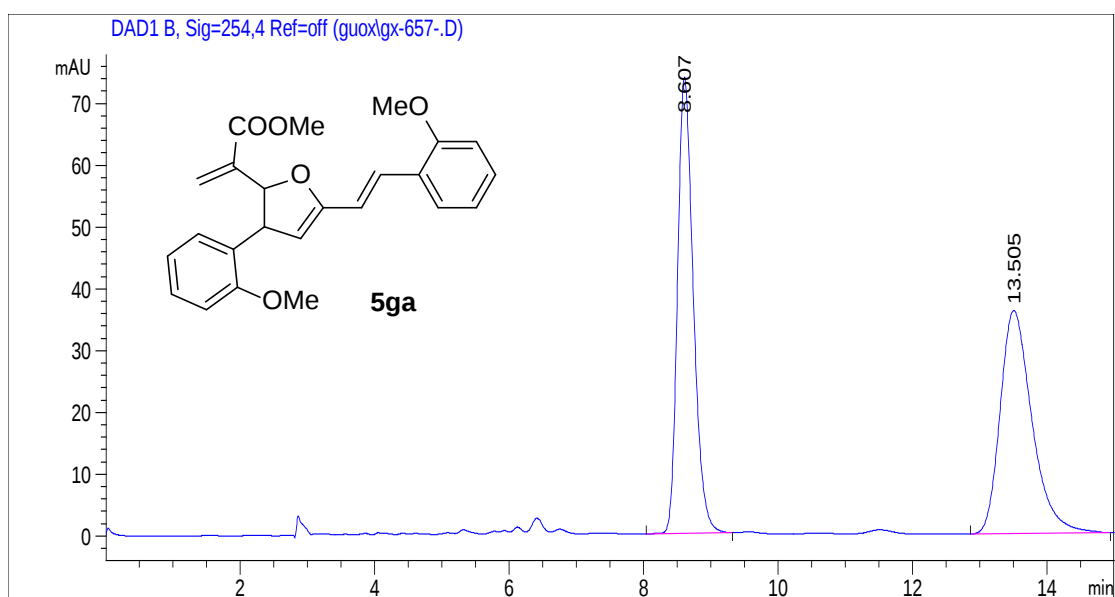


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.238	BVR	6177.2	651.4	0.1415	50.069	0.721
2	5.253	VVR	6160.1	539.4	0.1707	49.931	0.73

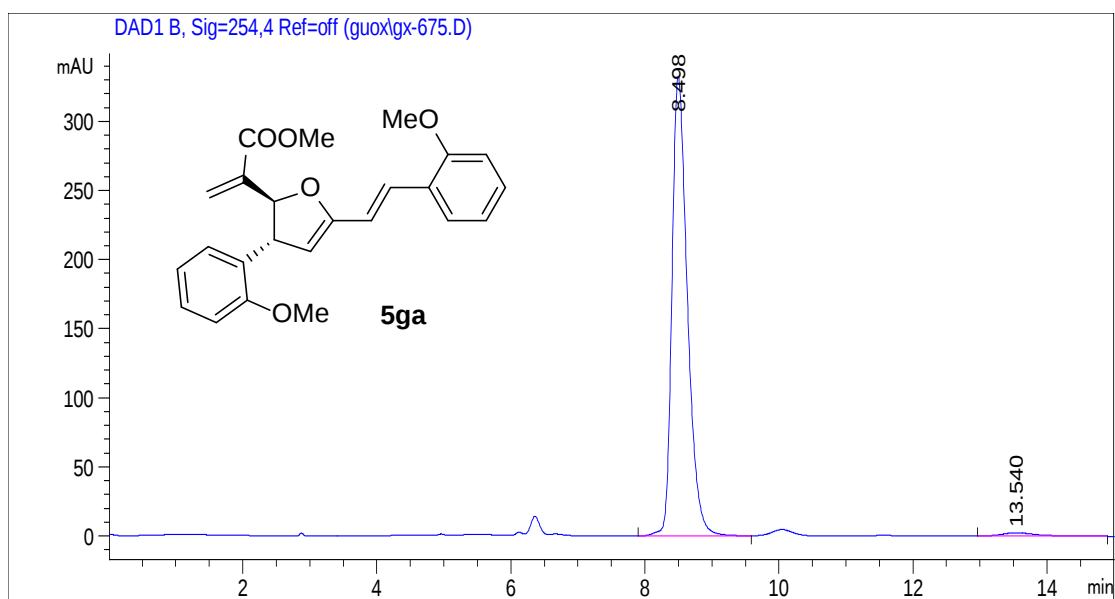


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.262	BVR	10070.5	1322.2	0.1147	98.472	0.687
2	5.3	VB	156.3	15.8	0.1492	1.528	0.755

5ga: OD-H, 90/10, 1.0 ml/min, 254 nm

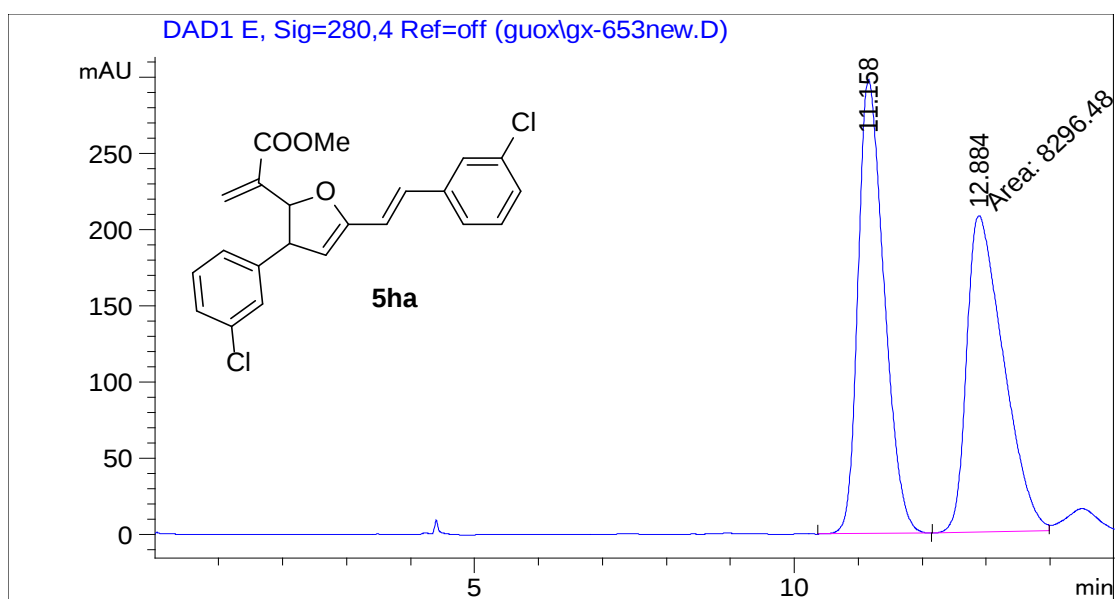


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	8.607	BB	1202.7	73.8	0.2501	50.288	0.729
2	13.505	BB	1188.9	36.1	0.5041	49.712	0.693

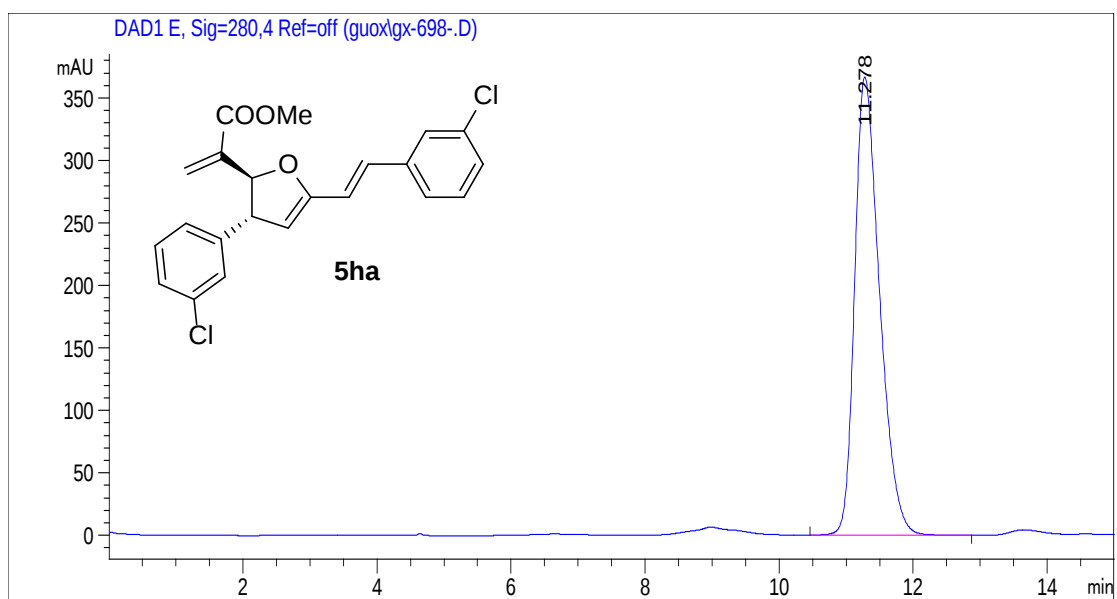


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	8.498	BB	5314.4	332.3	0.2446	98.513	0.645
2	13.54	BBA	80.2	2.3	0.4958	1.487	0.621

5ha: AD-H, 99/1, 1.0 ml/min, 280 nm

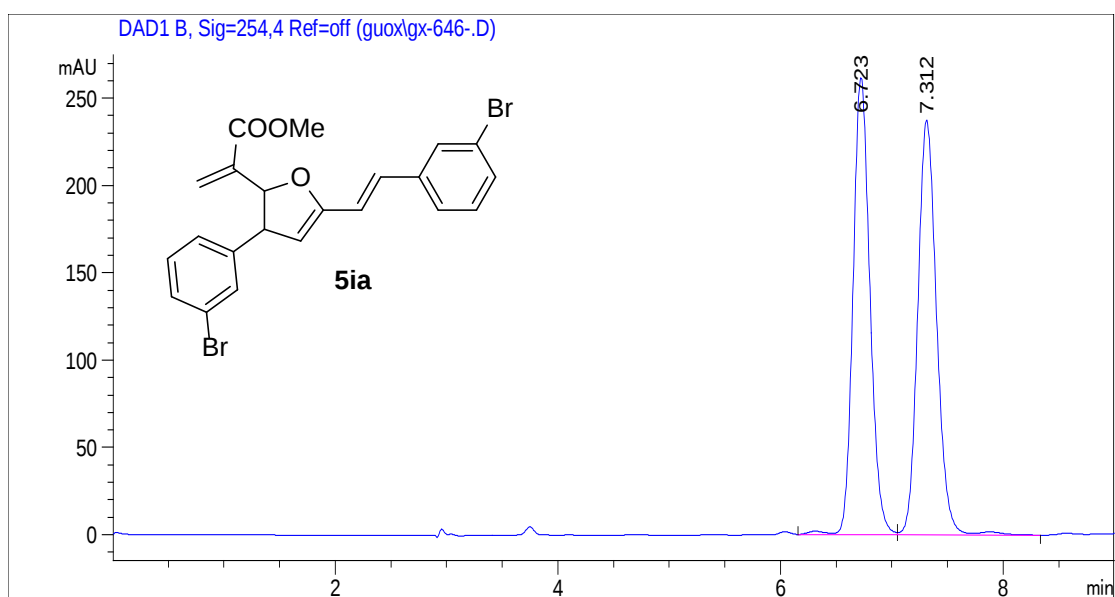


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	11.158	BB	8454.6	297.8	0.4372	50.472	0.636
2	12.884	MF	8296.5	207.7	0.6658	49.528	0.484

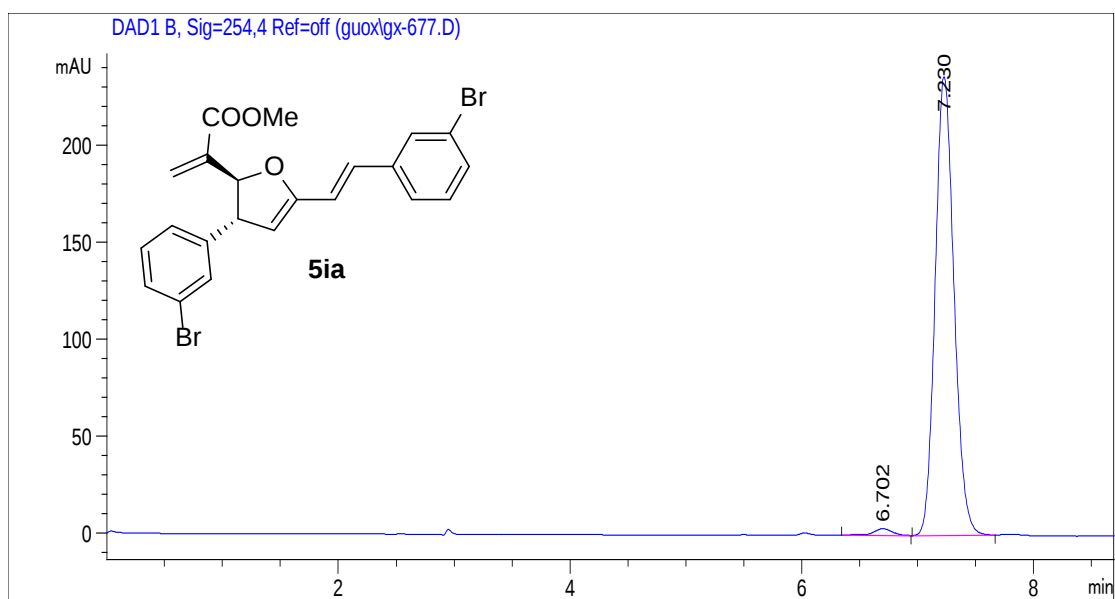


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	11.278	BB	9459.6	366.7	0.3929	100.000	0.64

5ia: OD-H, 95/5, 1.0 ml/min, 254 nm

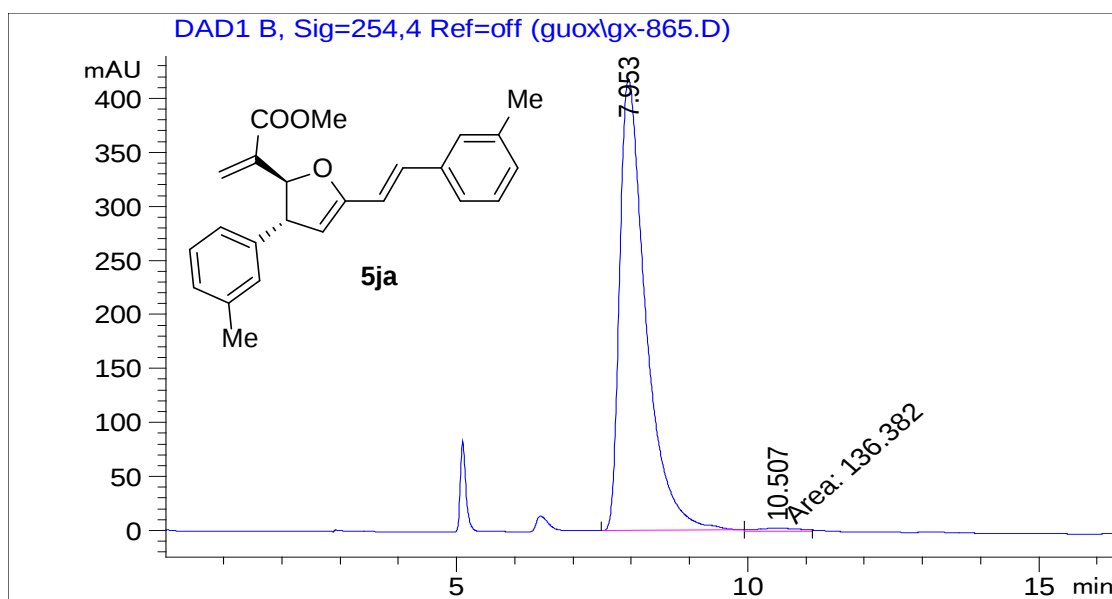
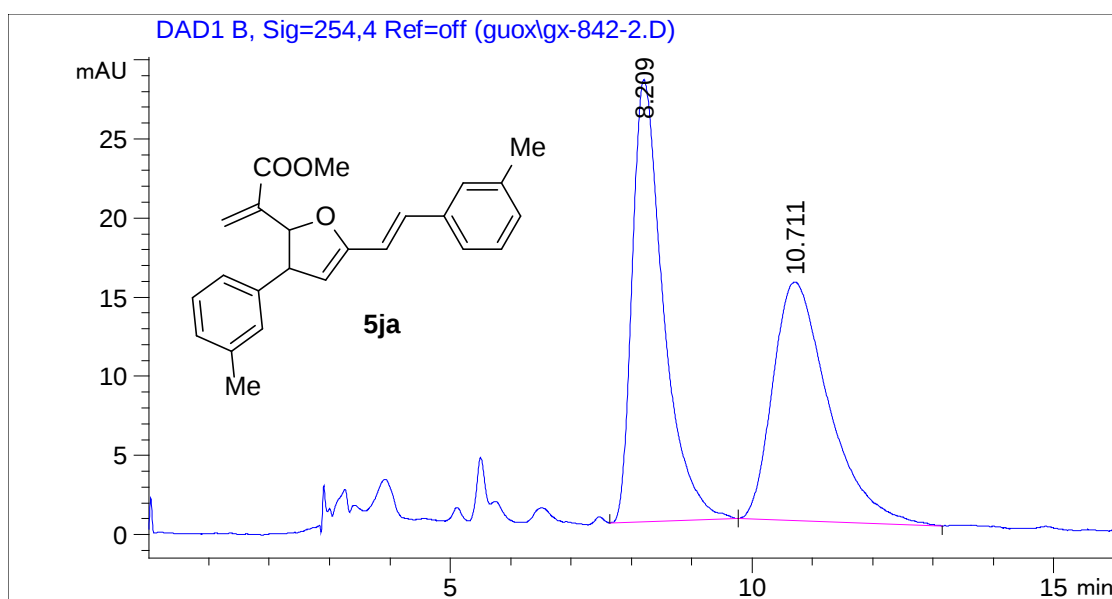


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.723	VVR	2762.3	261.7	0.1623	49.693	0.86
2	7.312	VVR	2796.4	237.5	0.18	50.307	0.842

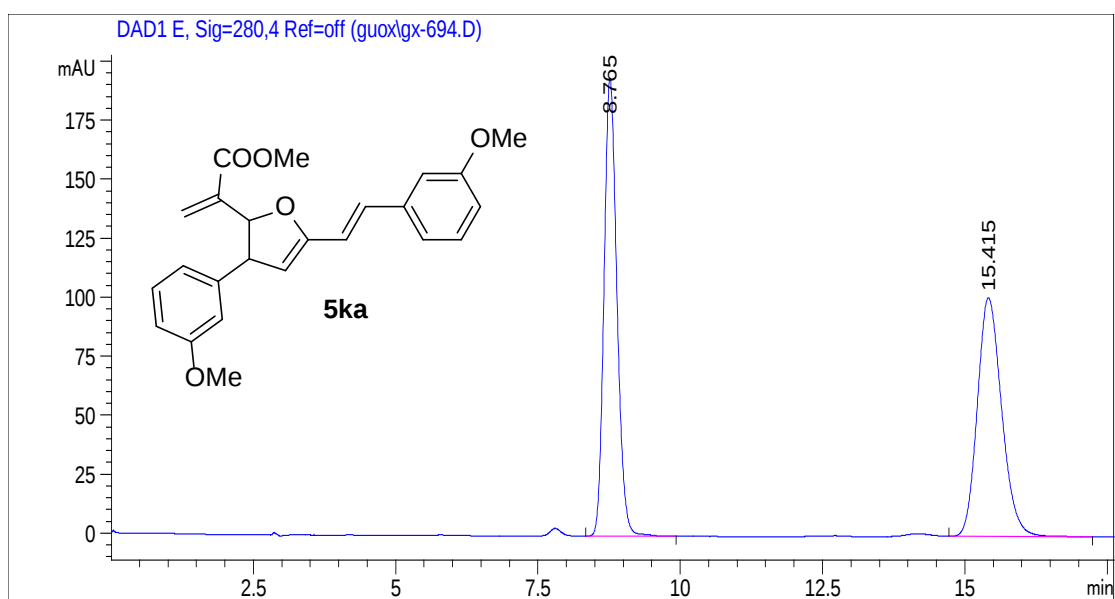


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.702	BB	41.1	3.5	0.1773	1.515	1.147
2	7.23	BB	2670.3	236.8	0.1756	98.485	0.844

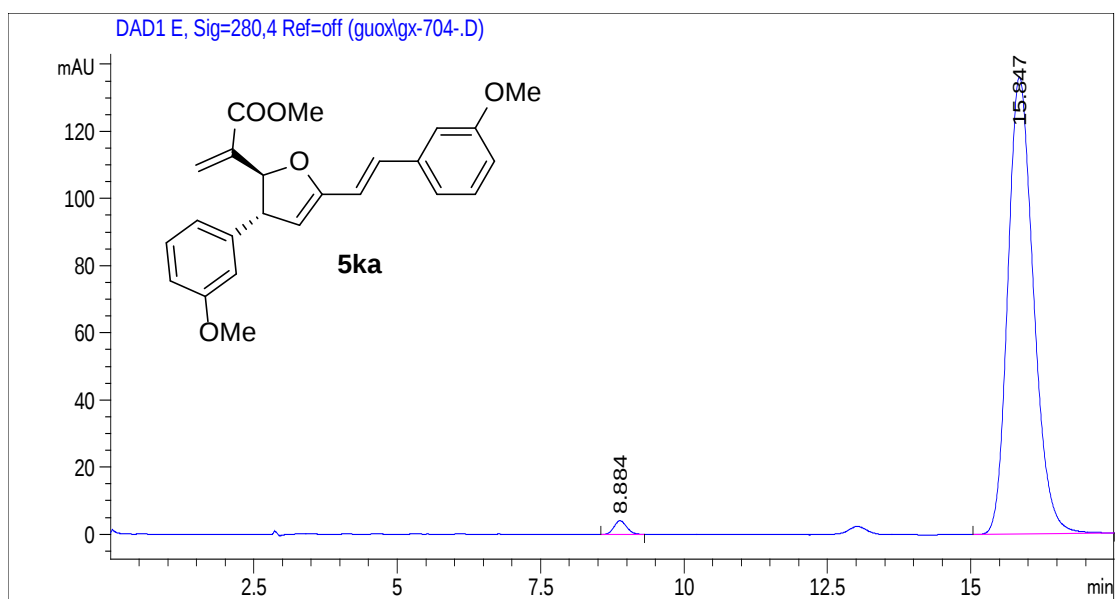
5ja: IJ, 90/10, 1.0 ml/min, 254 nm



5ka: OD-H, 90/10, 1.0 ml/min, 280 nm

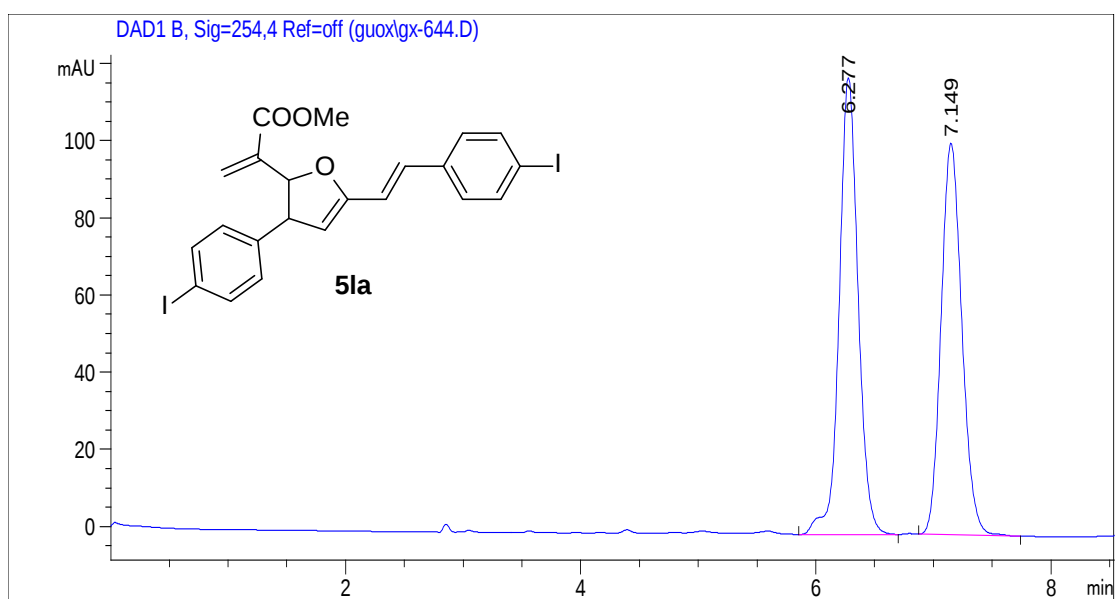


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	8.765	BB	3040.1	194.1	0.2408	50.231	0.803
2	15.415	BB	3012.1	101.2	0.4614	49.769	0.797

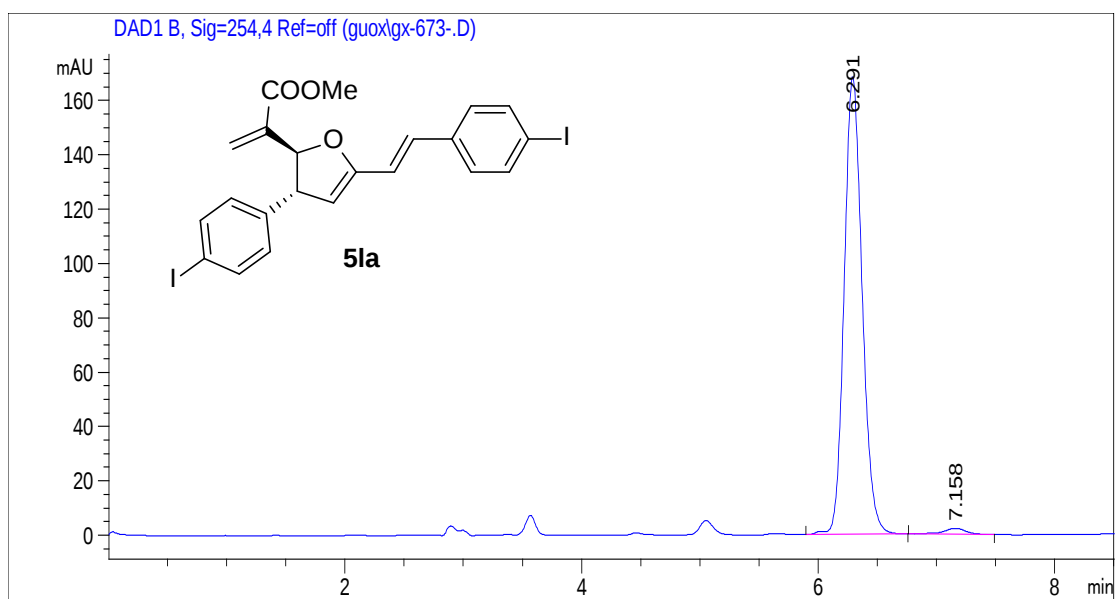


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	8.884	BB	62.8	4.1	0.2385	1.464	0.862
2	15.847	BBA	4227	136.2	0.4782	98.536	0.77

5la: OD-H, 90/10, 1.0 ml/min, 254 nm

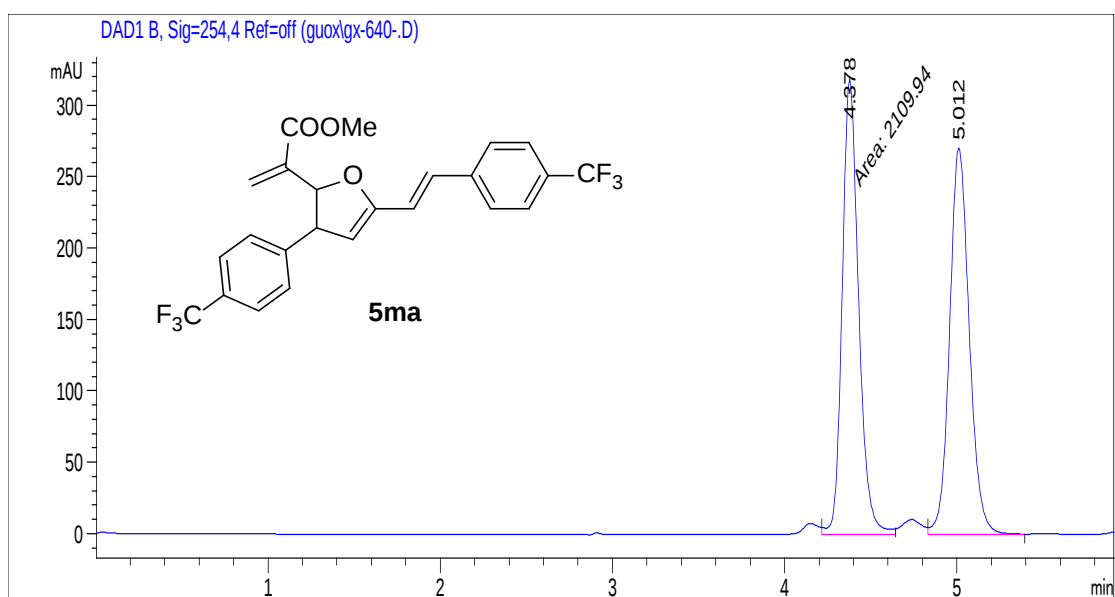


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.277	BB	1322.1	118.3	0.1703	51.504	0.925
2	7.149	BB	1244.9	101.5	0.1892	48.496	0.842

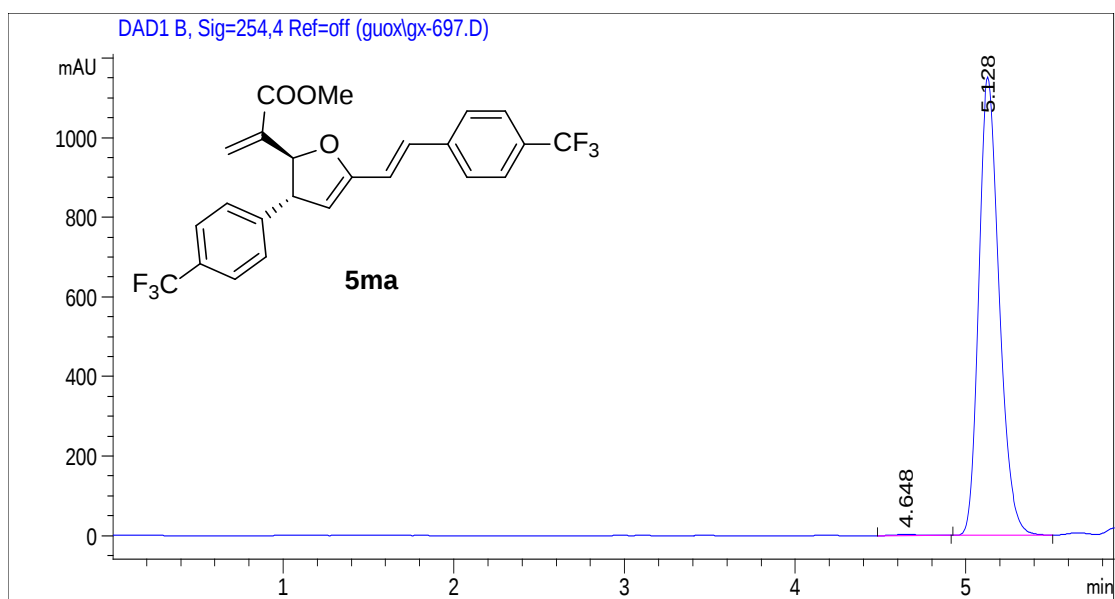


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	6.291	BB	1779.9	168.5	0.1633	98.281	0.846
2	7.158	BB	31.1	2.3	0.2045	1.719	1.141

5ma: OD-H, 97/3, 1.0 ml/min, 254 nm

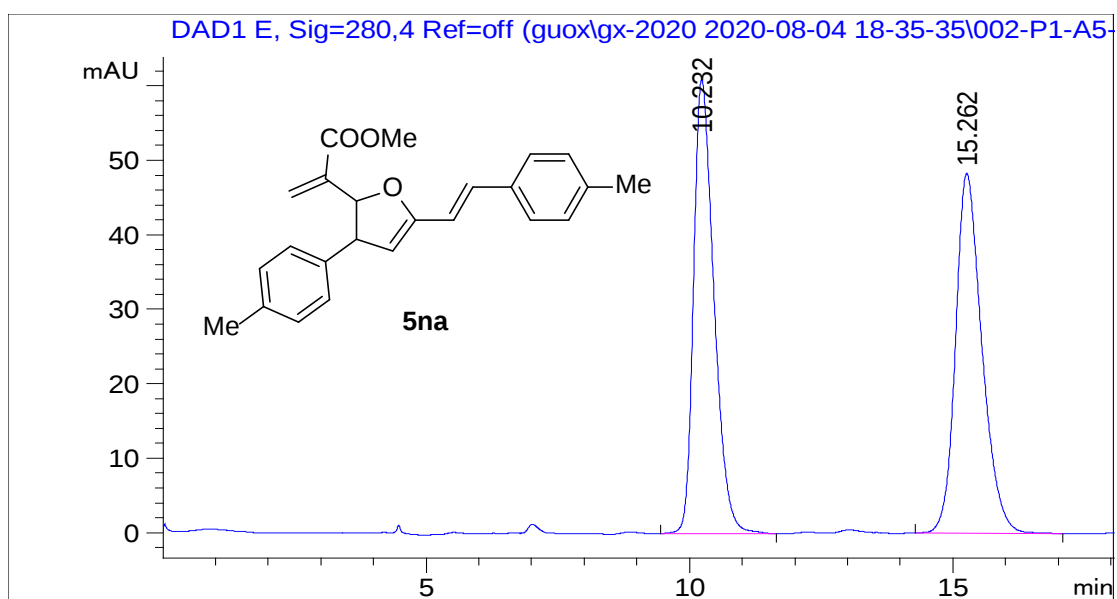


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.378	MF	2109.9	318.8	0.1103	49.620	0
2	5.012	VB	2142.3	270.8	0.1203	50.380	0.855

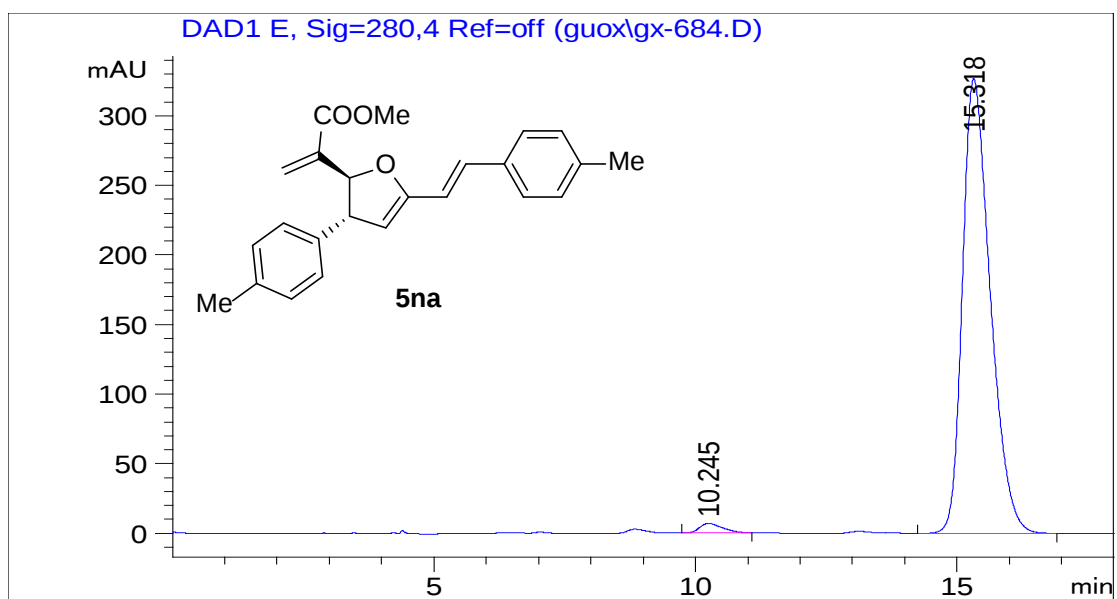


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.648	BB	27.6	3.6	0.1144	0.287	0.657
2	5.128	BB	9577.8	1151.8	0.127	99.713	0.751

5na: AD-H, 99/1, 1.0 ml/min, 280 nm

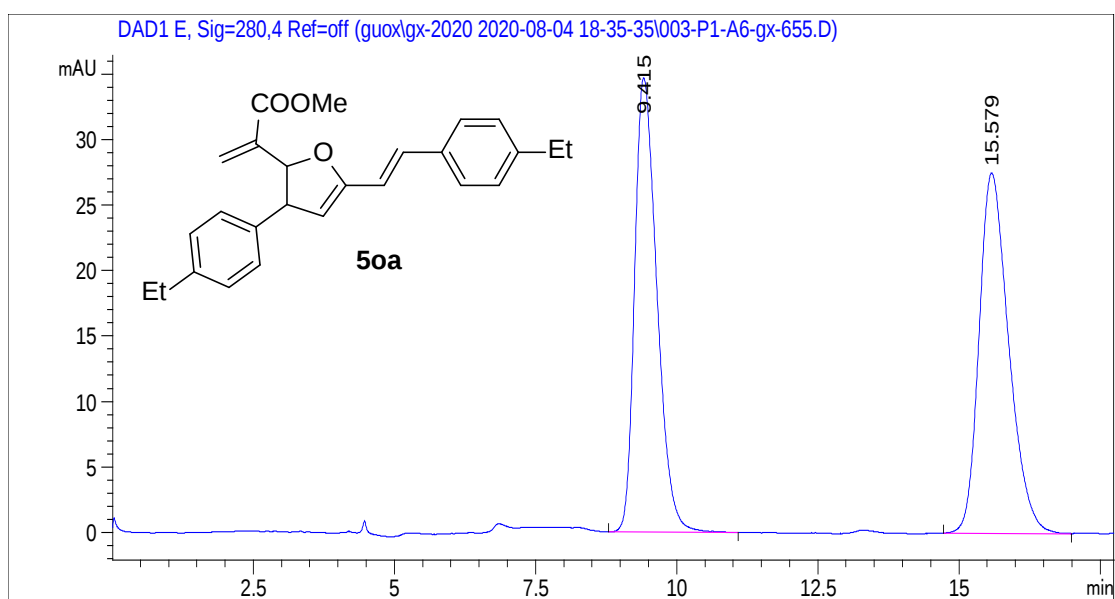


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	10.232	BB	1635.6	60.9	0.4132	49.240	0.628
2	15.262	BB	1686	48.3	0.5233	50.760	0.699

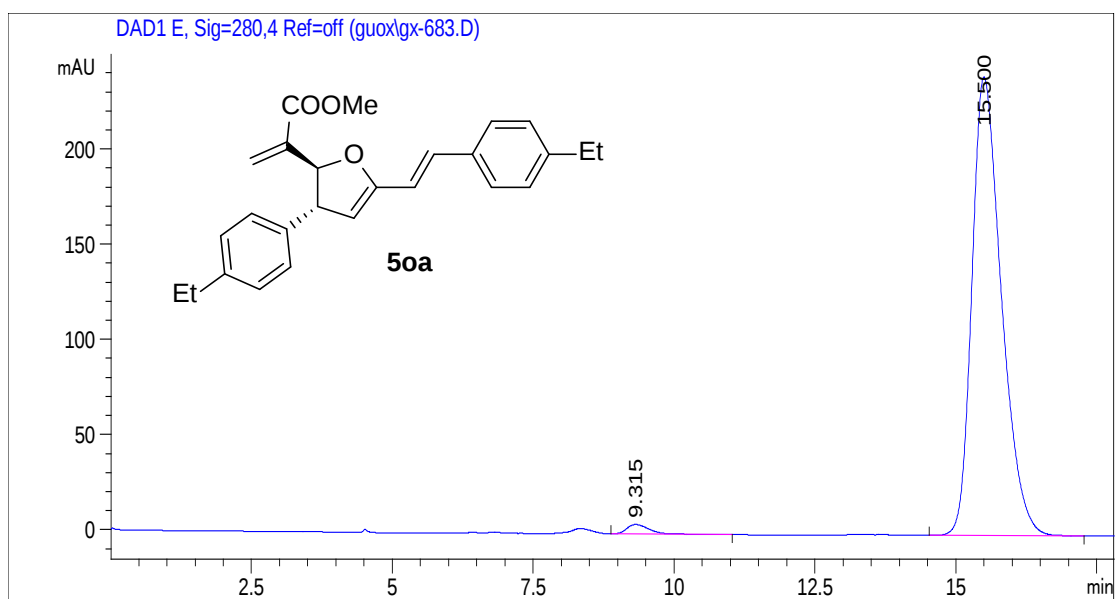


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	10.245	BB	212.4	6.9	0.4523	1.732	0.589
2	15.318	BB	12049.8	326.6	0.5624	98.268	0.643

50a: AD-H, 99/1, 1.0 ml/min, 280 nm

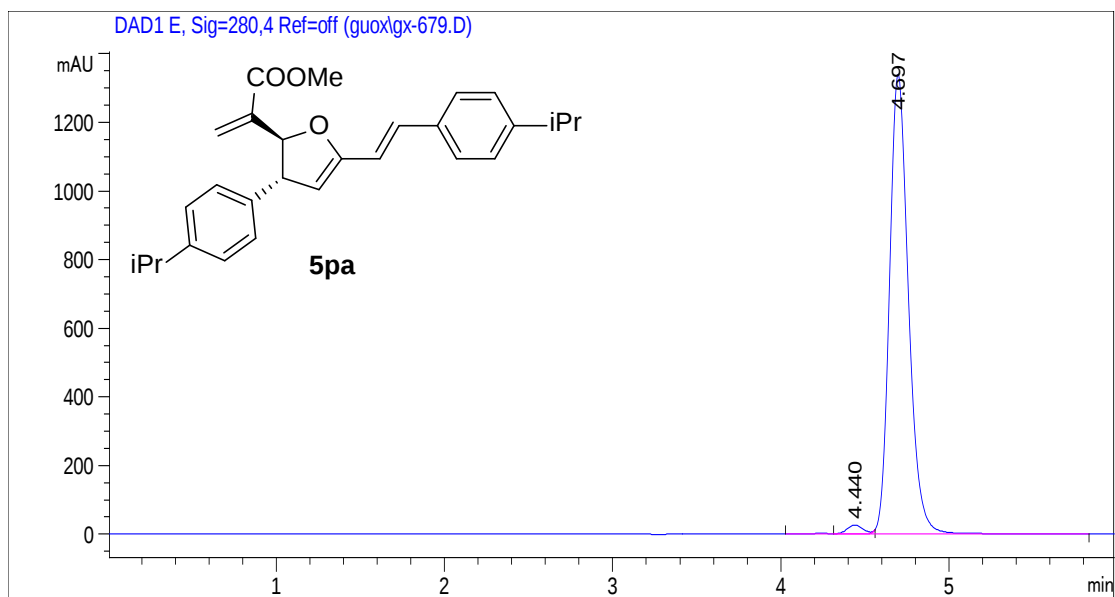
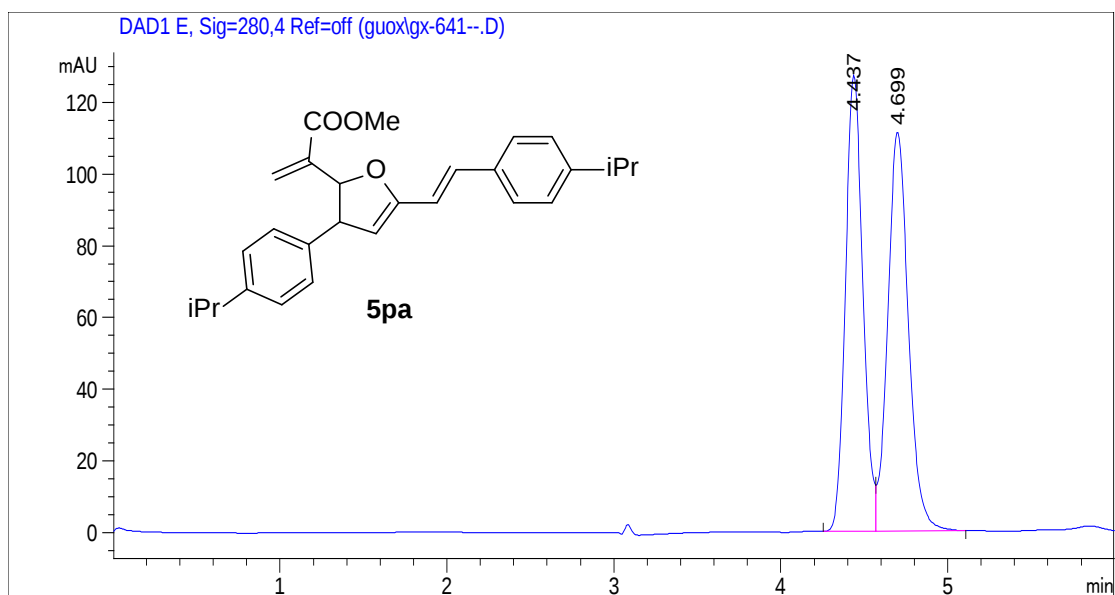


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	9.415	BB	950.7	34.7	0.4237	48.612	0.643
2	15.579	BB	1005	27.5	0.5541	51.388	0.697

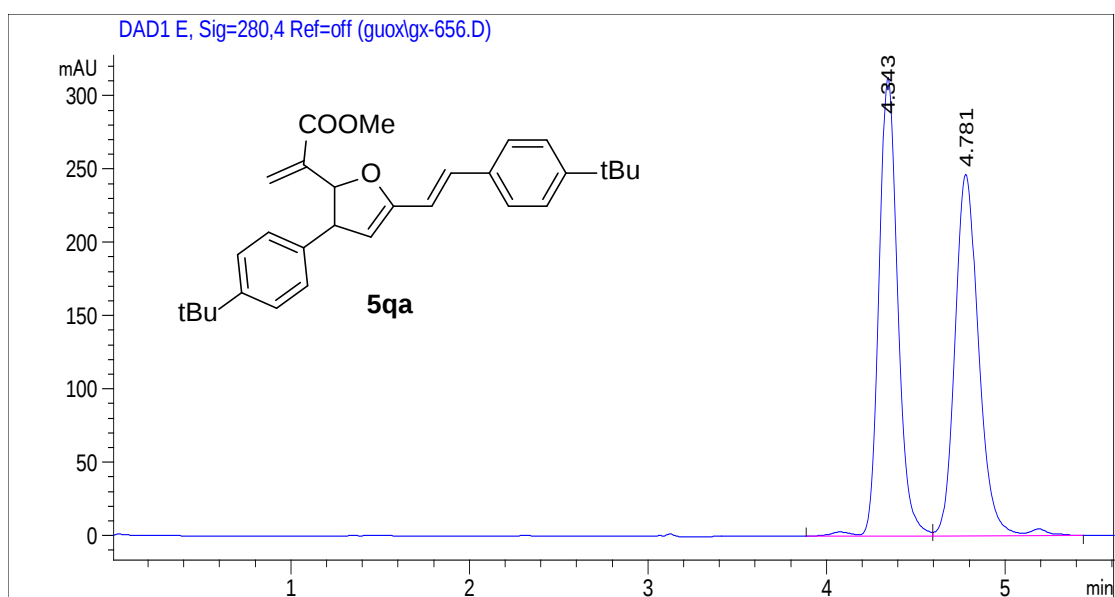


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	9.315	BB	144.4	5	0.428	1.624	0.575
2	15.5	BB	8747.6	240.9	0.5496	98.376	0.656

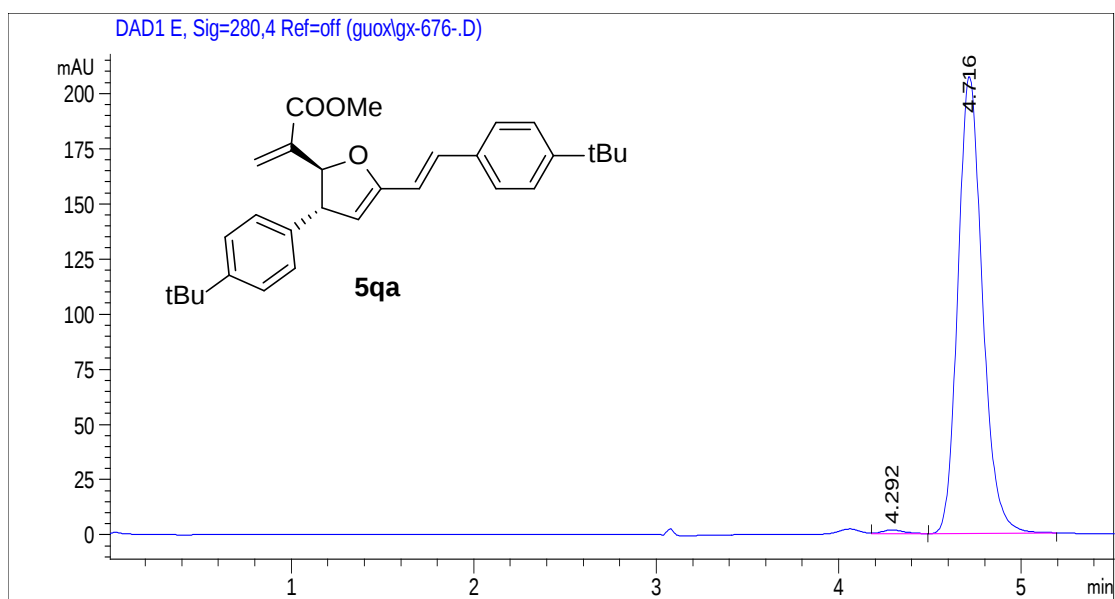
5pa: OD-H, 98/2, 1.0 ml/min, 280 nm



5qa: OD-H, 98/2, 1.0 ml/min, 280 nm

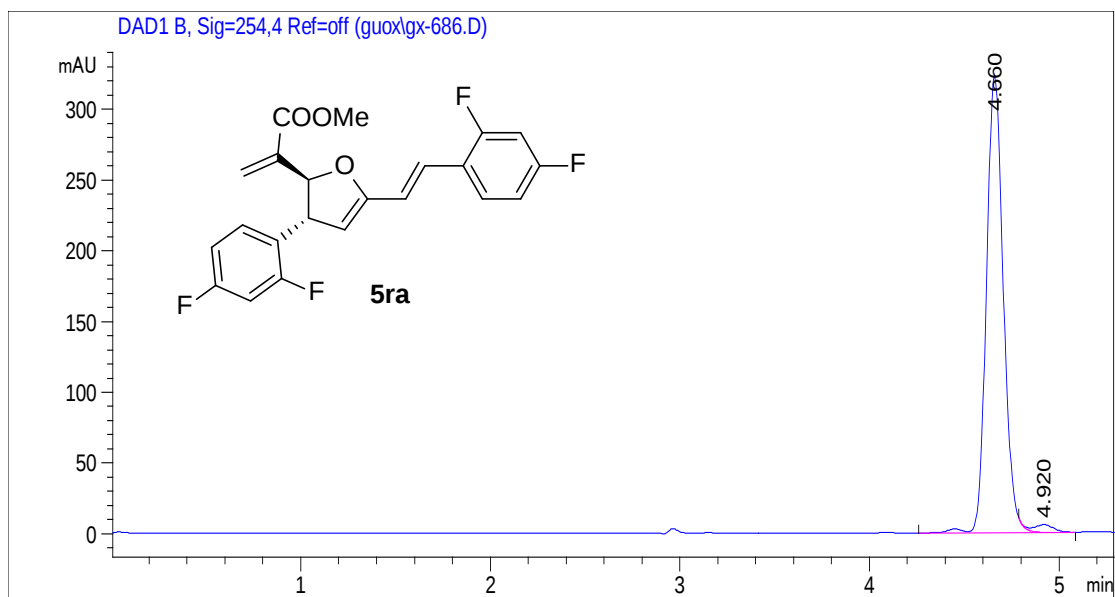
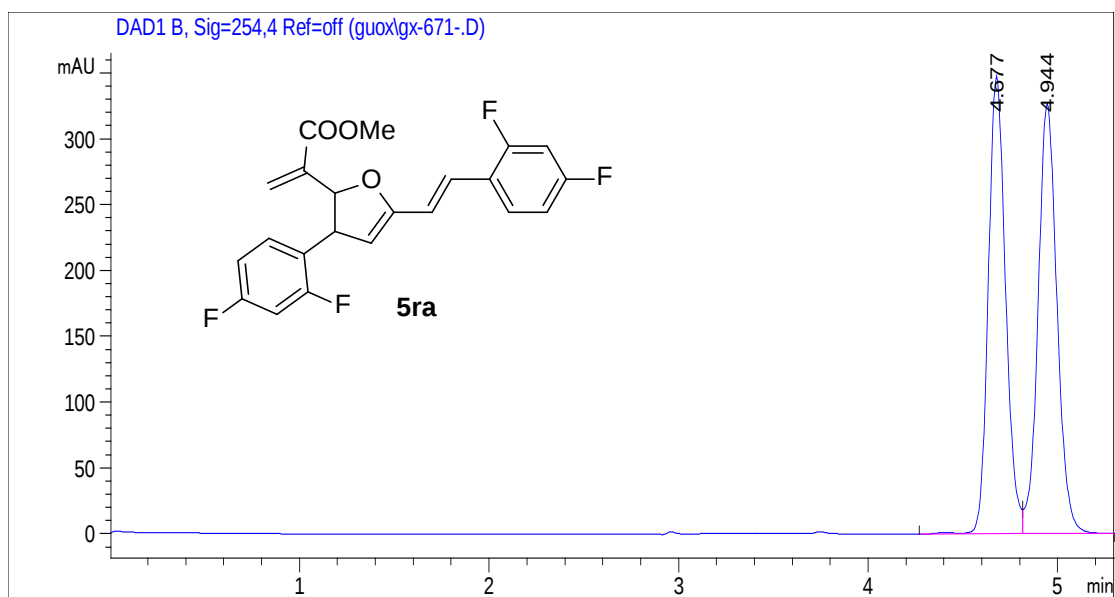


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.343	VVR	2288.8	312.7	0.1126	49.949	0.859
2	4.781	VVR	2293.5	246.7	0.1407	50.051	0.811

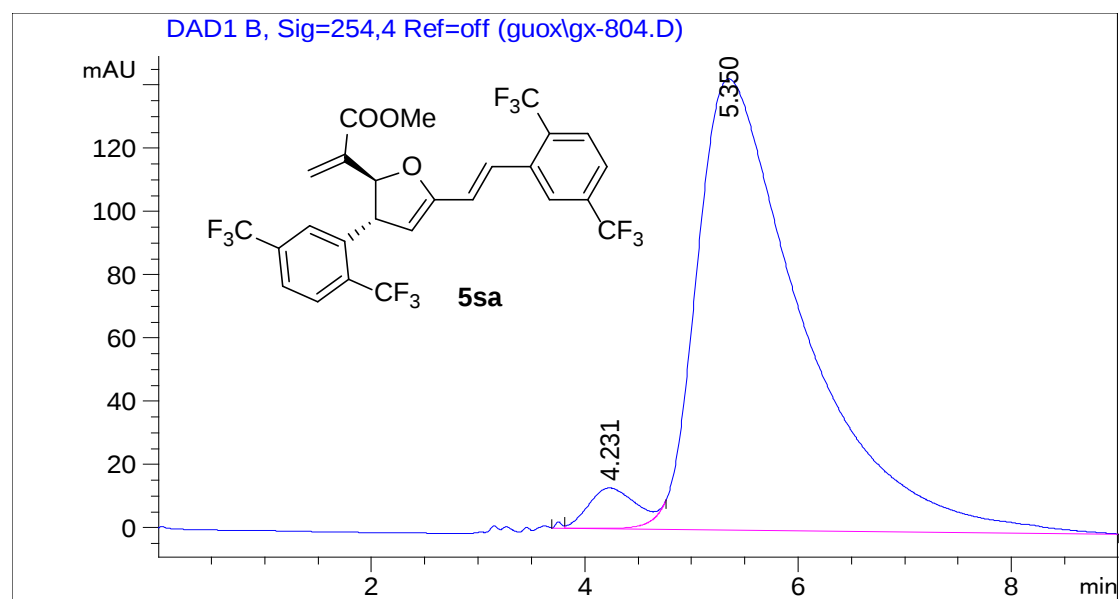
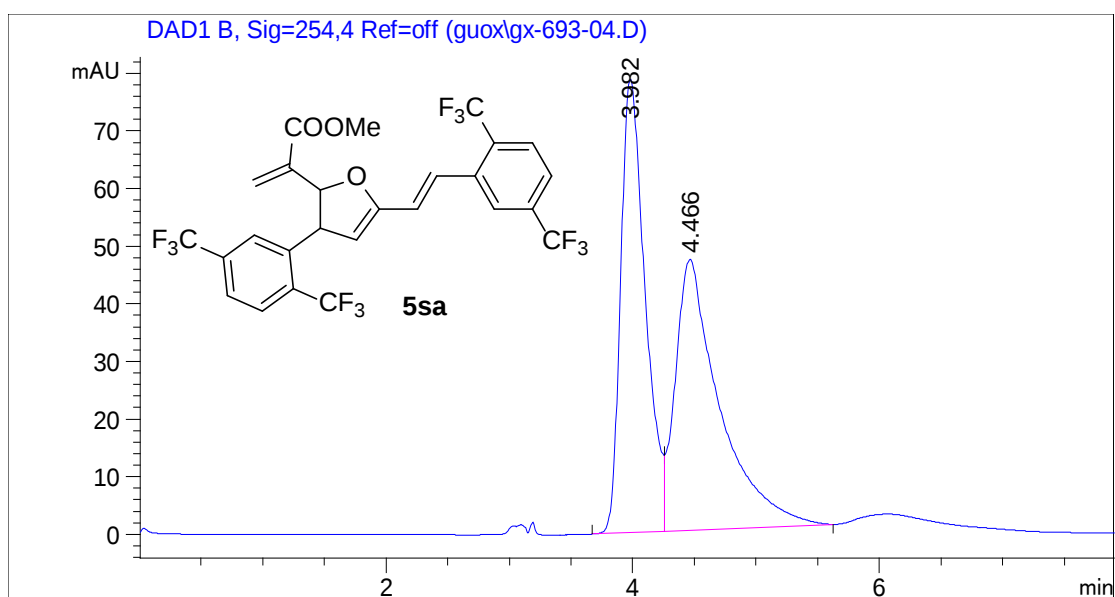


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	4.292	VB	15.3	1.8	0.1281	0.790	0.811
2	4.716	BB	1927.2	207.2	0.1445	99.210	0.814

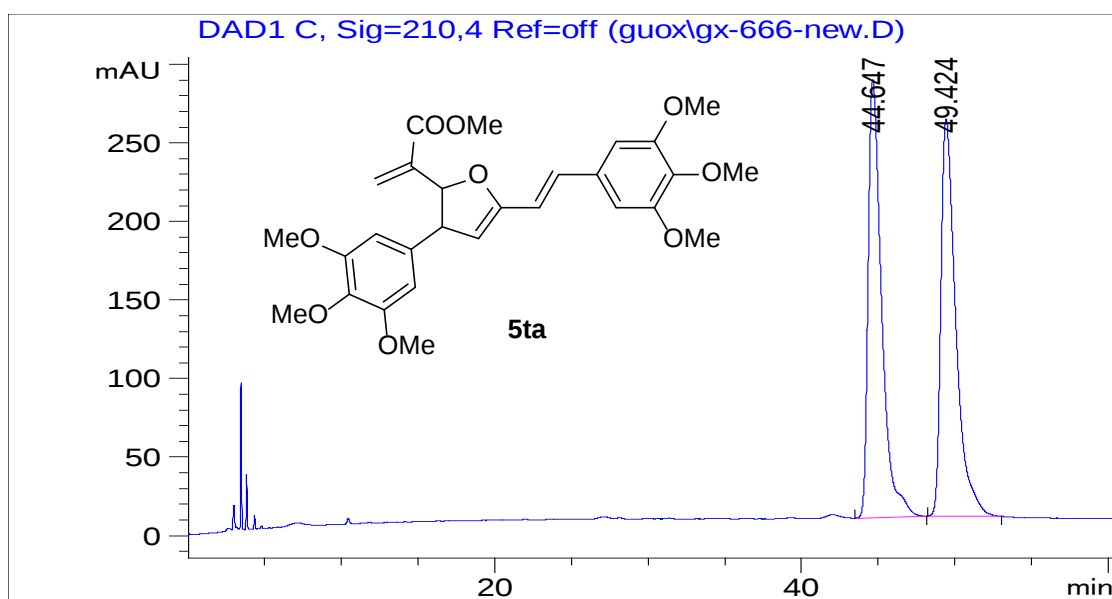
5ra: OD-H, 98/2, 1.0 ml/min, 254 nm



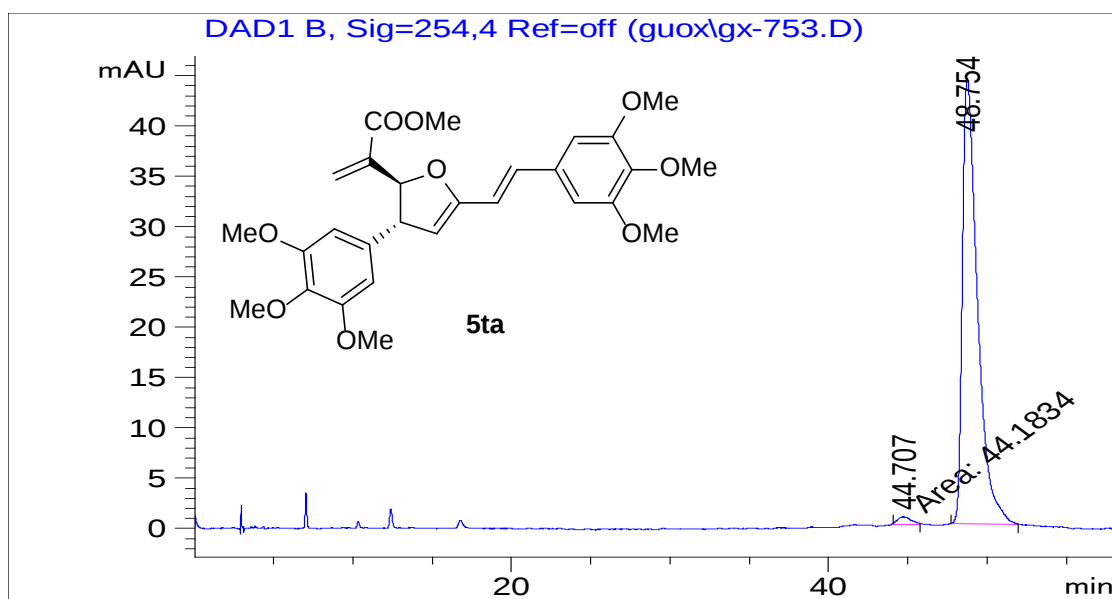
5sa: IJ, 99/1, 1.0 ml/min, 254 nm



5ta: IF-3, 90/10, 1.0 ml/min, 254 nm

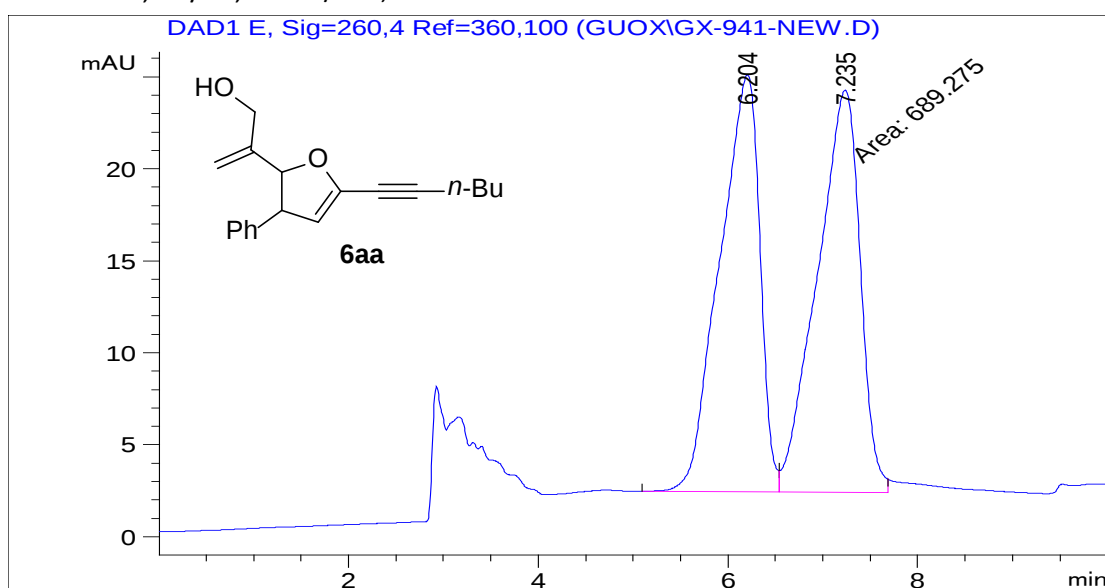


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	44.647	BB	16999.1	278.7	0.9136	49.855	0.483
2	49.424	BB	17098.3	252.8	1.005	50.145	0.489

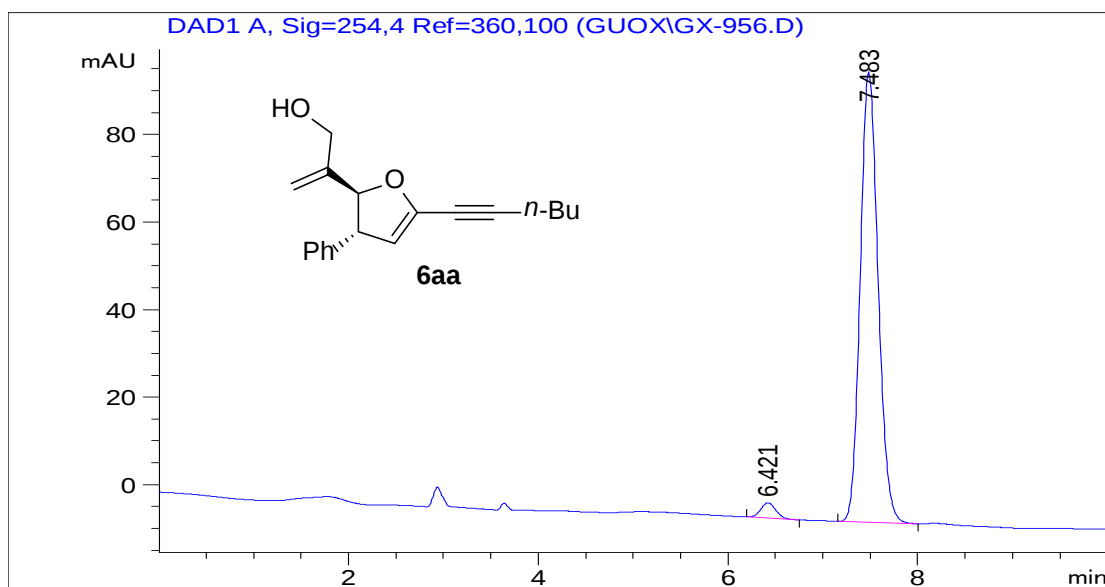


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	44.707	MM	44.2	7.3E-1	1.0121	1.485	0.673
2	48.754	BB	2930.3	44.2	0.9573	98.515	0.44

6aa: OD-H, 90/10, 1.0 ml/min, 254 nm

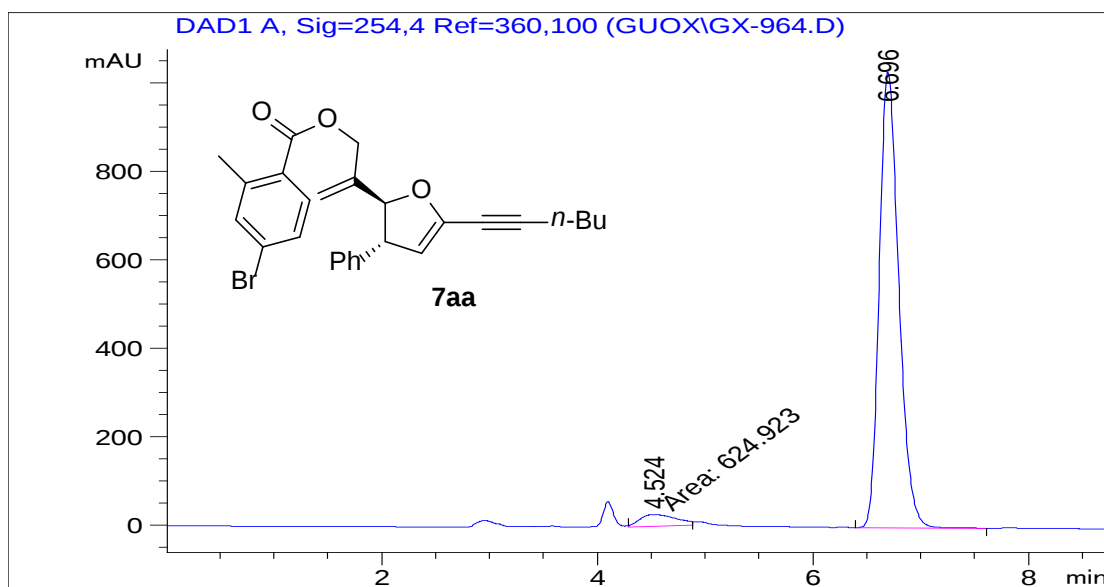
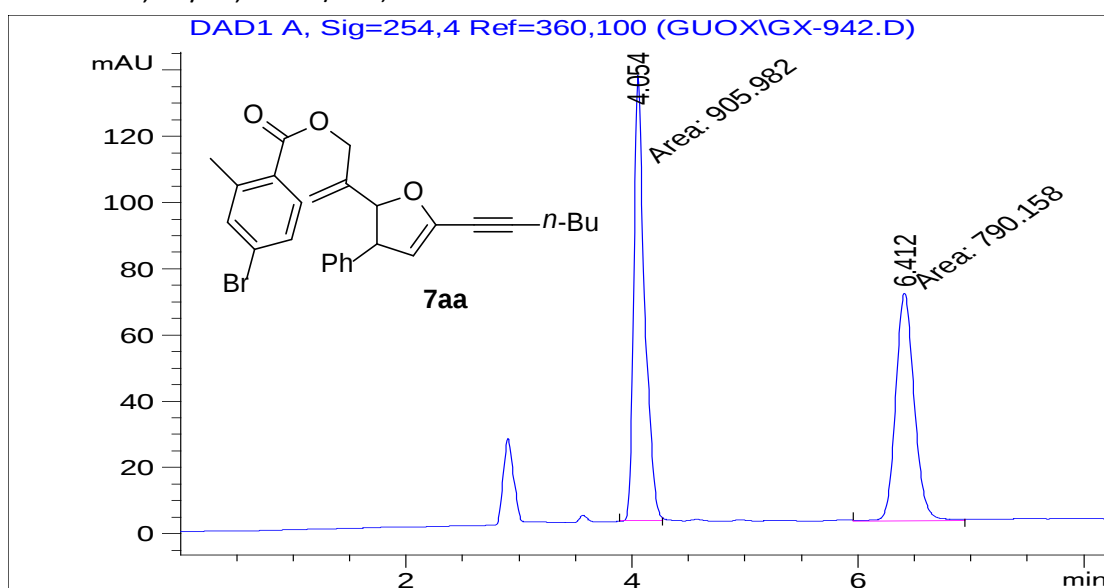


#	Time	Area	Height	Width	Area%	Symmetry
1	6.204	665.1	22.7	0.4303	49.106	2.119
2	7.235	689.3	21.9	0.5255	50.894	1.763



#	Time	Area	Height	Width	Area%	Symmetry
1	6.421	38.3	3.5	0.1688	2.779	0.865
2	7.483	1339.7	102.8	0.202	97.221	0.853

7aa: OD-H, 90/10, 1.0 ml/min, 254 nm



E: The absolute configuration of products

The absolute configuration of **3aa** was determined by ECD. Conformations of **(2S,3R)-3aa** was searched using Grimme's programs xTB 6.3. Next, Conformers within 5 kcal/mol were conducted at the M062X/6-311++G(d,p) level in MeCN solvent by a self-consistent reaction field (SCRF) using the SMD implicit solvent model with Gaussian 16. Then, conformers with distinct conformations were further subjected to TD-DFT calculation at the same level as aforementioned for dipole and rotational strengths of the first 30 excited states in the UV range. Next, ECD spectra of **(2S,3R)-3aa** (Figure 1) were calculated from excitation energies and rotational strengths as averages weighed on Boltzmann conformer relative populations as a sum of Gaussian functions centered at the wavelength of each transition with appropriate widths of the band at half-height using SpecDis (version 1.71), respectively.

Samples of compound **3aa** for ECD were dissolved in MeCN, and spectra were acquired in a 1.0-mm pathlength cuvette, respectively. The UV and ECD spectra were recorded using a Chirascan Spectrophotometer with the following instrumental parameters: 205–390 nm with a 1 nm step and a 2 nm bandwidth with data averaging over 1.0 sec per point. Three spectral acquisitions were taken for each sample and were averaged and smoothed thereafter.

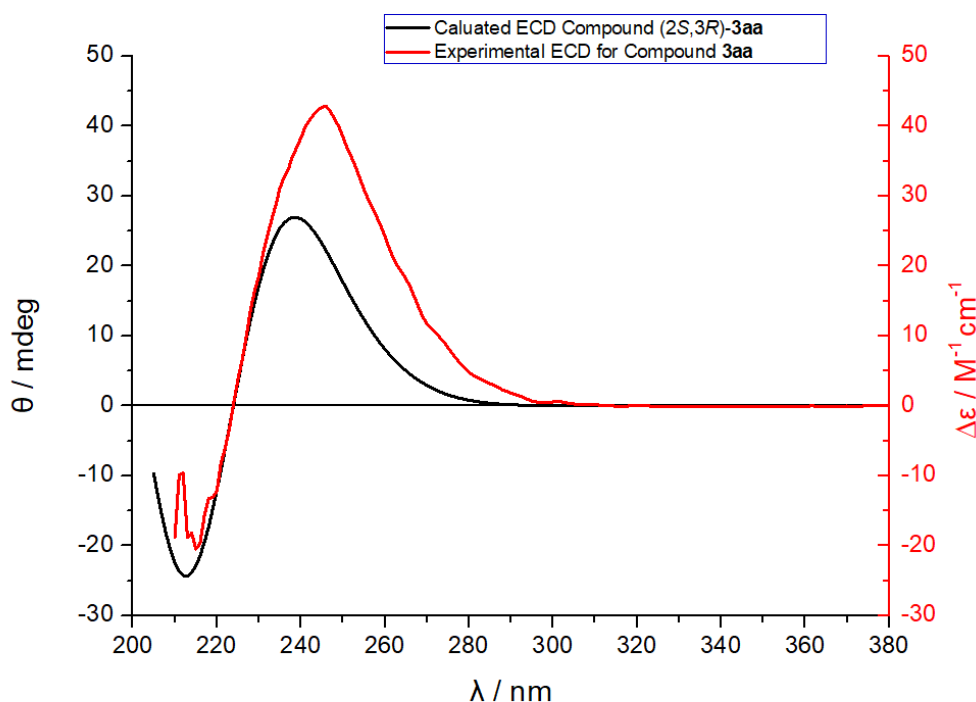


Figure S1. Comparison of the calculated ECD of compound (2S,3R)-3aa with the experimental one of compound 3aa. Width of the band at half-height σ : 0.33 eV; Shift: 0 nm.

The calculated spectrum for **(2*S*,3*R*)-3aa** was same to the experimental one, and thus, the absolute configuration of compound **3aa** was assigned to **2*S*,3*R*** accordingly. The absolute configurations of other chiral products were assigned by analogue to that of **3aa**.

Table S1. Energies of calculated conformers of (2*S*,3*R*)-3aa. Energies (E) (in Hartree) of the structures calculated at the SMD_(MeCN)/M06-2X/6-311+G(d,p) level of theory.

Structure (2 <i>S</i> ,3 <i>R</i>)-3aa	E _(solv-M06-2X)	G _(corr-solv-M06-2X)	G _(solv-M06-2X)	Boltzmann distribution(%)
conformer-1	-1000.833892	0.319043	-1000.514849	51.75%
conformer-2	-1000.831509	0.317024	-1000.514485	36.62%
conformer-3	-1000.833425	0.318092	-1000.513417	11.33%

F: Computational investigations

1. Computational Methods.

All of the DFT calculations were carried out with the Gaussian 16 series of programs ^[1]. The B3-LYP-D3 functional ^[2] with a Becke-Johnson (BJ) damping function ^[3] and the standard 6-31G(d) basis set was used for geometry optimizations. Harmonic vibrational frequency calculations were performed for all stationary points to determine whether they are local minima or transition structures and to derive thermochemical corrections for the enthalpies and free energies. The M06-2X ^[4] functional with the 6-311+G(d,P) basis set was used to calculate the single-point energies and give more accurate energy information. The solvent effects were considered by single-point calculations of the gas-phase stationary points with the SMD solvation model ^[5] in Acetonitrile (MeCN) solvent. In our computational studies, non-covalent interactions (NCI) analyses of key transition states were obtained with the Multiwfn^[6]. The 3D diagrams of molecules were generated using CYLView ^[7]. The global reactivity index (GRI) values were also calculated using M06-2X functional and the 6-311+G(d,P) basis set for all atoms. The ω (electrophilicity index) ^[8] values were calculated according to eq 1. In eq 1, the μ (electronic chemical potential) value could be obtained by $\mu = (\epsilon_{\text{HOMO}} + \epsilon_{\text{LUMO}})/2$ and the η (chemical hardness) value could be obtained by $\eta = \epsilon_{\text{HOMO}} - \epsilon_{\text{LUMO}}$. ^[9]

$$\omega = (\mu)^2 / 2\eta \quad (1)$$

The ϵ_{HOMO} values refer to the orbital energies of the highest occupied molecular orbital (HOMO), and the corresponding orbital and the ϵ_{LUMO} values refer to the orbital energies of the lowest unoccupied molecular orbital (LUMO).

2. Free energy profile for the [1,5]-proton transfer assisted by water.

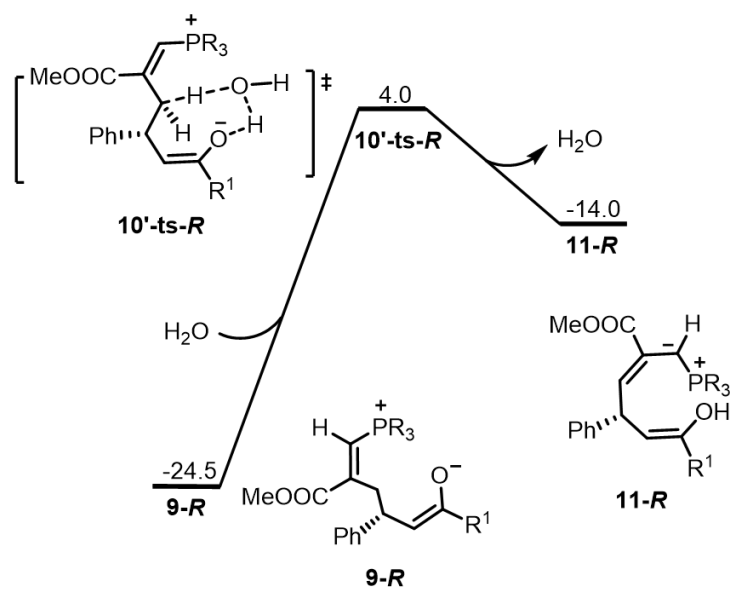


Fig. S2: Free energy profile for the [1,5]-proton transfer assisted by water. The energy values are in given kcal/mol and represent the relative free energies calculated with the DFT/M06-2X method in acetonitrile.

3. Comparison of different configurations of the key transition states and intermediates

The exploration of conformers and isomers are indeed important, especially for the investigation of selectivity-related problems. We have done a systematic conformational search for the key transition states and intermediates to ensure that they represent the corresponding lowest energy conformations.

3.1. Comparison of different configurations of the transition states TS1, TS3 and intermediate III.

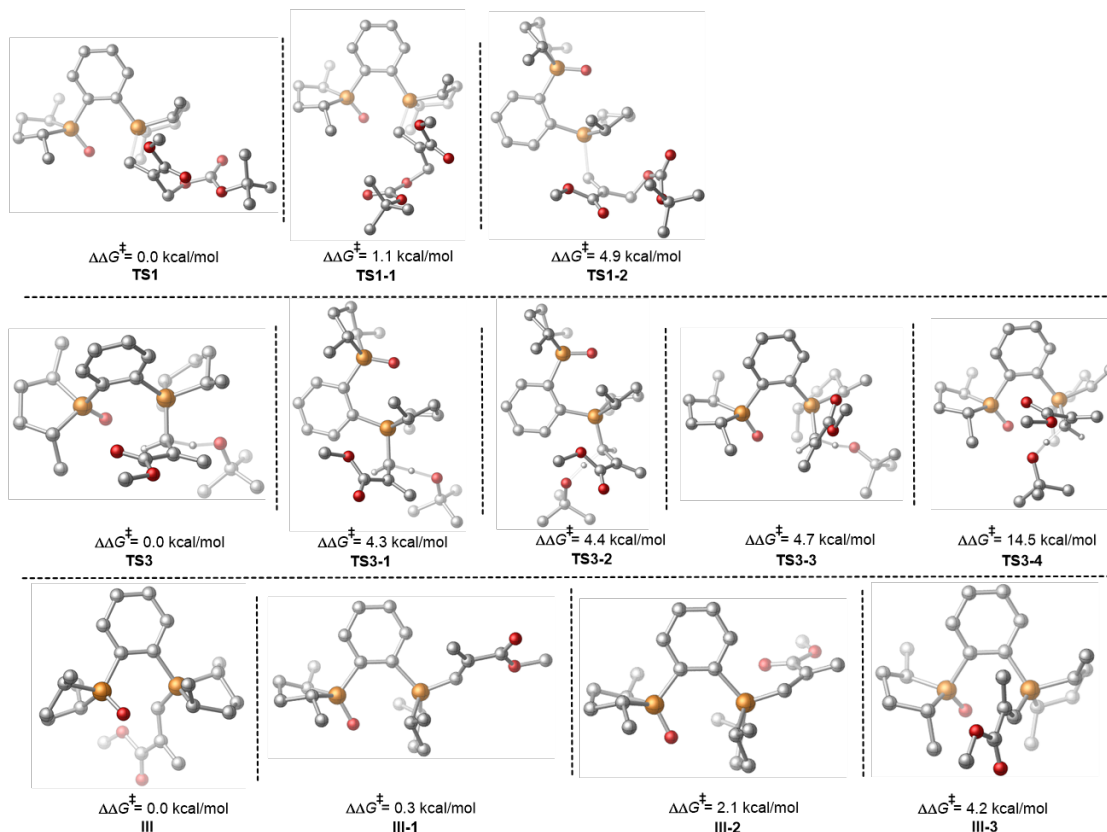


Fig. S3: Different configurations of the transition states TS1, TS3 and the intermediate III. Values are given in kcal/mol.

3.2. Comparison of different configurations of the transition states *Si*-TS4 and *Re*-TS4.

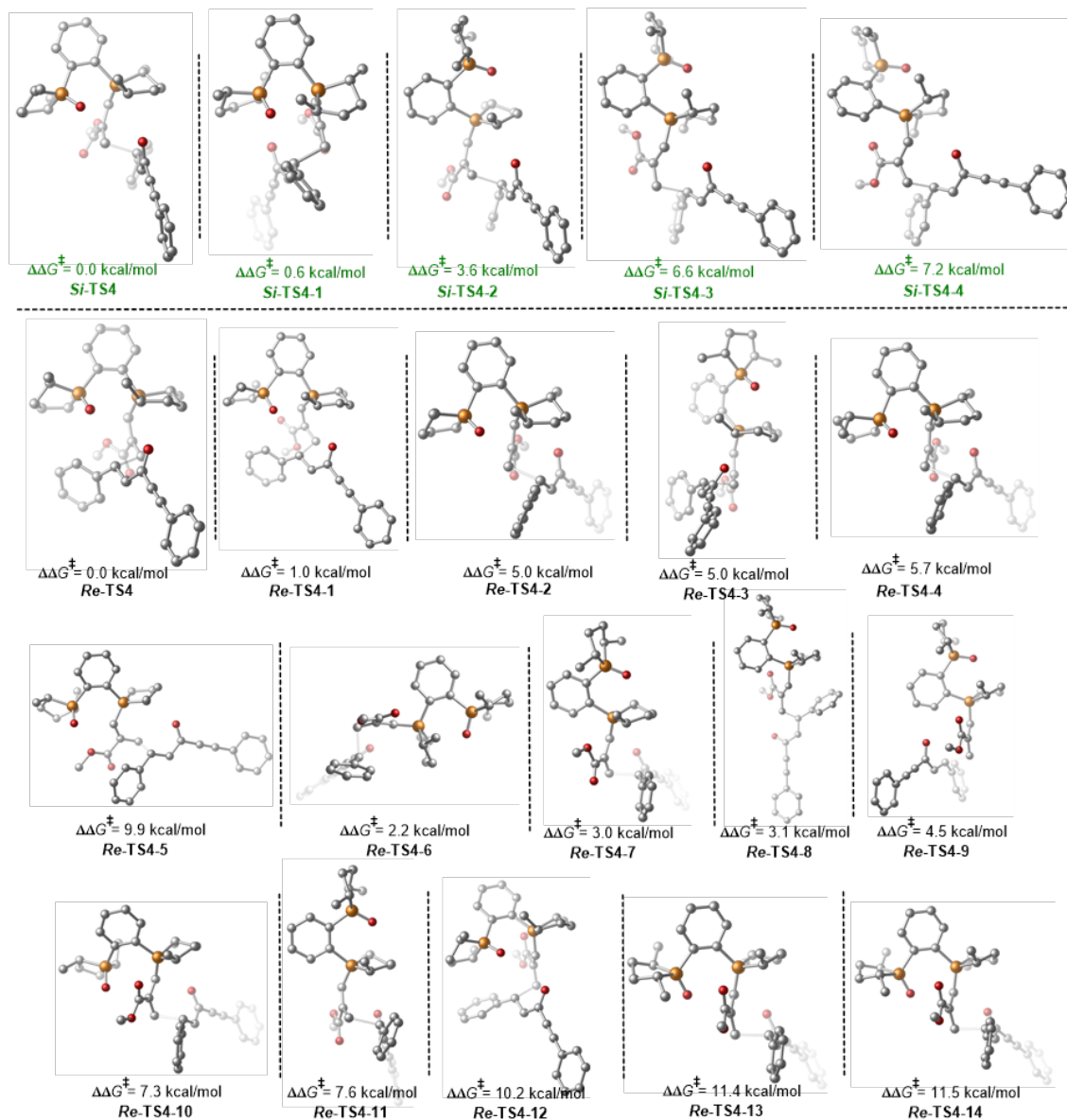


Fig. S4: Different configurations of the transition states *Si*-TS4 and *Re*-TS4. Values are given in kcal/mol.

3.3. Comparison of different configurations of the transition states 3S-TS5, 3R-TS5, 3R-TS6, and the intermediates 3R-V, 3R-VI.

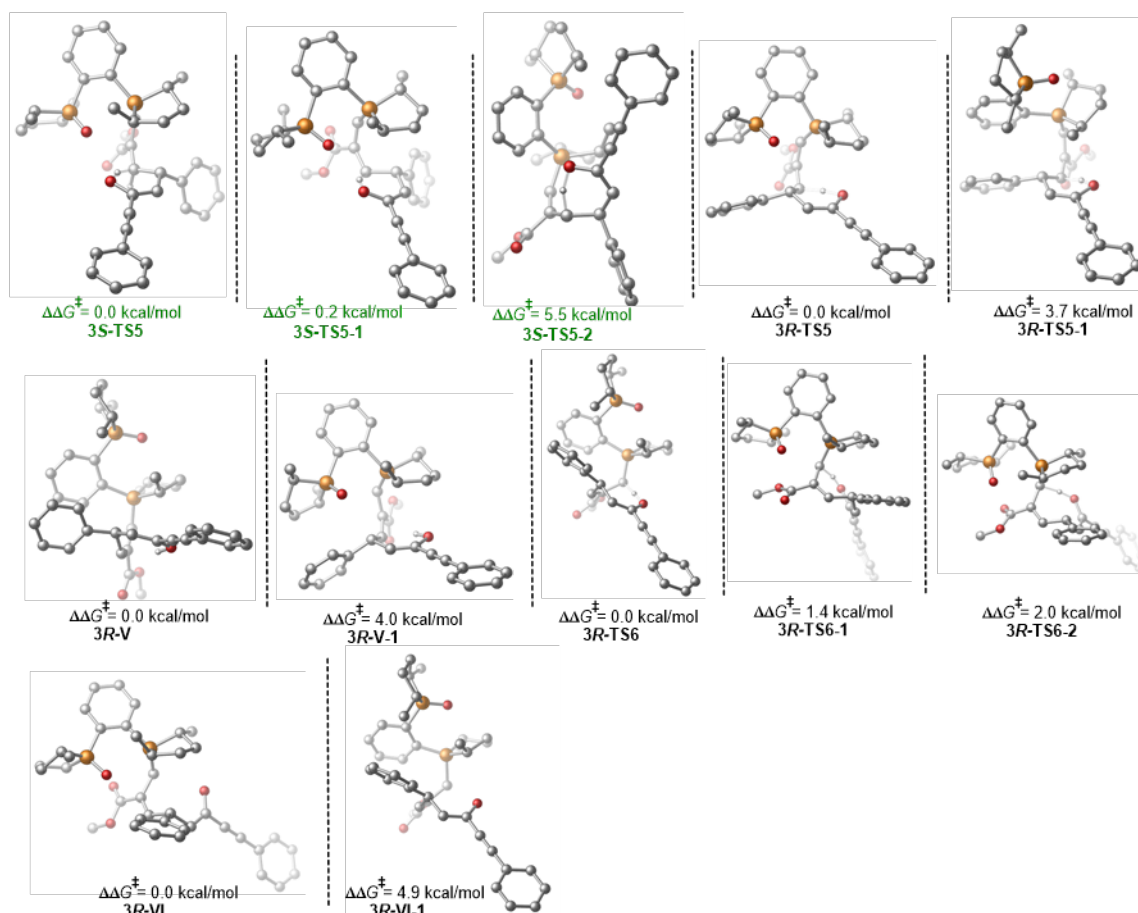


Fig. S5: Different configurations of the transition states 3S-TS5, 3R-TS5, 3R-TS6, and the intermediates 3R-V, 3R-VI. Values are given in kcal/mol.

3.4. Comparison of different configurations of the transition states 2*S*,3*R*-TS7, 2*R*,3*R*-TS7, 2*S*,3*R*-TS8, and 2*R*,3*R*-TS8.

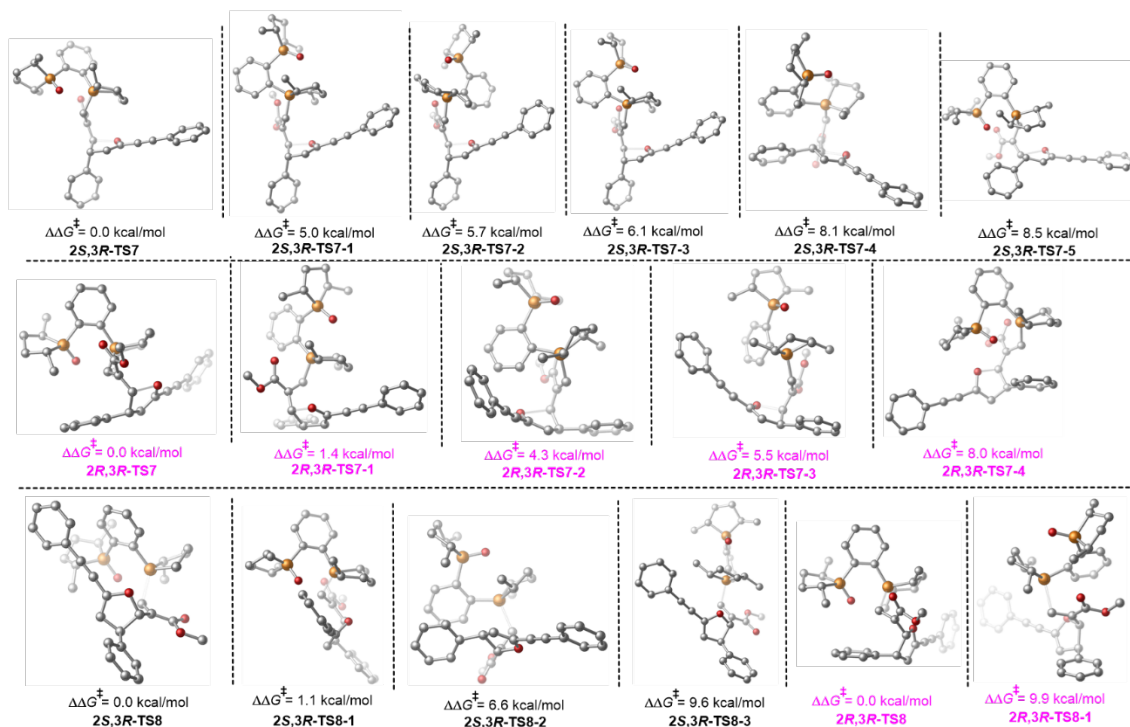


Fig. S6: Different configurations of the transition states 2*S*,3*R*-TS7, 2*R*,3*R*-TS7, 2*S*,3*R*-TS8, and 2*R*,3*R*-TS8. Values are given in kcal/mol.

3.5. Comparison of different configurations of the transition states TS4-a, TS5-a, and the intermediate IV-a.

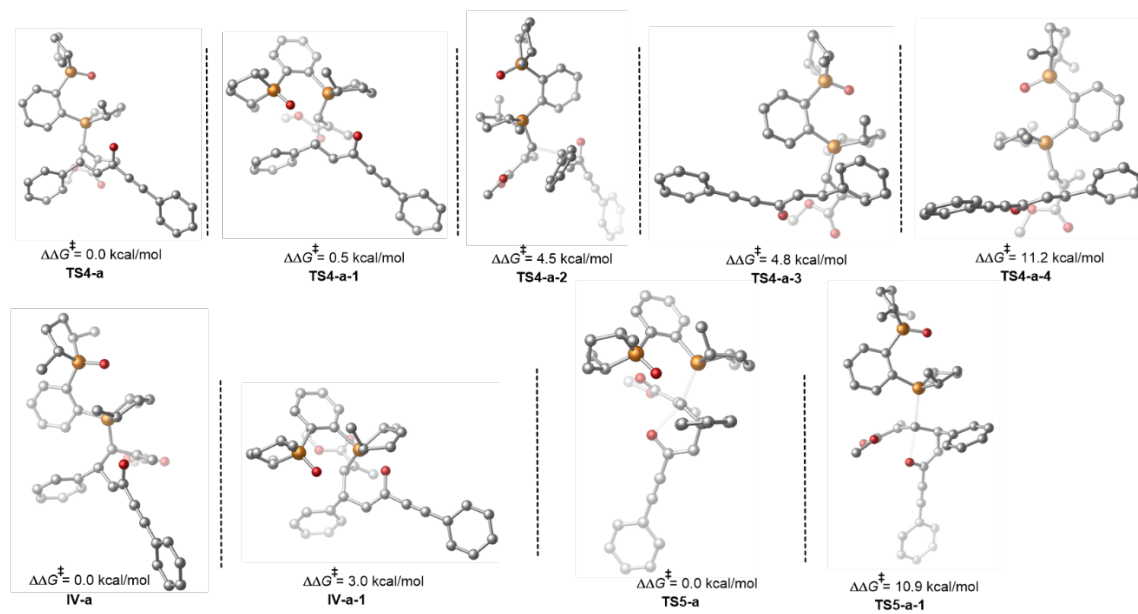


Fig. S7: Different configurations of the transition states TS4-a, TS5-a, and the intermediate IV-a. Values are given in kcal/mol.

4. SMD_(acetonitrile)/M06-2X/6-311+G(d,p)//B3LYP-D3(BJ)/6-31G(d) calculated absolute energies of all structures. Values are given in Hartree.

Table S2. SMD_(acetonitrile)/M06-2X/6-311+G(d,p)//B3LYP-D3(BJ)/6-31G(d) calculated absolute energies of all structures. Values are given in Hartree.

Geometry	E _(elec-B3-LYP-D3BJ) ¹	H _(corr-B3-LYP-D3BJ) ²	G _(corr-B3-LYP-D3BJ) ³	E _(solv-M06-2X) ⁴	IF ⁵
P4	-1460.865413	0.451991	0.378196	-1460.607277	-
2a	-766.876404	0.275558	0.211968	-766.750551	-
TS1	-2227.749487	0.729407	0.616140	-2227.347201	133.99 <i>i</i>
I	-2227.748999	0.730321	0.617433	-2227.356860	-
TS2	-2227.744925	0.728730	0.616580	-2227.350937	261.41 <i>i</i>
BocO⁻	-421.711722	0.148035	0.105293	-421.745727	-
II	-1805.903573	0.578529	0.485942	-1805.618076	-
^tBuO⁻	-233.056015	0.127883	0.091735	-233.112502	-
TS3	-2039.132350	0.705551	0.594937	-2038.741877	1327.03 <i>i</i>
^tBuOH	-233.689074	0.144011	0.107451	-233.639971	-
III	-1805.434714	0.563848	0.472257	-1805.119611	-
1g	-730.246895	0.251586	0.188716	-730.085317	-
Re-TS4	-2535.700599	0.817335	0.688071	-2535.211192	445.30 <i>i</i>
3R-IV	-2535.710202	0.819208	0.690028	-2535.241098	-
3R-TS5	-2535.693470	0.814676	0.687387	-2535.208441	1318.01 <i>i</i>
3R-V	-2535.708303	0.819734	0.689819	-2535.224174	-
3R-TS6	-2535.699468	0.814635	0.687864	-2535.218276	1534.74 <i>i</i>
3R-VI	-2535.722899	0.820209	0.690986	-2535.247235	-
2S,3R-TS7	-2535.715510	0.818768	0.689725	-2535.229058	213.46 <i>i</i>
2S,3R-VII	-2535.722978	0.820164	0.689733	-2535.238293	-
2S,3R-TS8	-2535.726519	0.819322	0.690416	-2535.229780	133.23 <i>i</i>
3ga	-1074.852372	0.365518	0.286416	-1074.633337	-
2R,3R-TS7	-2535.720191	0.819128	0.691071	-2535.227608	118.24 <i>i</i>
2R,3R-VII	-2535.727645	0.820409	0.693718	-2535.235505	-
2R,3R-TS8	-2535.722140	0.819261	0.690844	-2535.228295	121.38 <i>i</i>
2R,3R-3ga	-1074.852836	0.365446	0.286974	-1074.634550	-
Si-TS4	-2535.697269	0.816911	0.686813	-2535.211611	434.52 <i>i</i>
3S-IV	-2535.705963	0.818894	0.688381	-2535.241132	-
3S-TS5	-2535.678560	0.814002	0.685085	-2535.200508	1409.51 <i>i</i>
TS4-a	-2535.691509	0.817941	0.687785	-2535.206615	404.04 <i>i</i>
IV-a	-2535.698436	0.820070	0.690329	-2535.222089	-
TS5-a	-2535.683199	0.817968	0.690111	-2535.193958	353.71 <i>i</i>
1g-b	-462.336130	0.183028	0.134921	-462.232104	-
TS4-b	-2267.785310	0.748963	0.634041	-2267.349010	469.89 <i>i</i>
IV-b	-2267.792297	0.750737	0.636840	-2267.373323	-

H₂O	-76.409528	0.024945	0.002845	-76.429687	-
3R-TS5-a	-2612.119937	0.841828	0.709012	-2611.641532	1030.93i
TS1-1	-2227.738387	0.728942	0.615680	-2227.345015	110.90i
TS1-2	-2227.742523	0.729254	0.615416	-2227.338682	169.87i
TS3-1	-2039.122841	0.705734	0.597139	-2038.737255	473.04i
TS3-2	-2039.125938	0.705470	0.597513	-2038.737495	769.55i
TS3-3	-2039.129065	0.707140	0.598914	-2038.738407	29.23i
TS3-4	-2039.108300	0.704985	0.597798	-2038.721612	762.34i
III-1	-1805.435512	0.563912	0.471670	-1805.118585	-
III-2	-1805.440215	0.564162	0.473049	-1805.117077	-
III-3	-1805.429513	0.564224	0.471838	-1805.112518	-
Si-TS4-1	-2535.703562	0.817424	0.689547	-2535.213402	456.08i
Si-TS4-2	-2535.691252	0.817467	0.685901	-2535.205000	462.76i
Si-TS4-3	-2535.692654	0.817322	0.685166	-2535.199388	396.42i
Si-TS4-4	-2535.687904	0.817068	0.684927	-2535.198192	401.22i
Re-TS4-1	-2535.703466	0.817282	0.688125	-2535.209728	417.96i
Re-TS4-2	-2535.695520	0.816893	0.687391	-2535.202600	272.13i
Re-TS4-3	-2535.689731	0.817410	0.686016	-2535.201212	395.89i
Re-TS4-4	-2535.694612	0.817106	0.688336	-2535.202369	276.02i
Re-TS4-5	-2535.683834	0.817853	0.688895	-2535.196223	470.15i
Re-TS4-6	-2535.698399	0.817600	0.686628	-2535.206252	426.69i
Re-TS4-7	-2535.690808	0.817404	0.685884	-2535.204288	442.73i
Re-TS4-8	-2535.688581	0.817276	0.685088	-2535.203323	449.16i
Re-TS4-9	-2535.703953	0.817307	0.687466	-2535.203412	220.78i
Re-TS4-10	-2535.687061	0.817625	0.687380	-2535.198937	461.19i
Re-TS4-11	-2535.686992	0.817291	0.686479	-2535.197559	335.91i
Re-TS4-12	-2535.692040	0.817321	0.687572	-2535.194474	266.65i
Re-TS4-13	-2535.680724	0.816968	0.685803	-2535.190807	382.92i
Re-TS4-14	-2535.680732	0.816988	0.686020	-2535.190821	383.87i
3S-TS5-1	-2535.679870	0.814152	0.685060	-2535.200155	1355.38i
3S-TS5-2	-2535.679326	0.814753	0.685267	-2535.191958	1484.76i
3R-TS5-1	-2535.689752	0.814822	0.686822	-2535.201935	1187.50i
3R-V-1	-2535.708118	0.820045	0.690586	-2535.218557	-
3R-TS6-1	-2535.689333	0.814592	0.686674	-2535.214916	1666.07i
3R-TS6-2	-2535.693687	0.814556	0.686871	-2535.214037	1658.06i
3R-VI-1	-2535.716147	0.820053	0.692122	-2535.240605	-
2S,3R-TS7-1	-2535.699405	0.818423	0.690137	-2535.221547	255.13i
2S,3R-TS7-2	-2535.719378	0.819032	0.692491	-2535.222794	198.11i
2S,3R-TS7-3	-2535.709231	0.818623	0.691382	-2535.221056	96.82i
2S,3R-TS7-4	-2535.700854	0.818753	0.693560	-2535.219952	79.05i
2S,3R-TS7-5	-2535.694822	0.818906	0.690753	-2535.216583	120.02i

2R,3R-TS7-1	-2535.717777	0.819173	0.692425	-2535.226777	27.79i
2R,3R-TS7-2	-2535.718001	0.818705	0.692181	-2535.221887	72.13i
2R,3R-TS7-3	-2535.708953	0.818529	0.692373	-2535.220160	309.66i
2R,3R-TS7-4	-2535.715757	0.819021	0.693635	-2535.217436	262.42i
2S,3R-TS8-1	-2535.722064	0.819504	0.693659	-2535.231235	66.05i
2S,3R-TS8-2	-2535.707556	0.819053	0.691984	-2535.220814	170.62i
2S,3R-TS8-3	-2535.705164	0.819512	0.691287	-2535.215309	117.02i
2R,3R-TS8-1	-2535.709017	0.819034	0.689660	-2535.211365	175.21i
TS4-a-1	-2535.695668	0.817920	0.689666	-2535.207677	370.79i
TS4-a-2	-2535.686633	0.817884	0.687940	-2535.199525	375.59i
TS4-a-3	-2535.685868	0.818370	0.689215	-2535.200471	407.18i
TS4-a-4	-2535.681349	0.818042	0.688492	-2535.189426	376.53i
IV-a-1	-2535.717443	0.821550	0.696733	-2535.223772	-
TS5-a-1	-2535.663975	0.817879	0.688028	-2535.174554	330.09i

¹The electronic energy calculated by B3LYP-D3(BJ) in gas phase. ²The thermal correction to enthalpy calculated by B3LYP-D3(BJ) in gas phase. ³The thermal correction to Gibbs free energy calculated by B3LYP-D3(BJ) in gas phase.

⁴The electronic energy calculated by M06-2X in acetonitrile solvent. ⁵The B3LYP-D3(BJ) calculated imaginary frequencies for the transition states.

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6. Cartesian coordinates for DFT-optimized structures for all the optimized compounds and transition states

P4

C	0.61736000	-0.94577200	-0.51091600
C	-0.78676600	-0.76612700	-0.57109500
C	-1.54565300	-1.73854800	-1.23640300
C	-0.95233000	-2.85350700	-1.82882100
C	0.42821600	-3.02207700	-1.76546200
C	1.20424600	-2.07139600	-1.10449700
H	-2.62394600	-1.63932800	-1.28991300
H	-1.57193400	-3.59088700	-2.33192000
H	0.89996400	-3.88812800	-2.22062500
H	2.27693100	-2.21928600	-1.04941300
C	-2.36779700	-0.01589200	1.76530100
C	-3.16057000	0.98063600	-0.68136800
C	-3.79021800	-0.37645800	1.30762600
H	-2.43290300	0.82477500	2.46947800
C	-4.26563700	0.73397900	0.36786700
H	-3.24511800	0.22527700	-1.46913200
H	-3.76687800	-1.33675800	0.77425000
H	-4.46209400	-0.50691000	2.16613100
H	-5.22237900	0.49705800	-0.11417300
H	-4.42269900	1.65449400	0.94783400
P	-1.51980800	0.74297100	0.24442600
C	-1.60707000	-1.15429700	2.44145900
C	-3.24423100	2.36285300	-1.33483800
H	-2.47308600	2.49200600	-2.10246000
H	-4.22130500	2.51163700	-1.81242800
H	-3.10805000	3.15785500	-0.59237800
H	-0.59180500	-0.84350500	2.69999000
H	-2.13068700	-1.46618800	3.35422600
H	-1.53925800	-2.02497100	1.77964600
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C	1.20272600	1.89489200	-1.88366100
C	3.81401300	-1.27547000	1.44789300
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H	4.89776900	-1.44071600	1.45683200
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H	0.11469700	1.87794900	-1.78354200
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H	1.49884600	1.05958800	-2.52862300

2a

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C	-4.10326600	1.20901200	2.94996400
C	-4.27843000	0.52379700	1.75226100
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C	5.33194700	0.26021000	1.30638300
C	6.52789200	-1.52470600	0.00296700
C	6.79288600	0.89722400	-0.68002100
H	7.11144300	0.58305800	-1.67977200

H	6.29134200	1.86315100	-0.75579600
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H	4.62498800	-0.49545200	1.66071500

I

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C	1.65803300	-0.49392300	-1.42536200
C	3.44100900	0.41901700	0.08575800
H	2.74541200	-1.05026900	1.46856900
C	3.17782900	-0.46165500	-1.14056200
H	1.36569300	0.44647000	-1.90915600
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H	4.46605000	0.30735100	0.45462800
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H	3.52073000	-1.48212500	-0.92698400
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C	2.46718000	0.78747700	2.46999500
C	1.22135600	-1.66979500	-2.29950200
H	0.13874400	-1.68750100	-2.43084100
H	1.70853000	-1.59579300	-3.27891800
H	1.52671400	-2.62228000	-1.85257800
H	1.71210700	0.43670900	3.17419000
H	3.44353500	0.64401000	2.93915100
H	2.31595700	1.85731200	2.30785900

C	-3.73583900	-0.93314400	0.85614900
C	-3.90118200	0.19412100	-1.65628200
C	-5.12543700	-0.92115400	0.18014700
H	-3.70469800	-0.14595800	1.61993500
C	-5.18620400	0.25331800	-0.81138300
H	-3.97124800	-0.69505100	-2.30032800
H	-5.26345700	-1.86289500	-0.36762900
H	-5.92096700	-0.86888100	0.93120400
H	-6.07642700	0.20273600	-1.44868900
H	-5.24313600	1.20581300	-0.26690600
P	-2.57517700	-0.37947900	-0.48906800
O	-1.65278700	-1.39422500	-1.12072800
C	-3.60551800	1.39844900	-2.54815900
C	-3.36100300	-2.27201400	1.49294600
H	-2.43431900	-2.19367500	2.06450000
H	-4.15644900	-2.59352900	2.17527300
H	-3.23509300	-3.04580300	0.72861200
H	-2.66402800	1.26342800	-3.09092300
H	-4.40404400	1.52261000	-3.28837000
H	-3.53167800	2.32823800	-1.97807800
C	0.28108600	-2.06527300	0.97900000
H	-0.75271000	-2.13858300	0.65646600
H	0.84188000	-2.78201700	0.36567100
C	0.55998400	-2.27238500	2.42056200
C	-0.00214800	-1.41923400	3.38252600
O	-0.81246500	-0.42610000	2.75419700
C	-1.35871700	0.53783900	3.64351600
H	-0.57413000	1.04865000	4.21045400
H	-1.89196400	1.25667300	3.01670500
H	-2.04594300	0.07350000	4.35819700
O	0.12479600	-1.38579100	4.61153300
C	1.52889200	-3.29034100	2.83452100
H	1.39402100	-3.58355200	3.87162600
H	1.53928500	-4.16953700	2.18597700
O	2.98185400	-2.83220900	2.69323300
C	3.60283700	-2.25447100	3.72438800
O	4.53528100	-1.48685300	3.55916100
O	3.09810800	-2.64866300	4.89984200
C	3.39590800	-1.93720300	6.15029800
C	3.07497200	-0.44958200	6.00022600
C	4.85151800	-2.18991100	6.54047800

C	2.41930900	-2.59224700	7.12611800
H	5.04455100	-3.26573000	6.61330400
H	5.52678300	-1.75864000	5.79927100
H	5.05695300	-1.73754000	7.51731600
H	2.52620100	-2.14844800	8.12170300
H	1.39624000	-2.44234800	6.77016800
H	2.61540800	-3.66709100	7.20153600
H	3.13869700	0.03191900	6.98259900
H	3.78065500	0.04003000	5.32744800
H	2.05653500	-0.33717000	5.61725300

TS2

C	-1.74150500	1.22074000	0.38991800
C	-0.49573200	1.04675700	1.03382100
C	-0.05405900	2.06017800	1.89979900
C	-0.84847000	3.16145700	2.21130200
C	-2.12499500	3.26651900	1.66813200
C	-2.55001200	2.30721800	0.75234200
H	0.92541800	1.98914200	2.35042600
H	-0.47193500	3.91927000	2.89139000
H	-2.77366400	4.09686800	1.92976300
H	-3.52906600	2.41645300	0.29722800
C	1.70338300	-0.51559300	2.44661500
C	2.00726200	0.00428200	-0.24782200
C	3.02712000	0.15312700	2.03718300
H	1.90316000	-1.59763900	2.45447000
C	3.28930800	-0.24613700	0.58099900
H	1.89844000	1.08339300	-0.41649900
H	2.97922900	1.24705400	2.13614100
H	3.81567300	-0.20598800	2.70595400
H	4.13222600	0.29596800	0.13834600
H	3.53392700	-1.31522400	0.54653100
P	0.62811700	-0.41329900	0.94289300
C	1.18643700	-0.17276400	3.84373300
C	1.98025300	-0.72336900	-1.59189300
H	1.02863100	-0.58018500	-2.10611700
H	2.79607300	-0.35092100	-2.22212900
H	2.13722900	-1.79885200	-1.45621200
H	0.25055500	-0.68578100	4.06774800

H	1.93234900	-0.53745800	4.55358900
H	1.03981400	0.89770200	4.00802100
C	-3.86711900	-0.66710800	-0.48885200
C	-3.09585600	1.26655000	-2.29899800
C	-4.87843800	-0.30042400	-1.59750300
H	-4.17725800	-0.18272000	0.44611000
C	-4.60999000	1.14546100	-2.04894500
H	-2.86074700	0.67499000	-3.19612600
H	-4.73640600	-0.97824200	-2.44971900
H	-5.90649700	-0.43911800	-1.24614600
H	-5.17692400	1.40282900	-2.95076100
H	-4.92564800	1.84992900	-1.26716200
P	-2.30064200	0.19025700	-1.01061200
O	-1.17181800	-0.63997900	-1.57123100
C	-2.54268400	2.67529500	-2.50593100
C	-3.70380500	-2.16882800	-0.25287300
H	-3.07495500	-2.36549900	0.61784100
H	-4.68322700	-2.62797000	-0.07626100
H	-3.25181300	-2.65396500	-1.12396900
H	-1.45834200	2.65385800	-2.65720600
H	-2.99578900	3.12917700	-3.39444700
H	-2.74828500	3.33041200	-1.65531900
C	-0.09506800	-2.12201400	0.69454000
H	-0.95255000	-1.99409600	0.04209600
H	0.67278400	-2.61965900	0.09123200
C	-0.33041100	-2.88694400	1.95685200
C	-1.24217500	-2.38018100	2.93015400
O	-1.83161600	-1.18557700	2.46897000
C	-2.71461900	-0.55660200	3.39297900
H	-2.20729600	-0.33896600	4.33729300
H	-3.03235600	0.37232800	2.91479000
H	-3.57825200	-1.19399200	3.60494900
O	-1.53933100	-2.81483100	4.03741900
C	0.44018900	-4.02301100	2.24839100
H	0.13240600	-4.62507400	3.09337900
H	0.87281400	-4.57516500	1.42016100
O	2.12669500	-3.56572500	2.84191200
C	2.30290400	-3.44007000	4.12679100
O	3.08023700	-2.64068500	4.64642200
O	1.52466200	-4.30694700	4.83406800
C	1.34764000	-4.17676500	6.27625600

C	0.85357300	-2.77259700	6.63597700
C	2.65078800	-4.53508300	6.99282000
C	0.25102700	-5.20408900	6.56315800
H	2.97640800	-5.54077900	6.70473700
H	3.43365200	-3.82172800	6.73041900
H	2.49885300	-4.52065300	8.07848700
H	0.02260700	-5.22937700	7.63425300
H	-0.65644000	-4.93916300	6.01180300
H	0.57241900	-6.20353800	6.25150200
H	0.54707600	-2.75224300	7.68834700
H	1.64013200	-2.03239200	6.48583100
H	-0.01145300	-2.51980900	6.01523300

BocO⁻

O	7.44401800	-0.72970400	0.07738900
C	7.61395100	-0.84247300	-1.13970000
O	7.14136800	-1.62528000	-1.99152600
O	8.57092300	0.16975800	-1.62863300
C	8.92662400	0.23864900	-3.00458800
C	7.70423700	0.55157100	-3.88581500
C	9.61627200	-1.05524500	-3.47224300
C	9.92247600	1.40640600	-3.07222100
H	10.49403600	-1.25174400	-2.84363400
H	8.91411600	-1.88308900	-3.36519600
H	9.94997000	-0.97431200	-4.51699100
H	10.28052900	1.56852700	-4.09838100
H	9.44621900	2.32747900	-2.71693300
H	10.78513200	1.20258400	-2.42746300
H	7.99241000	0.67020000	-4.94047200
H	6.98293200	-0.26014800	-3.78264500
H	7.23725800	1.48548600	-3.54828900

II

C	-2.03928000	1.04559200	1.06197700
C	-0.66597900	1.02136900	1.40115600
C	-0.15391500	2.06774500	2.18328300
C	-0.96972300	3.10183500	2.64184500

C	-2.32445800	3.10762800	2.32726400
C	-2.84473200	2.08422200	1.53668000
H	0.88978700	2.09048900	2.44946800
H	-0.53904200	3.89495800	3.24453800
H	-2.97171100	3.90186700	2.68545400
H	-3.90131600	2.09639800	1.28851800
C	2.21449600	0.06921400	1.53887500
C	0.97676200	-0.36806700	-0.84585600
C	2.73337000	0.98690200	0.41675500
H	2.67993300	-0.91721900	1.38609100
C	2.37427900	0.31878400	-0.91877300
H	0.21417500	0.22566100	-1.35416600
H	2.26643400	1.97598700	0.50181300
H	3.81366700	1.13614900	0.51158100
H	2.39823400	1.03339800	-1.74599900
H	3.12187800	-0.45064500	-1.14038700
P	0.49508800	-0.33059300	0.95588500
C	2.55363000	0.52177200	2.97066900
C	0.99263900	-1.77865900	-1.44671900
H	0.00237600	-2.23059900	-1.41565300
H	1.31770200	-1.70900400	-2.49022000
H	1.71094400	-2.42556600	-0.92942700
H	1.81020700	0.22060400	3.71019300
H	3.51010900	0.08188800	3.26820300
H	2.67849600	1.60705800	3.02733300
C	-4.33112800	-0.87132500	0.78474000
C	-3.59667000	0.60106700	-1.44490000
C	-5.41853100	-0.62822600	-0.28885900
H	-4.52771000	-0.23746200	1.65783500
C	-5.08597100	0.66578400	-1.05133500
H	-3.48279400	-0.15683600	-2.23379500
H	-5.41940700	-1.47162500	-0.99126900
H	-6.41218600	-0.59199600	0.16814500
H	-5.71673500	0.78921300	-1.93760400
H	-5.26635800	1.54148100	-0.41315300
P	-2.78457000	-0.22869400	-0.00538500
O	-1.70773400	-1.23314900	-0.36608400
C	-2.97177000	1.91183900	-1.92092800
C	-4.20121900	-2.32800600	1.23436500
H	-3.47198700	-2.42223300	2.04159300
H	-5.16824700	-2.69011100	1.59955700

H	-3.88955100	-2.96878700	0.40369100
H	-1.91065200	1.78599400	-2.16379900
H	-3.47870000	2.26456100	-2.82484800
H	-3.05286800	2.69701200	-1.16316600
C	0.07777800	-1.95786400	1.72849300
H	-0.90424900	-2.23737800	1.34992600
H	0.81610300	-2.66280000	1.33486300
C	0.13120500	-1.91448600	3.23155600
C	-0.98984900	-1.17302700	3.88413500
O	-0.70998500	-0.79474000	5.13731000
C	-1.76307400	-0.08165900	5.81968000
H	-1.36310900	0.14818600	6.80592400
H	-2.00633300	0.83249500	5.27265500
H	-2.65472400	-0.70723800	5.89722100
O	-2.04041300	-0.92288500	3.31885500
C	1.06968300	-2.53841400	3.95340500
H	1.06164000	-2.50416900	5.03686600
H	1.85959400	-3.11409600	3.47924100

^tBuO⁻

O	8.54687700	0.01846400	-1.66079000
C	8.92190600	0.21149000	-2.91590800
C	7.70270400	0.54253200	-3.86066100
C	9.63407500	-1.05562800	-3.52924900
C	9.93794400	1.40942400	-3.05918100
H	10.50625500	-1.30004600	-2.90663500
H	8.94120700	-1.90667200	-3.46892100
H	9.97129300	-0.95389600	-4.57751300
H	10.28701600	1.61825700	-4.08743900
H	9.46321500	2.31810300	-2.66293500
H	10.81510900	1.19904700	-2.43120000
H	7.95456700	0.71356000	-4.92377100
H	6.98413800	-0.28714000	-3.80353100
H	7.19702000	1.43934600	-3.47573900

TS3

C	-2.09611700	1.22943200	1.15443000
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C	-0.69770200	1.04523000	1.28214600
C	0.04425300	2.07804300	1.87635500
C	-0.55534700	3.23512700	2.37078200
C	-1.93541600	3.38372800	2.29173500
C	-2.68803600	2.38619900	1.67649100
H	1.11443800	1.98363600	1.96344800
H	0.05965100	4.00724300	2.82366200
H	-2.42390300	4.26733800	2.69173600
H	-3.76244400	2.51711400	1.60044600
C	2.00291200	-0.33916600	1.31618300
C	0.48008600	-0.70826800	-0.93129400
C	2.57129400	0.34301300	0.06093000
H	2.27967500	-1.40421100	1.26067100
C	1.99459100	-0.41891300	-1.13687200
H	-0.12845600	0.07832800	-1.38914300
H	2.28825300	1.40482100	0.03190500
H	3.66690100	0.30403000	0.06814600
H	2.15205400	0.11064500	-2.08265200
H	2.50736500	-1.38392000	-1.20536500
P	0.20076300	-0.53729400	0.90854200
C	2.51911300	0.20649700	2.65634200
C	0.09876700	-2.07498300	-1.50838100
H	-0.97259000	-2.24941800	-1.43109500
H	0.39339100	-2.10309600	-2.56514500
H	0.64369300	-2.85498200	-0.97042900
H	1.80525000	0.07670800	3.47214100
H	3.43030500	-0.33515900	2.93136600
H	2.78764800	1.26706800	2.59868300
C	-4.75945900	-0.18179900	1.13394300
C	-3.93171800	1.13539800	-1.15163000
C	-5.86341000	0.37303700	0.20187800
H	-4.70750700	0.40901400	2.05491600
C	-5.30831200	1.55709200	-0.60897300
H	-4.08906300	0.37980600	-1.93491600
H	-6.16461500	-0.42154800	-0.49345800
H	-6.75615000	0.64934900	0.77360700
H	-5.98396400	1.83978600	-1.42466300
H	-5.20301600	2.44413700	0.02955800
P	-3.17725200	0.10464300	0.20097700
O	-2.45123900	-1.11251300	-0.30702500
C	-3.06658500	2.25937000	-1.71820700

C	-4.95094700	-1.65761200	1.49077000
H	-4.18986100	-1.98391500	2.20030900
H	-5.93990900	-1.80685900	1.94066400
H	-4.88138300	-2.28620500	0.59755300
H	-2.09578200	1.88035100	-2.05651000
H	-3.56071800	2.72687800	-2.57762800
H	-2.88002400	3.03731900	-0.97154500
C	-0.39080900	-1.99176200	1.73398800
H	-1.37411400	-2.23251400	1.33322100
C	-0.36855500	-1.89309500	3.22825500
C	-1.55941100	-1.29394400	3.89663700
O	-1.49841000	-1.31472400	5.24771300
C	-2.61624300	-0.72011100	5.91691700
H	-2.40095600	-0.80819300	6.98221300
H	-2.72264400	0.33012800	5.63065200
H	-3.54062600	-1.24841900	5.66742200
O	-2.51148400	-0.80855200	3.30510700
C	0.67980700	-2.32072800	3.95445300
H	0.69789500	-2.24215600	5.03579600
H	1.53007000	-2.75827300	3.44038800
H	0.58909700	-2.84852000	1.37744100
C	1.82554500	-4.77131200	1.02698700
C	2.53262800	-5.30399600	2.29043500
C	2.66185900	-5.14078100	-0.21351600
C	0.42901700	-5.41624100	0.91758600
H	3.63845700	-4.64604300	-0.15833400
H	2.82449900	-6.22318200	-0.30108600
H	2.15882100	-4.79308700	-1.12324800
H	-0.17624700	-5.15749800	1.79458600
H	-0.09298500	-5.04746600	0.02723500
H	0.48768700	-6.51028400	0.85355000
H	3.50531300	-4.81098600	2.40200100
H	1.93351800	-5.07954100	3.18101100
H	2.69493100	-6.38939600	2.25392000
O	1.72367200	-3.37462800	1.09363500

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O	8.50483900	0.06910100	-1.67044100
C	8.96880400	0.24646700	-3.01963100

C	7.70898500	0.54396800	-3.83237600
C	9.64080300	-1.04374300	-3.50706600
C	9.94685900	1.42705500	-3.07695900
H	10.52741400	-1.27231200	-2.90120500
H	8.94549100	-1.88533900	-3.42654900
H	9.96525100	-0.95653300	-4.55022300
H	10.28421400	1.61801700	-4.10204600
H	9.46806300	2.33313700	-2.69222500
H	10.83667900	1.22396500	-2.46670300
H	7.95455700	0.69686700	-4.88847900
H	7.00319600	-0.28896900	-3.75341400
H	7.21849900	1.44567400	-3.45225300
H	9.28316100	-0.12201400	-1.12302500

III

C	-1.93654900	0.69287400	0.43158900
C	-0.56538900	1.04817600	0.47662700
C	-0.08401200	2.02636900	-0.40164800
C	-0.92080000	2.64301800	-1.33248100
C	-2.26313100	2.28604800	-1.38963800
C	-2.76093800	1.32626300	-0.50764400
H	0.96148900	2.30711600	-0.37415700
H	-0.51927200	3.39241900	-2.00815500
H	-2.92773200	2.75402300	-2.11003400
H	-3.81432700	1.07722300	-0.55544400
C	0.55321700	0.79667800	3.35302000
C	2.31910800	0.89301400	1.28606800
C	2.04549400	0.99034100	3.75496900
H	0.05591100	0.01575800	3.92666800
C	2.97827600	0.51362300	2.62392100
H	2.26905900	1.98955700	1.22517900
H	2.22279800	2.05724700	3.93705200
H	2.26364400	0.46843500	4.69203000
H	3.97736100	0.95562400	2.71223900
H	3.10138600	-0.57575200	2.66374900
P	0.60773300	0.19022700	1.59486300
C	-0.25806100	2.09090400	3.48734200
C	3.01028900	0.30812100	0.05913300
H	2.52883200	0.62509100	-0.87293900

H	4.06122700	0.61708900	0.01829000
H	2.97180000	-0.78592300	0.09581400
H	-1.31185500	1.90471800	3.27851000
H	-0.17069400	2.46577500	4.51389300
H	0.11253400	2.87615800	2.81662200
C	-4.52590000	-0.17514700	1.67298400
C	-2.85161700	-2.18788600	0.95904900
C	-4.98080400	-1.54568600	2.21004500
H	-4.91482000	-0.07301500	0.65117700
C	-4.30013400	-2.62516400	1.34127200
H	-2.10229900	-2.77809100	1.48798100
H	-4.66455300	-1.63952500	3.25567200
H	-6.07241700	-1.64030300	2.18748500
H	-4.29138300	-3.59442600	1.84895800
H	-4.87999800	-2.75354400	0.41867400
P	-2.69893600	-0.47222300	1.64193700
O	-2.13633900	-0.32901000	3.03361300
C	-2.59996100	-2.28457800	-0.54833400
C	-4.92911800	1.02577900	2.52273900
H	-4.59647400	1.96526000	2.06640700
H	-6.01774000	1.07434100	2.64246300
H	-4.47139700	0.95351300	3.51370200
H	-1.57879100	-2.00035900	-0.80590100
H	-2.75847500	-3.31542500	-0.88457700
H	-3.28957000	-1.64366900	-1.11115300
C	0.42287600	-1.47778600	1.31593900
H	0.23050500	-1.70640700	0.27633200
C	0.76579700	-2.57539900	2.18939100
C	0.54626500	-3.96155700	1.64275000
O	-0.03436900	-3.95808600	0.40933000
C	-0.26094500	-5.25336300	-0.15299900
H	-0.92818200	-5.84024900	0.48444800
H	-0.71961700	-5.07423100	-1.12650300
H	0.68105000	-5.79707100	-0.26523500
O	0.83384400	-5.00252000	2.19952400
C	1.24024200	-2.57040500	3.46207100
H	1.38369700	-3.50772200	3.98288300
H	1.46558800	-1.65950700	4.00055000

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C	3.62734800	-1.28327000	-0.00003700
C	3.66329400	0.12436200	0.00001200
C	4.91821900	0.75901700	0.00006400
C	6.09736400	0.01831000	0.00006600
C	6.04387300	-1.37568500	0.00001500
C	4.80376500	-2.02270100	-0.00003600
H	2.67183000	-1.79821300	-0.00007700
H	4.95861900	1.84507800	0.00010500
H	7.05639700	0.52810800	0.00010700
H	6.96120700	-1.95730200	0.00001400
H	4.75789200	-3.10799100	-0.00007600
C	2.46197700	0.95155100	0.00001500
H	2.61963200	2.02912400	0.00008700
C	1.17798900	0.54277200	-0.00004500
H	0.89626200	-0.50616400	-0.00010900
C	0.07946900	1.53301800	-0.00002700
O	0.26101800	2.74898700	-0.00002400
C	-1.25680700	0.97218800	-0.00005400
C	-2.37736800	0.50008600	-0.00007500
C	-3.69799400	-0.02827100	-0.00002800
C	-4.80807100	0.83846900	0.00001100
C	-3.91083300	-1.42014300	-0.00002200
C	-6.09880100	0.31980200	0.00005400
H	-4.63958500	1.91026900	0.00000500
C	-5.20526400	-1.92952500	0.00002400
H	-3.05358000	-2.08551200	-0.00005200
C	-6.30067200	-1.06256900	0.00006100
H	-6.95005900	0.99415000	0.00008300
H	-5.36161900	-3.00424600	0.00002900
H	-7.31006200	-1.46366000	0.00009600

Re-TS4

C	-1.92964400	0.67147900	0.43295600
C	-0.55185800	1.00041400	0.49912400
C	-0.04226500	1.93954300	-0.40800700
C	-0.85368300	2.54660400	-1.36600800
C	-2.20279800	2.21809700	-1.43551200
C	-2.72711800	1.28761500	-0.54026800

H	1.00751600	2.20102800	-0.38632600
H	-0.42472100	3.26801300	-2.05472800
H	-2.84701900	2.68028500	-2.17736500
H	-3.78112400	1.04131600	-0.60430300
C	0.56048600	0.93679800	3.40134400
C	2.34430700	0.78373000	1.30569900
C	1.99189600	1.47726400	3.64610000
H	0.38787400	0.11048800	4.09430000
C	2.98228900	0.77853300	2.70653500
H	2.28247200	1.83485200	0.99629200
H	2.01377500	2.55744900	3.44629700
H	2.23824500	1.30712400	4.69615200
H	3.95269500	1.28733300	2.68413000
H	3.16735900	-0.25054900	3.03202800
P	0.60820000	0.20879500	1.68700200
C	-0.51762200	2.00321500	3.60056800
C	3.06197300	-0.04123400	0.24308700
H	2.56036000	0.02391900	-0.72910100
H	4.09090300	0.31469400	0.11908400
H	3.09282700	-1.09577700	0.53139500
H	-1.51348500	1.56705300	3.52443500
H	-0.40021900	2.42505500	4.60455900
H	-0.42117200	2.82353500	2.87836200
C	-4.50822600	-0.12886200	1.79755700
C	-2.99866800	-2.14756000	0.69471400
C	-5.06509800	-1.54774500	2.03553200
H	-4.93454600	0.24709400	0.85882600
C	-4.50944500	-2.44229600	0.91311700
H	-2.38139100	-2.86463200	1.24213300
H	-4.72974300	-1.90816500	3.01632100
H	-6.16051700	-1.54526600	2.04839500
H	-4.66767700	-3.50463300	1.12366700
H	-5.04943600	-2.21672000	-0.01599100
P	-2.71924000	-0.53201000	1.57474000
O	-2.01762400	-0.60306300	2.90868300
C	-2.60859000	-2.18885100	-0.78470000
C	-4.74949100	0.86862000	2.92777400
H	-4.34253700	1.85530000	2.68019400
H	-5.82214900	0.98265500	3.12041200
H	-4.26321600	0.52603800	3.84536700
H	-1.53822400	-2.03258700	-0.93599600

H	-2.86020800	-3.17121500	-1.20065300
H	-3.14828400	-1.43484000	-1.36846900
C	0.42623700	-1.50789700	1.40539700
H	-0.07950000	-1.71797900	0.47324800
C	0.93586900	-2.57659200	2.13220700
C	0.75409700	-3.94782000	1.54542300
O	-0.22810300	-3.99925500	0.60760000
C	-0.50830200	-5.31318200	0.10558300
H	-0.84523700	-5.95795700	0.92073400
H	-1.30027300	-5.17949600	-0.63253000
H	0.38073600	-5.74845700	-0.35747800
O	1.39479700	-4.92794500	1.86364200
C	1.51300800	-2.58535300	3.42523800
H	2.08908100	-3.46919200	3.66862300
H	1.88487400	-1.66005200	3.85096700
C	-0.25695200	-5.27437500	4.53871400
C	-0.74363100	-3.97036700	4.36757800
C	-2.00077700	-3.79893500	3.76955600
C	-2.75131100	-4.90003800	3.35705700
C	-2.25486400	-6.19358600	3.52878300
C	-1.00275000	-6.37436900	4.12231800
H	0.72663800	-5.42237500	4.97341800
H	-2.37196900	-2.78802500	3.63999200
H	-3.73170300	-4.74907700	2.91108100
H	-2.83811400	-7.05302300	3.20858400
H	-0.60273300	-7.37604800	4.25352700
C	0.03769800	-2.77606200	4.77978600
C	0.68180000	-2.76455000	6.04243100
H	0.78623700	-3.67978800	6.61583300
C	1.29423700	-1.58494700	6.52478400
O	1.36664700	-0.49926600	5.88209300
C	1.89294800	-1.66247700	7.84787800
C	2.40344900	-1.69216900	8.95159000
C	3.00126400	-1.72955800	10.24209100
C	3.60594200	-0.57881300	10.78568000
C	2.99985800	-2.91689000	11.00063500
C	4.18942400	-0.61871500	12.04827900
H	3.60770600	0.33679300	10.20307800
C	3.58610300	-2.94849300	12.26220100
H	2.53412800	-3.80453000	10.58456400
C	4.18263600	-1.80158900	12.79135700

H	4.65188500	0.27640400	12.45526600
H	3.57768300	-3.87122800	12.83594400
H	4.63921700	-1.82941500	13.77676500
H	-0.42790400	-1.83972800	4.47974100

3R-IV

C	-2.13170400	0.60736600	0.59138200
C	-0.77530200	1.01703300	0.63213300
C	-0.34691300	1.99687500	-0.27422200
C	-1.22072400	2.56218100	-1.20321800
C	-2.54774300	2.14813700	-1.24933200
C	-2.99210500	1.17684900	-0.35382700
H	0.68319300	2.32794400	-0.27451800
H	-0.85593500	3.31992700	-1.88975600
H	-3.23536900	2.57771800	-1.97140200
H	-4.03046100	0.86366600	-0.39054500
C	0.56070600	0.94080800	3.48917200
C	2.16129100	0.84449800	1.24430800
C	2.00048700	1.50080100	3.61254600
H	0.49545000	0.09437100	4.18670800
C	2.90813400	0.80821900	2.59093800
H	2.06581600	1.90356500	0.97421400
H	1.99907800	2.58266100	3.42009100
H	2.32749900	1.31334600	4.63728300
H	3.88007100	1.30495300	2.49625000
H	3.10298700	-0.22682700	2.89265000
P	0.46979300	0.26457300	1.76603000
C	-0.51910800	1.97110100	3.81688200
C	2.80260800	0.06747700	0.09908100
H	2.21404900	0.13792300	-0.82285600
H	3.80256500	0.46431200	-0.10748400
H	2.90169000	-0.99091700	0.35566400
H	-1.50840200	1.51440400	3.80553700
H	-0.32345500	2.35078100	4.82508500
H	-0.50161500	2.82358600	3.12593200
C	-4.53724400	-0.24759700	2.20557600
C	-3.09736000	-2.25108400	0.97546700
C	-5.05869500	-1.67516800	2.47126000
H	-5.04805500	0.14348100	1.31551000

C	-4.58306800	-2.56105100	1.30603000
H	-2.43881900	-2.94272200	1.50990300
H	-4.64519000	-2.03900100	3.41992100
H	-6.14957000	-1.68380900	2.56978000
H	-4.70611000	-3.62451600	1.53164700
H	-5.19579000	-2.34227700	0.42138700
P	-2.77913500	-0.61400400	1.79035900
O	-1.88770600	-0.63100300	3.00878500
C	-2.79994100	-2.32670100	-0.52338600
C	-4.67612400	0.73042100	3.37007000
H	-4.29906900	1.72358600	3.10280700
H	-5.72673800	0.83364300	3.66296300
H	-4.10634700	0.37730900	4.23424400
H	-1.74359200	-2.15726800	-0.74242900
H	-3.05805200	-3.32391800	-0.89723000
H	-3.38878900	-1.59829700	-1.09204700
C	0.38419400	-1.48362600	1.40823700
H	-0.03549100	-1.65334600	0.42150600
C	0.86236900	-2.54920200	2.09745000
C	0.80141700	-3.88370900	1.41194100
O	-0.28104500	-4.01316500	0.60639800
C	-0.43407700	-5.30993200	0.00785500
H	-0.56778900	-6.06087200	0.78999300
H	-1.32685600	-5.23917300	-0.61392700
H	0.44056700	-5.56329200	-0.59591200
O	1.62825800	-4.75950200	1.55153400
C	1.36408300	-2.59730400	3.48814100
H	2.04331400	-3.44202900	3.60233000
H	1.87119300	-1.68468600	3.80836200
C	-0.24720400	-5.21119000	4.05932700
C	-0.74274000	-3.91304200	4.23894200
C	-2.12598400	-3.71376500	4.13891200
C	-2.98789700	-4.77110700	3.84328000
C	-2.47837800	-6.05459200	3.63845000
C	-1.10346300	-6.27034300	3.75378600
H	0.81962200	-5.39207700	4.14101000
H	-2.51237700	-2.71128200	4.29025100
H	-4.05962000	-4.59505300	3.78219300
H	-3.14551200	-6.88029100	3.40516500
H	-0.69494400	-7.26784900	3.61289100
C	0.16477800	-2.74267900	4.54512600

C	0.72798500	-2.76478300	5.92223800
H	0.68581100	-3.67197900	6.51454900
C	1.39133800	-1.64146300	6.38919400
O	1.56060300	-0.55588500	5.72017700
C	1.94727300	-1.71528100	7.73159800
C	2.43060800	-1.72852800	8.84861000
C	2.99544700	-1.75422700	10.15330400
C	3.67710900	-0.63143100	10.66570200
C	2.88793500	-2.90215000	10.96476800
C	4.22954600	-0.65982400	11.94257400
H	3.76279700	0.25508200	10.04534100
C	3.44320200	-2.92264600	12.24059300
H	2.36411400	-3.76972600	10.57602100
C	4.11637300	-1.80361000	12.73667200
H	4.75175800	0.21506300	12.32123900
H	3.35067600	-3.81650400	12.85206400
H	4.54892200	-1.82273300	13.73321400
H	-0.41921500	-1.82901800	4.39964900

3R-TS5

C	-1.65693400	1.59946100	0.85125400
C	-1.07143000	2.06982100	2.05207400
C	-1.00007400	3.45986800	2.25056100
C	-1.45734500	4.36709200	1.29963400
C	-1.99397200	3.90251100	0.10524300
C	-2.09416600	2.53031300	-0.10451100
H	-0.55457100	3.83314600	3.16310800
H	-1.34787200	5.42972100	1.48373800
H	-2.33017600	4.59611400	-0.65932700
H	-2.51969600	2.17694300	-1.03876100
C	0.82685500	-0.31402500	3.30534900
C	-1.73489600	0.14237500	4.33739000
C	0.12413500	-1.48329700	4.04490100
H	1.66661500	0.05271500	3.90139600
C	-0.90487400	-0.94388500	5.05148000
H	-2.29083200	-0.33129500	3.52491200
H	-0.39054200	-2.09615300	3.30211600
H	0.88333300	-2.09866300	4.53892700
H	-1.56133700	-1.74164100	5.41734800

H	-0.40165500	-0.50543500	5.92290200
P	-0.39985500	1.09190000	3.48534300
C	1.39684900	-0.71966000	1.95069700
C	-2.67772100	0.94456900	5.23015300
H	-3.14859800	1.77117900	4.68634500
H	-3.47621200	0.29015800	5.59763100
H	-2.16488700	1.35643900	6.10463800
H	1.85217000	0.11931100	1.42134200
H	2.20645800	-1.43366500	2.13598900
H	0.63924500	-1.19927100	1.33296600
C	-3.57438600	-0.35633500	-0.33678900
C	-0.91517400	-0.55109900	-1.09983600
C	-3.27579400	-1.20822100	-1.58745600
H	-3.92976200	0.62848200	-0.66080800
C	-1.97900600	-0.67013400	-2.21353700
H	-0.52310500	-1.55326000	-0.88001100
H	-3.13568300	-2.25550300	-1.28809500
H	-4.11448600	-1.18362300	-2.29177600
H	-1.61917500	-1.30751000	-3.02851600
H	-2.16403900	0.32314500	-2.64606500
P	-1.89661300	-0.15884300	0.43457300
O	-1.66875700	-1.07946500	1.60830500
C	0.24884600	0.38317900	-1.43449400
C	-4.57855200	-0.96528600	0.64100800
H	-4.78025700	-0.28647300	1.47654800
H	-5.52849500	-1.17085000	0.13479700
H	-4.19458000	-1.90033400	1.05835600
H	0.98019600	0.42465200	-0.62359400
H	0.76473400	0.03035700	-2.33446800
H	-0.09876500	1.40350300	-1.62374600
C	0.22107200	2.21864800	4.69042800
H	-0.46705300	2.39454400	5.50605600
C	1.45674100	2.83818800	4.76052800
C	1.68853100	3.67123400	6.00167000
O	0.95330200	3.26642200	7.06248900
C	1.11518900	4.05894600	8.24757100
H	0.81618800	5.09424900	8.06222200
H	0.46995600	3.59924400	8.99672200
H	2.15760600	4.04616300	8.57543000
O	2.44033000	4.62383100	6.05565400
C	2.57601900	2.80796200	3.87812000

H	3.34202000	3.53260500	4.15125600
H	3.20890800	1.63915500	4.04127000
C	1.93458600	5.20690800	2.30058400
C	2.05858600	3.98084000	1.63973700
C	1.80092500	3.93706400	0.26159300
C	1.42617000	5.08033300	-0.43803500
C	1.30305300	6.30091800	0.23159700
C	1.55992400	6.35780500	1.60107700
H	2.12719300	5.26381000	3.36691300
H	1.88255500	2.98689000	-0.26055900
H	1.22558300	5.02067800	-1.50483600
H	1.01402400	7.19730600	-0.31073600
H	1.47418600	7.30242900	2.13213500
C	2.41304300	2.68449100	2.35694000
C	3.62957700	2.01442700	1.76096500
H	4.02026000	2.34681200	0.80742600
C	4.26490300	1.02256200	2.45324600
O	3.87446000	0.61023600	3.65756200
C	5.41304000	0.37367300	1.88861900
C	6.36776300	-0.20987000	1.41273800
C	7.48818100	-0.88607400	0.85636100
C	8.15254000	-1.89314300	1.58466700
C	7.95552800	-0.56399700	-0.43345600
C	9.24776100	-2.55366800	1.03661800
H	7.79613000	-2.14255400	2.57892300
C	9.05155500	-1.22969800	-0.97369600
H	7.44784300	0.21257500	-0.99680100
C	9.70240700	-2.22655400	-0.24310500
H	9.75029700	-3.32735000	1.61081600
H	9.40095800	-0.96919400	-1.96918000
H	10.55826600	-2.74391100	-0.66743400
H	1.54887800	2.02067400	2.17417900

3R-V

C	-1.65654000	1.62753300	0.87910100
C	-1.01549300	2.05662700	2.06760300
C	-0.89474600	3.44117400	2.28178900
C	-1.34302700	4.38023800	1.35857000
C	-1.94041200	3.95455300	0.17827100

C	-2.10211900	2.59075700	-0.04326300
H	-0.42415000	3.77541000	3.19864900
H	-1.19097000	5.43609700	1.55297200
H	-2.28070000	4.67110700	-0.56304900
H	-2.58647600	2.26950100	-0.96063400
C	0.93025900	-0.28123200	3.08528000
C	-1.57457800	-0.01560700	4.28652000
C	0.31712200	-1.54343100	3.75254600
H	1.79900500	0.04254400	3.66428700
C	-0.68432200	-1.14293600	4.84858500
H	-2.15145900	-0.42443300	3.45375300
H	-0.21196600	-2.10905700	2.98318100
H	1.11997600	-2.17111900	4.15428100
H	-1.30089800	-1.99801700	5.15001100
H	-0.16044600	-0.77968300	5.74133300
P	-0.30739400	1.06988400	3.49854800
C	1.38776800	-0.54152700	1.65136200
C	-2.50247700	0.64851800	5.29954000
H	-3.03843000	1.49859800	4.86336900
H	-3.24830900	-0.07800000	5.64247500
H	-1.95958300	1.00326400	6.18064500
H	1.73055100	0.36559100	1.14826400
H	2.24233200	-1.22724300	1.67657800
H	0.59069500	-1.00640600	1.07275200
C	-3.78747400	-0.17519700	-0.14205500
C	-1.26433600	-0.45814800	-1.25169300
C	-3.69938000	-0.96881400	-1.46133000
H	-4.12272900	0.84376800	-0.36659200
C	-2.46371100	-0.46369300	-2.22439500
H	-0.91563800	-1.49200800	-1.12394700
H	-3.58218700	-2.03697800	-1.23467800
H	-4.61776200	-0.86288800	-2.04931800
H	-2.24640100	-1.07569900	-3.10685200
H	-2.64559700	0.55823400	-2.58541900
P	-2.01671100	-0.10194600	0.41796800
O	-1.68959000	-1.12033400	1.48128400
C	-0.08891100	0.41357100	-1.69460400
C	-4.69196900	-0.78782600	0.92626900
H	-4.74352500	-0.14959100	1.81499200
H	-5.71009700	-0.91415400	0.54075600
H	-4.31263200	-1.76419200	1.24077600

H	0.74186200	0.35444500	-0.98670800
H	0.27743500	0.08081700	-2.67250700
H	-0.37668800	1.46549100	-1.78234300
C	0.29645000	2.11193300	4.72689500
H	-0.33401300	2.13847200	5.60227900
C	1.46995000	2.92085800	4.76844000
C	1.74080400	3.61105500	6.08994700
O	0.96159600	3.15134600	7.09893600
C	1.17441700	3.78975600	8.36311400
H	0.97426900	4.86254400	8.29304800
H	0.47732800	3.31250400	9.05299300
H	2.20554000	3.64689900	8.69707100
O	2.56040700	4.49130900	6.26630400
C	2.43222900	3.20875600	3.82653900
H	3.23337500	3.86994100	4.13929700
C	2.02189700	5.28359300	1.81968000
C	2.09747900	3.95069600	1.41040400
C	1.81394900	3.64240300	0.07330600
C	1.45442100	4.63696700	-0.83196400
C	1.38100200	5.96812500	-0.41394600
C	1.66964800	6.28650600	0.91287200
H	2.21900400	5.53132600	2.85761800
H	1.85391400	2.60597500	-0.25354600
H	1.22504300	4.37422300	-1.86150100
H	1.10180200	6.74836000	-1.11688300
H	1.61852300	7.31923500	1.24807000
C	2.42942900	2.80847300	2.37394000
C	3.71006100	2.11250000	1.94513900
H	4.10082400	2.32339600	0.95628500
C	4.37939000	1.21006200	2.69858600
O	4.02851100	0.85225300	3.97289100
C	5.51830400	0.51766200	2.19968100
C	6.47660800	-0.09105400	1.76667400
C	7.59857000	-0.80219700	1.25941900
C	8.27575100	-1.73765000	2.06622800
C	8.05011200	-0.58464800	-0.05704200
C	9.37178000	-2.43331700	1.56568300
H	7.92970100	-1.90525200	3.08100000
C	9.14778400	-1.28454300	-0.54816400
H	7.53054200	0.13662400	-0.67974600
C	9.81237100	-2.21073700	0.25895600

H	9.88563400	-3.15195200	2.19799200
H	9.48692200	-1.10679400	-1.56491300
H	10.66899600	-2.75527500	-0.12779600
H	1.61739200	2.08577600	2.22115600
H	3.41631100	1.56033500	4.29525100

3R-TS6

C	-1.57907600	1.34820200	0.95532000
C	-0.79073200	1.31853300	2.13080800
C	-0.80502100	2.46004400	2.95354000
C	-1.46204600	3.63061000	2.58159100
C	-2.10983800	3.69908800	1.35208600
C	-2.18895800	2.55166500	0.56876100
H	-0.30032900	2.42940200	3.90796300
H	-1.44226400	4.48818300	3.24706800
H	-2.58493000	4.61845400	1.02333700
H	-2.76273900	2.58657400	-0.35229400
C	1.19651100	-1.29535300	1.70268200
C	-0.66119200	-1.22398600	3.76204700
C	0.63211200	-2.64671300	2.19890500
H	2.21145500	-1.19163000	2.10084900
C	0.19140300	-2.50304400	3.66322300
H	-1.55672300	-1.36760300	3.14831300
H	-0.22448100	-2.92432700	1.58280000
H	1.40695300	-3.41401000	2.09056500
H	-0.38769000	-3.37154300	3.99751000
H	1.06519200	-2.41798000	4.32267500
P	0.33664500	-0.00946100	2.78489800
C	1.29148100	-1.18758000	0.18397000
C	-1.04437300	-0.78185700	5.17061100
H	-1.58971600	0.16817200	5.16050100
H	-1.69234900	-1.53648700	5.63083500
H	-0.16758400	-0.65918700	5.81320100
H	1.60224900	-0.19500100	-0.15055100
H	2.05640100	-1.89300900	-0.16080600
H	0.34772900	-1.45400100	-0.28738600
C	-3.94413600	-0.03874800	-0.17847000
C	-1.65552200	-0.06623200	-1.73809800
C	-4.11049100	-0.56609300	-1.61669200

H	-4.23726900	1.01739000	-0.16112600
C	-3.01190500	0.09229600	-2.46587200
H	-1.26065000	-1.06991700	-1.94239100
H	-3.98681100	-1.65730700	-1.62247000
H	-5.11302500	-0.35222000	-2.00347400
H	-2.96140600	-0.32825600	-3.47592700
H	-3.23369500	1.16277100	-2.57838300
P	-2.10787200	-0.15607600	0.06764500
O	-1.70806200	-1.41245200	0.80142200
C	-0.61665700	0.98313400	-2.13541300
C	-4.71296300	-0.80444800	0.89613600
H	-4.58131500	-0.34296000	1.88077100
H	-5.78464600	-0.81460900	0.66716300
H	-4.35829400	-1.83674000	0.96231400
H	0.33101600	0.85589500	-1.60971700
H	-0.41280600	0.91908100	-3.21008200
H	-0.96521400	1.99779300	-1.92607800
C	1.60407500	0.71671800	3.82817500
H	1.36986400	0.45774000	4.85844600
C	2.03865300	2.13955800	3.71494300
C	1.94766700	3.04410500	4.89294000
O	1.15101500	2.52656500	5.87545200
C	1.01866700	3.35255000	7.03812300
H	0.57751400	4.31890400	6.77834600
H	0.36660600	2.80176000	7.71726800
H	1.99473500	3.52692700	7.49826600
O	2.46536100	4.13933700	5.00145500
C	2.59200200	2.67416100	2.60516100
H	2.94471400	3.70057100	2.63328700
C	1.41569800	3.54730000	0.08656800
C	2.42758700	2.57885700	0.07655300
C	2.98863900	2.21313400	-1.15362600
C	2.55845300	2.80871000	-2.34017700
C	1.55684000	3.78039500	-2.31701100
C	0.98464400	4.14464900	-1.09702900
H	0.96016200	3.82920800	1.03017000
H	3.76489300	1.45419300	-1.17469000
H	3.00959900	2.51401300	-3.28396300
H	1.22583900	4.24822200	-3.24020800
H	0.20019200	4.89644800	-1.06383400
C	2.82943300	1.87159600	1.36056700

C	4.24941300	1.35025800	1.38483200
H	4.99840100	1.84890900	0.78060000
C	4.63821700	0.32219700	2.19496400
O	3.89599600	-0.35159800	3.07018700
C	5.99560400	-0.13834800	2.08976800
C	7.13721200	-0.54862200	2.01064300
C	8.47351100	-1.02698000	1.91908900
C	8.89562200	-2.12699600	2.69204400
C	9.40040500	-0.41181100	1.05434300
C	10.20314600	-2.59376000	2.59890000
H	8.18433300	-2.60180200	3.36017900
C	10.70650000	-0.88414700	0.96864400
H	9.07926800	0.43641900	0.45813400
C	11.11397000	-1.97601700	1.73859000
H	10.51425000	-3.44298400	3.20125300
H	11.41036100	-0.39857200	0.29811700
H	12.13430600	-2.34248200	1.66920900
H	2.18125700	0.99185100	1.41918900
H	2.83098700	0.11334800	3.42489000

3R-VI

C	2.91508500	0.87230300	1.54763100
C	2.60676400	0.32598500	2.81789100
C	3.54162200	0.50501800	3.85239600
C	4.72633400	1.21365500	3.65796700
C	5.00429900	1.77804600	2.41735400
C	4.09929800	1.59828000	1.37440200
H	3.35480900	0.08960300	4.83266100
H	5.42263200	1.32646000	4.48327000
H	5.91674200	2.34421000	2.25761900
H	4.32479000	2.02484500	0.40131900
C	-0.46205800	0.48718200	3.18084300
C	1.02774800	-0.72438400	5.12307000
C	-1.21189900	0.25247900	4.52765700
H	-1.04117900	0.14612400	2.32478200
C	-0.48908100	-0.78939900	5.40266500
H	1.41470700	0.22897100	5.50717500
H	-1.26285500	1.21123300	5.05636300
H	-2.24092900	-0.05687200	4.32301700

H	-0.66965400	-0.60339800	6.46731200
H	-0.83558300	-1.80849900	5.19091700
P	1.05561300	-0.57644300	3.27038000
C	-0.11163700	1.96565300	2.99208500
C	1.78670300	-1.90553100	5.74014400
H	2.83283500	-1.95957100	5.41891200
H	1.77763900	-1.80598400	6.83119900
H	1.29225600	-2.84869700	5.49262400
H	0.40959400	2.14430600	2.05417400
H	-1.03970100	2.54724400	2.98055500
H	0.51020900	2.34205700	3.81257500
C	1.63273800	2.16071200	-0.86999500
C	2.85885800	-0.29640300	-1.21637500
C	1.78527400	1.67275700	-2.32527600
H	2.47368300	2.82845900	-0.63936600
C	2.98992100	0.72513600	-2.36749600
H	2.17343400	-1.09813200	-1.51534900
H	0.87380500	1.13712700	-2.62294200
H	1.89991600	2.52023800	-3.00996300
H	3.07934700	0.21297500	-3.33158700
H	3.91299100	1.30537400	-2.22944600
P	1.86130000	0.58349100	0.08900100
O	0.57090000	-0.07467400	0.51378300
C	4.18998300	-0.91738200	-0.79059600
C	0.30726500	2.86961000	-0.59204700
H	0.31423500	3.38325200	0.37271700
H	0.11421700	3.62031100	-1.36679400
H	-0.52101700	2.15459100	-0.58738300
H	4.05303200	-1.62011400	0.03089100
H	4.61827900	-1.46845600	-1.63582200
H	4.91300200	-0.15023500	-0.49591000
C	0.94126800	-2.32953700	2.70738300
H	1.98092300	-2.67084200	2.69964400
C	0.26804600	-2.72513600	1.42636200
C	1.17136700	-3.11069700	0.34279900
O	0.54103400	-3.54293600	-0.77914500
C	1.39658800	-4.03514900	-1.81241100
H	2.01555300	-3.23342900	-2.22792200
H	2.05418600	-4.82123200	-1.43206000
H	0.73019400	-4.43006700	-2.58023600
O	2.39503100	-3.06042600	0.41204700

C	-1.07481000	-2.82454500	1.30317100
H	-1.47999300	-3.20281600	0.36939800
C	-2.98083600	-0.68264400	0.86523400
C	-3.18955600	-1.60014500	1.90529500
C	-4.42612300	-1.60361300	2.56131300
C	-5.43017300	-0.70923400	2.19164700
C	-5.21495300	0.20213200	1.15514200
C	-3.98646700	0.21167600	0.49380800
H	-2.02097800	-0.66228900	0.35426700
H	-4.58499000	-2.32111000	3.36158600
H	-6.38506300	-0.72595300	2.71090800
H	-5.99956400	0.89565500	0.86437300
H	-3.80902000	0.91529100	-0.31609900
C	-2.07016000	-2.51276700	2.37532900
C	-2.48202000	-3.84429400	2.94490300
H	-3.27365300	-4.41189100	2.46875400
C	-1.76965600	-4.37013900	4.01129500
O	-0.76550200	-3.81981400	4.60422100
C	-2.22901800	-5.65313100	4.51764000
C	-2.57798200	-6.72737500	4.97001800
C	-2.98909900	-7.98391400	5.49450900
C	-2.34953100	-8.53694200	6.62240600
C	-4.04425400	-8.70413400	4.89885200
C	-2.75421800	-9.76642800	7.13332200
H	-1.53622900	-7.98619200	7.08412400
C	-4.44252500	-9.93342100	5.41536300
H	-4.54022200	-8.28284900	4.03009800
C	-3.80112200	-10.47085000	6.53387500
H	-2.25029500	-10.17837100	8.00376300
H	-5.25781900	-10.47555300	4.94349300
H	-4.11447900	-11.43072600	6.93503600
H	-1.55409000	-1.99599300	3.18830000
H	0.40597800	-2.83345700	3.53678000

2S,3R-TS7

C	-4.40265300	4.96921700	2.45479800
C	-3.36741900	4.14408000	1.95977000
C	-2.99030400	4.28470000	0.61546700
C	-3.60671000	5.20885300	-0.22263600

C	-4.63282200	6.01388900	0.26349000
C	-5.02409200	5.88292800	1.59202200
H	-2.22519200	3.64559000	0.19712000
H	-3.28989400	5.28555900	-1.25828800
H	-5.12814900	6.73184600	-0.38299300
H	-5.83629000	6.50098700	1.96134500
C	-1.28690400	3.70686200	4.15636300
C	-1.06843300	2.19087200	1.89601700
C	0.10028000	3.04977600	3.89681000
H	-1.68095600	3.43666500	5.13777600
C	-0.06519500	1.81477000	3.00383900
H	-0.65315000	3.06752200	1.37780700
H	0.74142700	3.78017100	3.38732500
H	0.58755800	2.80127900	4.84468400
H	0.88313800	1.49043500	2.56463100
H	-0.44481200	0.96775100	3.58069400
P	-2.43664200	2.88859100	2.92854200
C	-1.22997100	5.23202600	4.05471900
C	-1.36412100	1.08248100	0.88510000
H	-2.19836000	1.34217700	0.22772100
H	-0.47139800	0.92775400	0.26748100
H	-1.59545400	0.14158600	1.39021700
H	-2.18025500	5.68137000	4.34174500
H	-0.45567700	5.60869400	4.73310200
H	-0.97274000	5.56088200	3.04130900
C	-5.55200300	6.49132500	4.78874500
C	-6.73881300	4.07953500	4.11059100
C	-6.88674200	6.16557900	5.49102300
H	-5.76335600	7.14681100	3.93521600
C	-7.67299200	5.22549500	4.56321900
H	-6.68547500	3.32371700	4.90585900
H	-6.68042700	5.66426300	6.44606400
H	-7.44415900	7.08053000	5.72006500
H	-8.57348800	4.82940400	5.04458700
H	-8.00506700	5.78482100	3.67757800
P	-5.03673100	4.82602800	4.15762800
O	-4.04840900	4.12135500	5.05809000
C	-7.14846500	3.41073200	2.79649000
C	-4.48982900	7.13302700	5.68006600
H	-3.60130500	7.41127800	5.10374100
H	-4.88374800	8.04078400	6.15100800

H	-4.17500700	6.43982600	6.46525000
H	-6.40795400	2.68486600	2.44936900
H	-8.11133600	2.90253800	2.92251900
H	-7.26632100	4.15554400	2.00176600
C	-3.35865900	1.53345400	3.80682000
H	-2.65612500	1.24472000	4.59548000
C	-3.78524100	0.33314800	3.01204800
C	-4.44780000	0.61319100	1.79187900
O	-4.87639700	-0.47130800	1.08120300
C	-5.52135900	-0.17448100	-0.15379500
H	-6.42588000	0.42208500	0.00338400
H	-4.85604300	0.37760500	-0.82505700
H	-5.77856500	-1.14145700	-0.58990700
O	-4.63076200	1.76790300	1.35137700
C	-3.50647300	-0.98007700	3.42520300
H	-4.04718800	-1.74727300	2.88554400
C	-4.67310800	-2.73470200	6.38628900
C	-3.77313100	-2.64446900	5.32202100
C	-3.39355700	-3.81974900	4.65739000
C	-3.91064000	-5.05152200	5.04993700
C	-4.80849800	-5.13296200	6.11867200
C	-5.18759400	-3.97031900	6.78710700
H	-4.97443100	-1.82822700	6.90720300
H	-2.69530900	-3.75312100	3.82841900
H	-3.61070900	-5.95353500	4.52275700
H	-5.20791200	-6.09591700	6.42552400
H	-5.88499000	-4.02129100	7.61947000
C	-3.19872200	-1.29883900	4.89795200
C	-1.69381800	-1.26001000	5.03864300
H	-1.18801200	-1.22664000	5.99503500
C	-1.08006900	-1.45345800	3.83944200
O	-1.82851800	-1.55604200	2.75028900
C	0.34082600	-1.51615000	3.68107400
C	1.54230000	-1.52475500	3.49426800
C	2.94698500	-1.51441100	3.27375600
C	3.46334000	-1.52701500	1.96245400
C	3.84765800	-1.48000600	4.35676800
C	4.83770800	-1.50519800	1.74619500
H	2.77123500	-1.55688400	1.12689500
C	5.22053600	-1.45858900	4.13094500
H	3.45335300	-1.47230300	5.36794700

C	5.72186100	-1.47052600	2.82716500
H	5.22169800	-1.51704200	0.72977600
H	5.90337600	-1.43365500	4.97578600
H	6.79427400	-1.45468900	2.65478300
H	-3.67016700	-0.53048000	5.52455800
H	-4.17433900	2.06418400	4.30261600

2S,3R-VII

C	-4.05376800	4.86576400	2.43819100
C	-3.29371700	3.96332200	1.65839500
C	-3.31329500	4.11327700	0.26296500
C	-4.04354000	5.12409900	-0.35306500
C	-4.79534300	6.00854800	0.41630000
C	-4.80057900	5.86649700	1.79967800
H	-2.77658000	3.41555100	-0.36430200
H	-4.03385600	5.20716900	-1.43564500
H	-5.37762700	6.79534400	-0.05361300
H	-5.40552900	6.54500900	2.39219800
C	-0.74746400	3.17176600	3.18071500
C	-1.36764200	1.77703800	0.92828400
C	0.41414600	2.33994100	2.56113700
H	-0.89409800	2.92751700	4.23377400
C	-0.14255900	1.22008700	1.67221800
H	-1.02298400	2.64323100	0.34438400
H	1.03098200	3.01050000	1.94987800
H	1.05803300	1.93746300	3.34840400
H	0.60460700	0.87227800	0.94891200
H	-0.44714900	0.35032100	2.25725100
P	-2.30127300	2.56867300	2.32595400
C	-0.50506800	4.67813800	3.06085700
C	-2.04219000	0.77318300	-0.00572000
H	-2.99937000	1.14147300	-0.37927300
H	-1.37593000	0.57914000	-0.85488500
H	-2.22711600	-0.16690900	0.51329400
H	-1.27551700	5.24168300	3.58740400
H	0.46506000	4.92402200	3.50861200
H	-0.47943000	5.00174500	2.01361500
C	-4.44504400	6.36045500	5.03324500
C	-5.86618300	4.00912700	4.65286800

C	-5.53289300	6.04497400	6.08098900
H	-4.87066200	7.05004500	4.29459600
C	-6.58635600	5.16210700	5.39141100
H	-5.63021200	3.21252600	5.37127200
H	-5.07966200	5.50255000	6.92144100
H	-5.96811700	6.96499300	6.48686500
H	-7.32528400	4.77303700	6.10010700
H	-7.13700400	5.76487600	4.65607900
P	-4.18731100	4.70229300	4.24863500
O	-3.01452500	3.94801100	4.82949800
C	-6.65492200	3.42447700	3.47698000
C	-3.14697600	6.94070500	5.59237700
H	-2.44697000	7.19335800	4.78864000
H	-3.34918700	7.85354400	6.16420200
H	-2.65351100	6.21776100	6.24792900
H	-6.08402400	2.68559800	2.90498100
H	-7.57203700	2.95024800	3.84523700
H	-6.94752600	4.21557500	2.77770600
C	-3.20860500	1.35495300	3.44539800
H	-2.49019600	1.13486500	4.23980800
C	-3.72948100	0.13480600	2.77962800
C	-4.57560400	0.38275600	1.70612100
O	-5.09946800	-0.72536700	1.06571100
C	-5.92060700	-0.44082200	-0.05813900
H	-6.74982500	0.22200500	0.20885800
H	-5.35159300	0.03429000	-0.86594000
H	-6.30411500	-1.40637400	-0.39678500
O	-4.84729100	1.53999800	1.28156100
C	-3.28614700	-1.19783500	3.20944900
H	-3.71500800	-1.96317600	2.56528300
C	-5.39123300	-3.10308700	5.42803200
C	-4.09473500	-2.94094000	4.93090200
C	-3.35754600	-4.08368700	4.59182300
C	-3.90642000	-5.35477700	4.74531100
C	-5.20204100	-5.50619700	5.24609100
C	-5.94333100	-4.37536800	5.58708400
H	-5.97361300	-2.22243100	5.68900900
H	-2.34826600	-3.96797700	4.20700300
H	-3.32171300	-6.23055900	4.47601800
H	-5.62874200	-6.49796300	5.36866900
H	-6.95252100	-4.48144200	5.97659400

C	-3.51006500	-1.55575700	4.72865100
C	-2.12871300	-1.40068800	5.30401300
H	-1.88579400	-1.39018600	6.35765400
C	-1.23959800	-1.29954700	4.29623800
O	-1.78529700	-1.33592000	3.04161000
C	0.15882000	-1.09114700	4.37029900
C	1.34988400	-0.84886600	4.38733500
C	2.73535600	-0.53084100	4.38265900
C	3.37240400	-0.17033300	3.17822900
C	3.48788000	-0.55361400	5.57278300
C	4.72396600	0.15910400	3.17052700
H	2.79280800	-0.15572500	2.26077700
C	4.83946100	-0.22348500	5.55409300
H	2.99878900	-0.83095100	6.50097500
C	5.46234500	0.13424200	4.35610200
H	5.20421400	0.43532500	2.23603300
H	5.40998800	-0.24504200	6.47827600
H	6.51754100	0.39146800	4.34637200
H	-4.20747100	-0.82447600	5.15394000
H	-3.97884200	1.98422900	3.89452000

2S,3R-TS8

C	-2.00351500	1.42512100	2.12021700
C	-0.70114800	1.04271300	2.52536100
C	-0.29782900	1.39969700	3.82430600
C	-1.10989600	2.15252700	4.66753700
C	-2.37231100	2.56085300	4.24336700
C	-2.81425400	2.17719700	2.98211800
H	0.67309900	1.09708700	4.18348500
H	-0.74964800	2.42068600	5.65686300
H	-3.01830000	3.14251800	4.89208000
H	-3.81691300	2.45716000	2.67330800
C	2.08247000	-0.05681900	2.31971700
C	1.08285500	1.27129500	0.17778600
C	2.69550200	1.34126600	2.14382700
H	2.59522700	-0.71938900	1.61059200
C	2.48471300	1.73172500	0.67445700
H	0.38182200	2.11221200	0.17876200
H	2.20616800	2.06045200	2.81248200

H	3.76161700	1.33637600	2.40401300
H	2.61580800	2.80765700	0.51405300
H	3.24357900	1.22383200	0.06791700
P	0.43320100	0.04431700	1.45744500
C	2.21880100	-0.68851100	3.71630900
C	1.15204500	0.66614900	-1.22823100
H	0.15977500	0.37329900	-1.57496200
H	1.57274900	1.40100300	-1.92643500
H	1.80787800	-0.21213800	-1.23526500
H	2.34974700	0.07329600	4.49381700
H	1.35892200	-1.30394400	3.98571900
H	3.10788500	-1.32700100	3.74662600
C	-4.38470700	0.23361800	0.81979700
C	-3.29331100	2.47161000	-0.37787400
C	-5.30957600	1.04095500	-0.11510800
H	-4.64452800	0.46435000	1.85843100
C	-4.81555800	2.49814300	-0.13530600
H	-3.11586000	2.20166400	-1.42853300
H	-5.25331100	0.62275100	-1.12904800
H	-6.35477800	0.96661300	0.20557100
H	-5.32521400	3.09295200	-0.90187600
H	-5.02849000	2.97761600	0.83002600
P	-2.70126300	0.94791200	0.50739800
O	-1.76031800	0.08242500	-0.29467900
C	-2.55221600	3.77062500	-0.06652800
C	-4.41675700	-1.27946200	0.60815800
H	-3.76954600	-1.79526900	1.32229300
H	-5.43760200	-1.65971700	0.73691500
H	-4.07747500	-1.53801400	-0.39938400
H	-1.47974700	3.67397400	-0.26773900
H	-2.93650300	4.58810400	-0.68728000
H	-2.66947300	4.05849200	0.98264500
C	0.09410300	-2.03911900	0.73265500
C	0.83078800	-2.96971100	1.47806200
C	2.19501700	-3.19841200	1.11392000
O	2.77692600	-4.22174300	1.83563600
C	4.14944500	-4.46272700	1.53648700
H	4.28321300	-4.72533700	0.48291400
H	4.76113400	-3.57986300	1.75007800
H	4.45001000	-5.29423800	2.17715600
O	2.83936200	-2.59013100	0.25230600

C	0.21799700	-3.60383800	2.68419600
H	0.98117600	-4.00165300	3.35068100
C	0.37695500	-6.87644300	2.63565900
C	-0.60107000	-5.99933300	3.12370100
C	-1.25463900	-6.31718300	4.31755300
C	-0.94911000	-7.49384300	5.00406700
C	0.02075100	-8.36444100	4.50775300
C	0.68717400	-8.04886800	3.32124800
H	0.90951500	-6.62031100	1.72325000
H	-2.00489500	-5.63625800	4.70918400
H	-1.46945700	-7.72846500	5.92908200
H	0.25858800	-9.28060700	5.04141800
H	1.44879400	-8.71803700	2.92961600
C	-0.86578600	-4.70482800	2.37391000
C	-2.13854000	-3.99468500	2.73752400
H	-3.13873700	-4.36662600	2.56157600
C	-1.84410600	-2.83589200	3.35768700
O	-0.50531700	-2.56894200	3.46705900
C	-2.75072700	-1.88795400	3.89020100
C	-3.58369800	-1.11814400	4.32559700
C	-4.57942600	-0.22736600	4.81121800
C	-5.83505000	-0.15231600	4.17680200
C	-4.32581500	0.60085000	5.92041300
C	-6.79813800	0.74643800	4.62725200
H	-6.04055200	-0.80638300	3.33550700
C	-5.29656400	1.49137200	6.36799200
H	-3.35984900	0.54100400	6.40939600
C	-6.53217100	1.57365000	5.72064400
H	-7.76103200	0.79760500	4.12699300
H	-5.08923100	2.12516400	7.22571200
H	-7.28581600	2.27257600	6.07142400
H	-0.82410900	-4.92006200	1.29947800
H	0.45212400	-1.80827000	-0.26558900
H	-0.98721400	-2.02502900	0.80336300

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C	-1.42490000	-0.50701200	0.59377500
C	-1.61462500	0.44118200	-0.64483900
C	-0.18606300	0.56123000	-1.11000300

C	0.63562600	0.07852600	-0.16267000
H	-2.24338400	-0.05682300	-1.38941300
H	0.12844500	1.02893800	-2.03214200
H	-1.99098100	-0.14075800	1.45235400
C	2.04628600	0.03041300	-0.12773000
C	3.25985800	-0.01669700	-0.09239900
C	4.68041100	-0.06843200	-0.05665200
C	5.34464200	-0.63873200	1.04657600
C	5.44129600	0.44929100	-1.12268800
C	6.73465000	-0.68734800	1.07774400
H	4.75785000	-1.03664100	1.86808100
C	6.83086800	0.39518800	-1.08185000
H	4.92941900	0.88920100	-1.97245600
C	7.48190600	-0.17204000	0.01606000
H	7.23747500	-1.12872100	1.93341600
H	7.40861500	0.79726300	-1.90912500
H	8.56691800	-0.21203000	0.04430800
O	-0.02432400	-0.44173000	0.93816100
C	-2.26612900	1.76801500	-0.28641900
C	-3.64345700	1.93961100	-0.46646900
C	-1.51960300	2.81467500	0.26609900
C	-4.26118700	3.13717100	-0.10814500
H	-4.23136800	1.12050800	-0.86854700
C	-2.13685900	4.01247500	0.62676600
H	-0.44979300	2.69067500	0.40538000
C	-3.50943800	4.17861000	0.43846200
H	-5.33131100	3.25632600	-0.25499700
H	-1.54372700	4.81719400	1.05294000
H	-3.99019100	5.11263000	0.71615200
C	-1.80551200	-1.94111500	0.29013900
C	-0.91739700	-2.93518500	0.19547300
H	0.13699800	-2.74702000	0.36256600
H	-1.23095100	-3.94612600	-0.03670000
C	-3.26398100	-2.15713600	0.10046400
O	-3.58927700	-3.43805500	-0.17193600
C	-4.99140900	-3.68361300	-0.35564900
H	-5.07487100	-4.74984300	-0.56620600
H	-5.54788300	-3.42370500	0.54854000
H	-5.37774800	-3.09369900	-1.19098900
O	-4.09182600	-1.26669400	0.18634500

2R,3R-TS7

C	-1.87846900	1.91573100	1.16721100
C	-0.94730900	1.33378600	2.05566700
C	-0.65477000	2.02164500	3.24371400
C	-1.28598000	3.21808100	3.57346900
C	-2.25174000	3.75228600	2.72592800
C	-2.53600100	3.09814300	1.53153400
H	0.06314300	1.61711800	3.94001600
H	-1.03196100	3.71707100	4.50378700
H	-2.77242300	4.66922000	2.98478600
H	-3.28535600	3.51769600	0.86715100
C	0.81686000	-0.73813800	3.34660300
C	1.39872900	-0.07004400	0.74822200
C	2.15883200	-0.00084300	3.17946100
H	0.99245100	-1.80605500	3.16240300
C	2.60690300	-0.17947900	1.72266100
H	1.31472400	0.94114000	0.33884500
H	2.05429300	1.06270200	3.42983700
H	2.90049500	-0.42012900	3.86823400
H	3.38446200	0.53952300	1.44474700
H	3.03600100	-1.17914400	1.61645700
P	-0.11613100	-0.29578000	1.82164500
C	0.15277700	-0.66060200	4.73555600
C	1.50951300	-1.07525000	-0.40328600
H	0.66141000	-0.98937600	-1.08250900
H	2.43479800	-0.87699800	-0.95721800
H	1.57057700	-2.09958700	-0.01966800
H	0.68852300	0.04202500	5.38507700
H	-0.89285000	-0.35239400	4.69343900
H	0.19045100	-1.65037000	5.19643900
C	-4.05900400	0.75242800	-0.44381100
C	-2.41025000	2.53266500	-1.75356500
C	-4.59154300	1.35167200	-1.76156500
H	-4.49196300	1.31992900	0.39081900
C	-3.92562700	2.72565200	-1.95486800
H	-2.02313300	1.98860500	-2.62720500
H	-4.32441500	0.69101600	-2.59737700
H	-5.68459900	1.42239200	-1.74389300
H	-4.13816900	3.15149700	-2.94204800

H	-4.31613900	3.43539300	-1.21205900
P	-2.25789300	1.20350800	-0.46379000
O	-1.24693900	0.14830300	-0.84106200
C	-1.57911600	3.80205700	-1.57640100
C	-4.33438600	-0.73635000	-0.23363200
H	-4.07665500	-1.03730900	0.78529000
H	-5.39929200	-0.94655700	-0.38777600
H	-3.76327900	-1.35600700	-0.93125200
H	-0.52104000	3.56333600	-1.42522400
H	-1.65618100	4.43058700	-2.47086900
H	-1.91147400	4.39669700	-0.72120200
C	-1.18499000	-1.73014600	1.34121900
H	-1.95673400	-1.33532500	0.69090200
C	-1.69544700	-2.52647500	2.49763300
C	-2.56601600	-1.81450000	3.36976800
O	-3.07169000	-2.53555100	4.41905600
C	-3.93496500	-1.81017600	5.29000200
H	-4.79877900	-1.41117700	4.74930900
H	-4.25964400	-2.52691100	6.04684900
H	-3.40975500	-0.97475200	5.76456900
O	-2.87225000	-0.61831400	3.21618700
C	-1.29110200	-3.84683900	2.71492700
H	-1.74360800	-4.32153900	3.57738600
C	-3.26853200	-4.78481300	0.53731500
C	-1.89050300	-4.59290300	0.36012700
C	-1.43867800	-4.17705200	-0.89515700
C	-2.33424900	-3.95108500	-1.94367100
C	-3.70116500	-4.14260200	-1.75277300
C	-4.16625800	-4.56267100	-0.50309700
H	-3.63817500	-5.09896300	1.51014900
H	-0.37864300	-4.00744100	-1.05282700
H	-1.95784600	-3.62097400	-2.90819800
H	-4.39951400	-3.96844200	-2.56699600
H	-5.23004000	-4.71463900	-0.34015800
C	-0.95563700	-4.81233300	1.54531200
C	0.51806600	-4.69372500	1.26927800
H	0.99986100	-5.05935600	0.37239600
C	1.18399700	-4.18561200	2.34163200
O	0.49829500	-3.84147000	3.42129000
C	2.58701600	-3.90098100	2.33925900
C	3.75528000	-3.56485700	2.38774800

C	5.10527700	-3.12095300	2.43482800
C	5.56685000	-2.37051700	3.53515700
C	5.99651500	-3.39557800	1.37909100
C	6.87874700	-1.90871900	3.57257600
H	4.88314400	-2.16394900	4.35265800
C	7.30760900	-2.93169200	1.42634200
H	5.64398900	-3.97240600	0.53004200
C	7.75433200	-2.18638600	2.52007700
H	7.22106000	-1.33169500	4.42722400
H	7.98470300	-3.15178900	0.60562100
H	8.77834400	-1.82553600	2.55261600
H	-1.16918500	-5.82498200	1.92720700
H	-0.52504700	-2.32671500	0.71283500

2R,3R-VII

C	-1.76978100	2.04264800	1.19794600
C	-0.60278300	1.57633000	1.83952400
C	0.04399100	2.42182700	2.75218500
C	-0.49203800	3.65702200	3.11237700
C	-1.70352000	4.06417300	2.56582300
C	-2.31851100	3.26343700	1.60458500
H	0.97722000	2.11285800	3.20553400
H	0.03199300	4.28261500	3.82884100
H	-2.15654500	5.00618300	2.85996200
H	-3.24183500	3.60896100	1.15596900
C	0.97714500	-0.57238300	3.30643200
C	1.76714600	0.19094700	0.76549300
C	2.47773500	-0.27258100	3.11312500
H	0.84145200	-1.66023100	3.26528200
C	2.82420500	-0.51632200	1.63884600
H	1.93608300	1.27439800	0.81329400
H	2.69863100	0.76926800	3.38570300
H	3.07688300	-0.90959900	3.77261900
H	3.83072800	-0.16348800	1.38709300
H	2.80404300	-1.59307700	1.43741600
P	0.17534100	-0.08437500	1.69797600
C	0.35965000	-0.10475600	4.62686800
C	1.75646300	-0.24957200	-0.69919800
H	0.92541200	0.20194500	-1.24523200

H	2.70268800	0.03133500	-1.17628000
H	1.65756900	-1.33755600	-0.77856900
H	0.70230000	0.89241900	4.91836400
H	-0.73026600	-0.08465600	4.56159800
H	0.64964100	-0.80014000	5.42179900
C	-4.07020800	0.36110000	0.22051300
C	-3.23478800	2.42594500	-1.39193000
C	-5.15721500	1.09536300	-0.60554900
H	-4.19205900	0.55140500	1.29138700
C	-4.70140100	2.52674100	-0.94220900
H	-3.22389100	1.84597900	-2.32789000
H	-5.30569300	0.54761600	-1.54548300
H	-6.11711100	1.08536800	-0.07806300
H	-5.32392700	2.97263800	-1.72704800
H	-4.79548800	3.17642600	-0.06275300
P	-2.46822000	1.17785100	-0.25506900
O	-1.39043000	0.36007300	-0.93074300
C	-2.48315600	3.73057700	-1.64855200
C	-4.06957400	-1.14905600	-0.02708200
H	-3.37392900	-1.67750500	0.62521900
H	-5.07246100	-1.55204300	0.15885300
H	-3.80253600	-1.38211200	-1.06177600
H	-1.44756600	3.52869500	-1.94198600
H	-2.96066000	4.28758700	-2.46307900
H	-2.45989200	4.37960400	-0.76964400
C	-0.62151200	-1.65130800	1.08434100
H	-1.17075300	-1.37840400	0.18434700
C	-1.38241100	-2.39342600	2.13641800
C	-2.23670100	-1.61889800	2.91057900
O	-2.96232800	-2.27556400	3.88586600
C	-3.77831500	-1.44337100	4.69835700
H	-4.49736800	-0.87646600	4.09799900
H	-4.30674500	-2.11878400	5.37552700
H	-3.18095800	-0.73100000	5.27875400
O	-2.35961500	-0.36623500	2.78148800
C	-1.01773500	-3.76937700	2.49299400
H	-1.67291900	-4.12770900	3.28311500
C	-3.11273600	-4.81406700	0.17954500
C	-1.73792000	-4.54935700	0.12738200
C	-1.20869000	-4.01885600	-1.05267700
C	-2.02821000	-3.75441200	-2.15116800

C	-3.39418100	-4.02503200	-2.08750700
C	-3.93532900	-4.55579200	-0.91399400
H	-3.53872100	-5.22434400	1.09202300
H	-0.14582600	-3.80505400	-1.11186000
H	-1.59589700	-3.33485100	-3.05532700
H	-4.03332600	-3.82398100	-2.94295600
H	-4.99926000	-4.76842600	-0.85168100
C	-0.88266600	-4.84060900	1.34305600
C	0.60640600	-4.90797900	1.13444800
H	1.10781000	-5.38675600	0.30471800
C	1.21919100	-4.32484500	2.18452600
O	0.37570400	-3.79658800	3.11979900
C	2.60231800	-4.13216700	2.41699400
C	3.76930700	-3.87870800	2.64463700
C	5.12585700	-3.53928200	2.89979700
C	5.47830900	-2.88122800	4.09491400
C	6.13234900	-3.83357700	1.95983200
C	6.80144300	-2.52557600	4.33641800
H	4.70398400	-2.66170700	4.82311200
C	7.45312500	-3.47552600	2.21158800
H	5.86223300	-4.34014800	1.03890000
C	7.79285500	-2.82025100	3.39750300
H	7.06113700	-2.01861100	5.26139800
H	8.22118900	-3.70772900	1.47933900
H	8.82498800	-2.54191100	3.58954400
H	-1.22620900	-5.80354900	1.75351100
H	0.25433000	-2.22390700	0.76021600

2R,3R-TS8

C	-1.91551500	2.18696600	1.40371000
C	-1.07760900	1.63717500	2.40469700
C	-0.82137700	2.42936400	3.53782700
C	-1.40133700	3.68304800	3.71272600
C	-2.27242300	4.18854100	2.75028200
C	-2.51264200	3.44107600	1.60194600
H	-0.14922800	2.06521200	4.29972000
H	-1.17371900	4.25924100	4.60496800
H	-2.74706600	5.15606500	2.88315000
H	-3.17292600	3.84609400	0.84020000

C	0.24697600	-0.53938100	4.02345200
C	1.29153200	0.05220100	1.54876700
C	1.69895800	-0.03488700	4.03707600
H	0.29351300	-1.62917800	3.89027200
C	2.28835300	-0.35806500	2.65995700
H	1.40711100	1.12098900	1.33109600
H	1.73454600	1.04620900	4.22949800
H	2.26874500	-0.51961700	4.84011100
H	3.25471800	0.13418400	2.49483600
H	2.45475500	-1.43732600	2.59113800
P	-0.42085500	-0.09823400	2.34027100
C	-0.57915800	-0.29454400	5.29009500
C	1.48323300	-0.75427700	0.26350900
H	0.81140800	-0.41031600	-0.52272900
H	2.52341400	-0.66426400	-0.07411300
H	1.28287800	-1.81144300	0.44736600
H	-0.49310400	0.72776000	5.66811300
H	-1.63670700	-0.51887500	5.12874300
H	-0.21450000	-0.95923400	6.08254700
C	-4.01845900	1.24512700	-0.47531400
C	-1.88629600	2.61323800	-1.57385200
C	-4.22011300	1.82825100	-1.88978200
H	-4.49433400	1.91918700	0.24886200
C	-3.29077800	3.04569800	-2.03707400
H	-1.46176000	1.95485500	-2.34512600
H	-3.94994200	1.06791200	-2.63497900
H	-5.27065700	2.08768900	-2.06099800
H	-3.26672500	3.42187700	-3.06621700
H	-3.65451600	3.86989400	-1.40757500
P	-2.18523500	1.38214500	-0.21089500
O	-1.37390900	0.12192700	-0.37281700
C	-0.89322800	3.74032800	-1.29734500
C	-4.54419400	-0.17670400	-0.28261000
H	-4.48750000	-0.48653100	0.76485300
H	-5.59345000	-0.23807500	-0.59465900
H	-3.96299700	-0.89407800	-0.86748900
H	0.06968200	3.34464000	-0.95696200
H	-0.71417000	4.32047500	-2.20985600
H	-1.26023500	4.42705500	-0.52918800
C	-1.83625200	-1.73390300	1.85797200
H	-2.72709900	-1.12308800	1.96989000

C	-1.73895600	-2.82445900	2.74457900
C	-2.54739300	-2.76083000	3.92665600
O	-2.45234800	-3.88232300	4.72635100
C	-3.22583500	-3.82918700	5.92113500
H	-4.28802100	-3.68923000	5.69912100
H	-3.06529600	-4.78687400	6.42113900
H	-2.89991600	-3.00751900	6.56775000
O	-3.28826300	-1.82627000	4.24819000
C	-0.76066100	-3.92112200	2.53563800
H	-0.71865500	-4.55412200	3.42422600
C	-3.01389000	-4.40412600	0.03242000
C	-1.61747900	-4.32319800	0.09559200
C	-0.93820400	-3.65378800	-0.92794500
C	-1.63629600	-3.07223100	-1.98619700
C	-3.02676900	-3.16544200	-2.04334700
C	-3.71511800	-3.83402800	-1.02831200
H	-3.55188500	-4.90715700	0.83165800
H	0.14325700	-3.57475300	-0.88463600
H	-1.09235900	-2.53955000	-2.76082000
H	-3.57195500	-2.71879800	-2.87079800
H	-4.79901400	-3.90708200	-1.06115000
C	-0.89398100	-4.89295200	1.30315200
C	0.55849600	-5.20833500	1.04815700
H	0.92896400	-5.97825700	0.38482800
C	1.32037100	-4.27234300	1.64556200
O	0.61036000	-3.36248400	2.39304300
C	2.71628200	-4.06103900	1.57226400
C	3.90319600	-3.80675500	1.51451200
C	5.28727600	-3.48975300	1.44644900
C	6.17551900	-4.29268400	0.70547900
C	5.78650500	-2.35705400	2.11917200
C	7.52697700	-3.96775800	0.64233500
H	5.79122300	-5.16488500	0.18657100
C	7.13917900	-2.04014300	2.04828700
H	5.10113200	-1.73853900	2.68931800
C	8.01373200	-2.84254100	1.31158300
H	8.20367000	-4.59447600	0.06847500
H	7.51369300	-1.16415800	2.57036400
H	9.06938100	-2.59229300	1.25939100
H	-1.45731500	-5.76738200	1.64885500
H	-1.51820800	-1.83182100	0.82977700

2R,3R-3ga

C	-1.03872200	-1.11568200	2.52686900
H	-1.78435400	-0.32897300	2.48940100
C	-1.39067900	-2.34798000	2.90224600
C	-2.81488600	-2.59596900	3.26404900
O	-2.98816700	-3.85433400	3.74369100
C	-4.34556000	-4.20366300	4.04758900
H	-4.95594000	-4.15851700	3.14163800
H	-4.30650200	-5.22161900	4.43626000
H	-4.76058100	-3.52038500	4.79225700
O	-3.72177900	-1.79772700	3.16102300
C	-0.43130200	-3.50579300	2.97193100
H	-0.44116300	-3.93502600	3.98038300
C	-2.88673000	-4.91864500	0.71589700
C	-1.61555600	-4.34074300	0.79114900
C	-1.23202200	-3.42533800	-0.19605500
C	-2.10540100	-3.08754500	-1.22776900
C	-3.37514100	-3.66516300	-1.29087500
C	-3.76347900	-4.58502100	-0.31692300
H	-3.19042700	-5.63284900	1.47673800
H	-0.24409300	-2.97729100	-0.14969100
H	-1.79541100	-2.37133800	-1.98372300
H	-4.05608800	-3.40077700	-2.09490000
H	-4.74717800	-5.04449200	-0.36129900
C	-0.68701300	-4.67744700	1.94450700
C	0.72901600	-4.95655800	1.50631200
H	1.02221700	-5.76701000	0.85407500
C	1.54297800	-3.98284200	1.94911400
O	0.91310900	-3.03244300	2.72824700
C	2.92290900	-3.79070800	1.71770900
C	4.10871100	-3.62030500	1.51588000
C	5.49687900	-3.42514500	1.27726600
C	6.21098600	-4.31219300	0.44869300
C	6.17513300	-2.34077700	1.86685400
C	7.56899200	-4.11570000	0.21909100
H	5.68818100	-5.14753500	-0.00576000
C	7.53310400	-2.15281700	1.63012200
H	5.62441100	-1.65794800	2.50556000

C	8.23415200	-3.03750100	0.80733900
H	8.11088500	-4.80567600	-0.42131400
H	8.04712100	-1.31336800	2.08937300
H	9.29433100	-2.88734300	0.62535700
H	-1.12192700	-5.51921900	2.49155400
H	-0.01497000	-0.88733000	2.25682100

Si-TS4

C	-2.88757000	-0.35623600	2.53535000
C	-1.52213200	-0.00096000	2.66620700
C	-1.07144600	0.45465600	3.91275600
C	-1.93501100	0.57165800	5.00355900
C	-3.27795900	0.24082700	4.86405300
C	-3.74250900	-0.22527700	3.63370500
H	-0.03577800	0.73722900	4.04863000
H	-1.55195900	0.92851100	5.95496100
H	-3.96110000	0.33738800	5.70248300
H	-4.79003800	-0.49135900	3.53531600
C	0.46785000	-1.49611100	0.73512100
C	1.17594000	0.92419400	1.80262800
C	1.98624900	-1.16947600	0.77641600
H	0.19297400	-1.71857400	-0.29583200
C	2.20258800	0.34872600	0.81165200
H	1.41767300	0.50222000	2.78657300
H	2.42555200	-1.61114400	1.68031400
H	2.45141000	-1.63162700	-0.09707400
H	3.22139800	0.61274600	1.11673500
H	2.03852300	0.78460200	-0.18058700
P	-0.37566500	0.08370600	1.20847400
C	0.09530300	-2.67956700	1.63068000
C	1.13321900	2.44739000	1.87969100
H	0.36773500	2.80327100	2.57870000
H	2.10180900	2.83394700	2.21575800
H	0.91787800	2.87694200	0.89683900
H	-0.95615900	-2.93923500	1.51047200
H	0.70366200	-3.53965000	1.33122400
H	0.30175900	-2.47400100	2.68871900
C	-4.83930300	-2.29481300	1.32409200
C	-4.60084600	0.15423300	0.06630800

C	-5.79965200	-2.05482700	0.14200400
H	-5.36061800	-2.01228300	2.24769700
C	-5.98778000	-0.53385400	0.02145100
H	-4.16859100	0.17932000	-0.94071100
H	-5.35196400	-2.45502100	-0.77700000
H	-6.75164200	-2.57552000	0.29336200
H	-6.52660000	-0.25677300	-0.89050300
H	-6.58960900	-0.17971900	0.87001200
P	-3.51251100	-1.05751300	0.96529000
O	-2.36537200	-1.65110700	0.18687800
C	-4.64615300	1.57417900	0.63308300
C	-4.28718800	-3.71335900	1.44859100
H	-3.64248800	-3.81189500	2.32877600
H	-5.10427600	-4.43742500	1.54346200
H	-3.69088900	-3.97028100	0.56873100
H	-3.65843800	2.03883700	0.63921500
H	-5.30827400	2.19578300	0.01959800
H	-5.03458900	1.58243600	1.65778700
C	-1.09359500	1.16133400	0.03260100
H	-1.23790100	2.13872100	0.48095400
C	-1.55842200	0.99134300	-1.26819500
C	-2.29402900	2.15209700	-1.87417900
O	-2.14811900	3.30728300	-1.17890100
C	-2.79525000	4.44469400	-1.76239100
H	-3.87305800	4.27818300	-1.84017100
H	-2.58195600	5.27765600	-1.09129900
H	-2.38615000	4.63642500	-2.75696600
O	-2.98533600	2.08138200	-2.87221500
C	-1.32099600	-0.07286000	-2.16563100
C	-0.20792300	2.01980100	-4.66645000
C	0.39486400	1.71740100	-3.43586200
C	0.86238200	2.78049900	-2.64870400
C	0.73669300	4.10188600	-3.07559700
C	0.13726800	4.38692300	-4.30283700
C	-0.33515800	3.33756200	-5.09582300
H	-0.60582700	1.21349300	-5.27457400
H	1.32581700	2.56324400	-1.69093100
H	1.10847000	4.90842800	-2.44892400
H	0.03982400	5.41537100	-4.64018600
H	-0.81276700	3.54863600	-6.04867800
C	0.49651100	0.32406900	-2.93596700

C	0.82325300	-0.73262300	-3.81389900
H	0.76215100	-0.60446500	-4.88916800
C	1.16917900	-2.00658200	-3.29549400
O	1.19013000	-2.30525100	-2.07118500
C	1.52301900	-3.02128200	-4.27668700
C	1.82269000	-3.89120400	-5.07224900
C	2.17198700	-4.90998300	-6.00201800
C	2.53527800	-6.19526100	-5.55338500
C	2.16120700	-4.65316000	-7.38723700
C	2.87642200	-7.18947700	-6.46516500
H	2.54389200	-6.39463000	-4.48667200
C	2.50348700	-5.65304400	-8.29240500
H	1.88208800	-3.66373300	-7.73518400
C	2.86214900	-6.92377200	-7.83652400
H	3.15472400	-8.17629200	-6.10539400
H	2.49092900	-5.44098600	-9.35802000
H	3.12904500	-7.70228400	-8.54572000
H	0.95195000	0.24381100	-1.94858000
H	-1.92979700	-0.07449000	-3.06204000
H	-1.08097600	-1.04836700	-1.76735200

3S-IV

C	-2.94567100	-0.11545600	2.59449100
C	-1.55534300	0.14992100	2.65952400
C	-1.03826100	0.71938300	3.83105500
C	-1.86211400	1.03247800	4.91325300
C	-3.22947000	0.79103400	4.83726200
C	-3.75963900	0.21674900	3.68222800
H	0.01846900	0.93780200	3.91250300
H	-1.42937100	1.47163500	5.80692200
H	-3.88116800	1.04103600	5.66888200
H	-4.82658700	0.02350700	3.63331000
C	0.28715300	-1.74587300	0.90855800
C	1.18315700	0.76295100	1.61129200
C	1.82204200	-1.53578100	0.97517200
H	0.05375800	-2.03330500	-0.12424600
C	2.15620400	-0.05846800	0.74520800
H	1.41425000	0.52037800	2.65605900
H	2.19688300	-1.84163200	1.96121000

H	2.26176200	-2.17898200	0.20891300
H	3.19237300	0.17903400	1.01015600
H	2.02327300	0.20073800	-0.31110700
P	-0.43098200	-0.06985000	1.20682200
C	-0.21190100	-2.82382500	1.87049900
C	1.23356400	2.27378100	1.39865300
H	0.50861500	2.80283300	2.02804300
H	2.23159100	2.65108900	1.64702400
H	1.02432400	2.52716500	0.35498300
H	-1.27631000	-3.00758900	1.72902500
H	0.33215100	-3.74695200	1.64577600
H	-0.02008200	-2.56424300	2.91963300
C	-5.02897300	-2.07599800	1.67029000
C	-4.73316200	0.21860700	0.15070700
C	-6.04969100	-1.88640000	0.52991100
H	-5.47372400	-1.68756000	2.59558000
C	-6.15808800	-0.37536100	0.27012300
H	-4.36798500	0.09162000	-0.87549800
H	-5.68799500	-2.39941700	-0.37062700
H	-7.01756100	-2.32896800	0.78913700
H	-6.74399500	-0.15269000	-0.62745600
H	-6.67418600	0.09872800	1.11678100
P	-3.66697100	-0.94818500	1.13236600
O	-2.57214900	-1.65983300	0.37814800
C	-4.66073500	1.69910400	0.52719700
C	-4.53997200	-3.50709400	1.88667400
H	-3.84380100	-3.56580700	2.73021900
H	-5.38470000	-4.17259500	2.09649600
H	-4.01793700	-3.87294400	0.99826200
H	-3.65075200	2.10004700	0.41870500
H	-5.32256900	2.27768300	-0.12659100
H	-4.98052400	1.86617000	1.56174400
C	-1.16451600	0.93597000	-0.06626400
H	-1.33084700	1.93874500	0.31932400
C	-1.56716200	0.66766400	-1.33491400
C	-2.32353300	1.75325000	-2.04108800
O	-1.95131900	2.99534200	-1.66541200
C	-2.61885500	4.06217600	-2.35711700
H	-3.69604800	4.02592200	-2.17349500
H	-2.18858000	4.98069400	-1.95780900
H	-2.42770200	3.98255500	-3.42914700

O	-3.21577000	1.53826700	-2.83877700
C	-1.25915300	-0.51999100	-2.15508800
C	-0.45087200	1.22407300	-4.67023700
C	0.30576000	0.97733000	-3.51637400
C	1.09750300	2.01577700	-3.01225800
C	1.12890000	3.26674100	-3.62943600
C	0.36404400	3.50086000	-4.77230400
C	-0.42417000	2.47112300	-5.29271800
H	-1.07835900	0.43360000	-5.07127500
H	1.69638500	1.83860100	-2.12245300
H	1.75152300	4.05725400	-3.21810600
H	0.38593100	4.47299100	-5.25772300
H	-1.02092300	2.64013300	-6.18524900
C	0.21271800	-0.34481200	-2.79113400
C	0.58582600	-1.52722200	-3.59549300
H	0.58494000	-1.47835600	-4.67850500
C	0.89221500	-2.71205900	-2.93777100
O	0.88366000	-2.87902800	-1.66792800
C	1.26224500	-3.84402300	-3.77719600
C	1.57617700	-4.81780000	-4.43630400
C	1.94101000	-5.95280100	-5.21165300
C	2.26880800	-7.17471700	-4.58948100
C	1.98361300	-5.88303100	-6.61902600
C	2.62557400	-8.28370100	-5.35061500
H	2.23749800	-7.23367600	-3.50616600
C	2.34126500	-6.99654900	-7.37316400
H	1.73273000	-4.94473000	-7.10365300
C	2.66390200	-8.20168400	-6.74468900
H	2.87534500	-9.21785800	-4.85419000
H	2.36894400	-6.92450500	-8.45734600
H	2.94294200	-9.06935000	-7.33618000
H	0.85769400	-0.30583100	-1.90240300
H	-1.98044400	-0.61166600	-2.96730200
H	-1.24354200	-1.44269600	-1.58109500

3S-TS5

C	-2.94567100	-0.11545600	2.59449100
C	-1.55534300	0.14992100	2.65952400
C	-1.03826100	0.71938300	3.83105500

C	-1.86211400	1.03247800	4.91325300
C	-3.22947000	0.79103400	4.83726200
C	-3.75963900	0.21674900	3.68222800
H	0.01846900	0.93780200	3.91250300
H	-1.42937100	1.47163500	5.80692200
H	-3.88116800	1.04103600	5.66888200
H	-4.82658700	0.02350700	3.63331000
C	0.28715300	-1.74587300	0.90855800
C	1.18315700	0.76295100	1.61129200
C	1.82204200	-1.53578100	0.97517200
H	0.05375800	-2.03330500	-0.12424600
C	2.15620400	-0.05846800	0.74520800
H	1.41425000	0.52037800	2.65605900
H	2.19688300	-1.84163200	1.96121000
H	2.26176200	-2.17898200	0.20891300
H	3.19237300	0.17903400	1.01015600
H	2.02327300	0.20073800	-0.31110700
P	-0.43098200	-0.06985000	1.20682200
C	-0.21190100	-2.82382500	1.87049900
C	1.23356400	2.27378100	1.39865300
H	0.50861500	2.80283300	2.02804300
H	2.23159100	2.65108900	1.64702400
H	1.02432400	2.52716500	0.35498300
H	-1.27631000	-3.00758900	1.72902500
H	0.33215100	-3.74695200	1.64577600
H	-0.02008200	-2.56424300	2.91963300
C	-5.02897300	-2.07599800	1.67029000
C	-4.73316200	0.21860700	0.15070700
C	-6.04969100	-1.88640000	0.52991100
H	-5.47372400	-1.68756000	2.59558000
C	-6.15808800	-0.37536100	0.27012300
H	-4.36798500	0.09162000	-0.87549800
H	-5.68799500	-2.39941700	-0.37062700
H	-7.01756100	-2.32896800	0.78913700
H	-6.74399500	-0.15269000	-0.62745600
H	-6.67418600	0.09872800	1.11678100
P	-3.66697100	-0.94818500	1.13236600
O	-2.57214900	-1.65983300	0.37814800
C	-4.66073500	1.69910400	0.52719700
C	-4.53997200	-3.50709400	1.88667400
H	-3.84380100	-3.56580700	2.73021900

H	-5.38470000	-4.17259500	2.09649600
H	-4.01793700	-3.87294400	0.99826200
H	-3.65075200	2.10004700	0.41870500
H	-5.32256900	2.27768300	-0.12659100
H	-4.98052400	1.86617000	1.56174400
C	-1.16451600	0.93597000	-0.06626400
H	-1.33084700	1.93874500	0.31932400
C	-1.56716200	0.66766400	-1.33491400
C	-2.32353300	1.75325000	-2.04108800
O	-1.95131900	2.99534200	-1.66541200
C	-2.61885500	4.06217600	-2.35711700
H	-3.69604800	4.02592200	-2.17349500
H	-2.18858000	4.98069400	-1.95780900
H	-2.42770200	3.98255500	-3.42914700
O	-3.21577000	1.53826700	-2.83877700
C	-1.25915300	-0.51999100	-2.15508800
C	-0.45087200	1.22407300	-4.67023700
C	0.30576000	0.97733000	-3.51637400
C	1.09750300	2.01577700	-3.01225800
C	1.12890000	3.26674100	-3.62943600
C	0.36404400	3.50086000	-4.77230400
C	-0.42417000	2.47112300	-5.29271800
H	-1.07835900	0.43360000	-5.07127500
H	1.69638500	1.83860100	-2.12245300
H	1.75152300	4.05725400	-3.21810600
H	0.38593100	4.47299100	-5.25772300
H	-1.02092300	2.64013300	-6.18524900
C	0.21271800	-0.34481200	-2.79113400
C	0.58582600	-1.52722200	-3.59549300
H	0.58494000	-1.47835600	-4.67850500
C	0.89221500	-2.71205900	-2.93777100
O	0.88366000	-2.87902800	-1.66792800
C	1.26224500	-3.84402300	-3.77719600
C	1.57617700	-4.81780000	-4.43630400
C	1.94101000	-5.95280100	-5.21165300
C	2.26880800	-7.17471700	-4.58948100
C	1.98361300	-5.88303100	-6.61902600
C	2.62557400	-8.28370100	-5.35061500
H	2.23749800	-7.23367600	-3.50616600
C	2.34126500	-6.99654900	-7.37316400
H	1.73273000	-4.94473000	-7.10365300

C	2.66390200	-8.20168400	-6.74468900
H	2.87534500	-9.21785800	-4.85419000
H	2.36894400	-6.92450500	-8.45734600
H	2.94294200	-9.06935000	-7.33618000
H	0.85769400	-0.30583100	-1.90240300
H	-1.98044400	-0.61166600	-2.96730200
H	-1.24354200	-1.44269600	-1.58109500

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C	-2.50910600	0.59579300	0.30745000
C	-1.36740200	1.20567800	0.89493900
C	-1.14966300	2.56751200	0.62368500
C	-1.99507600	3.32051800	-0.18524800
C	-3.11538500	2.72483800	-0.75016500
C	-3.35733300	1.37901500	-0.49452900
H	-0.29669000	3.07400900	1.04144800
H	-1.76167800	4.36654600	-0.35799700
H	-3.79448500	3.29075900	-1.38062300
H	-4.23464300	0.92206900	-0.94092700
C	0.86278100	-0.97717000	1.32568100
C	-0.88776200	-0.46768300	3.43377800
C	0.62916500	-2.13694900	2.32888300
H	1.89420600	-0.61456000	1.35425900
C	0.15010900	-1.58560100	3.68736700
H	-1.77581000	-0.94022900	3.01127000
H	-0.13747800	-2.79796900	1.92281000
H	1.55671100	-2.70783800	2.44357400
H	-0.30700900	-2.37707800	4.29190600
H	0.98911400	-1.17692300	4.25934100
P	-0.11034500	0.43175300	2.01582000
C	0.61979100	-1.33145500	-0.14059700
C	-1.26146900	0.38115200	4.64463900
H	-1.97103000	1.17282100	4.37841200
H	-1.73782600	-0.25512300	5.39949100
H	-0.39025900	0.85521900	5.09853100
H	0.76017500	-0.45968500	-0.78506300
H	1.36965300	-2.06878600	-0.44226200
H	-0.37190800	-1.76087100	-0.28739900
C	-4.84282400	-1.12546900	0.93863100

C	-3.33518500	-1.83622400	-1.27577800
C	-5.49133600	-2.11757100	-0.04941500
H	-5.24213900	-0.12313300	0.74470200
C	-4.87034100	-1.87289500	-1.43554300
H	-2.97799900	-2.86643900	-1.14050900
H	-5.27467500	-3.14394000	0.27503500
H	-6.58105000	-2.00657700	-0.06164000
H	-5.16673200	-2.64118900	-2.15809300
H	-5.22269100	-0.91197000	-1.83572400
P	-3.05473800	-1.15341500	0.43540800
O	-2.19698300	-2.03899800	1.29978600
C	-2.57503200	-1.20294200	-2.44068400
C	-5.01936300	-1.47121400	2.41671600
H	-4.57404900	-0.70440000	3.06012500
H	-6.08306200	-1.54704100	2.66868900
H	-4.53566600	-2.42367000	2.65145400
H	-1.49557600	-1.20514000	-2.26507300
H	-2.76752600	-1.76566300	-3.36100000
H	-2.88308800	-0.16746000	-2.61209900
C	0.95802300	1.77846900	2.57722500
H	0.30099500	2.61638900	2.79614000
C	1.82705300	1.52727400	3.74061800
C	1.78826200	2.50103300	4.86596300
O	0.65265400	3.25666000	4.86441900
C	0.60961500	4.28649300	5.85641400
H	1.40843300	5.01401400	5.68491100
H	-0.36575600	4.76148200	5.74451500
H	0.72402000	3.86533900	6.85821000
O	2.64729100	2.63716100	5.71686200
C	2.86538400	0.65462600	3.74325300
H	3.55821500	0.65134900	4.57716500
H	2.99245600	-0.10864600	2.99075400
C	2.37237300	4.65890200	2.35437700
C	1.98437800	3.90767600	1.23218100
C	1.39657200	4.58858400	0.15532500
C	1.17663400	5.96621100	0.20462200
C	1.54567800	6.69423000	1.33552200
C	2.15215800	6.03278800	2.40659200
H	2.86171200	4.16232200	3.18598200
H	1.12087900	4.02878800	-0.73496800
H	0.72771300	6.47090900	-0.64726800

H	1.37557000	7.76630700	1.37814400
H	2.46074800	6.59205500	3.28601300
C	2.20240300	2.42973300	1.17678700
C	3.54670800	2.00247000	1.41805400
H	4.21910900	2.63968300	1.97998700
C	4.06765500	0.81818800	0.84952300
O	3.40928600	-0.03212100	0.19104900
C	5.48552400	0.57419100	1.08884000
C	6.66066500	0.32971100	1.28240400
C	8.03675300	0.04789600	1.51271300
C	8.64384400	-1.08330800	0.93292000
C	8.81582300	0.89403600	2.32599500
C	9.98917500	-1.35592000	1.16166300
H	8.04487900	-1.73587300	0.30589400
C	10.16030500	0.61389600	2.55047300
H	8.34977100	1.76587200	2.77389900
C	10.75234600	-0.51033300	1.97022100
H	10.44502600	-2.23163500	0.70775800
H	10.74934100	1.27488400	3.18037800
H	11.80232400	-0.72616600	2.14706200
H	1.76888200	1.96067700	0.29325600

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C	-2.62973300	0.75348600	0.52083300
C	-1.50626200	1.27390300	1.22278800
C	-1.26834500	2.65541400	1.11981600
C	-2.05043500	3.50171800	0.33727300
C	-3.13247300	2.98560500	-0.36160200
C	-3.41393800	1.62717700	-0.24983300
H	-0.44192600	3.11113600	1.63501800
H	-1.78912100	4.55334000	0.28148200
H	-3.75656900	3.62289200	-0.98064000
H	-4.27274400	1.23493400	-0.78517300
C	0.59764800	-1.08061400	1.50121400
C	-1.11669100	-0.58479300	3.64566100
C	0.27283800	-2.29400800	2.41052200
H	1.66112300	-0.79592200	1.59546400
C	-0.19719000	-1.82022500	3.80090200
H	-2.04358200	-0.92928100	3.18239500

H	-0.51804900	-2.88147700	1.94427100
H	1.16951900	-2.91637000	2.49833300
H	-0.74604500	-2.61433900	4.31915000
H	0.65824500	-1.54979200	4.42674400
P	-0.29418600	0.33254800	2.26974800
C	0.39410300	-1.32578300	0.00732500
C	-1.42555600	0.16945800	4.93926500
H	-1.86118800	1.15702100	4.75269900
H	-2.15075900	-0.40834400	5.52324600
H	-0.53593400	0.29659600	5.55807100
H	0.51703900	-0.40677200	-0.57520000
H	1.16810300	-2.02180700	-0.33011900
H	-0.58506800	-1.76204400	-0.19655200
C	-5.05792800	-0.90206800	0.92387600
C	-3.46081500	-1.55446400	-1.24616600
C	-5.68353300	-1.82921400	-0.13856500
H	-5.41478400	0.12012200	0.75243400
C	-4.98764100	-1.53752600	-1.47875500
H	-3.13534700	-2.60010800	-1.15773200
H	-5.51157600	-2.87538200	0.14710500
H	-6.76776800	-1.68531300	-0.19857100
H	-5.26947400	-2.25940400	-2.25299300
H	-5.29177500	-0.54713900	-1.84546100
P	-3.24778000	-0.97356200	0.51193400
O	-2.47393200	-1.92714000	1.38313300
C	-2.63695600	-0.87267800	-2.33846400
C	-5.32280400	-1.30207500	2.37461900
H	-4.88753800	-0.57772600	3.07189500
H	-6.40015400	-1.35124100	2.56830400
H	-4.88323300	-2.27946200	2.59282700
H	-1.56570300	-0.92133700	-2.12579000
H	-2.81198200	-1.36848200	-3.29980000
H	-2.90739200	0.18108900	-2.45291600
C	0.96793500	1.55783500	2.85772200
H	0.39182200	2.43914800	3.12816100
C	1.64483700	1.10211100	4.12089100
C	1.38799100	1.83250400	5.38387900
O	0.62265500	2.95077600	5.20277200
C	0.33403400	3.68389700	6.39902700
H	1.25767900	4.01200300	6.88209700
H	-0.26023700	4.54130300	6.08090700

H	-0.22898400	3.06352900	7.10183100
O	1.78264600	1.50091500	6.48618800
C	2.61403100	0.16532500	4.14034700
H	3.12982200	-0.03658100	5.07395600
H	2.87000000	-0.43910100	3.27872100
C	1.77198800	4.42866200	2.18597500
C	1.80659600	3.39571700	1.23812100
C	1.65974000	3.72919900	-0.11444300
C	1.46168600	5.05054600	-0.51154400
C	1.41107300	6.07006500	0.44217000
C	1.57325300	5.75264900	1.79181900
H	1.88437400	4.19300200	3.24038000
H	1.69526400	2.93759000	-0.85848300
H	1.34533700	5.28474200	-1.56651900
H	1.25482800	7.10069600	0.13604000
H	1.54638700	6.53834900	2.54239400
C	2.00912100	1.95027000	1.64574200
C	3.45619400	1.70908200	1.90224300
H	4.05696600	2.52104000	2.29553100
C	4.06179200	0.51891300	1.51672400
O	3.45330500	-0.53034000	1.10695900
C	5.51023200	0.46067900	1.65402900
C	6.71835900	0.36524800	1.75775000
C	8.13179800	0.25671700	1.87948300
C	8.79591400	-0.92962000	1.50835300
C	8.89745100	1.33141800	2.37412400
C	10.17841700	-1.03309900	1.62897800
H	8.20960700	-1.75950900	1.12701000
C	10.27952900	1.21969700	2.49268000
H	8.39020700	2.24717500	2.66092300
C	10.92671400	0.03888600	2.12121300
H	10.67542100	-1.95479000	1.33807900
H	10.85536600	2.05775300	2.87639000
H	12.00590200	-0.04530400	2.21462900
H	1.73952000	1.31464500	0.79467900

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C	8.24951900	1.22050300	-1.20444500
C	7.78894800	1.31284900	0.13422000

C	8.74788400	1.53722200	1.13453500
C	10.10121200	1.70045000	0.83756200
C	10.53350300	1.66485900	-0.48390700
C	9.60239500	1.42604700	-1.49237300
H	8.44695300	1.59297500	2.17211700
H	10.80897200	1.87073100	1.64376800
H	11.58061700	1.81342300	-0.73007300
H	9.93999300	1.38683300	-2.52350400
C	5.07239200	2.66587200	0.03219100
C	5.96365000	1.75008700	2.42780200
C	4.33605400	3.23631500	1.27822000
H	4.36793800	2.29365200	-0.71032100
C	4.54053800	2.32629400	2.49779700
H	6.66563100	2.59208000	2.50439800
H	4.74808200	4.22703300	1.50541200
H	3.27373800	3.36846300	1.05684000
H	4.38902000	2.86886300	3.43860700
H	3.81817300	1.50260400	2.48731400
P	6.01259500	1.14830800	0.64886600
C	5.96898800	3.72922600	-0.60626700
C	6.25417300	0.73546300	3.53218900
H	7.22725000	0.24870000	3.41714300
H	6.23556300	1.23186000	4.51002400
H	5.50133700	-0.05536800	3.54231200
H	6.48144700	3.35970400	-1.49405800
H	5.35497000	4.58784700	-0.90517000
H	6.72951700	4.08927400	0.09631300
C	7.41267400	1.95033700	-4.00647000
C	7.64365200	-0.76780800	-3.46979300
C	7.88345600	1.03694100	-5.16571400
H	8.18249300	2.68261900	-3.74065700
C	7.31330900	-0.37480700	-4.92673200
H	6.97826300	-1.54661900	-3.08703700
H	7.56404700	1.44249000	-6.13207200
H	8.97831500	0.99004400	-5.18763500
H	6.22656400	-0.36430400	-5.07356500
H	7.72837600	-1.10418100	-5.63124000
P	7.13149200	0.77619400	-2.57570600
O	5.69826700	0.76542900	-2.09450100
C	9.09735900	-1.22817100	-3.31276300
C	6.10588700	2.68322700	-4.34411700

H	5.75028900	3.29324600	-3.51103700
H	6.26368200	3.33720100	-5.20935400
H	5.30737900	1.97554700	-4.58438400
H	9.34481400	-1.39166100	-2.26476300
H	9.22562700	-2.17573700	-3.84901800
H	9.81105800	-0.51653200	-3.74116800
C	5.18581400	-1.05646500	0.24233800
C	3.80827800	-3.30556300	-0.17998700
C	3.16332500	-2.41514200	0.63502900
C	3.71999400	-1.00162900	0.66164700
H	2.23887200	-2.63710200	1.15476300
O	4.88905100	-2.97356700	-0.82798400
C	3.32408800	-4.65883700	-0.29514500
C	2.94153500	-5.80554900	-0.42592700
C	2.48842700	-7.14604000	-0.57096000
C	1.29888300	-7.57561000	0.05057500
C	3.22099600	-8.07232100	-1.33994900
C	0.86012800	-8.88819800	-0.09449500
H	0.73099300	-6.86533700	0.64311100
C	2.77539300	-9.38317300	-1.47952300
H	4.13719600	-7.74483500	-1.82081700
C	1.59468000	-9.79782300	-0.85878500
H	-0.05964500	-9.20372400	0.39074800
H	3.35148500	-10.08549700	-2.07609400
H	1.24938000	-10.82186600	-0.97017100
H	3.66476900	-0.62438700	1.69310700
C	2.88761400	-0.07343600	-0.20747000
C	2.94292100	-0.16677000	-1.60417400
C	2.01827900	0.85513000	0.37157100
C	2.18826000	0.69270300	-2.39674000
H	3.59293400	-0.90517100	-2.05807600
C	1.25029600	1.71155400	-0.42125700
H	1.93736200	0.90836800	1.45478200
C	1.34488700	1.64144900	-1.81043300
H	2.25894000	0.62355000	-3.47880800
H	0.58131600	2.42890000	0.04732900
H	0.75807400	2.31138900	-2.43310200
C	6.10267100	-1.87975800	1.04799300
C	5.78273200	-2.37169500	2.25965900
H	4.83958100	-2.13984600	2.73610700
H	6.45177700	-3.04628500	2.77948300

C	7.38577000	-2.21214300	0.39266400
O	8.10286500	-3.14431300	1.05297200
C	9.35299500	-3.48988900	0.44620200
H	10.00861000	-2.61577100	0.38989400
H	9.78840300	-4.25506700	1.08939300
H	9.19349000	-3.88100900	-0.56196100
O	7.79105000	-1.68050800	-0.62708500
H	5.45303500	-0.83327100	-0.77209700

1g-b

C	3.77566700	-11.43245100	4.81612200
C	3.35620300	-10.11787400	4.53677500
C	2.32374100	-9.93335600	3.60030400
C	1.72888100	-11.01957500	2.96335300
C	2.15664600	-12.31559400	3.25178700
C	3.18253400	-12.51683800	4.18093400
H	4.57078800	-11.60356400	5.53505100
H	1.99110900	-8.92323600	3.37616500
H	0.93280200	-10.85474800	2.24309400
H	1.69551400	-13.16570200	2.75735500
H	3.51866500	-13.52442900	4.40851600
C	3.94190400	-8.94170800	5.17238000
C	4.93035000	-8.89771600	6.08589500
H	5.41300100	-9.79901500	6.45623600
C	5.40159100	-7.59873800	6.62615500
O	4.92225000	-6.52989900	6.27264100
C	6.52032100	-7.66672500	7.65023800
H	3.53019000	-7.97873000	4.87218700
H	7.40188900	-8.15952000	7.22067800
H	6.78607000	-6.66013900	7.97730700
H	6.20982000	-8.26565600	8.51591600

TS4-b

C	-1.92940900	0.66696400	0.42872200
C	-0.55202600	0.99674700	0.50561800
C	-0.03717500	1.93877200	-0.39556800
C	-0.84151500	2.54711000	-1.35859200

C	-2.18955500	2.21697900	-1.43951800
C	-2.71953700	1.28441700	-0.54991300
H	1.01212600	2.20120500	-0.36566200
H	-0.40783300	3.27040600	-2.04241000
H	-2.82866900	2.67971600	-2.18547200
H	-3.77283300	1.03788400	-0.62238200
C	0.54817400	0.93320100	3.41240000
C	2.34095100	0.77172500	1.32455700
C	1.97483200	1.48514400	3.65613700
H	0.38655700	0.10515400	4.10676200
C	2.97209700	0.78159100	2.72797700
H	2.28299000	1.81942900	1.00340800
H	1.99166300	2.56351000	3.44544900
H	2.21868000	1.32571000	4.70842300
H	3.94104000	1.29346400	2.70563300
H	3.15791100	-0.24343100	3.06513200
P	0.60007400	0.20076000	1.69858400
C	-0.53768100	1.99158000	3.61200500
C	3.06262100	-0.06547700	0.27438700
H	2.56516200	-0.01009100	-0.70051500
H	4.09269200	0.28768500	0.15108400
H	3.09028200	-1.11695500	0.57392400
H	-1.53016600	1.54740000	3.53887200
H	-0.42116000	2.41816100	4.61426500
H	-0.44912100	2.81056900	2.88716000
C	-4.52651700	-0.13497500	1.75574000
C	-2.99579200	-2.15542000	0.69230600
C	-5.07749800	-1.55309600	2.01061100
H	-4.94266200	0.22122700	0.80483400
C	-4.50519200	-2.46155300	0.90766600
H	-2.37388200	-2.86628900	1.24240100
H	-4.74951300	-1.89583300	3.00013900
H	-6.17305100	-1.55727700	2.01235500
H	-4.65356400	-3.52145300	1.13634400
H	-5.04193100	-2.25807700	-0.02835600
P	-2.73239300	-0.53363800	1.56540800
O	-2.05720000	-0.59285300	2.91330400
C	-2.60434300	-2.19633100	-0.78694000
C	-4.78957400	0.88030800	2.86481600
H	-4.38496800	1.86504200	2.60569300
H	-5.86544200	0.99118900	3.04107200

H	-4.31369700	0.55633300	3.79455900
H	-1.53514300	-2.03279400	-0.93851000
H	-2.84897100	-3.18110500	-1.20135200
H	-3.14931500	-1.44709200	-1.37212200
C	0.40713300	-1.51222500	1.41556000
H	-0.10552000	-1.71749400	0.48636700
C	0.93286000	-2.58469000	2.12842000
C	0.75782700	-3.95137300	1.53331000
O	-0.22941300	-4.00344500	0.59964600
C	-0.50517000	-5.31599900	0.09298400
H	-0.83415000	-5.96686100	0.90664500
H	-1.30207600	-5.18338800	-0.64009300
H	0.38340600	-5.74466800	-0.37724100
O	1.40697500	-4.93042300	1.83931700
C	1.51148900	-2.59793200	3.42133200
H	2.09541700	-3.47997000	3.65359000
H	1.89099700	-1.67348700	3.84319700
C	-0.25025500	-5.27107100	4.50724800
C	-0.73237900	-3.96315000	4.35533200
C	-1.99972000	-3.78097600	3.78285400
C	-2.76400400	-4.87529600	3.37669600
C	-2.27147000	-6.17276900	3.52829000
C	-1.00921300	-6.36433800	4.09637800
H	0.74056400	-5.42716400	4.92223300
H	-2.36832300	-2.76734400	3.66630200
H	-3.75225300	-4.71572700	2.95145000
H	-2.86525200	-7.02663700	3.21236900
H	-0.61175200	-7.36905600	4.21209700
C	0.06558000	-2.77580100	4.76317500
C	0.70187800	-2.77106200	6.03208800
H	0.79159600	-3.69701000	6.59195200
C	1.32344000	-1.60103700	6.52536000
O	1.40202400	-0.52787200	5.86911500
C	1.94842400	-1.63330200	7.91506800
H	-0.40248500	-1.83767000	4.47081800
H	3.01640300	-1.39375800	7.84356100
H	1.48939400	-0.85671400	8.53835800
H	1.83376100	-2.60068800	8.41413500

IV-b

C	-2.13685300	0.59903400	0.60810700
C	-0.78313600	1.01850900	0.64984600
C	-0.36257700	2.00871900	-0.24875200
C	-1.23991200	2.57362500	-1.17448300
C	-2.56325900	2.14839000	-1.22434400
C	-3.00046200	1.16861500	-0.33464100
H	0.66520700	2.34705300	-0.24605100
H	-0.88082200	3.33879800	-1.85585600
H	-3.25413700	2.57655400	-1.94423900
H	-4.03671300	0.84952900	-0.37354900
C	0.57106900	0.92535400	3.49832600
C	2.15549200	0.84738500	1.24378900
C	2.01516500	1.47446400	3.62056800
H	0.50118300	0.07575900	4.19102800
C	2.91325300	0.79292600	2.58279400
H	2.05905800	1.90980200	0.98691000
H	2.01903900	2.55907200	3.44381900
H	2.34765300	1.27044400	4.64039100
H	3.88580400	1.28866300	2.48725900
H	3.10745800	-0.24663200	2.86901400
P	0.46708600	0.25771600	1.77085600
C	-0.49938100	1.96350400	3.83300300
C	2.78479600	0.08196200	0.08455600
H	2.18903300	0.16654200	-0.83153400
H	3.78542000	0.47580300	-0.12527200
H	2.87884000	-0.98009400	0.32767900
H	-1.49218800	1.51439800	3.82111400
H	-0.29887900	2.33969200	4.84172600
H	-0.47610800	2.81789200	3.14437600
C	-4.55910700	-0.27805300	2.18117900
C	-3.06772100	-2.27223600	1.00980600
C	-5.04771900	-1.70781600	2.49196600
H	-5.06608000	0.06550600	1.26965700
C	-4.54110900	-2.62165000	1.36140500
H	-2.38247500	-2.94475200	1.53416000
H	-4.63237100	-2.02805500	3.45514000
H	-6.13897200	-1.74054700	2.58251100
H	-4.62332200	-3.67825500	1.63166200
H	-5.16381400	-2.46127000	0.47138300
P	-2.78612800	-0.62138900	1.80996600

O	-1.93124600	-0.60747900	3.05367300
C	-2.79627400	-2.34067000	-0.49466300
C	-4.74104200	0.73790700	3.30617300
H	-4.38460700	1.72993900	3.00770200
H	-5.79822500	0.82524100	3.58048800
H	-4.17528700	0.43067800	4.19032500
H	-1.74975700	-2.14288500	-0.73503600
H	-3.03510800	-3.34476100	-0.86286000
H	-3.41616700	-1.62884900	-1.05158700
C	0.36564000	-1.48155600	1.40966300
H	-0.06635300	-1.64466500	0.42788200
C	0.87826500	-2.55383700	2.07600400
C	0.83081100	-3.87618700	1.37217900
O	-0.22280900	-3.98797500	0.52323100
C	-0.35898400	-5.27369600	-0.09897800
H	-0.53111600	-6.03590200	0.66504000
H	-1.22363200	-5.18834700	-0.75788800
H	0.53881700	-5.52677500	-0.66807600
O	1.64405000	-4.76413000	1.52510600
C	1.38187100	-2.61344300	3.45977500
H	2.04986600	-3.46604400	3.57635900
H	1.89265200	-1.70678000	3.79124100
C	-0.29620800	-5.18907000	3.97242600
C	-0.76138000	-3.89075300	4.22019000
C	-2.14578600	-3.67260400	4.20726200
C	-3.03774500	-4.71048100	3.93266700
C	-2.55928100	-5.99291600	3.65694200
C	-1.18324700	-6.22764100	3.68296600
H	0.77023500	-5.38672100	3.98754400
H	-2.50952000	-2.67052500	4.40939200
H	-4.10870700	-4.52021100	3.94226700
H	-3.25050800	-6.80259300	3.43773100
H	-0.79679200	-7.22470800	3.48646300
C	0.17315700	-2.74273500	4.52664000
C	0.73021700	-2.78502300	5.90098300
H	0.68767800	-3.71215300	6.46356100
C	1.40653300	-1.67913100	6.39298000
O	1.57965800	-0.59799700	5.72663300
C	1.99794000	-1.72703000	7.79660900
H	-0.38858900	-1.81624500	4.37669300
H	3.08189400	-1.56103500	7.74847500

H	1.58022300	-0.91211300	8.40131300
H	1.80864800	-2.67735500	8.30732700

H₂O

O	-0.37844700	-8.39679000	0.00000000
H	0.58894100	-8.34746900	0.00000000
H	-0.65487600	-7.46842600	0.00000000

3R-TS5-a

C	2.95121800	-1.38983900	0.49081200
C	2.41073500	-0.09930300	0.26212700
C	2.36537500	0.79906900	1.34163600
C	2.82254900	0.45499200	2.61044100
C	3.33264800	-0.81742900	2.83776500
C	3.39385900	-1.72138300	1.78158700
H	1.94486000	1.78315300	1.18531800
H	2.75073400	1.17846500	3.41377300
H	3.68104500	-1.10931300	3.82396800
H	3.79869000	-2.71127100	1.96906700
C	0.40628300	-0.24735300	-2.23449700
C	3.00784600	0.64802000	-2.69056700
C	0.97149800	-0.41710400	-3.66876200
H	-0.36782700	0.51895200	-2.30542600
C	2.06344400	0.63634900	-3.91385700
H	3.50853200	-0.32067200	-2.63625500
H	1.39804400	-1.41582000	-3.77072800
H	0.14554800	-0.30122700	-4.37721400
H	2.63514300	0.41961800	-4.82336200
H	1.61113100	1.62905200	-4.03446800
P	1.76319300	0.62161400	-1.32185200
C	-0.18296200	-1.52089600	-1.62306800
C	4.02586400	1.78485900	-2.67201100
H	4.59534600	1.81132800	-1.73558700
H	4.74121700	1.64278500	-3.48985500
H	3.54944800	2.75943500	-2.81429300
H	-0.25245500	-1.45898000	-0.53228400
H	-1.20251000	-1.65527100	-1.99346900

H	0.42848200	-2.38515400	-1.88441800
C	4.87678500	-3.37624600	-0.59343700
C	2.27697800	-4.24598700	-0.18652700
C	4.65232700	-4.90215600	-0.59607700
H	5.26988200	-3.08115300	0.38639900
C	3.41277400	-5.18914200	0.26718400
H	1.86288200	-4.62784400	-1.12973000
H	4.47250300	-5.24056000	-1.62519400
H	5.53903700	-5.43286300	-0.23250100
H	3.09770300	-6.23615000	0.19951400
H	3.64638400	-4.99705800	1.32377400
P	3.15273900	-2.70495000	-0.76126300
O	2.81250000	-2.27123300	-2.16439000
C	1.14271500	-4.08206000	0.82531100
C	5.79787400	-2.85160700	-1.69399400
H	5.94708400	-1.77005200	-1.60440800
H	6.77985600	-3.33437000	-1.63462800
H	5.37106000	-3.04720800	-2.68177600
H	0.35276100	-3.43103600	0.44283500
H	0.69634200	-5.05813600	1.04612300
H	1.50031700	-3.65585100	1.76746600
C	1.39374600	2.32448200	-1.01881200
H	2.28363100	2.92924500	-1.14157200
C	0.23459600	3.01516300	-0.73577800
C	0.41241400	4.52003400	-0.67592900
O	1.43298300	4.97355500	-1.44044700
C	1.65745800	6.38925000	-1.37145200
H	1.90139200	6.69092800	-0.34919800
H	2.49474300	6.58496100	-2.04183200
H	0.76690000	6.93280500	-1.69658100
O	-0.27385100	5.26253900	-0.00301200
C	-1.12693600	2.60262900	-0.53923200
H	-1.74085700	3.43700900	-0.20199900
C	-0.53969300	2.35814900	2.36707900
C	-0.91521400	1.22744400	1.63371200
C	-0.83606500	-0.02786700	2.25344000
C	-0.38861500	-0.15640800	3.56555700
C	-0.01869400	0.97894300	4.29110000
C	-0.09573300	2.23407600	3.68646300
H	-0.59674000	3.33924200	1.90592100
H	-1.14873700	-0.90820100	1.69689700

H	-0.33060300	-1.14011100	4.02428700
H	0.32336800	0.88514900	5.31854200
H	0.18279800	3.12475400	4.24427300
C	-1.47530300	1.31051100	0.21586200
C	-2.96967200	1.08633100	0.29356800
H	-3.48951200	1.49744800	1.15323100
C	-3.69097000	0.36794000	-0.60202000
O	-3.20256700	-0.16090200	-1.74989000
C	-5.07452600	0.09930000	-0.35099200
C	-6.24633800	-0.14990900	-0.14333300
C	-7.61752600	-0.43637800	0.10071000
C	-8.37896900	-1.15502600	-0.84248400
C	-8.24123100	-0.00750200	1.28928600
C	-9.72040700	-1.43395900	-0.59990000
H	-7.90153400	-1.48607100	-1.75914300
C	-9.58370900	-0.28951300	1.52263300
H	-7.65792100	0.54628700	2.01806200
C	-10.32910700	-1.00329400	0.58135500
H	-10.29483800	-1.98928300	-1.33641300
H	-10.05119300	0.04871200	2.44343700
H	-11.37694100	-1.22201700	0.76683400
H	-1.07478300	0.45856600	-0.33519500
H	-1.53643600	2.29913300	-1.76152000
H	-2.65858600	0.57395800	-2.24959000
O	-1.87203000	1.68443500	-2.86923900
H	-2.50994900	2.26356600	-3.31608000

TS1-1

C	2.94528000	-0.07916100	-0.89070400
C	2.49199800	1.22176000	-0.55628600
C	3.12601200	2.31071100	-1.17960800
C	4.11722500	2.13358500	-2.14260800
C	4.49950700	0.84855300	-2.52158600
C	3.92073400	-0.24508100	-1.88285800
H	2.84825600	3.31833900	-0.90487600
H	4.58359100	3.00207000	-2.59867900
H	5.25321900	0.69800800	-3.28850700
H	4.24389300	-1.24631100	-2.15388200
C	0.38298500	3.24403400	0.18552000

C	1.55780000	1.88467300	2.25294100
C	1.13313300	4.13507400	1.18491000
H	-0.64294700	3.11449900	0.57274600
C	1.15778000	3.35966100	2.50727300
H	2.65053900	1.80254900	2.22005800
H	2.15579600	4.34003100	0.84043000
H	0.63457700	5.10593600	1.29686300
H	1.83040000	3.81092100	3.24522700
H	0.15054800	3.37533700	2.94328800
P	0.99115100	1.51491400	0.49145700
C	0.21453400	3.76198300	-1.24386300
C	1.00856400	0.93670600	3.32167800
H	1.36841500	-0.07981000	3.16962900
H	1.31741000	1.29016500	4.31336100
H	-0.08590600	0.90604500	3.30282000
H	-0.29731100	3.01976000	-1.86117800
H	-0.40870600	4.66369200	-1.22637300
H	1.15874900	4.02573800	-1.72558800
C	1.69741300	-2.79703000	-1.12613200
C	3.89269700	-2.55204800	0.53294100
C	2.46932200	-4.09132400	-0.78754900
H	1.98376500	-2.47541200	-2.13660300
C	3.92769800	-3.71506200	-0.47568600
H	3.55244800	-2.95280000	1.49883600
H	2.01530900	-4.55829300	0.09632300
H	2.39499500	-4.81424400	-1.60703200
H	4.49314100	-4.56435300	-0.07589000
H	4.43919300	-3.39931100	-1.39587500
P	2.40654500	-1.54662500	0.05172500
O	1.55334100	-1.14177000	1.22747300
C	5.20766100	-1.80753300	0.75480600
C	0.17480000	-2.92315000	-1.03191300
H	-0.32678100	-2.04026900	-1.43542600
H	-0.16517900	-3.79224500	-1.60664400
H	-0.15720800	-3.04220400	0.00401700
H	5.08128800	-0.98485500	1.46653700
H	5.96324200	-2.48942400	1.16098400
H	5.60121500	-1.38653000	-0.17468400
C	-0.79559100	0.34514200	0.13541700
H	-0.57688500	0.09104000	-0.89888900
H	-0.53905700	-0.45387900	0.82267800

C	-1.99613100	1.05752300	0.36033700
C	-2.74633200	1.64978000	-0.70205400
O	-2.12933000	1.49997400	-1.94581800
C	-2.87105700	2.03768400	-3.03760500
H	-3.08333900	3.10044700	-2.88793700
H	-2.24358400	1.89602700	-3.92064400
H	-3.82255200	1.51195400	-3.16577800
O	-3.83405500	2.21912800	-0.62283800
C	-2.60691500	1.04700500	1.72336600
H	-2.05026300	1.62143700	2.47436600
H	-3.63244800	1.41408000	1.68242100
O	-2.56484500	-0.30202700	2.31128700
C	-3.13085300	-1.29578300	1.60342300
O	-2.71890500	-2.43540700	1.65618200
O	-4.18207800	-0.85208500	0.89968600
C	-4.75730900	-1.64289600	-0.19595400
C	-5.40694500	-2.91106300	0.35876200
C	-5.80191200	-0.68872300	-0.77389900
C	-3.66840200	-1.95268800	-1.22664900
H	-3.19868700	-1.02857100	-1.57661900
H	-2.90151600	-2.60100500	-0.79813600
H	-4.11648700	-2.46342200	-2.08614200
H	-6.27227800	-1.13812200	-1.65521200
H	-6.58088700	-0.48358300	-0.03233100
H	-5.33761700	0.26197100	-1.05031000
H	-5.93541900	-3.43464300	-0.44605200
H	-4.65738700	-3.57657800	0.78866400
H	-6.13577200	-2.65157200	1.13389300

TS1-2

C	3.13034000	0.86033800	-0.15355800
C	1.81622300	1.16240300	-0.59316300
C	1.50899000	2.51469800	-0.85107000
C	2.45945600	3.52684800	-0.74907900
C	3.77211300	3.20905900	-0.41213300
C	4.08838600	1.88877500	-0.10947100
H	0.49373300	2.77903900	-1.11727900
H	2.17462900	4.55469000	-0.95427000
H	4.53781300	3.97771200	-0.36451600

H	5.10560600	1.65774000	0.19231700
C	-0.50816900	-0.57062100	0.45735200
C	0.89625700	-1.62273100	-1.70667900
C	-0.41821500	-2.11290400	0.36519100
H	-1.54098500	-0.26253400	0.25061800
C	-0.22079800	-2.50739500	-1.10599900
H	1.83765000	-1.91528600	-1.24230000
H	0.44321600	-2.44702500	0.94707500
H	-1.33341000	-2.55502400	0.76634400
H	0.05144000	-3.56470100	-1.20628200
H	-1.15901600	-2.35622700	-1.65285300
P	0.40610300	0.04077200	-1.03437500
C	-0.07499500	0.01853700	1.79714000
C	1.00692600	-1.67835700	-3.22944300
H	1.77551100	-0.99469600	-3.60928300
H	1.27807200	-2.69235000	-3.54707300
H	0.05930100	-1.42589400	-3.71760900
H	-0.12886900	1.11249500	1.79268900
H	-0.73885100	-0.34834700	2.58876400
H	0.94631900	-0.28772700	2.04131400
C	5.23023400	-1.22304400	-0.37980500
C	4.56388000	-0.39786900	2.17191400
C	6.24965900	-1.53242000	0.73685600
H	5.57431300	-0.34243000	-0.93653900
C	6.06884700	-0.48389400	1.84941400
H	4.28325200	-1.30602500	2.72353600
H	6.04698000	-2.53282200	1.14180200
H	7.27289800	-1.54501100	0.34547800
H	6.64635500	-0.73734100	2.74566300
H	6.43538900	0.49315800	1.50533600
P	3.70045700	-0.73204000	0.55520000
O	2.64997400	-1.80200100	0.68475900
C	4.11985000	0.81588700	2.98603700
C	4.96403000	-2.37339700	-1.35017000
H	4.27165800	-2.07211100	-2.14379100
H	5.89619800	-2.70389800	-1.82233800
H	4.51748900	-3.22425200	-0.82707000
H	3.03730600	0.80751000	3.15073100
H	4.60905900	0.81111100	3.96677600
H	4.37298200	1.75658300	2.48916600
C	-1.25296200	1.03515800	-2.34286700

H	-0.70982500	1.96530500	-2.45367500
H	-1.14898500	0.38133700	-3.20649800
C	-2.49759000	1.04170800	-1.69540000
C	-2.76932600	1.98610500	-0.64454700
O	-1.63672500	2.71578400	-0.30447300
C	-1.82434200	3.66104600	0.74738300
H	-2.13030900	3.16157600	1.67143600
H	-0.85477800	4.14480200	0.88525000
H	-2.58631900	4.39975100	0.48286900
O	-3.82657600	2.17799900	-0.05132700
C	-3.53165300	0.01915000	-2.00820400
H	-4.53258600	0.40262200	-1.82516300
H	-3.44709400	-0.33076700	-3.03915700
O	-3.36721900	-1.23618100	-1.23409700
C	-4.03760900	-1.43807000	-0.08914300
O	-3.68660800	-2.29447500	0.69823100
O	-5.09623400	-0.63242300	0.03020500
C	-5.76517600	-0.44589200	1.32996600
C	-4.73861700	0.00051000	2.37259000
C	-6.74947000	0.68170100	1.02550600
C	-6.48624900	-1.73424600	1.72425300
H	-7.17405500	-2.04197200	0.92925300
H	-5.77218700	-2.53875700	1.90549500
H	-7.07113700	-1.56237000	2.63482500
H	-7.31139900	0.94143400	1.92893800
H	-6.20407500	1.56008000	0.67191300
H	-7.46068500	0.37076900	0.25288000
H	-5.25666200	0.25501200	3.30378300
H	-4.01919400	-0.79372900	2.58091600
H	-4.21291200	0.88769200	2.00843700

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C	-2.41625800	1.28093000	0.61224100
C	-1.19137600	1.56940600	1.26400400
C	-1.09317200	2.80003300	1.93895100
C	-2.13150500	3.72513300	1.96788100
C	-3.32200300	3.44809200	1.30363600
C	-3.45046200	2.23432100	0.63957300
H	-0.17079000	3.05470400	2.43804400

H	-2.00087200	4.65959300	2.50516200
H	-4.14178200	4.16009800	1.30497700
H	-4.38346100	2.02296600	0.12685400
C	1.16909600	-0.28134000	-0.01775300
C	-0.15477700	-1.07733100	2.30566400
C	1.10337500	-1.80541100	0.26418500
H	2.19711800	0.05668900	0.14685100
C	0.93202600	-2.04401700	1.77706600
H	-1.11725500	-1.35877800	1.87241000
H	0.25500900	-2.22265900	-0.27865700
H	2.02186400	-2.27624900	-0.10419600
H	0.62631000	-3.07745000	1.97740500
H	1.86271700	-1.85284800	2.32652700
P	0.31862300	0.48325400	1.44969900
C	0.74527600	0.15047700	-1.41885500
C	-0.23200100	-0.97107100	3.82712600
H	-0.93659800	-0.19433600	4.14976300
H	-0.57666000	-1.92521400	4.24242700
H	0.76283000	-0.76302200	4.22719500
H	0.75958200	1.23995100	-1.52238700
H	1.44720700	-0.26476300	-2.15121700
H	-0.24921900	-0.22901100	-1.65336100
C	-4.51291700	-0.79806600	0.23249800
C	-3.32200100	0.22987200	-2.04945400
C	-5.24911000	-1.03816900	-1.10264300
H	-4.99931100	0.03098000	0.75904200
C	-4.85955000	0.09626200	-2.06621300
H	-2.89641500	-0.60172500	-2.62789400
H	-4.93110700	-2.00191200	-1.52194900
H	-6.33244300	-1.09494300	-0.95095300
H	-5.22422800	-0.08647800	-3.08305500
H	-5.31465600	1.03933200	-1.73273400
P	-2.82727100	-0.24273800	-0.31694800
O	-1.77874400	-1.31996100	-0.24890000
C	-2.77653500	1.54706600	-2.60054900
C	-4.43055800	-2.01285500	1.15659300
H	-3.94026300	-1.75935500	2.10250800
H	-5.43433900	-2.38822700	1.38524500
H	-3.85383200	-2.81640700	0.69002600
H	-1.68377500	1.57948500	-2.55123600
H	-3.07007300	1.66747600	-3.64941600

H	-3.16195400	2.40670700	-2.04381700
C	1.63323600	1.30439600	2.36278600
H	1.22314000	1.96545400	3.13049200
H	2.22908300	0.41046500	3.03587400
C	2.72427600	1.96974900	1.55364000
C	2.48101300	3.11214600	0.62534900
O	1.17036700	3.17247100	0.25145100
C	0.83059100	4.21328800	-0.67046000
H	1.34296100	4.06254200	-1.62458900
H	-0.25072900	4.14694200	-0.79745300
H	1.11430700	5.18909400	-0.26857600
O	3.30903200	3.88644100	0.19271500
C	3.98574300	1.51364700	1.62429800
H	4.77987700	2.00265900	1.06805800
H	4.19247000	0.64296600	2.24344300
C	3.54657800	-0.36449000	4.89698300
C	5.08940300	-0.34203200	4.80654100
C	3.12811500	-1.52551400	5.82608100
C	3.06615500	0.97043300	5.51158800
H	3.42973800	-2.47774400	5.37539700
H	3.58241600	-1.45173500	6.82359000
H	2.03868200	-1.54338400	5.94788900
H	3.35433200	1.80940100	4.86604900
H	1.97294400	0.97514500	5.60882300
H	3.49423100	1.14587100	6.50709800
H	5.43676300	-1.25908400	4.31749200
H	5.42299800	0.51019700	4.20217500
H	5.56977000	-0.26759100	5.79167200
O	3.00153400	-0.56418200	3.62822400

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C	-2.32930100	0.98312600	0.63659900
C	-1.01594200	1.22763900	1.12819000
C	-0.75984200	2.46129200	1.75209600
C	-1.74954800	3.43503400	1.88130100
C	-3.03017800	3.20436900	1.39767500
C	-3.30450500	1.98379500	0.78823800
H	0.22013500	2.71610500	2.16255700
H	-1.49344800	4.37086300	2.36968700

H	-3.81191100	3.95271200	1.49187100
H	-4.30943800	1.80850800	0.41731200
C	1.01287300	-0.57350700	-0.53839200
C	-0.01891400	-1.57683100	1.84347300
C	0.96260300	-2.11706900	-0.38646200
H	2.06018000	-0.25911200	-0.53474200
C	0.98242800	-2.49332900	1.10741800
H	-1.01388900	-1.80970300	1.46143400
H	0.03578500	-2.48013800	-0.83160200
H	1.80790900	-2.56712800	-0.91883100
H	0.70976500	-3.54417000	1.25659500
H	1.98806400	-2.35612300	1.52719600
P	0.42141000	0.06148800	1.11198200
C	0.35756200	-0.02373900	-1.80178200
C	-0.00934100	-1.66777800	3.36739500
H	-0.68488200	-0.93336900	3.81976400
H	-0.34432900	-2.66486000	3.67509400
H	0.98776800	-1.51277500	3.79045500
H	0.38337900	1.06947500	-1.81267800
H	0.91036900	-0.38070000	-2.67872900
H	-0.67060400	-0.37445800	-1.88918700
C	-4.53697300	-1.00609400	0.65268800
C	-3.78035200	-0.00463400	-1.81719900
C	-5.52375900	-1.22320900	-0.51347400
H	-4.88261800	-0.15820700	1.25475600
C	-5.29557600	-0.09809000	-1.53780800
H	-3.49732300	-0.84806500	-2.46204200
H	-5.32019700	-2.19480500	-0.98301100
H	-6.55864200	-1.24902600	-0.15511600
H	-5.85218500	-0.27047200	-2.46567700
H	-5.65459700	0.85587600	-1.12755500
P	-2.97124500	-0.50694900	-0.21476500
O	-1.99052600	-1.64049700	-0.37975400
C	-3.31843800	1.29515800	-2.47479900
C	-4.32049600	-2.22050200	1.55461000
H	-3.64618100	-1.98265600	2.38470200
H	-5.27244400	-2.55782900	1.97983100
H	-3.87679400	-3.04658600	0.99146400
H	-2.23773100	1.29620400	-2.64535800
H	-3.81265900	1.42077500	-3.44483300
H	-3.55840400	2.16737600	-1.86013000

C	1.85288800	0.66989400	2.03396500
H	1.74845700	1.83571000	2.55969700
H	2.05715500	-0.06880200	2.81112700
C	3.08321100	0.93941000	1.23174400
C	3.05455700	2.17858100	0.39100700
O	1.78322900	2.43816400	-0.02101100
C	1.53938000	3.79225000	-0.42632400
H	0.50535900	3.81561700	-0.77310700
H	1.66788800	4.42836900	0.45305600
H	2.22586400	4.08698800	-1.22272500
O	4.00995700	2.84771900	0.06850700
C	4.24207700	0.27507400	1.34036300
H	5.13231700	0.63610700	0.83616000
H	4.33266300	-0.61066700	1.96267700
C	2.41350500	3.59650700	3.93748900
C	3.86318000	3.08671700	4.07460500
C	1.56145000	3.06338200	5.10935600
C	2.40880100	5.13597100	3.95978400
H	1.54829500	1.96614400	5.09784000
H	1.94095700	3.38776700	6.08728900
H	0.52689300	3.41365300	5.00775700
H	3.00384000	5.51692900	3.12222800
H	1.38226900	5.50352700	3.84010000
H	2.81775400	5.54419900	4.89351300
H	3.88190600	1.99024800	4.09361400
H	4.44635300	3.41250100	3.20685200
H	4.35100400	3.45206900	4.98798200
O	1.87509500	3.17889000	2.71814200

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C	-1.79182700	1.15847500	1.29949900
C	-0.43435500	0.77827500	1.41803800
C	0.45031900	1.66925800	2.04679700
C	0.03272900	2.90061500	2.54028800
C	-1.30408500	3.27274300	2.42716600
C	-2.19833100	2.40174700	1.81464000
H	1.48439300	1.38694900	2.16398000
H	0.75152100	3.55975100	3.01771500
H	-1.65006500	4.22783400	2.81100600

H	-3.23786300	2.70187100	1.72917900
C	2.15725900	-0.77815200	0.84065000
C	0.21853200	-0.77993100	-1.05284600
C	2.49012500	0.13406400	-0.34926000
H	2.29011300	-1.84093800	0.52298700
C	1.64666400	-0.37642600	-1.52570600
H	-0.50393300	0.00107100	-1.30806400
H	2.27230200	1.18798300	-0.12549700
H	3.56036200	0.07304600	-0.57731800
H	1.58514000	0.35255600	-2.34078700
H	2.12793300	-1.27640700	-1.92106800
P	0.31087300	-0.80168000	0.81786300
C	3.02628600	-0.61912400	2.08332200
C	-0.21554100	-2.11555800	-1.67114300
H	-1.26768500	-2.31637300	-1.46680000
H	-0.07971100	-2.05270500	-2.75815900
H	0.40940600	-2.92912600	-1.28063800
H	2.74965500	-1.34207000	2.84936200
H	4.06265200	-0.81955900	1.78549800
H	3.00575300	0.37630300	2.53719800
C	-4.59578300	0.20047000	1.56559800
C	-3.82818900	1.23389800	-0.88510600
C	-5.72413600	0.67952400	0.62674500
H	-4.43568000	0.95784700	2.34190300
C	-5.15023200	1.76710200	-0.29795000
H	-4.06830600	0.47381000	-1.64162900
H	-6.06987800	-0.16850800	0.02080000
H	-6.58694600	1.03830300	1.19853800
H	-5.85188600	2.03766100	-1.09502100
H	-4.95784200	2.68377300	0.27659300
P	-3.09769600	0.18042800	0.46474000
O	-2.65693100	-1.18148900	0.00375800
C	-2.91565200	2.28567400	-1.51343800
C	-4.84066800	-1.15800000	2.22139000
H	-4.02246900	-1.42745700	2.89573900
H	-5.77364600	-1.14076800	2.79649100
H	-4.91226100	-1.94477200	1.46465000
H	-1.99713700	1.83484800	-1.90453500
H	-3.42512500	2.78122000	-2.34762000
H	-2.62789900	3.05429900	-0.78970500
C	-0.37234600	-2.34579600	1.45876900

H	-1.15396100	-2.62195300	0.75453200
C	-0.91366500	-2.44661800	2.83821800
C	-0.22444600	-1.69907800	3.91802500
O	-0.61676700	-2.02881200	5.16323700
C	0.01708300	-1.29174800	6.21803700
H	-0.41063900	-1.68045800	7.14222000
H	1.09851000	-1.44918300	6.19782600
H	-0.18784100	-0.22247500	6.11662900
O	0.61136300	-0.83333200	3.70777400
C	-1.97134000	-3.22586100	3.13280100
H	-2.30739000	-3.36378300	4.15331700
H	-2.50609800	-3.75047700	2.34773900
H	0.54855800	-3.05627400	1.19925100
C	2.29023100	-4.78805500	0.84822000
C	2.92449300	-4.56720500	2.24283300
C	3.38336700	-5.25804400	-0.13497800
C	1.20296400	-5.88184700	0.96045800
H	4.15395800	-4.48275200	-0.22443700
H	3.86639200	-6.19400900	0.17826900
H	2.94230400	-5.40776600	-1.12723300
H	0.42959600	-5.56850800	1.67390300
H	0.72305500	-6.02015000	-0.01527500
H	1.60258700	-6.84961500	1.29358700
H	3.69759900	-3.79171200	2.17935600
H	2.15807800	-4.22204400	2.94934000
H	3.38217300	-5.47688700	2.65570400
O	1.73307200	-3.61026300	0.37885000

TS3-4

C	-1.71715100	1.19861100	1.04701400
C	-0.38138600	0.98842400	1.46193700
C	0.19747600	1.91882900	2.33726000
C	-0.50560300	3.02435500	2.81098600
C	-1.82580300	3.21420300	2.42241000
C	-2.41344800	2.30381500	1.54766800
H	1.21045800	1.78144100	2.67544300
H	-0.02054400	3.71876500	3.49027600
H	-2.39879700	4.05794600	2.79546400
H	-3.44834100	2.45292800	1.26317800

C	2.42524500	-0.17052300	1.50390500
C	1.04623100	-0.60950700	-0.75416100
C	2.91865600	0.72039100	0.35811800
H	2.80462600	-1.18443400	1.30043900
C	2.44742700	0.04497400	-0.94221400
H	0.27335000	-0.04615900	-1.27408400
H	2.49309000	1.72707200	0.46062000
H	4.00928200	0.82997600	0.37948400
H	2.42793600	0.75087000	-1.77833700
H	3.16501500	-0.74059400	-1.20668500
P	0.63354300	-0.48908100	1.06261800
C	2.90264600	0.19437800	2.91504700
C	0.98936900	-2.06063000	-1.24621900
H	-0.00904300	-2.47252000	-1.10036700
H	1.23198200	-2.08653700	-2.31489100
H	1.72220900	-2.69045400	-0.72777100
H	2.25396700	-0.22084000	3.69036800
H	3.91071400	-0.20624400	3.06959900
H	2.97413100	1.27617600	3.06254100
C	-4.28335800	-0.25519900	0.51037200
C	-3.15581700	1.23855000	-1.52276300
C	-5.26071200	0.47248900	-0.45041500
H	-4.32385900	0.17915700	1.51472000
C	-4.57536600	1.67637900	-1.12524200
H	-3.23756400	0.53032700	-2.36054500
H	-5.55976900	-0.23885400	-1.23041800
H	-6.17634000	0.76871200	0.07303200
H	-5.14098900	2.01719200	-2.00069400
H	-4.52472700	2.53304800	-0.44154600
P	-2.59008800	0.11788500	-0.15080200
O	-1.70667100	-1.00690500	-0.61714100
C	-2.19927900	2.36169000	-1.91769800
C	-4.54014400	-1.76213400	0.60366600
H	-3.75931300	-2.28364600	1.17135700
H	-5.52191500	-1.93476200	1.06349500
H	-4.55755100	-2.20545700	-0.39875800
H	-1.20582900	1.96892000	-2.16355600
H	-2.57305300	2.89605200	-2.79881800
H	-2.08067600	3.08871100	-1.10793800
C	0.10399000	-2.01133300	1.82815300
H	-0.93926200	-2.59702600	1.42171200

C	-0.23128800	-1.97329900	3.29249300
C	-1.66047900	-1.62544300	3.57950300
O	-2.15903000	-2.30248700	4.63246300
C	-3.56589300	-2.12650600	4.83314000
H	-3.81824500	-2.74196100	5.69741700
H	-3.80692100	-1.07672600	5.02277500
H	-4.10127800	-2.47118100	3.94492000
O	-2.28430200	-0.75994800	2.99093000
C	0.59143400	-2.35478200	4.27940000
H	0.24335200	-2.44867900	5.30230700
H	1.62429400	-2.62599900	4.07730400
H	0.94540500	-2.69369300	1.66288400
C	-2.05544700	-4.68614000	1.55304100
C	-2.65485900	-5.07342100	0.18366000
C	-2.89234500	-5.31858000	2.68467300
C	-0.61155000	-5.23583900	1.63904500
H	-3.92261500	-4.94699800	2.62950500
H	-2.91732500	-6.41567500	2.63241500
H	-2.47686100	-5.02061800	3.65381700
H	-0.00123000	-4.83694700	0.81888900
H	-0.15199300	-4.93675900	2.58834900
H	-0.58492500	-6.33115600	1.57367400
H	-3.69440700	-4.73252300	0.12207700
H	-2.09401100	-4.57401800	-0.61499700
H	-2.63429900	-6.15739800	0.00341600
O	-2.08869500	-3.30345600	1.70541100

III-1

C	-2.35835100	1.36302600	0.42995400
C	-1.01225900	1.65815000	0.75935600
C	-0.69886300	2.98166600	1.11740100
C	-1.66577000	3.98126400	1.18899500
C	-2.99495900	3.67537900	0.91589200
C	-3.32550900	2.37845500	0.53487000
H	0.33304900	3.20778300	1.36027100
H	-1.37789100	4.98766600	1.47780800
H	-3.76836400	4.43451800	0.98854500
H	-4.36211000	2.15752300	0.29901300
C	1.12515200	-0.10325600	-0.70062500

C	0.05175300	-1.10026100	1.67661900
C	1.05856300	-1.64449500	-0.55224700
H	2.17151000	0.22118200	-0.69529300
C	1.07072100	-2.00350200	0.94269500
H	-0.94547900	-1.37940900	1.33749500
H	0.12473100	-1.99521300	-0.99461700
H	1.89396100	-2.11233700	-1.08561800
H	0.81898200	-3.05781600	1.10492200
H	2.06819300	-1.83246000	1.36878300
P	0.48990400	0.53988900	0.92045500
C	0.44272400	0.44208800	-1.95549600
C	0.16398800	-1.17211400	3.19696700
H	-0.62555300	-0.59962000	3.69320900
H	0.07638900	-2.21653900	3.52121500
H	1.12508200	-0.78124700	3.54131400
H	0.46581700	1.53680500	-1.98589000
H	0.95875100	0.06931100	-2.84817600
H	-0.59438900	0.10404500	-2.00176000
C	-4.41081400	-0.73733300	0.83193500
C	-4.03999000	0.14921100	-1.75909700
C	-5.54424100	-1.03693900	-0.17158000
H	-4.69887200	0.12900000	1.44003200
C	-5.49897200	0.03753100	-1.27301500
H	-3.81552700	-0.74197200	-2.36186500
H	-5.37753700	-2.02597300	-0.61884700
H	-6.51741400	-1.07068500	0.33047800
H	-6.17026500	-0.20304300	-2.10518500
H	-5.83367900	1.00218300	-0.86752500
P	-2.99973100	-0.20930100	-0.25556200
O	-1.96394400	-1.27052200	-0.52413800
C	-3.70246500	1.38889800	-2.58536300
C	-4.02720100	-1.90132400	1.74490300
H	-3.25363400	-1.60578300	2.46188100
H	-4.89795700	-2.24965600	2.31187500
H	-3.63449600	-2.73840900	1.16000000
H	-2.64769100	1.39452100	-2.87939900
H	-4.30630800	1.40824900	-3.49984300
H	-3.89752600	2.31282900	-2.03409000
C	1.79891600	1.33893600	1.67187800
H	2.69272400	1.40294900	1.06862400
C	1.80839000	1.93195700	2.98481600

C	3.12377900	2.46126100	3.48945000
O	4.13713300	2.28603800	2.60045400
C	5.40828200	2.77654000	3.03469700
H	6.10106700	2.56123800	2.21977800
H	5.36393100	3.85229800	3.22746300
H	5.72512600	2.27168400	3.95166900
O	3.30765200	2.99637900	4.56581300
C	0.77367200	2.10348300	3.85128100
H	0.94694500	2.55491500	4.81915800
H	-0.23559000	1.78621400	3.61457200

III-2

C	-2.33415100	1.31132100	0.55636100
C	-1.08063000	1.56391400	1.16420500
C	-0.91160600	2.79796200	1.81635900
C	-1.90635900	3.76838000	1.85305600
C	-3.13384200	3.52146300	1.24368000
C	-3.33683800	2.29980700	0.61432400
H	0.03124400	2.97727900	2.31964300
H	-1.72198100	4.71017600	2.36199100
H	-3.92778400	4.26244400	1.26460600
H	-4.30227900	2.11182000	0.15418400
C	1.17553700	-0.16432900	-0.24134400
C	-0.03001600	-1.17135700	2.04934700
C	1.14695500	-1.70800400	-0.08140500
H	2.20632500	0.19037500	-0.15734800
C	1.03113700	-2.08792900	1.40550900
H	-0.99141200	-1.41003800	1.59067100
H	0.27143500	-2.08928500	-0.60921200
H	2.04226600	-2.14768000	-0.53619700
H	0.74588400	-3.14057400	1.52161900
H	1.99003600	-1.94463600	1.91909500
P	0.45138300	0.47499500	1.36059300
C	0.60176000	0.32720000	-1.56846600
C	-0.13497600	-1.28029500	3.56767200
H	-0.84311800	-0.55293600	3.98025200
H	-0.48622500	-2.28234500	3.84128300
H	0.83314500	-1.12706800	4.05390700
H	0.57408700	1.41809600	-1.60460100

H	1.23745900	-0.02599900	-2.39032000
H	-0.39674800	-0.08041800	-1.72754300
C	-4.50552000	-0.70550900	0.36031200
C	-3.47601100	0.25557100	-2.02452600
C	-5.34419600	-0.96489300	-0.90790400
H	-4.93211900	0.14993900	0.89626400
C	-5.01201300	0.14273300	-1.92243500
H	-3.10628300	-0.58974500	-2.62094800
H	-5.07121000	-1.94224900	-1.32785000
H	-6.41426900	-1.00178900	-0.67490400
H	-5.45513600	-0.05484800	-2.90508300
H	-5.42803000	1.09882600	-1.57545500
P	-2.85180000	-0.20518400	-0.32824900
O	-1.85409400	-1.33476100	-0.34659500
C	-2.96256700	1.55729400	-2.63896300
C	-4.38222700	-1.89526900	1.31112400
H	-3.81339200	-1.62758300	2.20826400
H	-5.37344700	-2.23878100	1.62880400
H	-3.86239200	-2.72579700	0.82507300
H	-1.86975800	1.57674000	-2.68094300
H	-3.34318800	1.66637100	-3.66118600
H	-3.28706400	2.42976400	-2.06442400
C	1.61650900	1.13078200	2.42466100
H	1.57498900	0.72489100	3.42864000
C	2.56653400	2.19040400	2.21023400
C	2.50129400	2.88538200	0.89480500
O	3.51765500	3.73719700	0.64883300
C	3.43972700	4.43488000	-0.59909100
H	2.53020700	5.04023600	-0.64867500
H	4.32552600	5.06988900	-0.63377900
H	3.43860300	3.73054700	-1.43558300
O	1.59878400	2.72168700	0.08307300
C	3.48355000	2.62678000	3.11696800
H	4.16284900	3.43689600	2.89088000
H	3.55293700	2.16801600	4.09874100

III-3

C	0.94912100	-0.30142600	1.02238700
C	-0.33157700	-0.91001100	1.01498400

C	-0.95606300	-1.17959800	2.23878500
C	-0.39320900	-0.79376600	3.45456100
C	0.81065000	-0.10036600	3.45613700
C	1.47425900	0.12071400	2.24965300
H	-1.90997600	-1.68503500	2.25244400
H	-0.90809500	-1.01545100	4.38472900
H	1.24839600	0.24948300	4.38645600
H	2.42839800	0.62806900	2.27911600
C	-3.03738200	-1.60068900	-0.12741000
C	-0.90852900	-2.72464300	-1.38519300
C	-2.94358500	-3.11468400	0.10747000
H	-3.46924300	-1.47209400	-1.13242500
C	-2.10428600	-3.66499700	-1.06187200
H	0.00839100	-3.07361500	-0.90617800
H	-2.46384100	-3.33868600	1.06815900
H	-3.93774400	-3.57740400	0.13387500
H	-1.74609100	-4.68066700	-0.86436700
H	-2.74786300	-3.72182500	-1.94853000
P	-1.28542500	-1.09840000	-0.55708800
C	-3.90007800	-0.75252200	0.80842300
C	-0.64333700	-2.59189100	-2.88675700
H	0.23134200	-1.96439000	-3.05857900
H	-0.44918100	-3.58560700	-3.30797000
H	-1.50866700	-2.17064800	-3.41103200
H	-3.83565900	0.30365800	0.53089900
H	-4.94852600	-1.06331900	0.72334600
H	-3.62153800	-0.83664600	1.86098100
C	2.11654600	1.47319800	-1.17239600
C	3.79479000	-0.26495500	0.09752800
C	3.52257900	2.02287200	-0.79770600
H	1.32904300	2.05667000	-0.68549000
C	4.15993800	1.20613800	0.34416100
H	4.27676900	-0.55752500	-0.84874300
H	4.16775400	1.93662400	-1.68067100
H	3.46971700	3.08804100	-0.54948500
H	5.24785700	1.34252900	0.36531000
H	3.78975600	1.54944600	1.31712800
P	2.02908400	-0.25377200	-0.47894400
O	1.73867700	-1.40815600	-1.40454800
C	4.21155600	-1.28893300	1.15135400
C	1.90227000	1.47503600	-2.69025800

H	0.92574900	1.07859100	-2.96083800
H	1.97728300	2.49987800	-3.07290800
H	2.66746900	0.87011800	-3.18903100
H	3.88065200	-2.29166100	0.86110700
H	5.30341800	-1.31011200	1.24855800
H	3.79449100	-1.07272000	2.13811600
C	-1.12296400	0.28707300	-1.52207200
C	-1.28685500	1.63858300	-1.05984800
C	-1.22460200	2.63715300	-2.18267600
O	-1.02539900	3.91196000	-1.76171900
C	-0.98464000	4.88854500	-2.80670600
H	-0.81768900	5.84444000	-2.30828200
H	-0.17188900	4.67189000	-3.50585300
H	-1.92688800	4.90450300	-3.36178800
O	-1.32248600	2.36155900	-3.36365600
C	-1.47659800	2.11504300	0.20304800
H	-1.55317200	3.17698900	0.38896000
H	-1.56078700	1.45553000	1.05935400
H	-1.06084300	0.11934100	-2.58807700

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C	-1.42164200	1.52137800	0.86086300
C	-0.00981200	1.63407000	0.89738400
C	0.60501900	2.69923300	0.22598600
C	-0.14648900	3.64248800	-0.47561200
C	-1.53196200	3.52848000	-0.51727700
C	-2.15765800	2.47487100	0.14955000
H	1.68301400	2.80028800	0.23651700
H	0.35539600	4.45782800	-0.98761600
H	-2.12768400	4.25508000	-1.06168600
H	-3.23919500	2.40101400	0.11745200
C	1.21781200	0.59241000	3.56670900
C	2.83711600	0.80347900	1.38182800
C	2.74610300	0.50512100	3.84462900
H	0.67984800	-0.24021000	4.01084800
C	3.50197800	0.08398700	2.57045700
H	2.97714400	1.88398400	1.52365900
H	3.10256200	1.49299200	4.16010000
H	2.93537900	-0.18437400	4.67287900

H	4.56679900	0.33476700	2.62896500
H	3.43432400	-0.99991900	2.41829000
P	1.05394100	0.39254900	1.72958600
C	0.58892700	1.89030600	4.07934300
C	3.33724300	0.36828500	0.00817100
H	2.83714600	0.91285800	-0.80022800
H	4.41475000	0.54611200	-0.08016200
H	3.14937900	-0.69927300	-0.14237300
H	-0.48920900	1.88130200	3.91549200
H	0.77538700	1.96749900	5.15639700
H	1.02372400	2.77527200	3.59902500
C	-4.03477700	0.66399800	2.13395800
C	-2.70448600	-1.21716000	0.66809500
C	-4.63421100	-0.75456700	2.25888900
H	-4.47497800	1.14048400	1.24712300
C	-4.18050700	-1.56284500	1.02627100
H	-2.06761300	-2.04357800	0.98850900
H	-4.25388400	-1.22351000	3.17461800
H	-5.72592600	-0.71329200	2.34176200
H	-4.25439200	-2.63759300	1.20593400
H	-4.82513600	-1.30840900	0.17476500
P	-2.29184300	0.18991300	1.77951900
O	-1.53534900	-0.11031700	3.05677100
C	-2.50834500	-0.94317800	-0.82474600
C	-4.19128100	1.55794200	3.36011600
H	-3.75546800	2.54950400	3.19092600
H	-5.24958500	1.69165200	3.61111600
H	-3.68504000	1.11011100	4.22026600
H	-1.46556100	-0.73212800	-1.07524700
H	-2.81194400	-1.82793500	-1.39433200
H	-3.11722600	-0.09889800	-1.17189900
C	0.64863900	-1.17286000	1.08071500
H	0.27900800	-1.11958900	0.06463500
C	0.82502500	-2.43074400	1.64678300
C	0.46649100	-3.63203800	0.81963300
O	-0.17751300	-3.31702000	-0.32789300
C	-0.80844500	-4.43240100	-0.97576100
H	-1.58173500	-4.82505200	-0.31054900
H	-1.24510500	-4.02882400	-1.89071700
H	-0.07830900	-5.21164400	-1.20628300
O	0.73998900	-4.77133700	1.14302000

C	1.21177700	-2.76946700	2.97102500
H	1.62325400	-3.76407100	3.08710200
H	1.71208500	-2.01534600	3.56448100
C	0.96030600	-3.34765200	6.12487700
C	0.03693300	-2.59544100	5.38263200
C	-0.40361400	-1.36951000	5.90737700
C	0.07091600	-0.90842500	7.13629200
C	0.99362900	-1.66253600	7.86221200
C	1.43361200	-2.88686000	7.35139500
H	1.31687400	-4.29375600	5.72671000
H	-1.11874600	-0.78560400	5.33554700
H	-0.28544800	0.04116100	7.52816800
H	1.36547200	-1.30362800	8.81807600
H	2.15089800	-3.48228900	7.91036000
C	-0.46016200	-3.03936400	4.05041400
C	-0.94112500	-4.36432800	3.88886200
H	-0.63384000	-5.15553200	4.56495700
C	-1.76892500	-4.68739200	2.79363300
O	-2.13921500	-3.86471500	1.90394400
C	-2.20946900	-6.06681400	2.68730100
C	-2.60918700	-7.20752900	2.55209400
C	-3.06842500	-8.54516200	2.39904700
C	-3.92532100	-8.89207600	1.33572400
C	-2.67590700	-9.54851100	3.30700000
C	-4.37301100	-10.20133400	1.18864300
H	-4.22906400	-8.12090900	0.63502400
C	-3.12805100	-10.85543400	3.15296800
H	-2.01518700	-9.28439100	4.12645900
C	-3.97741000	-11.18791600	2.09499300
H	-5.03349400	-10.45426500	0.36363600
H	-2.81666000	-11.61880400	3.86081000
H	-4.32857700	-12.20926700	1.97749000
H	-1.05175600	-2.28317100	3.54242900

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C	-2.72679100	-0.51232200	2.24026500
C	-1.36768500	-0.19990200	2.49506900
C	-0.88863300	-0.36940200	3.80654200
C	-1.69761800	-0.83616800	4.83907400

C	-3.02037400	-1.17752100	4.57790200
C	-3.51659300	-1.01515200	3.28857400
H	0.14816800	-0.13597400	4.01420100
H	-1.28506900	-0.94067600	5.83791800
H	-3.66298000	-1.56181100	5.36434000
H	-4.55229300	-1.27834800	3.09665600
C	-0.35432700	2.11582600	0.68821000
C	0.04564300	-0.46548900	-0.30924000
C	-0.29775200	1.96000600	-0.85380300
H	0.50434700	2.71257400	1.00054000
C	0.51396000	0.70310900	-1.21080600
H	-0.97975000	-0.71179200	-0.58576000
H	-1.31322100	1.85290000	-1.23860000
H	0.15072300	2.86340600	-1.27801200
H	0.38809200	0.42848900	-2.26408400
H	1.58507500	0.87879900	-1.04345000
P	-0.05235400	0.41028000	1.31506400
C	-1.59084300	2.84237100	1.21361600
C	0.93692700	-1.70321900	-0.35760000
H	0.60322900	-2.47783400	0.34266800
H	0.90568600	-2.13229100	-1.36546400
H	1.97855400	-1.46007800	-0.12798400
H	-1.64136300	2.81762300	2.30779500
H	-1.50954900	3.89092100	0.91652100
H	-2.50611600	2.41397900	0.80010600
C	-4.45291500	-1.90558000	0.27281100
C	-5.19362900	0.66926100	0.97132000
C	-5.89668800	-1.48490700	-0.07247300
H	-4.47136800	-2.50604800	1.19029400
C	-6.31601200	-0.38905800	0.92265600
H	-5.24659600	1.26999300	0.05274500
H	-5.92162300	-1.08316600	-1.09412300
H	-6.57515200	-2.34461800	-0.04772100
H	-7.27137600	0.07067000	0.64657100
H	-6.45418200	-0.82723200	1.92093600
P	-3.62631600	-0.28789000	0.66023600
O	-2.79766800	0.27035200	-0.46722300
C	-5.23606000	1.60999200	2.17495000
C	-3.71721900	-2.66993500	-0.82703000
H	-2.71688800	-2.97333500	-0.49898400
H	-4.27065900	-3.57446000	-1.10320000

H	-3.59960500	-2.04685300	-1.71834500
H	-4.41445200	2.33147300	2.14945100
H	-6.17713100	2.17134500	2.17677000
H	-5.17094800	1.06346700	3.12023000
C	1.50215300	0.16635900	2.09196900
H	1.84158800	-0.85826200	1.99935800
C	2.22690800	0.98859700	2.95023800
C	3.39344900	0.36511200	3.66987200
O	3.68464300	-0.88454600	3.23599100
C	4.84566700	-1.47156800	3.83759800
H	4.71987600	-1.55570000	4.92028500
H	4.94187600	-2.45856700	3.38328800
H	5.72532000	-0.86011000	3.62306500
O	4.01467800	0.90384200	4.56413500
C	2.13143900	2.39169400	3.13488600
C	5.54845500	2.90414500	2.60336800
C	4.53263900	2.49394900	1.72727400
C	4.76708300	1.37126600	0.91938400
C	5.97891700	0.68372200	0.97744100
C	6.98282300	1.10804800	1.84865400
C	6.75970000	2.22146400	2.66292000
H	5.37392300	3.74811200	3.26291000
H	3.98403100	1.03491500	0.24593700
H	6.13889300	-0.18151600	0.33937800
H	7.93049900	0.57796300	1.89330000
H	7.53014100	2.55295000	3.35360400
C	3.21749700	3.18249200	1.66660300
C	3.14790000	4.59151000	1.80075400
H	3.98525900	5.15329200	2.19943800
C	1.95210000	5.28250200	1.49231900
O	0.88195000	4.73479700	1.10891800
C	1.98891700	6.72919600	1.64326700
C	1.98456600	7.93979300	1.76074000
C	1.97904300	9.35584300	1.89982100
C	0.82570000	10.10187800	1.58622200
C	3.12530800	10.03789500	2.35338300
C	0.82324400	11.48655100	1.72359900
H	-0.05790000	9.57799700	1.23618400
C	3.11444400	11.42279900	2.48826700
H	4.01517800	9.46544100	2.59493600
C	1.96538200	12.15250300	2.17461300

H	-0.07302800	12.04959000	1.47787600
H	4.00568500	11.93585000	2.83912600
H	1.96014300	13.23369400	2.28071300
H	2.56151000	2.76703800	0.89973700
H	2.65281500	2.78041500	4.00094400
H	1.20332200	2.90107000	2.89762000

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C	-1.44157300	0.55252500	-0.47177700
C	-0.69425100	1.46875400	0.30239000
C	-0.26586600	2.65757600	-0.31362700
C	-0.58822300	2.96598900	-1.63019900
C	-1.38264000	2.09418600	-2.36980300
C	-1.79711600	0.90293400	-1.78659200
H	0.31736100	3.36021800	0.26912400
H	-0.23587800	3.89656400	-2.06490900
H	-1.67057500	2.33129800	-3.38965200
H	-2.40778100	0.22285600	-2.37203100
C	1.22294400	0.15831900	2.33522200
C	-1.34901900	0.59964800	3.32982400
C	0.72572100	-0.79138300	3.45001700
H	2.01655100	0.79075600	2.74592200
C	-0.31512600	-0.03929300	4.28955500
H	-1.87042500	-0.20389600	2.81051700
H	0.26422300	-1.66824900	2.99088500
H	1.57181600	-1.11653400	4.06399600
H	-0.83617200	-0.70665400	4.98515200
H	0.17947300	0.74434200	4.87774500
P	-0.18507900	1.35547700	2.08600300
C	1.73455300	-0.54740500	1.08042200
C	-2.32824700	1.53146900	4.02835900
H	-3.07581800	1.93517300	3.34345600
H	-2.83863400	0.97470500	4.82319100
H	-1.80348900	2.36966800	4.49385000
H	2.03476700	0.16423700	0.30374300
H	2.61074600	-1.15404200	1.33615600
H	0.96926900	-1.21425300	0.67670400
C	-3.83003600	-1.13785300	-0.07124300
C	-1.68468900	-2.33817500	-1.32945700

C	-4.12783500	-2.42211800	-0.87338900
H	-4.12224300	-0.27002900	-0.67577500
C	-3.06623800	-2.54578100	-1.98175300
H	-1.45706500	-3.23360800	-0.73379800
H	-4.06030300	-3.29017500	-0.20415500
H	-5.14546700	-2.40668500	-1.27859200
H	-3.11621400	-3.51652400	-2.48763300
H	-3.23847900	-1.78048600	-2.75104800
P	-1.97711300	-1.11762200	0.04450400
O	-1.39131400	-1.58267900	1.35323100
C	-0.51695800	-2.08909300	-2.28265300
C	-4.49608100	-1.05537400	1.30165100
H	-4.27855300	-0.10012000	1.79138500
H	-5.58403000	-1.14666600	1.20769200
H	-4.13592700	-1.85529200	1.95570200
H	0.41841500	-1.94165000	-1.73288300
H	-0.38352500	-2.95103700	-2.94611200
H	-0.67688500	-1.20674700	-2.90808300
C	0.48387600	2.87804200	2.63760100
C	-0.08559200	4.12786500	2.83294700
C	-1.48837400	4.36322500	2.40987800
O	-1.95450700	5.57045700	2.77558100
C	-3.34396000	5.80847200	2.52809200
H	-3.95245100	5.03394400	3.00192100
H	-3.55354600	6.78050500	2.97338000
H	-3.54811500	5.81691600	1.45373600
O	-2.17495900	3.54948800	1.80439600
C	0.59293800	5.11037400	3.60892800
H	0.21442600	6.12529700	3.58922000
H	1.67228100	5.02194700	3.63684700
H	1.44882900	2.73948500	3.11605200
C	-0.49756400	6.78292600	6.35738300
C	-0.79734000	5.46638700	5.97212800
C	-2.14227600	5.06911100	5.97320600
C	-3.15503700	5.95214900	6.34523300
C	-2.84212600	7.25864900	6.72199500
C	-1.50631700	7.66845500	6.72745700
H	0.53683700	7.11457400	6.34667000
H	-2.39454900	4.05287000	5.68490400
H	-4.18931300	5.61719300	6.34474200
H	-3.62874400	7.95032300	7.01077200

H	-1.25088400	8.68393400	7.01876900
C	0.26286000	4.52540200	5.53174200
C	1.50409000	4.46199100	6.21302100
H	1.79035600	5.22464800	6.92986200
C	2.39454200	3.38860400	5.96019300
O	2.25633000	2.52800600	5.04430200
C	3.54357900	3.29248500	6.84787500
C	4.52048000	3.18638000	7.56506700
C	5.65996500	3.06100400	8.40773500
C	6.55114900	1.98070100	8.25230800
C	5.91876900	4.01345100	9.41325500
C	7.66381400	1.86010100	9.07913100
H	6.35374100	1.24613000	7.47823600
C	7.03476300	3.88655200	10.23465300
H	5.23335800	4.84598600	9.53598200
C	7.91102300	2.81090500	10.07223800
H	8.34215700	1.02132900	8.94855900
H	7.22189300	4.62880900	11.00585000
H	8.78096300	2.71410400	10.71574000
H	-0.09840200	3.54505800	5.22548700

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C	-1.38258700	0.57836100	-0.49644600
C	-0.72377300	1.54753700	0.29434400
C	-0.33309200	2.74868300	-0.32449100
C	-0.61141800	3.01829400	-1.65964900
C	-1.32201600	2.09135500	-2.41824400
C	-1.69509900	0.88704200	-1.83332200
H	0.17630000	3.49357900	0.27565100
H	-0.29134600	3.96002200	-2.09522700
H	-1.57493200	2.29582400	-3.45432500
H	-2.23440700	0.16220300	-2.43517500
C	1.14374200	0.39501100	2.47781300
C	-1.51333700	0.71982900	3.28751400
C	0.61972300	-0.55982700	3.57657500
H	1.86922200	1.07391700	2.93641800
C	-0.51849100	0.14461900	4.32628400
H	-1.96316200	-0.11692000	2.75365800
H	0.24540400	-1.47345700	3.10983300

H	1.43801100	-0.81439800	4.25717600
H	-1.05427100	-0.54207800	4.99121800
H	-0.10334600	0.95671700	4.93459500
P	-0.30323900	1.50566100	2.10859500
C	1.77406700	-0.30445400	1.27493700
C	-2.57944400	1.61659800	3.90174800
H	-3.34142700	1.91202300	3.17692700
H	-3.07692100	1.07045300	4.71155100
H	-2.14334500	2.52118700	4.33294400
H	2.09347900	0.40826100	0.50678300
H	2.65912700	-0.86120200	1.60285900
H	1.07389400	-1.01667100	0.83182000
C	-3.65980200	-1.28879600	-0.24001600
C	-1.33306900	-2.33272500	-1.30339000
C	-3.78996400	-2.61228000	-1.02287000
H	-3.97305000	-0.46387500	-0.89245300
C	-2.64157600	-2.66993500	-2.04674400
H	-1.06991500	-3.19559500	-0.67536900
H	-3.70067700	-3.45510200	-0.32469100
H	-4.77211100	-2.69300200	-1.50115400
H	-2.57374600	-3.65173600	-2.52834100
H	-2.81791800	-1.93809500	-2.84712800
P	-1.82864100	-1.11996000	0.01778800
O	-1.32026400	-1.51363000	1.38032000
C	-0.12925000	-1.99189900	-2.18028800
C	-4.43477900	-1.22773200	1.07566100
H	-4.32986400	-0.24755000	1.55398000
H	-5.50200200	-1.40686900	0.90374500
H	-4.06480100	-1.98017200	1.77844300
H	0.74952300	-1.75339800	-1.57239600
H	0.12520900	-2.84676200	-2.81683100
H	-0.32494400	-1.13583200	-2.83178600
C	0.22982200	3.08162000	2.65477400
C	-0.42292500	4.28022700	2.90697200
C	-1.82244700	4.55577800	2.48909800
O	-2.27817000	3.61732500	1.60993600
C	-3.60030300	3.81959400	1.10643100
H	-3.68627100	4.80452100	0.64113400
H	-3.75348900	3.02973900	0.36942100
H	-4.33570800	3.74508700	1.91258400
O	-2.50689200	5.49340800	2.84260000

C	0.19093600	5.26511100	3.73642000
H	-0.30255900	6.22918100	3.79727300
H	1.27308100	5.30113800	3.71071400
H	1.19323300	2.98981400	3.14961900
C	-0.59812400	6.63373300	6.80081400
C	-0.95274400	5.39473100	6.24300700
C	-2.30510400	5.02522300	6.26126100
C	-3.27074700	5.85403300	6.82892100
C	-2.90306200	7.07881600	7.38569900
C	-1.56080900	7.46543000	7.36607600
H	0.44047600	6.95037900	6.77692900
H	-2.60004400	4.07381700	5.82839800
H	-4.31218300	5.54339800	6.83326700
H	-3.65404300	7.72897500	7.82589400
H	-1.26388500	8.42064500	7.79119600
C	0.05615400	4.49976800	5.62189000
C	1.35121100	4.38036000	6.19185100
H	1.69700300	5.09905100	6.92740000
C	2.21362200	3.31135500	5.85218000
O	2.02024800	2.46524000	4.92964900
C	3.41512700	3.18999900	6.66389400
C	4.43613400	3.06052200	7.31261400
C	5.62777900	2.91069900	8.07525500
C	6.50428400	1.83459800	7.83198800
C	5.95425500	3.83481400	9.08752500
C	7.66858500	1.69058000	8.58021200
H	6.25483400	1.12177900	7.05259300
C	7.12146000	3.68461200	9.83000200
H	5.28035900	4.66400900	9.27786600
C	7.98269400	2.61344200	9.58073900
H	8.33497200	0.85541700	8.38226700
H	7.36054000	4.40516300	10.60738100
H	8.89281400	2.49847800	10.16272800
H	-0.34060800	3.54953000	5.26897000

Re-TS4-1

C	-1.85756700	0.64980700	0.38503100
C	-0.50159400	1.01199500	0.60499500
C	0.06145400	2.01638700	-0.19292000

C	-0.66658700	2.64887200	-1.19997500
C	-1.98629700	2.27941400	-1.43104200
C	-2.56724200	1.29056100	-0.63948000
H	1.09152000	2.31351800	-0.04537600
H	-0.19504900	3.42087300	-1.80035500
H	-2.56593100	2.75686500	-2.21525300
H	-3.60011500	1.01922900	-0.82561500
C	0.32418400	0.97495100	3.56135300
C	2.34298200	0.71783200	1.67754700
C	1.65111300	1.72322900	3.81888200
H	0.28154600	0.14289800	4.27021600
C	2.78868600	0.97079500	3.12881100
H	2.34777100	1.69098300	1.17396500
H	1.58419900	2.74621400	3.42097500
H	1.81010100	1.77662900	4.89780300
H	3.72765300	1.53592300	3.14212600
H	2.96650100	0.02899000	3.65662300
P	0.55113700	0.19613700	1.87433900
C	-0.89887100	1.87827600	3.71019000
C	3.19112800	-0.27206500	0.88423200
H	2.81516100	-0.40249300	-0.13578200
H	4.22420500	0.08915400	0.82574000
H	3.19625500	-1.25370300	1.36503300
H	-1.82030000	1.30306800	3.63319800
H	-0.85948600	2.35164500	4.69774000
H	-0.90519200	2.67730400	2.95853400
C	-4.56377500	-0.20267500	1.43287000
C	-2.93763300	-2.19613600	0.47170600
C	-5.12099000	-1.62621300	1.64061800
H	-4.89758400	0.14887800	0.44843900
C	-4.45373500	-2.52998100	0.58681400
H	-2.33667400	-2.91682800	1.03256800
H	-4.87021100	-1.96562300	2.65352600
H	-6.21302700	-1.63965800	1.55369400
H	-4.59766000	-3.59088100	0.81422100
H	-4.92757500	-2.34490100	-0.38590800
P	-2.75981100	-0.59533100	1.39909700
O	-2.21821500	-0.69927300	2.80488700
C	-2.45115800	-2.18775400	-0.98002800
C	-4.93148000	0.81054400	2.51338500
H	-4.50724500	1.79678300	2.29451000

H	-6.01935600	0.91822800	2.58918400
H	-4.54440600	0.48590700	3.48334500
H	-1.37890100	-1.99514200	-1.05499400
H	-2.63343000	-3.17038600	-1.42737400
H	-2.98060400	-1.43860100	-1.58014500
C	0.34577600	-1.50561100	1.53650700
H	-0.22079900	-1.68642900	0.63374200
C	0.86558200	-2.62035900	2.17676500
C	0.53240500	-3.90517400	1.47273900
O	1.12456700	-4.97644700	2.03001500
C	0.74967500	-6.24190800	1.47047100
H	1.03564400	-6.29479800	0.41657800
H	1.28735600	-6.98758900	2.05602500
H	-0.32822100	-6.38760200	1.56560100
O	-0.19049200	-3.99483000	0.49310100
C	1.51252700	-2.68760100	3.43410400
H	2.06400900	-3.59121700	3.65585300
H	1.93555300	-1.77768500	3.84696800
C	-0.37623300	-5.29277200	4.84791200
C	-0.74656300	-3.98405900	4.50284500
C	-1.92642600	-3.79392500	3.76695900
C	-2.71248700	-4.88225600	3.38883700
C	-2.33766200	-6.17975800	3.74151600
C	-1.16502900	-6.37865300	4.47583500
H	0.54643000	-5.45945800	5.39566900
H	-2.21193500	-2.78104900	3.50049300
H	-3.62660300	-4.71546400	2.82362500
H	-2.95204200	-7.02789900	3.45112400
H	-0.86260300	-7.38493600	4.75439900
C	0.08081500	-2.80624600	4.86267200
C	0.77480600	-2.76778500	6.09723500
H	0.86090600	-3.65735700	6.71193700
C	1.46254100	-1.60034900	6.50089400
O	1.56060100	-0.54817900	5.80608800
C	2.11585900	-1.65127600	7.79844500
C	2.67505500	-1.66012500	8.87869700
C	3.33033300	-1.67313600	10.14146700
C	4.03423700	-0.54010600	10.59538600
C	3.28815000	-2.81835700	10.96108500
C	4.67445200	-0.55639400	11.83070400
H	4.06748900	0.34308000	9.96560500

C	3.93142800	-2.82651100	12.19490000
H	2.74572900	-3.69206700	10.61417200
C	4.62649600	-1.69758000	12.63493700
H	5.21347500	0.32453800	12.16848000
H	3.89049900	-3.71663400	12.81671000
H	5.12747900	-1.70697200	13.59886100
H	-0.35800200	-1.86463800	4.53829000

Re-TS4-2

C	-3.71382600	-1.97619700	0.05442300
C	-3.41098600	-1.44530200	1.33281900
C	-4.34008900	-1.61196000	2.36675500
C	-5.55116400	-2.27494000	2.15609900
C	-5.85444800	-2.77745700	0.89633700
C	-4.93263200	-2.63175400	-0.14218900
H	-4.13726800	-1.20779300	3.35043400
H	-6.25390600	-2.38469900	2.97664500
H	-6.79783000	-3.28432300	0.71680000
H	-5.17564800	-3.03935100	-1.11755500
C	-0.36218200	-1.22403200	2.02161100
C	-2.14289000	0.46422200	3.25628900
C	0.09584700	-0.56814600	3.35656100
H	0.32970400	-0.99933900	1.21113200
C	-0.66977500	0.73927900	3.60435100
H	-2.51961700	-0.28954600	3.96068900
H	-0.11463300	-1.26876000	4.17476500
H	1.17850600	-0.40690400	3.34763800
H	-0.57779600	1.06754100	4.64577600
H	-0.30449500	1.55436100	2.96826100
P	-1.94535500	-0.34988600	1.59331100
C	-0.51510400	-2.74339000	2.13536700
C	-3.02715100	1.70962600	3.27205700
H	-4.04472200	1.49808700	2.92277700
H	-3.09803600	2.09885000	4.29392300
H	-2.59016000	2.48913600	2.64158100
H	-0.76223300	-3.17657300	1.16632400
H	0.43193600	-3.17227800	2.48268800
H	-1.28840000	-3.01547200	2.86377500
C	-2.70777400	-3.37195700	-2.40297200

C	-2.87572900	-0.62566200	-2.57974200
C	-2.27960200	-2.77475400	-3.75758700
H	-3.77476600	-3.62007700	-2.46985200
C	-3.01434300	-1.43168300	-3.89766700
H	-1.96701200	-0.01374700	-2.60665600
H	-1.19317600	-2.61747100	-3.75890700
H	-2.51138800	-3.45684600	-4.58319100
H	-2.64560000	-0.84760600	-4.74719200
H	-4.07947400	-1.62759500	-4.08212300
P	-2.47510500	-1.90909400	-1.29505200
O	-1.07936500	-1.87955300	-0.71589600
C	-4.08222800	0.27007600	-2.29405600
C	-1.91468400	-4.59011900	-1.93661900
H	-2.30013400	-4.97283500	-0.98500000
H	-1.97460500	-5.39698100	-2.67588300
H	-0.86367000	-4.32610300	-1.78978900
H	-3.91746900	0.88523000	-1.40838100
H	-4.25427700	0.93917300	-3.14492800
H	-4.99373800	-0.32106900	-2.14662000
C	-1.98609600	0.88881400	0.38845200
H	-2.84288200	1.52619400	0.58073100
C	-1.00697200	1.43597000	-0.44294200
C	-1.27265200	2.80253600	-0.99663600
O	-2.48950100	3.30058800	-0.66931700
C	-2.65316800	4.69503900	-0.95468100
H	-2.51462100	4.89442900	-2.02043500
H	-3.67043800	4.93999300	-0.64566400
H	-1.92467200	5.27512700	-0.38126500
O	-0.47401500	3.41943700	-1.67826800
C	0.25078700	0.91806800	-0.82039900
H	0.70167400	1.37300800	-1.69310100
H	0.41366100	-0.14545100	-0.70691100
C	3.58964900	1.13429900	-1.06432700
C	2.84164500	0.81235700	0.07964900
C	3.19032100	-0.34246400	0.79515300
C	4.25830400	-1.14335900	0.39403400
C	4.99732100	-0.80722200	-0.74042200
C	4.65625600	0.33562300	-1.46801400
H	3.31766300	2.01112600	-1.64463600
H	2.62332900	-0.60748400	1.68332600
H	4.51368400	-2.02956400	0.96902300

H	5.82847600	-1.43076200	-1.05769000
H	5.22110300	0.60211300	-2.35739600
C	1.69491100	1.64678500	0.51130600
C	1.77359700	3.05142900	0.45356000
H	2.57582600	3.54315500	-0.08514200
C	0.72771800	3.83832600	0.99199800
O	-0.32425500	3.34969200	1.49093600
C	0.85330900	5.28060400	0.89165500
C	0.89013400	6.49414100	0.81848300
C	0.94057800	7.91300900	0.72675600
C	-0.08038900	8.70327100	1.29073500
C	2.00923700	8.55321700	0.06901000
C	-0.03018700	10.09070800	1.19782700
H	-0.90391400	8.21144300	1.79859100
C	2.05162500	9.94121300	-0.01972100
H	2.79593000	7.94621000	-0.36731900
C	1.03416000	10.71522700	0.54324500
H	-0.82400900	10.68822300	1.63771000
H	2.88147700	10.42203400	-0.53031400
H	1.07048700	11.79866000	0.47225700
H	1.13444100	1.25545700	1.35601200

Re-TS4-3

C	-2.48829800	0.57625900	0.47211900
C	-1.43482400	1.18028300	1.20345100
C	-1.25853800	2.57184100	1.07360900
C	-2.10558100	3.35887600	0.29888900
C	-3.17359100	2.77132000	-0.37067500
C	-3.34801600	1.39446500	-0.28086100
H	-0.43773800	3.04521800	1.59842700
H	-1.92835100	4.42787900	0.23035500
H	-3.85607400	3.36938200	-0.96699300
H	-4.17150900	0.94201000	-0.82426000
C	1.04513300	-0.68725400	1.49863000
C	-0.88937900	-0.90827200	3.50278400
C	0.96283400	-2.03895100	2.25048300
H	2.01969800	-0.24648900	1.71166700
C	0.37034900	-1.79607400	3.65050800
H	-1.64549100	-1.47949700	2.96530500

H	0.31250600	-2.71974800	1.69747200
H	1.96930400	-2.46366100	2.30374900
H	0.10383900	-2.73620300	4.14611700
H	1.10226100	-1.28777100	4.29297300
P	-0.20907200	0.36857900	2.33965200
C	0.94525300	-0.78512500	-0.02287000
C	-1.43806500	-0.34218600	4.80788100
H	-2.31971400	0.28731000	4.63748300
H	-1.73758300	-1.16333500	5.46912800
H	-0.68812200	0.26158200	5.32772100
H	0.92090300	0.20489000	-0.49241500
H	1.84272900	-1.29733000	-0.38168200
H	0.06366800	-1.35273300	-0.32778300
C	-4.61556000	-1.46803100	0.75909100
C	-3.02400300	-1.64058000	-1.49807200
C	-5.15997300	-2.31786600	-0.40860400
H	-5.10668000	-0.48740000	0.73983800
C	-4.54548000	-1.77861800	-1.71259000
H	-2.58603600	-2.64851000	-1.50583500
H	-4.85653800	-3.36340500	-0.26557500
H	-6.25499000	-2.30063400	-0.43181600
H	-4.75967300	-2.43234100	-2.56531700
H	-4.97915200	-0.79769700	-1.95180300
P	-2.83214300	-1.21851900	0.30517700
O	-1.86183500	-2.12338200	1.01713800
C	-2.28359400	-0.78302200	-2.52326600
C	-4.76892000	-2.09311500	2.14525900
H	-4.40051500	-1.42077700	2.92783400
H	-5.82226600	-2.31021400	2.35494700
H	-4.20054300	-3.02524300	2.21424500
H	-1.21413700	-0.72717700	-2.29834500
H	-2.39437600	-1.21671400	-3.52340500
H	-2.67119800	0.23911500	-2.55722700
C	0.43116700	1.70407100	3.28350200
H	-0.35233200	2.39446500	3.57180200
C	1.67258000	1.91836100	3.87516400
C	1.79493900	3.15513900	4.73042400
O	0.73619300	3.99336500	4.61475700
C	0.86489500	5.22387200	5.33810600
H	1.72684400	5.78438700	4.96850500
H	-0.05954600	5.77134100	5.14928100

H	0.98931400	5.03382400	6.40735200
O	2.74236600	3.40477000	5.44790900
C	2.90719000	1.26167400	3.67044400
H	3.69993200	1.54937000	4.34937800
H	2.93965000	0.22812400	3.34653700
C	4.42057200	4.23914100	2.81176700
C	3.50061500	3.48690000	2.06579300
C	2.40955500	4.15513300	1.48920200
C	2.23780600	5.52881900	1.65434100
C	3.15994100	6.26377100	2.40013900
C	4.25362700	5.61119100	2.97617900
H	5.25168200	3.73369800	3.29307000
H	1.69691700	3.58517600	0.90024800
H	1.38628500	6.02606600	1.19657100
H	3.03118200	7.33500100	2.52975800
H	4.97280000	6.17295900	3.56579500
C	3.62473600	2.01703500	1.92239000
C	4.88316800	1.41320100	1.70133600
H	5.79853000	1.98392300	1.81601700
C	4.97095000	0.02621400	1.42578000
O	3.98806900	-0.76603500	1.40318800
C	6.30350700	-0.49556800	1.16819700
C	7.40423300	-0.96351200	0.94736800
C	8.69158700	-1.51244200	0.69081500
C	8.84112700	-2.88407400	0.40556100
C	9.83932200	-0.69586500	0.71715000
C	10.10134200	-3.41809100	0.15487900
H	7.95792300	-3.51434100	0.38543100
C	11.09597900	-1.23797000	0.46578900
H	9.72646500	0.36104900	0.93652400
C	11.23272000	-2.59921900	0.18382200
H	10.20243700	-4.47765700	-0.06363400
H	11.97279900	-0.59668800	0.48966200
H	12.21522200	-3.01944700	-0.01199900
H	2.79320100	1.57485400	1.37149300

Re-TS4-4

C	-2.24193900	0.79704800	1.17087400
C	-1.23026000	0.82893200	2.16100100

C	-1.04102800	2.00736700	2.89367500
C	-1.81602800	3.14368700	2.65392100
C	-2.79391700	3.11752300	1.66606900
C	-3.00562900	1.94502500	0.93888400
H	-0.26910200	2.05831000	3.65121400
H	-1.64293700	4.04532100	3.23380200
H	-3.39424600	3.99882700	1.46088600
H	-3.77898500	1.93442800	0.17774300
C	-0.55407700	-1.93361600	3.46669400
C	1.36482800	0.03376200	3.42438500
C	0.60209200	-2.05104700	4.50242300
H	-0.62059500	-2.82391100	2.84293800
C	1.84884600	-1.30615100	4.00510000
H	0.92784300	0.61912500	4.24458500
H	0.26616700	-1.60106600	5.44543300
H	0.81735300	-3.10359500	4.71220900
H	2.56497000	-1.13479200	4.81661800
H	2.37032100	-1.86253600	3.21710900
P	-0.02442500	-0.55769000	2.33544300
C	-1.91299300	-1.69092900	4.12939600
C	2.45438400	0.83099500	2.70985900
H	2.05619700	1.72913000	2.22300800
H	3.21265900	1.15057000	3.43345300
H	2.94451400	0.20674200	1.95743800
H	-2.70750600	-1.69101400	3.38345800
H	-2.10601000	-2.49335800	4.85071900
H	-1.92828700	-0.74167400	4.67822100
C	-4.42190900	-0.64822800	-0.24648300
C	-1.91924800	-0.71837400	-1.45426100
C	-4.36551200	-0.28768800	-1.74609400
H	-4.93653500	0.12317900	0.33402700
C	-3.14447800	-1.00515000	-2.35179200
H	-1.19838600	-1.53905000	-1.48661400
H	-5.29523600	-0.56947700	-2.25337700
H	-4.25004200	0.79684900	-1.87135600
H	-3.33470400	-2.08394900	-2.38487100
H	-2.95582600	-0.68139100	-3.38122100
P	-2.63078400	-0.75473200	0.26601800
O	-2.32844000	-1.95595600	1.12989200
C	-1.21043900	0.59124900	-1.81716000
C	-5.10462000	-1.99770000	0.02027500

H	-5.03955000	-2.27116200	1.07611600
H	-6.16071200	-1.94048500	-0.26711800
H	-4.63921200	-2.80769500	-0.54909800
H	-0.36830100	0.77699800	-1.14790300
H	-0.82241100	0.52415500	-2.83948500
H	-1.88459000	1.45367700	-1.77123900
C	0.62075000	-0.89159100	0.76740000
C	0.87117700	-2.08293100	0.08294800
C	1.89037900	-2.03631300	-1.01445100
O	2.39480200	-0.80022700	-1.24265100
C	3.55375100	-0.78165500	-2.08472900
H	3.33105000	-1.20976100	-3.06553000
H	3.83215600	0.26922800	-2.17707100
H	4.35824500	-1.35471400	-1.61519100
O	2.24215500	-3.01561100	-1.64730700
C	0.33127000	-3.37118400	0.28728800
C	0.65024900	-6.66269500	0.85640900
C	0.75315300	-5.62510800	1.79694100
C	-0.00414200	-5.72057400	2.97356000
C	-0.82607600	-6.82038800	3.21378600
C	-0.91268000	-7.84754200	2.27381800
C	-0.17069800	-7.76199400	1.09317800
H	1.21011500	-6.59289800	-0.07162500
H	0.06244100	-4.92738200	3.71312800
H	-1.39806600	-6.87504100	4.13628100
H	-1.55465700	-8.70475400	2.45635000
H	-0.23697000	-8.55333400	0.35126300
C	1.61281300	-4.44289900	1.54987900
C	2.88457100	-4.59575300	0.96473100
H	3.17816800	-5.53328200	0.50604100
C	3.74670900	-3.47926900	0.85313100
O	3.42096300	-2.31198400	1.20847900
C	5.03989800	-3.68842300	0.22923000
C	6.12849400	-3.79493600	-0.30271600
C	7.39934700	-3.92844600	-0.92821100
C	8.27733000	-2.82937800	-1.00657300
C	7.80183200	-5.15950100	-1.48228700
C	9.51885400	-2.96174900	-1.62076500
H	7.96892800	-1.88053600	-0.57926300
C	9.04496600	-5.28324500	-2.09505800
H	7.12635100	-6.00688700	-1.42413700

C	9.90788300	-4.18713400	-2.16704700
H	10.18654200	-2.10615600	-1.67385200
H	9.34263300	-6.23844400	-2.51876100
H	10.87780500	-4.28729800	-2.64600400
H	1.54836500	-3.66282800	2.30350900
H	0.43732200	-4.05909500	-0.54173700
H	-0.59192000	-3.44875200	0.84670100
H	1.21051300	-0.03813500	0.44874500

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C	-1.50519300	1.48646600	1.54306800
C	-0.11018100	1.22157800	1.61200900
C	0.73879700	2.25686100	2.04406000
C	0.26106700	3.49921100	2.44946700
C	-1.10732300	3.73705900	2.43912000
C	-1.96472900	2.73968700	1.98364100
H	1.80710700	2.09364200	2.06785200
H	0.95851500	4.26308900	2.77923100
H	-1.50999500	4.68931800	2.77067900
H	-3.02719800	2.94695400	1.97617600
C	2.30465200	-0.49477600	2.26672100
C	1.83317900	0.14368600	-0.36659300
C	3.47618700	0.19946300	1.54728100
H	2.53182100	-1.56279100	2.15119800
C	3.30416700	-0.08621200	0.04709500
H	1.65925200	1.22207400	-0.47420900
H	3.51162500	1.27815500	1.74818000
H	4.41080400	-0.23775800	1.90676800
H	3.96576900	0.53336300	-0.56850300
H	3.58063900	-1.13135200	-0.12262500
P	0.82474100	-0.30765200	1.15762100
C	2.10715800	-0.20874900	3.75160600
C	1.42786000	-0.56087000	-1.66076200
H	0.37695900	-0.39467600	-1.90857100
H	2.03511100	-0.17810800	-2.48902100
H	1.58817600	-1.63840900	-1.59109400
H	1.25830300	-0.77536600	4.15018900
H	3.00253400	-0.52226100	4.29825800
H	1.93323800	0.85051100	3.96321600

C	-4.36898000	1.30927000	0.57258400
C	-2.53430800	-0.13518400	-0.78698100
C	-4.93590800	0.60289500	-0.69987700
H	-4.09094700	2.33337200	0.30548700
C	-3.97195600	-0.50746300	-1.19524600
H	-1.87602000	-1.00322700	-0.82836300
H	-5.91879600	0.17535200	-0.47962900
H	-5.08637800	1.34951000	-1.48591600
H	-4.22887700	-1.46162700	-0.72487500
H	-4.04844100	-0.64707600	-2.27940900
P	-2.83266800	0.33657400	0.97237300
O	-3.11084400	-0.77686500	1.94919800
C	-1.96118100	1.02100400	-1.61684300
C	-5.34937000	1.32769200	1.74849700
H	-4.95093900	1.87959400	2.60705300
H	-6.29323700	1.79836100	1.45146200
H	-5.55309600	0.30767700	2.08585800
H	-0.97006800	1.32388000	-1.26810600
H	-1.87311700	0.71927200	-2.66677000
H	-2.60225800	1.90870100	-1.58433100
C	-0.23444900	-1.68182900	1.04791700
H	-1.23083100	-1.53419100	1.44848000
C	0.06863800	-2.92050200	0.47879800
C	-1.08019000	-3.84369500	0.18066300
O	-2.26479200	-3.32735700	0.56479300
C	-3.39166200	-4.20023100	0.44931500
H	-3.57302600	-4.46283500	-0.59697700
H	-4.22830500	-3.63670800	0.86274500
H	-3.21565000	-5.11350500	1.02356400
O	-0.97295200	-4.92334800	-0.36713200
C	1.34347800	-3.50598700	0.28872500
C	0.51761500	-6.51065500	1.94791900
C	0.63514800	-5.18950900	2.40250700
C	-0.40541700	-4.65672400	3.17838900
C	-1.52794300	-5.42064100	3.49500600
C	-1.62769600	-6.73696400	3.04205300
C	-0.59930700	-7.27755300	2.26659100
H	1.29369000	-6.92832600	1.31447800
H	-0.33655400	-3.62869500	3.52202500
H	-2.32225400	-4.98559700	4.09533800
H	-2.49945000	-7.33682100	3.28936400

H	-0.67418800	-8.29715200	1.89881400
C	1.78686900	-4.32778300	2.03637700
C	3.08756800	-4.87665700	1.89098100
H	3.23667800	-5.94923300	1.83905800
C	4.20079700	-4.02594900	1.71196000
O	4.13169000	-2.76378600	1.62819000
C	5.49849700	-4.66784900	1.60305300
C	6.60003200	-5.17484400	1.50842100
C	7.88672600	-5.77165200	1.39635000
C	9.03525800	-4.97243700	1.23200300
C	8.03531100	-7.17166500	1.44788700
C	10.29200300	-5.55963700	1.12301900
H	8.92223300	-3.89382700	1.19241200
C	9.29568600	-7.75079000	1.33766300
H	7.15186700	-7.78907500	1.57508600
C	10.42786400	-6.94894800	1.17507200
H	11.16976900	-4.93179600	0.99690600
H	9.39615300	-8.83183800	1.37904500
H	11.41051000	-7.40419900	1.08961700
H	1.75529800	-3.35947300	2.53681800
H	1.37803900	-4.36715300	-0.36790400
H	2.22457200	-2.87248500	0.26918100

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C	-2.31560100	0.88785600	1.09106300
C	-1.11847800	1.50899600	1.52083700
C	-1.01515900	2.90506300	1.39187600
C	-2.03921400	3.67606200	0.85224100
C	-3.21903600	3.06540000	0.43712100
C	-3.34646000	1.68698400	0.56500800
H	-0.11088600	3.38870500	1.73791500
H	-1.91309400	4.75104100	0.76610200
H	-4.03399400	3.65140100	0.02273300
H	-4.27266900	1.22043800	0.24377100
C	1.32265500	-0.51511800	1.33694800
C	-0.01617900	-0.32312100	3.78486400
C	1.38103100	-1.74898400	2.27432500
H	2.30940500	-0.05232100	1.27794100
C	1.17092000	-1.31224700	3.73457100

H	-0.91888500	-0.87032600	3.51046000
H	0.58208500	-2.43501000	1.98840900
H	2.34071300	-2.26344400	2.14712500
H	0.96341300	-2.17384000	4.37901000
H	2.06596600	-0.81677600	4.13029000
P	0.37468200	0.74877700	2.32887100
C	0.85497800	-0.82047100	-0.08379600
C	-0.19589700	0.37649100	5.13276400
H	-0.95749800	1.16335400	5.08654900
H	-0.52986400	-0.36189500	5.87096900
H	0.73599600	0.81428000	5.50351100
H	0.77804300	0.09424500	-0.67515600
H	1.58950800	-1.47655600	-0.56664700
H	-0.10071400	-1.34495800	-0.06872500
C	-4.33823900	-1.09461200	1.97038800
C	-3.25708900	-1.45375900	-0.55313900
C	-5.11007700	-2.02723500	1.01349600
H	-4.82995900	-0.11467300	1.98016100
C	-4.78884700	-1.59307400	-0.42734900
H	-2.82280000	-2.46231500	-0.59575400
H	-4.77524600	-3.06147300	1.16886700
H	-6.18554200	-2.00259300	1.22035100
H	-5.17719500	-2.30386300	-1.16523600
H	-5.26635600	-0.62640100	-0.63935700
P	-2.69139900	-0.90232800	1.13330800
O	-1.59873900	-1.76447100	1.71143200
C	-2.76838900	-0.65580300	-1.76143400
C	-4.19002700	-1.60889100	3.40186600
H	-3.67014000	-0.88070300	4.03373900
H	-5.17381100	-1.79959700	3.84521100
H	-3.61217100	-2.53741900	3.42158500
H	-1.67639700	-0.59095100	-1.78313600
H	-3.09659300	-1.13933500	-2.68852500
H	-3.16123100	0.36503000	-1.75820400
C	1.41109400	2.00088800	2.97345900
C	2.41864100	2.74075700	2.36007700
C	2.58422700	2.65168400	0.89254600
O	3.73237000	3.18688400	0.44631700
C	4.00745900	3.00210900	-0.94680100
H	3.23340100	3.47065900	-1.56040600
H	4.97683700	3.47072900	-1.11282400

H	4.06030100	1.93541000	-1.17854100
O	1.75720800	2.14433600	0.14173800
C	3.39650000	3.39080000	3.15560000
H	4.10983300	4.04504300	2.66832100
H	3.06990500	3.69017500	4.14491100
C	6.49380700	2.32610500	2.35223200
C	5.38967400	1.52333000	2.67430900
C	5.09660600	0.43361500	1.84142700
C	5.86812500	0.16086800	0.71217000
C	6.95521400	0.97684400	0.39570000
C	7.26719900	2.05732100	1.22570400
H	6.72605900	3.18125000	2.98089500
H	4.26084300	-0.21196000	2.09670500
H	5.62378000	-0.69212600	0.08411700
H	7.55843100	0.77015100	-0.48406500
H	8.11541800	2.69487400	0.99017300
C	4.49846600	1.83344300	3.81569800
C	4.99719200	2.16318900	5.09360800
H	6.04227600	2.39796100	5.26640700
C	4.06377100	2.22877500	6.16483500
O	2.81628500	2.11147100	6.01970000
C	4.61093700	2.45274300	7.49312800
C	5.04118200	2.64198600	8.61496100
C	5.54013200	2.86232200	9.92914700
C	4.66046600	2.92137400	11.02816800
C	6.92101900	3.02496700	10.15594200
C	5.15116200	3.13617600	12.31239500
H	3.59649700	2.79648200	10.85483600
C	7.40342300	3.24022100	11.44327800
H	7.60058600	2.97905800	9.31093700
C	6.52235900	3.29656100	12.52574300
H	4.46167900	3.17919100	13.15108800
H	8.47091000	3.36403800	11.60382800
H	6.90210200	3.46436600	13.52967900
H	3.60098000	1.21198400	3.85838800
H	1.35930400	2.09469900	4.05291300

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C	-2.36785100	0.86237600	1.12091800
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C	-1.16851500	1.50244100	1.51671600
C	-1.10490000	2.90423200	1.42489600
C	-2.16928200	3.66302900	0.94842700
C	-3.35025500	3.03329100	0.56602500
C	-3.43944400	1.64884600	0.66189500
H	-0.19637700	3.39805100	1.74656400
H	-2.07429500	4.74303200	0.88878800
H	-4.19644400	3.60921500	0.20333400
H	-4.36850600	1.16846600	0.37064900
C	1.30607000	-0.43223200	1.14905300
C	0.09272400	-0.36785200	3.67253800
C	1.46736200	-1.68963400	2.04622500
H	2.27362500	0.06247700	1.03672900
C	1.30812300	-1.31294800	3.53003200
H	-0.80392300	-0.93562500	3.42109300
H	0.68574500	-2.40174300	1.77600100
H	2.44040900	-2.15712100	1.85698500
H	1.15645400	-2.20553200	4.14706200
H	2.20358400	-0.80473900	3.90628800
P	0.38097600	0.76290800	2.23996100
C	0.74605100	-0.73514800	-0.23961400
C	-0.04563800	0.28319700	5.04905600
H	-0.84987100	1.02773500	5.06771400
H	-0.29964300	-0.49302600	5.78023400
H	0.87985500	0.76229200	5.38320900
H	0.49658300	0.17818900	-0.78445300
H	1.49860400	-1.27894500	-0.82247700
H	-0.14200900	-1.36230500	-0.16154800
C	-4.28916800	-1.18355400	2.07266600
C	-3.35363500	-1.46851500	-0.51693500
C	-5.09916600	-2.11056100	1.14204900
H	-4.79774700	-0.21397500	2.13348700
C	-4.87260700	-1.63954900	-0.30524300
H	-2.90533300	-2.46816100	-0.60273300
H	-4.73686600	-3.14110900	1.25388400
H	-6.16054800	-2.11133600	1.41273800
H	-5.29046900	-2.34236300	-1.03452100
H	-5.37987000	-0.67844300	-0.46737600
P	-2.70023400	-0.93753300	1.14397200
O	-1.55379200	-1.78460100	1.63419500
C	-2.94874900	-0.64254700	-1.73713100

C	-4.04611200	-1.72504600	3.48105500
H	-3.50284200	-1.00047900	4.09716900
H	-4.99812400	-1.94389600	3.97738800
H	-3.45184100	-2.64270900	3.44614800
H	-1.86050300	-0.56555700	-1.82340100
H	-3.32638100	-1.11305900	-2.65192400
H	-3.35216100	0.37318100	-1.69141800
C	1.42306000	2.01985000	2.84890100
C	2.46155700	2.73292300	2.24786100
C	2.70363100	2.78191600	0.78678000
O	1.59639600	2.40653300	0.07175500
C	1.73260400	2.51876700	-1.34980200
H	2.46130700	1.79517000	-1.72528400
H	0.74197400	2.31397100	-1.75755200
H	2.06208800	3.52415000	-1.62180400
O	3.71975800	3.15809400	0.24052300
C	3.45094500	3.33300000	3.06713100
H	4.19972100	3.94990700	2.58244800
H	3.11890100	3.65000100	4.04906300
C	6.51018900	2.04239300	2.34289400
C	5.34893400	1.32679300	2.66708000
C	5.02047100	0.20518900	1.89232400
C	5.82175500	-0.18955500	0.82193900
C	6.97093200	0.53524400	0.50655400
C	7.31249700	1.65124300	1.27448500
H	6.76845800	2.92285200	2.92465600
H	4.13800100	-0.37244300	2.15278700
H	5.55106100	-1.06584800	0.23814800
H	7.59612900	0.23492900	-0.32971100
H	8.20480900	2.22286600	1.03362200
C	4.45380200	1.73805500	3.77243400
C	4.95298000	2.07639100	5.04811500
H	6.00804900	2.25365400	5.22799700
C	4.01420000	2.22934300	6.10498400
O	2.76307800	2.17239100	5.94997300
C	4.55833800	2.47301800	7.43059500
C	4.98632100	2.67955800	8.55023300
C	5.48308400	2.92098300	9.86149900
C	4.59716500	3.05913700	10.94832300
C	6.86803100	3.02592600	10.09737400
C	5.08575500	3.29446400	12.22974500

H	3.53008100	2.97886000	10.76784200
C	7.34830100	3.26216100	11.38181900
H	7.55228100	2.91930200	9.26170100
C	6.46103500	3.39710700	12.45221300
H	4.39149600	3.39880800	13.05906100
H	8.41893700	3.34102300	11.54952900
H	6.83915400	3.58120300	13.45390500
H	3.51991100	1.17334100	3.81755000
H	1.37328500	2.11753300	3.92944200

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C	-2.35341200	1.26598800	0.12179500
C	-1.41438400	1.72435800	1.07368800
C	-1.37077500	3.10328200	1.34261900
C	-2.24006400	4.00466100	0.73893300
C	-3.21223800	3.54186100	-0.14342700
C	-3.25674100	2.18568600	-0.44170900
H	-0.65170000	3.46688200	2.06638600
H	-2.16995100	5.06096800	0.98050200
H	-3.92227900	4.22485600	-0.60001200
H	-4.01101100	1.83203700	-1.13746700
C	1.25483200	0.21781100	1.05294500
C	-0.67927300	-0.94464100	2.70092300
C	1.33196000	-1.31418300	1.24810000
H	2.11228400	0.68427100	1.55040600
C	0.68766900	-1.66253900	2.59512200
H	-1.33641400	-1.36230400	1.93926100
H	0.77630400	-1.79863300	0.44331300
H	2.37479100	-1.64775900	1.20299500
H	0.53327700	-2.74243800	2.70081000
H	1.32960700	-1.34264600	3.42361100
P	-0.19483500	0.75124500	2.09992600
C	1.22777900	0.66494000	-0.40862300
C	-1.30349800	-1.05538700	4.08647700
H	-2.31308700	-0.64390900	4.11316700
H	-1.34789500	-2.11601100	4.36280700
H	-0.69731000	-0.54394100	4.83799900
H	1.13091100	1.75154600	-0.50372900
H	2.16014300	0.36457300	-0.90056900

H	0.40015500	0.18691500	-0.93690400
C	-4.22368300	-1.00956900	-0.09509400
C	-2.77285800	-0.40850200	-2.36578500
C	-4.76293400	-1.56714400	-1.42915300
H	-4.80031600	-0.11454200	0.17032800
C	-4.28512500	-0.63729700	-2.55954100
H	-2.25650100	-1.34047800	-2.63653000
H	-4.35837500	-2.57539800	-1.58965600
H	-5.85428000	-1.65831100	-1.40537100
H	-4.49136600	-1.05974600	-3.54936900
H	-4.82148000	0.32007600	-2.50773000
P	-2.51015000	-0.43739600	-0.52338900
O	-1.38425500	-1.36046400	-0.13054700
C	-2.15099700	0.73130400	-3.17088900
C	-4.23300900	-1.99148500	1.07578200
H	-3.88551300	-1.51270800	1.99747900
H	-5.24632700	-2.36896100	1.25305800
H	-3.57640700	-2.84312000	0.87295500
H	-1.07989000	0.82437600	-2.96302600
H	-2.26844600	0.54050700	-4.24361700
H	-2.61667100	1.69518600	-2.94939400
C	0.53294800	1.77620000	3.31708100
C	-0.05330000	2.40597400	4.41808000
C	-1.50050800	2.19114800	4.65432400
O	-1.89855200	2.59344800	5.86986200
C	-3.29214700	2.44629100	6.16604100
H	-3.58017300	1.39164800	6.13450100
H	-3.41360800	2.85216300	7.16952100
H	-3.89713700	3.00206400	5.44463600
O	-2.26882800	1.69765500	3.83452800
C	0.66747000	3.19538700	5.35038100
H	0.11196200	3.92590200	5.93083900
H	1.65011800	3.52393100	5.02284000
C	3.05022800	0.98017700	5.73841600
C	1.82847000	0.92437600	6.42665700
C	1.23885500	-0.33069900	6.62650200
C	1.85944000	-1.49734300	6.17907500
C	3.07696600	-1.42769200	5.50134500
C	3.66712200	-0.18092800	5.27773800
H	3.51607300	1.94648600	5.56639900
H	0.29345700	-0.38947100	7.15981400

H	1.38796800	-2.46045700	6.35555600
H	3.56037400	-2.33428600	5.14790100
H	4.61415800	-0.11507100	4.74829200
C	1.16860100	2.15113700	6.94106100
C	1.91106300	3.04418200	7.75132100
H	2.99409800	2.98853000	7.79550100
C	1.23610800	4.11640100	8.40124700
O	0.01149000	4.35562600	8.27654500
C	2.06266500	4.97696400	9.24006900
C	2.72795200	5.71218600	9.94448600
C	3.50192900	6.57619000	10.76891200
C	2.89666800	7.65628400	11.44135600
C	4.88620300	6.36850500	10.92819700
C	3.65602900	8.49964700	12.24660600
H	1.83036300	7.81727600	11.32003100
C	5.63854400	7.21672500	11.73498900
H	5.35452900	5.53634500	10.41224000
C	5.02809600	8.28459000	12.39692700
H	3.17616100	9.32859800	12.75969700
H	6.70534700	7.04443300	11.84899900
H	5.61796100	8.94490600	13.02649600
H	0.13987700	2.01028700	7.26750300
H	1.58917800	1.95884700	3.15141800

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C	-0.83566700	-0.88053000	2.48983800
C	0.26512700	-0.05396300	2.14883700
C	1.47455700	-0.24587000	2.83193200
C	1.61527800	-1.19317800	3.84114100
C	0.54018100	-2.01003600	4.17265800
C	-0.66398200	-1.85257200	3.49206900
H	2.33691700	0.36270000	2.60659200
H	2.56826400	-1.25281200	4.35593300
H	0.62752300	-2.76174500	4.95197600
H	-1.49610700	-2.49764200	3.75792200
C	-0.78590100	2.72349400	0.94573000
C	-0.16713200	0.65157100	-0.79937900
C	-1.49212700	2.72510700	-0.43506100
H	-0.08023100	3.55674800	0.99994400

C	-0.64013200	1.96083200	-1.46467500
H	-1.05693900	0.05510100	-0.59042800
H	-2.45282200	2.21849200	-0.32859500
H	-1.67769000	3.75622200	-0.75627700
H	-1.21654900	1.74029200	-2.37065100
H	0.23143700	2.55623900	-1.76751400
P	0.38457200	1.26801100	0.85416900
C	-1.73552200	2.81625300	2.13734700
C	0.83207200	-0.17451700	-1.60545300
H	1.20751200	-1.02923900	-1.03187700
H	0.34149800	-0.56473700	-2.50465000
H	1.69176500	0.41642700	-1.93623800
H	-1.18677400	2.74478400	3.07839200
H	-2.24734200	3.78615900	2.11228100
H	-2.49581300	2.03706300	2.08089300
C	-2.98961400	-2.56370100	1.32885500
C	-3.76114500	-0.63648900	3.16137100
C	-4.39754700	-2.71663500	1.94067600
H	-2.30550800	-3.24865900	1.84276100
C	-4.38316000	-2.03985200	3.32226600
H	-4.50496300	0.01769400	2.68577700
H	-5.12961100	-2.21550600	1.29329000
H	-4.68998300	-3.77072600	2.00192600
H	-5.38692300	-1.97398500	3.75681400
H	-3.77569800	-2.63333000	4.01937200
P	-2.51963400	-0.82466300	1.78503700
O	-2.71673400	0.16609500	0.66387100
C	-3.28371900	0.01593700	4.45829700
C	-2.90741800	-2.79378200	-0.17950900
H	-1.87488100	-2.71246100	-0.53660400
H	-3.27618700	-3.79311200	-0.43728700
H	-3.50402300	-2.05119400	-0.71718600
H	-2.85101100	1.00369200	4.27453900
H	-4.12567000	0.13835100	5.14929000
H	-2.52284600	-0.59021100	4.95813500
C	2.03214500	1.80653500	0.58969600
C	2.82728500	2.64594100	1.36956400
C	2.29983900	3.04854100	2.70280900
O	3.12538300	3.83489200	3.40413100
C	2.76637000	4.01277600	4.78399300
H	1.79380600	4.50420300	4.86755100

H	2.73935800	3.03491500	5.26983200
H	3.55626300	4.62954300	5.21106800
O	1.19127300	2.71646700	3.10558500
C	4.12591600	3.04485400	0.99260800
H	4.59790500	3.85006600	1.53839500
H	4.37630700	2.98340500	-0.06102600
C	7.46033500	2.33910000	0.39029400
C	6.35860600	1.47232700	0.47180400
C	6.12286800	0.59630700	-0.60004800
C	6.96593300	0.57364200	-1.70909400
C	8.06157000	1.43583100	-1.77307300
C	8.30242700	2.31977600	-0.71847900
H	7.64813100	3.04105400	1.19713400
H	5.26903900	-0.07529700	-0.55152900
H	6.76841800	-0.11849700	-2.52337900
H	8.72015300	1.42202800	-2.63693800
H	9.14927900	2.99944300	-0.76233400
C	5.43465700	1.47152300	1.62673500
C	5.87585800	1.74607700	2.92982700
H	6.83330400	2.22276500	3.11080700
C	5.01797100	1.51102300	4.03188200
O	3.86036100	1.01669600	3.94485700
C	5.50633500	1.91864800	5.33765100
C	5.84736500	2.27816100	6.44878400
C	6.24550700	2.70250600	7.74708100
C	5.37532100	2.55411100	8.84521700
C	7.51207700	3.28235300	7.95731900
C	5.76387700	2.97490100	10.11326700
H	4.39978000	2.10636200	8.68466400
C	7.89309300	3.69953200	9.22888200
H	8.18392600	3.39717400	7.11275400
C	7.02225900	3.54845300	10.31059900
H	5.08344200	2.85478000	10.95174400
H	8.87298800	4.14458600	9.37759900
H	7.32277500	3.87552500	11.30193800
H	4.62263400	0.75140400	1.55350400
H	2.44804100	1.48256900	-0.35746500

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C	-1.86248700	1.29203000	0.93988200
C	-0.74676700	1.21793700	1.81035900
C	-0.44779000	2.31931000	2.62822800
C	-1.24832200	3.45759300	2.65726800
C	-2.38446700	3.50575600	1.85816800
C	-2.67055200	2.43935000	1.00842400
H	0.42901000	2.28889200	3.26639000
H	-0.98804500	4.28765100	3.30705100
H	-3.04021600	4.37099000	1.87933600
H	-3.55192800	2.50919900	0.38397000
C	0.69841900	-0.50029500	3.88644500
C	2.13507500	0.45336500	1.70881800
C	2.14932100	-0.03508900	4.13765800
H	0.67271000	-1.59448300	3.90626500
C	2.95676600	-0.18651400	2.84556400
H	2.07840700	1.53636800	1.87970300
H	2.14171700	1.02000000	4.44689400
H	2.58597200	-0.60363900	4.96625000
H	3.94080600	0.29004500	2.92011500
H	3.11930600	-1.24401800	2.60429800
P	0.41539600	-0.19214400	2.04533000
C	-0.30317600	0.02342500	4.91366100
C	2.73008200	0.18878200	0.32349200
H	2.07787600	0.53160800	-0.48386900
H	3.67739900	0.73381000	0.23756300
H	2.94657200	-0.87381000	0.18220000
H	-1.31461000	-0.30705900	4.68095600
H	-0.02478000	-0.36342800	5.90166700
H	-0.29531700	1.11490900	4.97897400
C	-3.49197500	0.87644700	-1.55944600
C	-0.99211300	-0.13393400	-1.57413200
C	-3.07472300	0.25775100	-2.93097700
H	-3.27819100	1.94911700	-1.58546700
C	-1.81316500	-0.63425900	-2.77887800
H	-0.28769000	-0.89178000	-1.23001300
H	-3.90141900	-0.33225800	-3.33802100
H	-2.88336100	1.06609100	-3.64379600
H	-2.11332300	-1.66982900	-2.59073500
H	-1.20839700	-0.62959800	-3.69259500
P	-2.35288900	0.04651200	-0.34109600

O	-2.96420500	-1.23177200	0.17124600
C	-0.26358300	1.18505800	-1.86061000
C	-4.96507300	0.64816600	-1.21191800
H	-5.24903000	1.14513800	-0.27729400
H	-5.61126300	1.03270500	-2.00913300
H	-5.15898400	-0.42045700	-1.08409000
H	0.23604200	1.57852300	-0.97145500
H	0.49540800	1.02984200	-2.63569000
H	-0.94669800	1.96213900	-2.22067500
C	0.27921900	-1.62683700	1.08445600
C	-0.62363000	-2.66602300	1.22152700
C	-1.77302700	-2.45097400	2.13451800
O	-2.65689800	-3.44569000	2.14053200
C	-3.79319300	-3.25390900	2.99107600
H	-4.32384300	-2.34631700	2.69451400
H	-4.41542800	-4.13678200	2.84693400
H	-3.47673100	-3.17681600	4.03459200
O	-1.86471300	-1.46068400	2.85347900
C	-0.31940700	-3.95971800	0.72588800
H	-1.11308700	-4.69817300	0.71594300
H	0.35716100	-3.99254600	-0.11991800
C	-0.27198700	-6.69881500	2.83276600
C	0.10199700	-5.36415000	3.04919300
C	-0.41095600	-4.70855400	4.17824900
C	-1.26687900	-5.35958500	5.06466400
C	-1.63030200	-6.68745800	4.83625800
C	-1.12737000	-7.35339300	3.71600800
H	0.10064500	-7.21874700	1.95492800
H	-0.13833600	-3.67137400	4.35761100
H	-1.64707400	-4.83081500	5.93504000
H	-2.29851500	-7.19920900	5.52328400
H	-1.40613600	-8.38696400	3.52844600
C	0.96914800	-4.62231000	2.10005300
C	2.06009500	-5.24641800	1.43719100
H	2.17097600	-6.32478200	1.40126100
C	3.00670100	-4.42421600	0.78377700
O	2.88905400	-3.17006600	0.63936200
C	4.18732600	-5.08665900	0.25471300
C	5.18310700	-5.60906700	-0.20942300
C	6.34789000	-6.22213900	-0.74947800
C	7.34205000	-5.44493200	-1.37638600

C	6.52932500	-7.61703300	-0.66843400
C	8.48012400	-6.04760900	-1.90342300
H	7.20402700	-4.37037900	-1.44031800
C	7.66965200	-8.21204100	-1.19932900
H	5.76555600	-8.21812100	-0.18542600
C	8.64911900	-7.43164300	-1.81808300
H	9.23891700	-5.43585200	-2.38376200
H	7.79603200	-9.28901500	-1.12986400
H	9.53855300	-7.89913500	-2.23110100
H	1.22508200	-3.61760300	2.43558800
H	1.18205700	-1.85157800	0.52756300

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C	-2.95824900	-0.24544300	2.15112100
C	-1.64401300	-0.00557100	2.62213900
C	-1.40798000	-0.12113800	4.00352800
C	-2.41265300	-0.47367500	4.90098600
C	-3.69293600	-0.74663800	4.43017400
C	-3.95079300	-0.63119200	3.06751900
H	-0.39881500	0.05579400	4.36315400
H	-2.18569100	-0.54605600	5.96038500
H	-4.48557000	-1.04315200	5.11069700
H	-4.95454000	-0.84117100	2.71056900
C	-0.07115200	2.05975400	0.85858700
C	0.20587900	-0.64069100	0.16084500
C	0.21983700	1.74003300	-0.63105100
H	0.80591800	2.53405600	1.29231900
C	0.94948900	0.38930500	-0.72419300
H	-0.76704900	-0.85097400	-0.28378900
H	-0.72800500	1.68516800	-1.16754900
H	0.82284500	2.54340400	-1.06900800
H	0.98208800	0.02717200	-1.75774700
H	1.98319300	0.47771600	-0.36668300
P	-0.08655700	0.39514400	1.66895400
C	-1.27586200	2.96535300	1.10737500
C	1.00585000	-1.91969300	0.40394800
H	0.50463900	-2.59314500	1.10976200
H	1.11538100	-2.45750900	-0.54475100
H	2.00612900	-1.69127500	0.78236200

H	-1.47188500	3.09795500	2.17706100
H	-1.07393700	3.95527400	0.68343300
H	-2.16725000	2.56080900	0.62509200
C	-4.34131300	-1.66483000	-0.05109700
C	-5.09198500	0.95951600	0.39373500
C	-5.69013200	-1.21882500	-0.65379400
H	-4.53643200	-2.22457500	0.87191800
C	-6.23186500	-0.06260700	0.20536100
H	-4.95619300	1.49682700	-0.55540800
H	-5.52765100	-0.86710900	-1.68126500
H	-6.39412200	-2.05627100	-0.70775500
H	-7.10770900	0.41086500	-0.25197900
H	-6.55519400	-0.44467200	1.18354300
P	-3.53551000	-0.06089200	0.42480600
O	-2.48306700	0.43657600	-0.53120500
C	-5.29698800	1.98448100	1.50830100
C	-3.45678100	-2.49632200	-0.97960000
H	-2.53793000	-2.81388700	-0.47497300
H	-3.98741200	-3.39545000	-1.31220000
H	-3.16760400	-1.91656300	-1.86109400
H	-4.44602000	2.66902700	1.58234500
H	-6.19275000	2.58308000	1.30823400
H	-5.42459300	1.50620700	2.48357200
C	1.25706000	0.12579900	2.73809300
H	1.46058500	-0.93445500	2.83665300
C	2.25341200	0.97359300	3.21193600
C	3.49600100	0.32775100	3.75441500
O	3.46556800	-1.02343300	3.73278700
C	4.73394900	-1.64788700	3.96710700
H	5.13915000	-1.35603500	4.93935900
H	4.54161300	-2.72137900	3.93590300
H	5.43500100	-1.35821100	3.17953800
O	4.44886800	0.95995800	4.17294500
C	2.33661500	2.39066700	3.20672800
H	3.04519800	2.81019500	3.90908800
H	1.41917900	2.96269100	3.10960600
C	3.73441400	5.29367600	2.48656400
C	3.07925500	4.45111600	1.57459300
C	2.11516100	5.01498000	0.72566900
C	1.81764100	6.37634400	0.77853700
C	2.47740500	7.20204300	1.68911800

C	3.43852900	6.65334000	2.54195200
H	4.47242900	4.86922700	3.16123700
H	1.60901100	4.38114900	0.00253000
H	1.07370600	6.79239500	0.10399800
H	2.24637100	8.26264500	1.73469300
H	3.95661000	7.28791200	3.25610700
C	3.37004300	2.99656900	1.52095400
C	4.70365200	2.53309900	1.54019300
H	5.52271500	3.17982000	1.83394900
C	4.95070600	1.16585400	1.27925700
O	4.03286600	0.31660900	1.09766500
C	6.33171600	0.71716300	1.29245500
C	7.46529000	0.27660600	1.31203700
C	8.79445000	-0.23035600	1.33823100
C	9.05200000	-1.58042000	1.02833200
C	9.87644300	0.60599500	1.67650300
C	10.35250500	-2.07451000	1.05661900
H	8.21966000	-2.22593900	0.76655900
C	11.17391900	0.10385000	1.70289800
H	9.68022500	1.64592600	1.91691700
C	11.41796100	-1.23629700	1.39355300
H	10.53672300	-3.11774500	0.81478900
H	11.99893100	0.76015800	1.96606000
H	12.43219200	-1.62504300	1.41492700
H	2.73219800	2.42638200	0.84993700

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C	-1.69624700	-0.03151400	1.39210900
C	-0.32059000	0.21223700	1.61123500
C	0.26089500	1.33901200	1.01129800
C	-0.48566500	2.22120000	0.23450200
C	-1.84268100	1.98838900	0.03207600
C	-2.43169800	0.86399000	0.60336200
H	1.31929500	1.52824600	1.12773600
H	-0.00107200	3.08277600	-0.21505300
H	-2.43722800	2.66786400	-0.57128800
H	-3.48507700	0.67655200	0.42274100
C	0.39028200	-0.62869700	4.47118400
C	2.45736400	-0.01464700	2.76884600

C	1.73708300	-0.21814500	5.12785900
H	0.08067900	-1.62574300	4.79266400
C	2.89637800	-0.50004500	4.16465800
H	2.29700000	1.06962900	2.83427300
H	1.71027800	0.85786000	5.34448200
H	1.86556700	-0.73717300	6.08247500
H	3.81730900	0.00854600	4.47152700
H	3.11074600	-1.57460400	4.12320400
P	0.78499500	-0.83562200	2.66100200
C	-0.72798500	0.36663100	4.78228000
C	3.45473400	-0.34418000	1.66289800
H	3.12658800	0.01665500	0.68584300
H	4.42707200	0.10432100	1.89799500
H	3.58904400	-1.42746600	1.58820500
H	-1.68657200	0.00062300	4.41563100
H	-0.80444800	0.49301100	5.86844600
H	-0.52896100	1.35277400	4.34610400
C	-4.32061900	-1.20646000	2.35371400
C	-2.82160700	-2.67066400	0.56348900
C	-4.94793700	-2.54076700	1.89674700
H	-4.68800900	-0.41229200	1.69114400
C	-4.35659200	-2.87204400	0.51638900
H	-2.35010100	-3.60323300	0.88111100
H	-4.68648300	-3.32780000	2.61608000
H	-6.04140300	-2.47374100	1.87053400
H	-4.59459700	-3.89225900	0.20078100
H	-4.78500400	-2.18912900	-0.23034300
P	-2.53324900	-1.53877300	2.00455300
O	-1.81550200	-2.13769800	3.18735900
C	-2.21849900	-2.23932500	-0.77369100
C	-4.57386400	-0.83230700	3.81222500
H	-4.14428200	0.14663400	4.05196300
H	-5.64944400	-0.78884400	4.01840800
H	-4.11888700	-1.57013600	4.47922000
H	-1.15263600	-2.01721800	-0.68892300
H	-2.34880300	-3.04198400	-1.50649500
H	-2.70942400	-1.33932300	-1.16050400
C	0.99271500	-2.54461700	2.41747600
C	1.29246600	-3.30924500	1.29444600
C	1.32790700	-2.63979100	-0.02218700
O	1.48504300	-3.48001500	-1.06862400

C	1.50667300	-2.85953400	-2.36032000
H	0.55648800	-2.35706500	-2.56134700
H	2.31548900	-2.12709400	-2.42063000
H	1.66780700	-3.67158300	-3.06951100
O	1.24166600	-1.42711900	-0.18071600
C	1.44324600	-4.71456000	1.41950200
H	1.70921600	-5.29497200	0.54402000
H	1.88017200	-5.05174900	2.34909200
C	-2.55001000	-6.46347800	1.33016900
C	-1.33374400	-5.82559900	1.02091100
C	-1.05890600	-5.56249700	-0.32918400
C	-1.96538000	-5.91806800	-1.32897100
C	-3.17158300	-6.54001300	-1.00619900
C	-3.45923000	-6.81238400	0.33251600
H	-2.78006600	-6.66298000	2.37198200
H	-0.13486800	-5.07102100	-0.60140400
H	-1.72239500	-5.70852100	-2.36787700
H	-3.87588200	-6.81418700	-1.78695700
H	-4.39290400	-7.29909900	0.60253700
C	-0.46086000	-5.38787500	2.15472300
C	-0.22879500	-6.28008500	3.20920200
H	-0.38906600	-7.34668400	3.08000900
C	0.32441600	-5.81951900	4.44165900
O	0.71047300	-4.64478600	4.66672000
C	0.44528300	-6.81692600	5.49447500
C	0.55721500	-7.63136000	6.39087000
C	0.69027300	-8.58128100	7.44182200
C	0.34419100	-9.93154600	7.23766200
C	1.17115900	-8.18739200	8.70617300
C	0.47685900	-10.85666800	8.26857300
H	-0.02634800	-10.23699000	6.26434600
C	1.29977800	-9.11863500	9.73203100
H	1.43835800	-7.14758100	8.86445000
C	0.95415600	-10.45518100	9.51845500
H	0.20686500	-11.89511700	8.09735500
H	1.67166900	-8.80156400	10.70247300
H	1.05632700	-11.17977100	10.32142400
H	-0.60457100	-4.35152900	2.46582100
H	0.84675600	-3.09881000	3.34397200

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C	-2.51071700	0.87990200	1.09600900
C	-1.13248300	1.12837000	1.27833900
C	-0.63731800	2.40854400	0.95709300
C	-1.45266400	3.43159700	0.48936700
C	-2.81427100	3.19405300	0.32847200
C	-3.31871100	1.93455900	0.62745300
H	0.41865400	2.61958700	1.08001000
H	-1.02479000	4.40244700	0.25841600
H	-3.47729400	3.97537000	-0.03063500
H	-4.37986200	1.76464100	0.48264500
C	1.18802800	0.96384200	3.22424100
C	1.55897100	0.09624700	0.60654500
C	2.53894700	1.29191000	2.54594600
H	1.35012500	0.16631900	3.95432900
C	2.83420000	0.24883200	1.46011100
H	1.39050800	1.02733600	0.05343100
H	2.47959700	2.29120400	2.09115600
H	3.33399600	1.33691200	3.29864600
H	3.68150600	0.54766600	0.83226800
H	3.07710100	-0.72440200	1.90213600
P	0.22216300	0.02274200	1.90509700
C	0.54466200	2.14588300	3.94580800
C	1.61097400	-1.06563100	-0.38904700
H	0.63609200	-1.25221800	-0.85264400
H	2.31910400	-0.81781800	-1.18820300
H	1.96139700	-1.98428600	0.08893700
H	-0.40881400	1.85837300	4.39030300
H	1.21733000	2.48126200	4.74485200
H	0.37691900	2.99808000	3.28159400
C	-4.94504600	-0.26599800	2.32968500
C	-4.36682300	-1.02701900	-0.26801200
C	-6.09753400	-0.89399900	1.51799900
H	-5.06598600	0.82328500	2.32773600
C	-5.82791600	-0.63023000	0.02560700
H	-4.31004500	-2.12358400	-0.29678800
H	-6.11696200	-1.97664000	1.70033200
H	-7.06750400	-0.49631600	1.83709400
H	-6.52079000	-1.18428800	-0.61807700

H	-5.97815400	0.43549000	-0.19728000
P	-3.44239000	-0.70088600	1.32133900
O	-2.68898600	-1.90305700	1.80081600
C	-3.77850800	-0.47971400	-1.56702700
C	-4.82026800	-0.75811600	3.77029900
H	-4.02754100	-0.21423300	4.29048500
H	-5.76295900	-0.61052100	4.31046500
H	-4.56384300	-1.82164000	3.79464500
H	-2.73563400	-0.79071200	-1.69186700
H	-4.34452000	-0.85524600	-2.42732100
H	-3.80644600	0.61356400	-1.60019500
C	0.10084700	-1.65834400	2.29007100
C	-0.40639200	-2.24085800	3.43599900
C	-1.17408900	-1.38186400	4.36092500
O	-1.54471500	-2.00080100	5.48897900
C	-2.11432000	-1.18486900	6.51859700
H	-3.13965200	-0.90584100	6.26272700
H	-2.09503400	-1.80149300	7.41664000
H	-1.51502700	-0.28373900	6.66413300
O	-1.42741200	-0.19920200	4.13766100
C	-0.00112000	-3.54080500	3.82815100
H	-0.52248300	-4.01934400	4.64862600
H	0.31832600	-4.19638700	3.02726700
C	1.36020300	-4.00816300	6.90865200
C	1.60421800	-2.95156300	6.01761100
C	1.54623500	-1.64137900	6.51551500
C	1.25101000	-1.38943900	7.85444700
C	1.00184500	-2.45006700	8.72657400
C	1.06085400	-3.76114300	8.24595200
H	1.38611400	-5.02870700	6.53715100
H	1.74413300	-0.81133500	5.84167500
H	1.21832900	-0.36505600	8.21707200
H	0.76882400	-2.25914900	9.77050400
H	0.86988200	-4.59414500	8.91743200
C	1.86519300	-3.18318400	4.57801200
C	2.72996900	-4.20727600	4.12623300
H	3.06485400	-5.00774000	4.77764200
C	3.13936800	-4.18533800	2.76837100
O	2.69166200	-3.37928700	1.90298300
C	4.14501200	-5.15977200	2.37824500
C	4.97878400	-5.96842800	2.01652100

C	5.95584600	-6.91233600	1.59409600
C	6.47266100	-7.86427800	2.49514500
C	6.42484400	-6.91234600	0.26537700
C	7.42772700	-8.78570100	2.07676600
H	6.11348400	-7.86617600	3.51932700
C	7.38104200	-7.83635200	-0.14456400
H	6.02727500	-6.18047700	-0.43035900
C	7.88607800	-8.77606700	0.75727300
H	7.81717100	-9.51439300	2.78247900
H	7.73388400	-7.82474900	-1.17222800
H	8.63211100	-9.49650500	0.43376600
H	1.96232300	-2.27181400	3.98827400
H	0.69164800	-2.29270600	1.64215700

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C	-2.38482300	1.00266500	1.08529600
C	-1.00405000	1.18964100	1.31553000
C	-0.43698400	2.43892300	0.99144000
C	-1.18461400	3.48975200	0.47476800
C	-2.54883700	3.31291100	0.26515400
C	-3.12346400	2.08457600	0.56694200
H	0.62243000	2.60270300	1.15111700
H	-0.70275500	4.43493600	0.24368300
H	-3.15994400	4.11713900	-0.13331500
H	-4.18534100	1.96180500	0.38473700
C	1.23416600	0.94913600	3.34878500
C	1.65729200	0.02081200	0.76012700
C	2.62303500	1.20087500	2.71604900
H	1.33125300	0.15766800	4.09679600
C	2.90676100	0.12684000	1.65762700
H	1.55391700	0.94959300	0.18749400
H	2.62858800	2.19408900	2.24446200
H	3.39148000	1.22048200	3.49693300
H	3.78950600	0.37455800	1.05695000
H	3.08642200	-0.84935200	2.12269200
P	0.27250400	0.03254200	2.00961100
C	0.62277400	2.17280100	4.02747900
C	1.68912400	-1.15842600	-0.21570900
H	0.72361200	-1.30618700	-0.71182200

H	2.43641600	-0.95754000	-0.99205800
H	1.97788400	-2.08462900	0.28821300
H	-0.35819300	1.93836300	4.44231300
H	1.28232800	2.49063400	4.84442200
H	0.51899400	3.01982600	3.34385300
C	-4.91556500	0.00404800	2.24908900
C	-4.28169500	-0.84230600	-0.30893000
C	-6.06728800	-0.58603500	1.40841500
H	-4.98303200	1.09754600	2.22007400
C	-5.73133800	-0.36921200	-0.07803400
H	-4.27758000	-1.94068900	-0.31337600
H	-6.14618600	-1.66210300	1.61236100
H	-7.02758600	-0.13511100	1.68286500
H	-6.42675200	-0.90359200	-0.73546500
H	-5.82099100	0.69723100	-0.32841400
P	-3.40067800	-0.52611300	1.30689600
O	-2.72689200	-1.75294500	1.83948800
C	-3.62076200	-0.35242500	-1.59589600
C	-4.86714100	-0.46068600	3.70336100
H	-4.06730200	0.05527000	4.24089000
H	-5.82000100	-0.25466700	4.20519600
H	-4.66516100	-1.53470000	3.75941500
H	-2.59025800	-0.71523600	-1.67534800
H	-4.17257300	-0.71957100	-2.46893800
H	-3.59475700	0.73996000	-1.65233400
C	0.05654300	-1.63443100	2.41440200
C	-0.51779100	-2.17310100	3.55000400
C	-1.27663200	-1.26360800	4.43322200
O	-1.71816300	-1.84612700	5.55508600
C	-2.28569000	-0.98730400	6.55042000
H	-3.28300100	-0.65755000	6.24845200
H	-2.33698200	-1.59185300	7.45539900
H	-1.64528900	-0.11753500	6.71109800
O	-1.46351200	-0.07379100	4.18424800
C	-0.18812800	-3.48360000	3.97674500
H	-0.76062600	-3.92341900	4.78473100
H	0.12843600	-4.16690800	3.19819100
C	1.04418500	-3.96744200	7.11146800
C	1.36355100	-2.93588100	6.21494100
C	1.34410800	-1.61692100	6.69224200
C	1.01401100	-1.33226000	8.01637000

C	0.69030000	-2.36795800	8.89396500
C	0.70990800	-3.68756200	8.43394600
H	1.03948400	-4.99376700	6.75535400
H	1.59982000	-0.80630100	6.01421600
H	1.01250700	-0.30195200	8.36335200
H	0.42993300	-2.15139100	9.92635900
H	0.46075100	-4.50140000	9.10984200
C	1.66450400	-3.20043100	4.78885000
C	2.49725600	-4.26943200	4.38282200
H	2.77178600	-5.07393900	5.05708100
C	2.95616700	-4.28683800	3.04097300
O	2.57670800	-3.47537100	2.14835600
C	3.93111800	-5.31031300	2.70185300
C	4.74148900	-6.15942900	2.38209100
C	5.69140800	-7.15053000	2.00867600
C	6.20545000	-7.19236400	0.69738900
C	6.13598700	-8.10813700	2.94168500
C	7.13507400	-8.16234200	0.33532600
H	5.86350400	-6.45616100	-0.02290200
C	7.06489500	-9.07562800	2.57111800
H	5.74207000	-8.07787300	3.95255900
C	7.56838500	-9.10722900	1.26852800
H	7.52325300	-8.18267100	-0.67938000
H	7.39856100	-9.80811500	3.30106300
H	8.29384600	-9.86360300	0.98241800
H	1.82465400	-2.30322900	4.19127100
H	0.64044200	-2.30625300	1.79878600

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C	-2.62055700	-0.62811500	2.11836900
C	-1.41258800	0.05486500	2.40576700
C	-1.16574400	0.42763400	3.73527900
C	-2.07416900	0.14887700	4.75720000
C	-3.26275200	-0.51072400	4.46731200
C	-3.52332800	-0.89610800	3.15338800
H	-0.25950000	0.95634800	3.99601500
H	-1.84756700	0.45608500	5.77369400
H	-3.98140700	-0.72756800	5.25182900
H	-4.45068400	-1.41538200	2.93352400

C	0.91624200	-0.69363100	0.43918200
C	1.10991800	1.55970000	1.98698000
C	2.35161600	-0.10020700	0.58714500
H	0.64057000	-0.87087400	-0.60173700
C	2.32516500	1.36746600	1.06409900
H	1.32367800	1.00984600	2.91200700
H	2.89677600	-0.70141800	1.32401400
H	2.87621500	-0.19428500	-0.36698000
H	3.24478000	1.62596700	1.60117900
H	2.25692300	2.05836400	0.21936600
P	-0.22170500	0.61081200	1.09303900
C	0.76269700	-2.02056900	1.19293100
C	0.76885700	3.01560800	2.29382900
H	-0.07233900	3.10453000	2.98992500
H	1.63134600	3.52458200	2.73816700
H	0.49413400	3.54302100	1.37489800
H	-0.21964100	-2.45407000	1.00827700
H	1.51926900	-2.71817000	0.81827200
H	0.91695800	-1.90532600	2.27316400
C	-3.87648500	-2.84425600	0.52239500
C	-4.44142000	-0.25898900	-0.28240900
C	-4.88772300	-2.70983400	-0.63364100
H	-4.43722400	-2.91064900	1.46360500
C	-5.54370700	-1.32629600	-0.49711100
H	-4.05379500	0.06770700	-1.25504500
H	-4.35473500	-2.78364800	-1.59038200
H	-5.62693600	-3.51815500	-0.60916200
H	-6.16167800	-1.07642700	-1.36606900
H	-6.20889000	-1.32941700	0.37760800
P	-3.00880000	-1.21244500	0.42697400
O	-1.76104200	-1.27093200	-0.40918800
C	-4.91926100	0.95444700	0.51723300
C	-2.90206000	-4.01514900	0.40685800
H	-2.24776000	-4.07373000	1.28368200
H	-3.44693700	-4.96272900	0.32767000
H	-2.26734900	-3.89770400	-0.47595400
H	-4.13719400	1.70741000	0.62537400
H	-5.76149000	1.43087000	0.00266900
H	-5.26281000	0.66087100	1.51521900
C	-1.14998200	1.64226200	0.02585900
H	-1.84435800	2.25166000	0.59861000

C	-1.32986600	1.64795900	-1.35152100
C	-2.59280500	2.37280500	-1.74030200
O	-3.07281100	1.97637600	-2.93876200
C	-4.26377100	2.64766400	-3.37007700
H	-4.08620600	3.72210200	-3.46238100
H	-4.50738300	2.21224400	-4.33923600
H	-5.07680600	2.48407300	-2.65693800
O	-3.15586600	3.21224500	-1.06044900
C	-0.51827800	1.11351700	-2.39507700
C	1.51986800	2.96992500	-4.25534000
C	1.28958800	2.77415400	-2.88837500
C	1.25354600	3.89760200	-2.05196800
C	1.44555500	5.18043600	-2.56313500
C	1.67799600	5.36265700	-3.92749900
C	1.71229500	4.25137900	-4.77146000
H	1.54519000	2.10440900	-4.91142600
H	1.05658200	3.76247400	-0.99178900
H	1.41553900	6.03812100	-1.89584500
H	1.83210400	6.36081000	-4.32847500
H	1.89144800	4.38206400	-5.83567900
C	1.01235500	1.39035200	-2.32476800
C	1.80837200	0.30332400	-2.98789900
H	2.77612900	0.54072200	-3.41419300
C	1.31383000	-0.96452300	-3.11236700
O	0.13875000	-1.35163800	-2.63024900
C	2.08336400	-1.96679200	-3.79576300
C	2.72884500	-2.83649800	-4.34846300
C	3.48310400	-3.85128800	-4.99920100
C	2.94491100	-5.14138500	-5.17880000
C	4.78300800	-3.58891400	-5.47599100
C	3.68580600	-6.13264400	-5.81492600
H	1.94377000	-5.34665900	-4.81349800
C	5.51722900	-4.58647800	-6.11015500
H	5.20100100	-2.59636200	-5.34086200
C	4.97379300	-5.86159500	-6.28297200
H	3.25664000	-7.12230000	-5.94672100
H	6.51826700	-4.36832400	-6.47246700
H	5.54937400	-6.63796100	-6.77915900
H	1.25814200	1.43260300	-1.25902500
H	-0.90406500	1.35151800	-3.38522900
H	-0.44432400	-0.22042200	-2.40788600

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C	-2.03327900	0.74658800	2.24949100
C	-0.68119300	0.35254800	2.41073500
C	-0.21327200	0.12512800	3.71551200
C	-1.01981300	0.29379300	4.83477400
C	-2.34095500	0.69783300	4.67798400
C	-2.83159700	0.91252600	3.39538100
H	0.81458300	-0.17544400	3.85776500
H	-0.60521300	0.12018100	5.82272800
H	-2.98596000	0.84408800	5.53920500
H	-3.86560500	1.22364700	3.28411300
C	0.93827200	1.49048200	-0.06498300
C	0.08286800	-1.15257100	-0.18300300
C	0.82662800	0.83992700	-1.47384000
H	1.97676000	1.73528100	0.14849500
C	0.94794100	-0.69031400	-1.37405900
H	-0.95511500	-0.89710200	-0.40462100
H	-0.15696400	1.08593800	-1.87826300
H	1.58884700	1.25972900	-2.13865200
H	0.60926200	-1.17435300	-2.29722900
H	1.99046500	-0.99155000	-1.20761800
P	0.60755600	0.07318400	1.09742400
C	0.11090600	2.76578600	0.10034000
C	0.19983500	-2.63298300	0.16836400
H	-0.33428800	-2.87717800	1.09363200
H	-0.24210000	-3.23085000	-0.63679500
H	1.24106500	-2.95067300	0.27874200
H	-0.07432200	2.98271000	1.15193600
H	0.66655100	3.61451900	-0.30836500
H	-0.83643100	2.67428800	-0.42807300
C	-4.53449900	0.18242400	0.74546800
C	-3.63408100	2.80735400	0.73156900
C	-5.53263400	1.24811500	0.24986800
H	-4.76389500	-0.05407700	1.79064800
C	-5.15176400	2.58038400	0.91547400
H	-3.45542300	3.14608000	-0.29804000
H	-5.45093300	1.34177800	-0.84126400
H	-6.56519900	0.95699500	0.47246700

H	-5.72066500	3.42256500	0.50646000
H	-5.38364000	2.53445300	1.98876700
P	-2.91248900	1.08616000	0.68062100
O	-2.13132900	0.77677700	-0.57345900
C	-3.03042800	3.82420800	1.70197200
C	-4.49699800	-1.10592700	-0.07483100
H	-3.79992700	-1.83166200	0.35845400
H	-5.48969400	-1.56915000	-0.10780700
H	-4.17115200	-0.90220400	-1.09871800
H	-1.96432200	3.98223400	1.52811400
H	-3.53034800	4.79212800	1.58588900
H	-3.15145500	3.50850700	2.74262500
C	2.02953700	-0.66594700	1.83249500
H	1.92519100	-1.74293400	1.79266500
C	3.00959000	-0.20620900	2.70735200
C	3.64179900	-1.26723100	3.57818500
O	3.64099300	-2.49543400	3.00277100
C	4.23186600	-3.53306600	3.79717100
H	3.67580200	-3.66883900	4.72889300
H	4.18205800	-4.43408300	3.18496700
H	5.26889300	-3.28680300	4.03903600
O	4.11132400	-1.06508400	4.67874800
C	3.43456000	1.12175300	3.00030800
C	5.97612200	3.23499700	2.65508600
C	5.36317100	2.24701900	1.87636400
C	6.17449100	1.36172100	1.15728100
C	7.56400200	1.46051400	1.20905300
C	8.16597300	2.45078000	1.98786200
C	7.36627300	3.33623900	2.71176400
H	5.35216400	3.92459100	3.21675200
H	5.70654000	0.58516100	0.55569800
H	8.17737600	0.76659700	0.63996100
H	9.24878200	2.53188600	2.02883100
H	7.82561800	4.10996200	3.32153000
C	3.85122000	2.08566700	1.84798200
C	3.11829200	3.40231700	1.89024900
H	3.54231800	4.25428000	1.37063400
C	1.94187300	3.54986800	2.55744800
O	1.33668400	2.55560100	3.21979000
C	1.21222200	4.78382700	2.53499000
C	0.46915100	5.74561300	2.48893300

C	-0.42910500	6.84603000	2.43082900
C	-1.63565000	6.81326100	3.15952400
C	-0.14939800	7.97349700	1.63438000
C	-2.53308500	7.87397000	3.08572500
H	-1.84989400	5.94750500	3.77784800
C	-1.05192700	9.03094200	1.56843500
H	0.77867300	8.00313100	1.07249400
C	-2.24671100	8.98651700	2.29056000
H	-3.45871500	7.83512900	3.65373400
H	-0.82255000	9.89433600	0.94998500
H	-2.94847900	9.81386900	2.23597800
H	3.62588900	1.56398900	0.90395500
H	4.13907300	1.15724100	3.82766200
H	2.28377400	1.75464900	3.33211000

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C	-0.98293000	1.93573700	0.85509100
C	-0.06227200	2.12614900	1.91667600
C	1.09434900	2.87573500	1.66786900
C	1.35646900	3.41772500	0.40784800
C	0.46490900	3.20536100	-0.63677100
C	-0.69977900	2.47300700	-0.40406700
H	1.81919500	3.03768500	2.45455700
H	2.26254000	3.99501200	0.25061800
H	0.66360600	3.61150100	-1.62399200
H	-1.40175900	2.32982600	-1.21871000
C	-1.20330200	2.08984900	4.88191900
C	1.41864000	1.43954500	4.41203400
C	-0.22610400	2.18634200	6.08853700
H	-2.03807800	1.43694200	5.12858900
C	0.97825500	1.26313300	5.87337800
H	1.73430600	2.48476100	4.29449600
H	0.11920500	3.22488900	6.17527700
H	-0.75610800	1.92059200	7.00464800
H	1.80378400	1.50612400	6.55207400
H	0.67637300	0.23088100	6.07070600
P	-0.21889000	1.24875100	3.54074500
C	-1.73555000	3.45764000	4.44312100

C	2.52482600	0.50074500	3.94093700
H	2.79315600	0.67694400	2.89272700
H	3.42409300	0.64973500	4.54881400
H	2.21403300	-0.54336500	4.03655200
H	-2.46806600	3.34977300	3.64363600
H	-2.21579700	3.93497400	5.30448800
H	-0.92572100	4.11788000	4.10892900
C	-3.87565500	1.82619700	0.02525000
C	-2.70996000	-0.60334900	0.56753900
C	-4.83939000	0.62451500	-0.04347900
H	-3.43388000	1.96583600	-0.97073900
C	-3.98599500	-0.62507900	-0.32035000
H	-2.88476000	-1.18787000	1.47488600
H	-5.35927300	0.51513200	0.91495500
H	-5.60162000	0.77463800	-0.81622200
H	-4.55341700	-1.54173800	-0.13788000
H	-3.68191200	-0.62506200	-1.37569100
P	-2.60374700	1.14732300	1.17352200
O	-2.96509800	1.39586200	2.61984900
C	-1.47488200	-1.13652500	-0.16186700
C	-4.48567600	3.13301600	0.52507800
H	-3.74707700	3.94242100	0.52879200
H	-5.32109100	3.43848600	-0.11487300
H	-4.85534600	3.01076200	1.54707600
H	-0.60216700	-1.17952700	0.49208600
H	-1.67518900	-2.15106800	-0.52526100
H	-1.22161200	-0.51884800	-1.03170600
C	-0.35008300	-0.44604100	3.09543800
H	0.42264000	-0.61086500	2.35097300
C	-0.92079600	-1.59280300	3.62601900
C	-0.36591800	-2.88945600	3.07080000
O	0.82101100	-2.74483800	2.42968400
C	1.33855900	-3.94416600	1.83691300
H	0.63966100	-4.33646800	1.09332200
H	2.27951100	-3.65552500	1.36769600
H	1.50544300	-4.70663200	2.60166400
O	-0.91923100	-3.96693100	3.15821800
C	-1.91318500	-1.77146600	4.63183200
H	-2.13334100	-2.82012900	4.81959200
H	-1.37457600	-1.30714700	5.74099100
C	-4.28903600	-2.63383400	3.14118600

C	-4.32595600	-1.41469900	3.82715600
C	-5.46442300	-0.60650100	3.67696700
C	-6.53508000	-1.00587500	2.88095400
C	-6.48832300	-2.22765900	2.20252000
C	-5.36057200	-3.03544700	2.33560200
H	-3.41577200	-3.27243300	3.21704100
H	-5.49287000	0.35772500	4.17618700
H	-7.40555300	-0.36156800	2.78359100
H	-7.32165200	-2.54263100	1.58009400
H	-5.30893300	-3.98902200	1.81585000
C	-3.16263800	-0.87602200	4.65430700
C	-3.55470100	-0.51489500	6.06908000
H	-4.59607300	-0.35147100	6.31817000
C	-2.60428900	-0.38937700	7.03936500
O	-1.30332500	-0.61629800	6.82881500
C	-2.96911900	0.01437200	8.36578400
C	-3.23698600	0.39828900	9.48860900
C	-3.56150800	0.83991900	10.80041700
C	-2.56758500	0.92389800	11.79625000
C	-4.88188700	1.20523100	11.13148200
C	-2.88802100	1.35946700	13.07831900
H	-1.54997100	0.64142500	11.54596000
C	-5.19333000	1.63935300	12.41629100
H	-5.65094600	1.14086900	10.36826700
C	-4.20009700	1.71925100	13.39523800
H	-2.11047400	1.41767400	13.83530500
H	-6.21645600	1.91640100	12.65592000
H	-4.44681600	2.05818900	14.39746500
H	-2.89803600	0.04514000	4.12582500

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C	-0.98406400	2.11583700	1.04258900
C	0.02998200	2.19643700	2.03070700
C	1.13671500	3.02048400	1.79741100
C	1.27030000	3.74490400	0.61127400
C	0.28851400	3.64828900	-0.36701200
C	-0.83195900	2.84702500	-0.14131900
H	1.92281100	3.09267600	2.53811200
H	2.14410000	4.37100700	0.45703100

H	0.38178600	4.19778300	-1.29913300
H	-1.60120100	2.80412500	-0.90340700
C	-0.92054200	1.74520900	4.98322000
C	1.68672200	1.28323200	4.33710600
C	0.08257800	1.65732000	6.17080600
H	-1.76851700	1.08471600	5.15025100
C	1.31935800	0.84520000	5.76228400
H	1.94945200	2.34936100	4.37920600
H	0.39697100	2.67472200	6.43552200
H	-0.40617500	1.22317400	7.04552800
H	2.15626600	1.00169800	6.45224800
H	1.08659900	-0.22550700	5.77821300
P	0.01602900	1.09626800	3.50993500
C	-1.44031400	3.17100900	4.76489100
C	2.80283900	0.47998500	3.67812400
H	3.03020300	0.85147200	2.67202200
H	3.72085800	0.53932500	4.27430600
H	2.51452200	-0.57134600	3.58514800
H	-2.19560100	3.18851000	3.97916300
H	-1.89015200	3.52957900	5.69789900
H	-0.62658100	3.85913500	4.50476900
C	-3.85060800	1.92867900	0.19655600
C	-2.68310100	-0.46666000	0.69182700
C	-4.87453000	0.78003000	0.26323700
H	-3.44203400	1.95898600	-0.82271000
C	-4.11330700	-0.55107600	0.07168200
H	-2.59200000	-1.13256900	1.55036900
H	-5.36030900	0.79214200	1.24407900
H	-5.65882200	0.90609600	-0.49170800
H	-4.67064400	-1.37918400	0.51625900
H	-4.01552300	-0.75861000	-1.00092200
P	-2.58019700	1.25661000	1.35703600
O	-3.01954300	1.46861700	2.79038100
C	-1.58477400	-0.79489400	-0.32463000
C	-4.38542700	3.29842500	0.60320700
H	-3.61631000	4.07338500	0.50892300
H	-5.23676400	3.58729800	-0.02394700
H	-4.71352400	3.27685500	1.64674200
H	-0.59367100	-0.75078800	0.13116600
H	-1.73685900	-1.80628400	-0.71832700
H	-1.60350200	-0.10466700	-1.17714600

C	-0.25378200	-0.46884500	2.86641000
H	0.47152500	-0.57894500	2.06311100
C	-0.68681100	-1.72888400	3.41874500
C	0.14992100	-2.94325000	3.07243500
O	1.34877600	-2.62096900	2.52242500
C	2.16211000	-3.74094000	2.15091900
H	1.64359900	-4.36798800	1.42067900
H	3.06777400	-3.31380500	1.71887800
H	2.40200500	-4.34855900	3.02737900
O	-0.17984500	-4.09997900	3.24894100
C	-1.79300800	-2.05060500	4.15445600
H	-1.88461400	-3.09024000	4.45397700
C	-4.40610400	-2.89916900	3.23027800
C	-4.24740200	-1.62232000	3.77709500
C	-5.31179800	-0.71471100	3.67440700
C	-6.50818100	-1.07860500	3.06023000
C	-6.66068000	-2.36000500	2.52458600
C	-5.60382300	-3.26536700	2.60941400
H	-3.58768700	-3.60987200	3.26669800
H	-5.17917000	0.29510300	4.05078200
H	-7.31895700	-0.35798500	2.98931500
H	-7.59116400	-2.64566300	2.04164500
H	-5.70612800	-4.26318700	2.19085500
C	-2.95352300	-1.14289100	4.44895900
C	-3.19675000	-0.87912800	5.92323600
H	-4.18954700	-0.54351000	6.20237200
C	-2.28471900	-0.95288200	6.91920100
O	-0.97969400	-1.35393200	6.77797800
C	-2.60624600	-0.56610000	8.25080600
C	-2.86459800	-0.20910700	9.38321200
C	-3.17613500	0.20776200	10.70653200
C	-2.21243400	0.11797500	11.73004800
C	-4.45190800	0.71936300	11.01472700
C	-2.52059800	0.52994600	13.02278400
H	-1.22966400	-0.27743700	11.49439100
C	-4.75072400	1.12782000	12.31079100
H	-5.19596300	0.78869600	10.22768600
C	-3.78847400	1.03577100	13.31903800
H	-1.76874900	0.45520000	13.80347200
H	-5.73870600	1.51975400	12.53575700
H	-4.02543100	1.35565800	14.32968400

H	-2.75592100	-0.17500900	3.97169100
H	-0.88701600	-1.69189200	5.85836400

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C	2.94200000	0.97958300	1.55185800
C	2.00647400	0.99145500	2.61319600
C	2.13322700	2.00946800	3.57647600
C	3.17255700	2.93618000	3.55106700
C	4.13701400	2.86118600	2.55352200
C	4.00369800	1.89643900	1.55965800
H	1.39892800	2.11206100	4.36339600
H	3.22093000	3.70731800	4.31392500
H	4.96775100	3.55979300	2.52828700
H	4.73406500	1.87592700	0.76023000
C	-0.96132000	0.87100100	2.66274200
C	0.46793300	-0.29663900	4.74803900
C	-1.34618500	1.31655400	4.08918400
H	-1.70988500	0.16520000	2.30356800
C	-0.95489300	0.21138200	5.08580000
H	1.18293400	0.43285500	5.13047600
H	-0.82495700	2.25140100	4.33485900
H	-2.42003200	1.52700000	4.13087200
H	-0.98330900	0.57481300	6.11943800
H	-1.67139200	-0.61234500	5.02615700
P	0.55321800	-0.17281600	2.87466900
C	-0.83559300	1.98256900	1.62175400
C	0.84357700	-1.64529600	5.36053400
H	1.87952000	-1.91107000	5.12050600
H	0.76611600	-1.57201000	6.45195800
H	0.21165700	-2.46481000	5.01564600
H	-0.50769700	1.57620000	0.66062000
H	-1.81048800	2.46429700	1.48733900
H	-0.11838700	2.74871900	1.93454000
C	3.77768300	0.51643100	-1.32085700
C	3.52768500	-1.70026000	0.30010900
C	4.13496800	-0.82879200	-1.98238100
H	4.70928700	0.93341800	-0.91989400
C	4.56350600	-1.77683700	-0.85128900
H	2.73645500	-2.43457800	0.13196700

H	3.25571000	-1.22673100	-2.50340900
H	4.92507600	-0.70101600	-2.73056300
H	4.67839300	-2.80844500	-1.20041900
H	5.54406700	-1.45708100	-0.47313500
P	2.68601200	-0.05260200	0.06359000
O	1.22637700	-0.02589200	-0.31609000
C	4.15351500	-1.92026800	1.68077200
C	3.08675200	1.53528500	-2.22381600
H	2.92201800	2.48224500	-1.69853700
H	3.69634000	1.73944200	-3.11134400
H	2.11061200	1.16063400	-2.54383200
H	3.40638500	-1.92088500	2.48029300
H	4.66241000	-2.89024800	1.70807300
H	4.89302000	-1.14619900	1.91481600
C	0.39488700	-1.78129700	2.08362900
H	1.35906300	-2.10956700	1.70650600
C	-0.69766100	-1.92546000	1.05843700
C	-0.42550600	-2.13492700	-0.39264200
O	0.71944500	-2.83970900	-0.61013300
C	1.00288700	-3.07801200	-1.99153200
H	0.22193800	-3.69286300	-2.44623600
H	1.06622100	-2.12998300	-2.53219900
H	1.95956500	-3.60349600	-2.01279500
O	-1.17915000	-1.83870100	-1.29633100
C	-1.99421500	-2.07977400	1.40422800
H	-2.71568700	-2.26255800	0.61264200
C	-4.25234300	-0.42714500	2.25536900
C	-3.73466800	-1.38473900	3.13530400
C	-4.34531100	-1.53989300	4.38812000
C	-5.43388800	-0.75241700	4.75611800
C	-5.93795900	0.20592400	3.87287900
C	-5.34515200	0.36298600	2.62089700
H	-3.79929500	-0.29507800	1.27707600
H	-3.95428300	-2.29091700	5.06955300
H	-5.89149900	-0.88689400	5.73269100
H	-6.78809000	0.81965400	4.15760800
H	-5.73330000	1.09888000	1.92169200
C	-2.48781100	-2.19127900	2.81943900
C	-2.59681700	-3.65878100	3.16431700
H	-3.56192000	-4.15012500	3.12997200
C	-1.47167300	-4.37050800	3.46390500

O	-0.22801200	-3.90594700	3.48753400
C	-1.61082600	-5.75334600	3.83096400
C	-1.70589000	-6.92251900	4.15040300
C	-1.82095900	-8.28998200	4.52406000
C	-0.68092800	-9.03075200	4.89476800
C	-3.07597200	-8.93067600	4.53225900
C	-0.79723800	-10.36793800	5.26169300
H	0.28720900	-8.54030800	4.88887000
C	-3.18303900	-10.26856400	4.89960200
H	-3.95643100	-8.36372400	4.24694100
C	-2.04643600	-10.99310000	5.26602600
H	0.09095100	-10.92611200	5.54538400
H	-4.15780100	-10.74885700	4.90041500
H	-2.13351400	-12.03737500	5.55261700
H	-1.69703000	-1.80149700	3.46835700
H	0.03674900	-2.81987100	2.94438300

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C	2.89546700	1.02342900	1.52243300
C	2.03317100	0.97671700	2.64208600
C	2.20081100	1.96507900	3.62885300
C	3.21673200	2.91638800	3.56369600
C	4.11165800	2.89949500	2.50021000
C	3.93338800	1.96462800	1.48455600
H	1.51680200	2.02753800	4.46435800
H	3.30089200	3.66338800	4.34726800
H	4.92130900	3.62070500	2.44331200
H	4.60473100	1.98588600	0.63404600
C	-0.92660300	0.77839200	2.82292000
C	0.62268700	-0.41898000	4.80566700
C	-1.30468100	1.09744300	4.28717100
H	-1.65947800	0.08775900	2.40975300
C	-0.82467300	-0.04366500	5.20109200
H	1.28191100	0.35994400	5.19047600
H	-0.82657200	2.04003900	4.58672700
H	-2.38681500	1.24571300	4.36458000
H	-0.85805500	0.24747700	6.25728400
H	-1.47869000	-0.91437700	5.09765700

P	0.62071100	-0.23374200	2.93978300
C	-0.85171900	1.97972500	1.88150800
C	1.13257300	-1.74960900	5.35937800
H	2.16432100	-1.93943100	5.04093700
H	1.13121800	-1.70085000	6.45495400
H	0.52190100	-2.59815300	5.04588100
H	-0.52831600	1.66637000	0.88484300
H	-1.84478500	2.43670600	1.80476100
H	-0.15493300	2.74048300	2.24833800
C	3.49907800	0.62467000	-1.42647800
C	3.45009000	-1.60924200	0.18653200
C	3.80900700	-0.71238300	-2.12986700
H	4.45757700	1.05106700	-1.10473700
C	4.37869200	-1.64901200	-1.05409300
H	2.66998800	-2.36546500	0.07003800
H	2.88352800	-1.13620500	-2.54124600
H	4.50474500	-0.56720300	-2.96378900
H	4.48457800	-2.67532000	-1.41951400
H	5.38163000	-1.30003400	-0.77101000
P	2.55086200	0.01499400	0.04036000
O	1.05976900	0.03341900	-0.20698900
C	4.19901900	-1.81843200	1.50544200
C	2.71546600	1.64313100	-2.25011400
H	2.58426200	2.58177500	-1.70080100
H	3.23932200	1.86667000	-3.18645000
H	1.72014100	1.25673200	-2.48621000
H	3.52478900	-1.83718100	2.36760100
H	4.72684500	-2.77838900	1.48236000
H	4.94143100	-1.03139800	1.68118800
C	0.43419500	-1.84323600	2.15808000
H	1.40157600	-2.22387400	1.83375000
C	-0.60837100	-1.98455700	1.08403900
C	-0.17420700	-2.25275000	-0.31427300
O	-1.06502800	-1.80988100	-1.22763600
C	-0.69888700	-2.04386600	-2.58995500
H	0.20942700	-1.48401900	-2.83158300
H	-0.52472100	-3.10724700	-2.77386500
H	-1.53747700	-1.68184600	-3.18629400
O	0.82575600	-2.87633600	-0.62879600
C	-1.92188900	-2.13245700	1.36070500
H	-2.60764300	-2.32982900	0.54192700

C	-4.18466000	-0.42536000	2.07184000
C	-3.73778300	-1.38415700	2.98872300
C	-4.41810200	-1.51014800	4.20834300
C	-5.50757900	-0.69506400	4.50719200
C	-5.94183800	0.26282700	3.58698100
C	-5.27786200	0.39254500	2.36806000
H	-3.67125700	-0.31154200	1.12134300
H	-4.08033400	-2.25992900	4.91887400
H	-6.02013800	-0.80705100	5.45901600
H	-6.79231800	0.89819700	3.81822900
H	-5.60966900	1.12982900	1.64174900
C	-2.49170300	-2.21783700	2.75076900
C	-2.63534600	-3.67415100	3.12311100
H	-3.59827000	-4.16411900	3.04066600
C	-1.53364900	-4.37530200	3.51854000
O	-0.29535100	-3.90358600	3.60695600
C	-1.69263300	-5.74731700	3.91552500
C	-1.80436200	-6.90720000	4.26213800
C	-1.93636400	-8.26473500	4.66529300
C	-0.81202700	-8.99741800	5.09523800
C	-3.19212600	-8.90353600	4.64329100
C	-0.94432000	-10.32516800	5.48991700
H	0.15670600	-8.50846800	5.11217400
C	-3.31519200	-10.23199400	5.03882200
H	-4.06048000	-8.34272000	4.31234300
C	-2.19410500	-10.94863700	5.46383300
H	-0.06810300	-10.87733200	5.81891700
H	-4.29027300	-10.71110400	5.01571000
H	-2.29359400	-11.98560800	5.77210300
H	-1.72911000	-1.82808500	3.43055200
H	0.00812400	-2.84627700	3.03312300

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C	-1.80408000	1.58739600	1.09031800
C	-0.96269000	1.49097300	2.22390600
C	-0.83479400	2.62104800	3.05147700
C	-1.40996900	3.84358900	2.71062500
C	-2.11764300	3.96864200	1.51905700
C	-2.33617900	2.83589000	0.73953400

H	-0.29059700	2.55289900	3.98163900
H	-1.28146000	4.69501200	3.37154000
H	-2.53260100	4.92575600	1.21825600
H	-2.95538300	2.92116500	-0.14813100
C	0.83238100	-1.25902100	1.68965500
C	-0.95331600	-1.09297900	3.82688200
C	0.24266900	-2.58024400	2.23644300
H	1.88515800	-1.16981000	2.01105600
C	-0.14345000	-2.40043800	3.71252400
H	-1.88031200	-1.21319300	3.25759100
H	-0.64347100	-2.84417100	1.65540800
H	0.99185700	-3.37016800	2.11696800
H	-0.73771200	-3.24401600	4.08101400
H	0.75567500	-2.33690700	4.33973200
P	0.04612400	0.05007800	2.77379500
C	0.83519900	-1.16940900	0.16714400
C	-1.25465600	-0.61491900	5.24426400
H	-1.74241000	0.36623900	5.24713700
H	-1.93073500	-1.32456300	5.73379000
H	-0.35035800	-0.54692100	5.85653900
H	1.12239000	-0.17966000	-0.19436900
H	1.58935000	-1.87144400	-0.20544000
H	-0.13224300	-1.44575800	-0.24836200
C	-4.30813900	0.34808300	0.10075100
C	-2.11992100	0.15408300	-1.58552700
C	-4.59136700	-0.18823600	-1.31581000
H	-4.52791600	1.42235800	0.11400400
C	-3.50434000	0.38635700	-2.23750000
H	-1.79820300	-0.87456300	-1.79367900
H	-4.53827100	-1.28511700	-1.30902100
H	-5.59896300	0.08474100	-1.64802600
H	-3.53761400	-0.05195300	-3.24049300
H	-3.66497500	1.46684800	-2.35719400
P	-2.47351500	0.11670600	0.24177900
O	-2.10098400	-1.14654400	0.98065800
C	-1.04509400	1.13295200	-2.05904900
C	-5.06163800	-0.34721900	1.23254000
H	-4.84020500	0.11738100	2.19950600
H	-6.14313400	-0.28599500	1.06722600
H	-4.77603500	-1.40095800	1.29576700
H	-0.07603400	0.95440200	-1.59077400

H	-0.91216300	1.04433300	-3.14284600
H	-1.31896200	2.16913900	-1.84469200
C	1.44668500	0.69813800	3.82329400
H	1.12663400	0.59283800	4.85856800
C	2.02943000	2.08113200	3.61712600
C	2.03212600	3.03475800	4.74053100
O	1.22330900	2.61882800	5.77239400
C	1.16942900	3.51338000	6.88917000
H	0.78682200	4.49152400	6.58460000
H	0.49769500	3.04471200	7.60976500
H	2.16411200	3.64743900	7.32182000
O	2.61400400	4.10305500	4.78468100
C	2.61044800	2.49546500	2.46571800
H	3.05827100	3.48583600	2.46048500
C	1.31754600	3.42206100	0.02631100
C	2.27988300	2.40656200	-0.03395600
C	2.76778900	2.02033200	-1.28851800
C	2.30820300	2.63641900	-2.45249600
C	1.35682500	3.65675500	-2.38076100
C	0.86249600	4.04633000	-1.13515800
H	0.92449100	3.72735000	0.99118000
H	3.51982300	1.23750000	-1.33159800
H	2.70081500	2.32616200	-3.41738400
H	1.00757100	4.14477000	-3.28678300
H	0.12156800	4.83894700	-1.06460400
C	2.74163400	1.68552500	1.22132600
C	4.16806200	1.20199400	1.21592300
H	4.93591400	1.83112600	0.78000500
C	4.50212600	0.01687000	1.85631300
O	3.71045100	-0.76694400	2.49866300
C	5.89846000	-0.38015700	1.75403400
C	7.05595800	-0.74932900	1.69190300
C	8.41061200	-1.17700700	1.61662800
C	8.80124900	-2.42460700	2.14337500
C	9.39097800	-0.36371800	1.01343600
C	10.12691300	-2.84079300	2.06653900
H	8.04960800	-3.05348400	2.60972800
C	10.71483000	-0.78658800	0.94165400
H	9.09525100	0.59833400	0.60702900
C	11.08968700	-2.02565600	1.46646600
H	10.41155700	-3.80579900	2.47757300

H	11.45851800	-0.14677600	0.47395300
H	12.12401000	-2.35321400	1.40874000
H	2.12488800	0.79149100	1.32942000
H	2.25638300	-0.01968100	3.61651500

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C	-4.29763200	4.63356900	2.45719000
C	-2.95865500	4.48795800	2.03889200
C	-2.41743800	5.47546100	1.19249800
C	-3.16597400	6.56730800	0.77011000
C	-4.47853900	6.72591200	1.21112500
C	-5.02544600	5.76793100	2.05419800
H	-1.37533100	5.43041600	0.90641100
H	-2.70785200	7.30846300	0.12271400
H	-5.06490100	7.58885500	0.91078400
H	-6.04049300	5.90386200	2.41343200
C	-2.20088700	1.59336900	1.49987300
C	-1.54942400	2.33808700	4.13619600
C	-2.20392800	0.47135400	2.56350700
H	-1.33404900	1.45878700	0.84079500
C	-1.26177800	0.87591300	3.70352200
H	-2.53002200	2.36726400	4.60842200
H	-3.21952000	0.36149200	2.94843700
H	-1.89678700	-0.47812200	2.11195900
H	-1.38499200	0.22366200	4.57470900
H	-0.21395100	0.78621500	3.39498800
P	-1.77165800	3.13381600	2.46500000
C	-3.46216000	1.65012300	0.63928600
C	-0.46780500	2.89642900	5.05970400
H	-0.71844000	3.89357600	5.42308800
H	-0.40038300	2.22654700	5.92611600
H	0.51852400	2.93519700	4.58860000
H	-3.44145200	2.48452200	-0.06956000
H	-3.55175600	0.72172100	0.06394300
H	-4.34841500	1.74279100	1.27002200
C	-5.56477900	4.40796400	5.10290800
C	-6.93508100	3.23560700	3.01174700
C	-7.06118200	4.11196400	5.33552400
H	-5.45362700	5.47306000	4.86180700

C	-7.76190100	4.12291900	3.96447200
H	-7.08682900	2.18899900	3.31260600
H	-7.16770800	3.11965800	5.79360600
H	-7.50265800	4.83577600	6.02882000
H	-8.79510800	3.76466100	4.03098600
H	-7.80794400	5.15014000	3.57723400
P	-5.17238600	3.46797700	3.55226700
O	-4.43293000	2.16506300	3.72590600
C	-7.25709600	3.35635700	1.52281400
C	-4.63184900	4.04172500	6.25658400
H	-3.59563300	4.31754600	6.03335600
H	-4.92961500	4.56427000	7.17228400
H	-4.65633500	2.96484100	6.44890500
H	-6.62169300	2.69549300	0.92436700
H	-8.29963800	3.07261000	1.34086500
H	-7.11892100	4.37534800	1.15182300
C	-0.13258700	3.55495700	1.78653200
H	0.37321400	2.58291700	1.85789500
C	0.76193200	4.61263600	2.39488100
C	0.33938900	5.59882100	3.33581100
O	-1.03398500	5.49262100	3.62468700
C	-1.56724900	6.48414700	4.49091700
H	-2.65473900	6.41408600	4.39531700
H	-1.26965500	6.30113200	5.52958100
H	-1.22025100	7.47892600	4.20265300
O	0.99594200	6.47500200	3.88308500
C	2.14984900	4.40175000	2.29458300
H	2.75041100	5.17660600	2.75739200
C	4.49659400	4.76187900	-0.46627100
C	4.18037000	4.21974800	0.78129100
C	5.18358400	4.14196800	1.75828400
C	6.46920500	4.60296800	1.48793200
C	6.77817600	5.14111800	0.23494300
C	5.78784900	5.21835000	-0.74256000
H	3.72422900	4.82816900	-1.22988500
H	4.93897300	3.72287700	2.72977900
H	7.23539400	4.54143700	2.25642900
H	7.78310100	5.49776700	0.02542500
H	6.01621500	5.63592200	-1.71996300
C	2.78082900	3.70067400	1.07823800
C	2.77479400	2.21991200	1.38182400

H	2.88985700	1.45361100	0.62633100
C	2.65828400	1.99294300	2.71806100
O	2.56544900	3.03455900	3.53354900
C	2.50978300	0.68977900	3.29155800
C	2.27050000	-0.37902600	3.82050600
C	1.93382100	-1.60935100	4.44841500
C	1.29894500	-1.60824800	5.70714800
C	2.20169400	-2.84347400	3.82479400
C	0.94311300	-2.80677900	6.31762500
H	1.09582200	-0.65748300	6.18993300
C	1.84383200	-4.03739600	4.44399300
H	2.69151000	-2.84803800	2.85626300
C	1.21310600	-4.02551500	5.69021500
H	0.45507700	-2.79115600	7.28834600
H	2.05820500	-4.98235100	3.95234200
H	0.93546000	-4.95965000	6.17010700
H	2.15339000	3.91274600	0.20039300
H	-0.30483600	3.67868000	0.70305300

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C	1.67091500	-0.09422500	7.46765500
C	1.50832300	0.56093800	6.22444400
C	2.65041700	0.80369800	5.44751000
C	3.92245500	0.43534700	5.88267100
C	4.08522300	-0.18538900	7.11549200
C	2.95967100	-0.44124100	7.89699900
H	2.60791800	1.32510300	4.50362700
H	4.76486900	0.65990200	5.23638100
H	5.07097700	-0.46920900	7.47239700
H	3.09292100	-0.91592100	8.86333300
C	-1.70737600	1.75621300	5.96740200
C	-0.76425000	-0.54803000	4.72494700
C	-2.74011400	0.66348700	5.61121500
H	-1.79013800	2.58366700	5.25290900
C	-2.23023700	-0.18114900	4.43290700
H	-0.75123800	-1.21544700	5.59189000
H	-2.87062400	0.02265500	6.48543000
H	-3.70298000	1.13512100	5.38254200
H	-2.83513000	-1.08486000	4.29765500

H	-2.29142000	0.38562900	3.49343800
P	-0.06363300	1.04167000	5.38408700
C	-1.89973400	2.34348700	7.35971100
C	-0.00127700	-1.18475200	3.56328500
H	1.06431300	-1.30372000	3.78760900
H	-0.41025500	-2.17917800	3.35141000
H	-0.08267700	-0.59357700	2.64571300
H	-1.13778600	3.09144100	7.57484900
H	-2.88161100	2.83266700	7.38949900
H	-1.89101900	1.55662400	8.11161800
C	0.59838500	-1.89482400	9.64229300
C	0.30000200	0.85010200	9.92411400
C	0.20385100	-1.38097300	11.04299500
H	1.67395200	-2.10411600	9.64324000
C	0.73934000	0.05421800	11.17300500
H	-0.75380200	1.13468900	10.03878700
H	-0.89077500	-1.37923500	11.13369500
H	0.59143100	-2.03939900	11.82810600
H	0.39442500	0.54216100	12.09114400
H	1.83708800	0.03130900	11.21745000
P	0.26507200	-0.42136800	8.56615500
O	-1.02361600	-0.53101800	7.78360900
C	1.14036200	2.09744200	9.63641000
C	-0.16032100	-3.13221400	9.16317000
H	0.20838600	-3.47097700	8.18940700
H	-0.03884200	-3.95444000	9.87743300
H	-1.22680200	-2.91552200	9.05608600
H	0.86659700	2.57873300	8.69331600
H	1.01865400	2.82585000	10.44640400
H	2.20334200	1.84099900	9.57331300
C	0.36133000	1.98893400	3.85979000
H	0.84620900	1.28893200	3.17570600
C	1.22240800	3.22084300	4.02235900
C	1.32781100	3.74898900	5.32973000
O	2.15382300	4.81741900	5.48766300
C	2.31734000	5.27703900	6.82798200
H	2.74763400	4.49475100	7.46148700
H	2.99960100	6.12626800	6.76376500
H	1.36148200	5.59051800	7.25833600
O	0.71569700	3.27849500	6.31962600
C	2.09197200	3.60542500	2.98788300

H	2.68130700	4.49321500	3.18288100
C	3.72196800	4.60928900	0.54426500
C	2.33368400	4.41740800	0.59715000
C	1.51315600	5.20934300	-0.20908600
C	2.06034900	6.17563500	-1.05693200
C	3.44066500	6.36306200	-1.10094200
C	4.26903700	5.57694100	-0.29431800
H	4.36100700	3.99550500	1.17199700
H	0.43487000	5.06886000	-0.17348300
H	1.40655700	6.78120400	-1.67936000
H	3.87018700	7.11501900	-1.75740000
H	5.34647200	5.71776800	-0.32246800
C	1.74071500	3.35348900	1.51054600
C	2.23376900	1.96343400	1.17519300
H	1.86759600	1.38844700	0.33480200
C	3.19444600	1.55498700	2.04312600
O	3.56724600	2.38529500	3.01514300
C	3.73828000	0.23110500	2.07952600
C	4.15315300	-0.89943300	2.24980500
C	4.61077000	-2.22890800	2.46945300
C	4.76197900	-2.71587200	3.78336900
C	4.90720700	-3.08306900	1.38985600
C	5.19897200	-4.01823300	4.00454400
H	4.52689800	-2.06155700	4.61680600
C	5.34413200	-4.38404100	1.62138700
H	4.79140500	-2.71064800	0.37707700
C	5.49237200	-4.85741500	2.92705500
H	5.31059900	-4.38155100	5.02267300
H	5.57067300	-5.03199200	0.77918000
H	5.83380000	-5.87345000	3.10346600
H	0.64721800	3.39913300	1.41193500
H	-0.62375100	2.19917500	3.41563800

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C	-4.22645500	4.53197800	2.26885400
C	-2.91752300	4.25998100	1.82461400
C	-2.38142500	5.07408400	0.81030600
C	-3.10812100	6.12212900	0.25489300
C	-4.38807500	6.41052800	0.72209900

C	-4.92794600	5.62285400	1.73129200
H	-1.36206200	4.93198100	0.47884000
H	-2.65623100	6.72814400	-0.52448900
H	-4.95434200	7.24219200	0.31419300
H	-5.91260600	5.86508700	2.11723300
C	-2.26572400	1.34547800	1.51866900
C	-1.51068500	2.16616500	4.09814200
C	-2.29780700	0.27842800	2.63320000
H	-1.41691300	1.13802300	0.85407800
C	-1.28662000	0.68319300	3.70930100
H	-2.47055400	2.24369600	4.60349800
H	-3.30139000	0.25652100	3.06505100
H	-2.07529900	-0.71186100	2.22087000
H	-1.38801100	0.06897300	4.61049200
H	-0.25726200	0.54539300	3.35563200
P	-1.77289700	2.92183500	2.40188400
C	-3.54324300	1.40938300	0.68240400
C	-0.38366800	2.71791000	4.96874800
H	-0.62937500	3.70430500	5.36115500
H	-0.26426600	2.03119800	5.81647300
H	0.58203600	2.77936800	4.45846800
H	-3.49416600	2.18374400	-0.08996900
H	-3.70243200	0.44584900	0.18468600
H	-4.40640400	1.60671000	1.32263700
C	-5.01494000	4.75385500	5.06547400
C	-6.86339800	3.51130500	3.44474300
C	-6.45240900	4.65083000	5.61312500
H	-4.88205000	5.75755900	4.64048400
C	-7.40365600	4.59236100	4.40225800
H	-7.03604600	2.53405900	3.91877800
H	-6.55545400	3.73302500	6.20748400
H	-6.68245600	5.49193300	6.27602100
H	-8.43427700	4.36941600	4.70010100
H	-7.42181700	5.56833300	3.89745400
P	-5.01675800	3.60050600	3.61428100
O	-4.38941200	2.23866100	3.79158500
C	-7.47057800	3.46496700	2.04311700
C	-3.88230400	4.47434700	6.05153600
H	-2.90979600	4.65390900	5.58180400
H	-3.96494200	5.13137500	6.92477600
H	-3.91180700	3.43694000	6.39980100

H	-7.00125300	2.68410500	1.43541400
H	-8.54128500	3.24075100	2.10617200
H	-7.36175200	4.41229300	1.50903300
C	-0.12468200	3.24896100	1.69353600
H	0.42381000	2.32566700	1.91685900
C	0.65664200	4.44196400	2.19662600
C	0.01976500	5.32264400	3.12619200
O	0.76730100	6.38206900	3.52696100
C	0.17759200	7.20881700	4.52995700
H	-0.00835700	6.64039900	5.44641900
H	0.90458300	7.99983100	4.71948600
H	-0.76804800	7.63463200	4.18172200
O	-1.13959900	5.17562600	3.56316900
C	2.03564600	4.44722200	2.05303700
H	2.56631700	5.29235600	2.47211500
C	4.44323400	4.70757100	-0.62356900
C	4.12908200	4.25218200	0.65861200
C	5.10262400	4.33752400	1.66515100
C	6.35722700	4.87365300	1.38736800
C	6.66517000	5.32441700	0.09983800
C	5.70472600	5.23805200	-0.90622300
H	3.69398500	4.64529900	-1.41039000
H	4.85578000	3.98250400	2.66128000
H	7.10154100	4.93751500	2.17702400
H	7.64678600	5.73848400	-0.11478900
H	5.93319300	5.58438500	-1.91109300
C	2.76276800	3.65510600	0.96730500
C	2.84403500	2.21363600	1.42246200
H	2.96547600	1.39046200	0.72975300
C	2.76717300	2.08441300	2.77953200
O	2.66097000	3.14650700	3.54250100
C	2.64470700	0.79555000	3.40839100
C	2.39866600	-0.24603600	3.98707200
C	2.05416200	-1.44443100	4.67042000
C	1.37020800	-1.38272200	5.90188000
C	2.35975500	-2.70823300	4.12882000
C	1.00339500	-2.54988700	6.56448400
H	1.13752500	-0.40923300	6.32208200
C	1.99115300	-3.87058800	4.79983500
H	2.88687200	-2.76035000	3.18146000
C	1.31131200	-3.79823100	6.01784600

H	0.47673400	-2.48644400	7.51291600
H	2.23527900	-4.83850000	4.37048100
H	1.02488800	-4.70783900	6.53808700
H	2.15724600	3.71668700	0.04988900
H	-0.24227400	3.23462600	0.59999200

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C	-1.79626800	1.22399000	0.65672100
C	-0.95786100	1.47136100	1.77138800
C	-0.71153100	2.80869900	2.13833200
C	-1.26172400	3.87271100	1.42981300
C	-2.06868200	3.62850800	0.32530900
C	-2.32971400	2.31330000	-0.04840900
H	-0.02606500	3.03009800	2.94742800
H	-1.01154000	4.88653700	1.72049500
H	-2.48274800	4.45041100	-0.25019400
H	-2.95626900	2.13233300	-0.91635600
C	0.98977200	-1.14292100	2.34596500
C	-1.38550500	-0.79991300	3.80319600
C	0.35601700	-2.39852700	3.00281200
H	1.92063600	-0.85043100	2.85128200
C	-0.51493100	-2.00858400	4.20796200
H	-2.09617400	-1.13288100	3.04474600
H	-0.27204000	-2.88903500	2.25587600
H	1.15334300	-3.09034300	3.29368400
H	-1.15511900	-2.84112400	4.52002400
H	0.10986400	-1.74516700	5.07104500
P	-0.16150100	0.23229700	2.87410000
C	1.32028900	-1.36932000	0.87213700
C	-2.11318800	-0.10468000	4.95171800
H	-2.64538900	0.79061300	4.61108400
H	-2.85486300	-0.78905900	5.37865100
H	-1.43196200	0.18807200	5.75607600
H	1.76198800	-0.48926400	0.40360500
H	2.08129000	-2.15616400	0.81980200
H	0.43970900	-1.70296700	0.32398400
C	-4.01273200	-0.46917400	-0.39902600
C	-1.57396500	-0.59727300	-1.71053000
C	-4.02184400	-1.06000700	-1.82465200

H	-4.37280800	0.56513100	-0.44509700
C	-2.83441300	-0.45202700	-2.58965700
H	-1.24599500	-1.64551100	-1.74158000
H	-3.90233700	-2.15004300	-1.76542100
H	-4.97688100	-0.86743200	-2.32516500
H	-2.68577400	-0.92887700	-3.56453500
H	-3.02404800	0.61287400	-2.78364600
P	-2.20695400	-0.43751200	0.03111300
O	-1.77837300	-1.53535500	0.97472400
C	-0.40544700	0.30629600	-2.10426900
C	-4.82841600	-1.24787800	0.63276100
H	-4.81857600	-0.74761300	1.60700100
H	-5.87124900	-1.33512500	0.30795400
H	-4.42076800	-2.25321400	0.77171700
H	0.46130100	0.14348700	-1.45804300
H	-0.09989500	0.09757300	-3.13554100
H	-0.67644300	1.36442300	-2.03966900
C	0.68971700	1.15806500	4.20113700
H	-0.10284500	1.70455100	4.72273200
C	1.88031500	2.05800500	3.96411400
C	2.29386400	2.85629200	5.09772500
O	1.46326400	2.68268700	6.19191900
C	1.78384100	3.50286400	7.31404700
H	1.72734900	4.56482400	7.05521200
H	1.04529200	3.25926700	8.08114100
H	2.79358700	3.29208900	7.67801000
O	3.22238000	3.65801300	5.14296500
C	2.77247300	2.01613500	2.89361200
H	3.64729200	2.63684000	3.07205200
C	2.19891800	4.50351800	1.51824500
C	2.08083900	3.29759900	0.81630000
C	1.57378700	3.33033900	-0.48998800
C	1.18319800	4.52812400	-1.08216200
C	1.29680200	5.72636100	-0.37254800
C	1.81032300	5.70735500	0.92425800
H	2.57821900	4.50826700	2.53497800
H	1.47331500	2.39807800	-1.03963000
H	0.78831700	4.52833200	-2.09511400
H	0.99405600	6.66489700	-0.82920100
H	1.91041300	6.63413800	1.48323800
C	2.42874300	1.94286300	1.41514600

C	3.57167100	1.23720700	0.73653400
H	3.83145800	1.36846300	-0.30512800
C	4.18712000	0.38151300	1.60110400
O	3.77399700	0.34780300	2.85773800
C	5.23788200	-0.50553200	1.20275700
C	6.10753100	-1.29316600	0.88331200
C	7.12762300	-2.20869900	0.50412000
C	7.71882300	-3.05913800	1.45962500
C	7.56525200	-2.28477300	-0.83314000
C	8.71462900	-3.95579700	1.08473800
H	7.38582400	-3.00061000	2.49086100
C	8.56224600	-3.18386900	-1.19899300
H	7.11364100	-1.62959200	-1.57131000
C	9.14077900	-4.02304100	-0.24388800
H	9.16217100	-4.60455600	1.83276200
H	8.89064300	-3.23007300	-2.23381500
H	9.91934900	-4.72347600	-0.53266300
H	1.51158100	1.33660200	1.29447900
H	0.96272500	0.34140200	4.88902900

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C	2.77752800	1.14974300	1.43067700
C	2.64913900	0.51864000	2.69060800
C	3.59085500	0.83340400	3.68369200
C	4.61016800	1.75782900	3.45682300
C	4.70928100	2.39907500	2.22586500
C	3.79675400	2.08507200	1.22147200
H	3.54430800	0.35645400	4.65305400
H	5.32082400	1.97433800	4.24853200
H	5.49301500	3.12788200	2.04348600
H	3.88573200	2.57031700	0.25366800
C	-0.34350500	0.14745600	3.30261800
C	1.48160400	-1.02792000	4.94641900
C	-0.89264200	-0.30465700	4.69053700
H	-0.96907500	-0.20158300	2.48413000
C	0.03077300	-1.34631900	5.34749300
H	1.74218200	-0.06290000	5.40019100
H	-0.96278100	0.57987800	5.33460700
H	-1.90530600	-0.70187500	4.57552200

H	-0.06286200	-1.32396200	6.43903100
H	-0.23631600	-2.36377300	5.03765800
P	1.31558100	-0.69038800	3.12029200
C	-0.21766900	1.67202800	3.21613100
C	2.48098400	-2.10043800	5.38967700
H	3.48106600	-1.95173800	4.96825900
H	2.57039800	-2.08262500	6.48136900
H	2.13801300	-3.10086100	5.10914200
H	0.14608500	1.99370000	2.24131100
H	-1.20713500	2.11542500	3.37319500
H	0.45371400	2.06994200	3.98551200
C	1.10791400	2.21129400	-0.85056300
C	2.72767900	0.01751300	-1.33974700
C	1.31227500	1.82244200	-2.32947700
H	1.79838100	3.03031600	-0.60818500
C	2.66343500	1.10357500	-2.43439800
H	2.16447500	-0.87091500	-1.64708800
H	0.50464500	1.14530400	-2.63842400
H	1.25864500	2.70520800	-2.97598900
H	2.81945400	0.66188500	-3.42446800
H	3.47552500	1.82826400	-2.27865000
P	1.68735900	0.68868800	0.04489300
O	0.57240800	-0.17630000	0.58971400
C	4.14517300	-0.43254400	-0.98524100
C	-0.32521600	2.61377600	-0.50275300
H	-0.39540200	3.04459600	0.49967900
H	-0.68805000	3.36417200	-1.21424700
H	-0.99176400	1.74703900	-0.54152100
H	4.12245300	-1.21958200	-0.23104800
H	4.62402200	-0.84759800	-1.87905700
H	4.76226600	0.39917300	-0.63021100
C	1.62274700	-2.33776600	2.29739600
H	2.59948000	-2.18883500	1.82673500
C	0.73785700	-3.04045700	1.31801600
C	1.33111300	-3.28870000	0.02626600
O	0.57159100	-4.08113700	-0.78302400
C	1.14247100	-4.37940200	-2.05416100
H	1.24457600	-3.47387000	-2.66196200
H	2.12908700	-4.83941300	-1.94681900
H	0.44871300	-5.07338300	-2.53161200
O	2.40304800	-2.82394900	-0.37265500

C	-0.37358500	-3.72432100	1.74977700
H	-0.77949100	-4.48486500	1.09098500
C	-2.48202300	-1.73844600	0.96858900
C	-2.60634400	-2.72385000	1.96182900
C	-3.86512500	-3.28302100	2.19840900
C	-4.98293500	-2.85005300	1.48188100
C	-4.85621000	-1.85503700	0.51267300
C	-3.59859900	-1.30484100	0.25554900
H	-1.50127000	-1.33401700	0.73326700
H	-3.96126400	-4.06815100	2.94108400
H	-5.95456500	-3.29484500	1.68146900
H	-5.72707000	-1.51767400	-0.04326400
H	-3.48364100	-0.54167400	-0.51065500
C	-1.36630900	-3.15705100	2.74504700
C	-1.58532800	-4.07547300	3.90704700
H	-2.41353300	-3.95242400	4.59404400
C	-0.55383400	-4.95502800	4.12502400
O	0.45647700	-5.04612800	3.31582300
C	-0.56788800	-5.79000500	5.30551200
C	-0.52977700	-6.48787600	6.30097000
C	-0.49168900	-7.30268500	7.46634100
C	0.57898200	-8.19264000	7.68601300
C	-1.52110100	-7.23644200	8.42670600
C	0.61505500	-8.98634400	8.82846500
H	1.37235700	-8.24870200	6.94755500
C	-1.47771200	-8.03401100	9.56626000
H	-2.34892500	-6.55415800	8.26095400
C	-0.41096500	-8.91166900	9.77357500
H	1.44711500	-9.66833300	8.98226200
H	-2.28036100	-7.97183400	10.29636200
H	-0.38020900	-9.53360000	10.66386500
H	-0.92052500	-2.21982000	3.10212300
H	1.74179900	-3.01599100	3.14706600

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C	-2.36319700	1.78047700	1.30605300
C	-1.04206600	1.71479000	1.80426000
C	-0.48284500	2.88777000	2.34426900
C	-1.19746100	4.07772400	2.41774500

C	-2.49946300	4.13905300	1.92866700
C	-3.06307300	2.99824500	1.37126200
H	0.54053900	2.88759400	2.68724500
H	-0.72536400	4.95722800	2.84458700
H	-3.06675300	5.06395100	1.97051000
H	-4.06781200	3.06001200	0.96610800
C	0.56076800	-0.95753900	0.58315600
C	-0.77932800	-1.02454900	3.03727000
C	0.06148500	-2.33560000	1.08250700
H	1.65383300	-0.92453700	0.69977900
C	-0.05838300	-2.32374900	2.61653500
H	-1.81422500	-1.08499100	2.69508300
H	-0.91490500	-2.53933500	0.64060300
H	0.77108900	-3.10347700	0.76197000
H	-0.61451600	-3.19593900	2.97737900
H	0.93751100	-2.36979400	3.07284800
P	0.03182500	0.21449900	1.92892000
C	0.21720800	-0.63987000	-0.86711300
C	-0.73189100	-0.69933100	4.52997800
H	-1.23446200	0.24911000	4.75300200
H	-1.24417700	-1.48746300	5.09348200
H	0.29248700	-0.63520500	4.90935600
H	0.54231700	0.36913400	-1.12964100
H	0.74833800	-1.34962000	-1.51200300
H	-0.85311100	-0.75081000	-1.04667600
C	-5.00638100	0.42848000	0.88541700
C	-3.42722800	0.92906100	-1.34013300
C	-5.70663000	0.37985500	-0.48963300
H	-5.24439800	1.38340200	1.36738400
C	-4.92311400	1.29270900	-1.44827600
H	-3.25625600	-0.01508000	-1.87549200
H	-5.68876100	-0.65132300	-0.86690300
H	-6.75855800	0.67425500	-0.40729700
H	-5.27469200	1.20088700	-2.48181400
H	-5.06452400	2.34310200	-1.15790900
P	-3.20477100	0.41635300	0.43342700
O	-2.53597400	-0.91927300	0.63249400
C	-2.46217700	1.99080300	-1.86864200
C	-5.35670300	-0.71966900	1.83211800
H	-4.86812400	-0.59571000	2.80437400
H	-6.43898500	-0.76008400	1.99933500

H	-5.03022400	-1.67765900	1.41791100
H	-1.41878400	1.69648700	-1.72441500
H	-2.62674000	2.14887200	-2.94047100
H	-2.60839700	2.94880700	-1.36028300
C	1.57878400	0.64350400	2.82366100
H	1.33681500	1.34431300	3.62941400
C	2.76107200	1.03866200	1.97293000
C	2.50030300	1.75879700	0.76803900
O	3.60412400	2.14870600	0.07118300
C	3.34674700	2.74100500	-1.20104800
H	2.71526200	3.62861900	-1.10241300
H	4.32532400	3.01226000	-1.60071600
H	2.85153100	2.03119300	-1.87151700
O	1.36121700	2.02422200	0.34060900
C	3.98254100	0.40406500	2.16457700
H	4.78113400	0.70834500	1.50110100
C	4.34969500	2.02487500	4.74093400
C	3.96805300	0.67659600	4.69183600
C	3.15914800	0.18306300	5.72010500
C	2.73199000	1.01140500	6.76124300
C	3.10952800	2.35259000	6.79125000
C	3.92498400	2.85657900	5.77415500
H	4.97342400	2.42740400	3.94706400
H	2.84425800	-0.85490300	5.69594200
H	2.10181600	0.60390400	7.54771500
H	2.77773600	2.99915400	7.59913000
H	4.22965700	3.89990400	5.78681400
C	4.42866700	-0.18824100	3.51877100
C	3.99437900	-1.63094300	3.56400500
H	4.03115200	-2.22958800	4.46485400
C	3.71940800	-2.14488600	2.32933100
O	3.79818400	-1.38507800	1.26295700
C	3.27408500	-3.50106100	2.16084700
C	2.83684200	-4.62087300	1.97683600
C	2.29585200	-5.91832400	1.76125500
C	1.81897400	-6.28975600	0.48819100
C	2.21131300	-6.85000000	2.81463600
C	1.27368200	-7.55294000	0.28064100
H	1.88569200	-5.57509300	-0.32599500
C	1.66619100	-8.11180300	2.59762700
H	2.57818600	-6.56748000	3.79628400

C	1.19460400	-8.46902000	1.33223700
H	0.90963600	-7.82510700	-0.70631300
H	1.60852900	-8.82045700	3.41934000
H	0.76932200	-9.45480700	1.16658500
H	5.53131400	-0.13857400	3.51882100
H	1.82148700	-0.29786100	3.32284800

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C	-2.22127100	1.39725700	0.88367300
C	-0.82793700	1.25138500	1.07295500
C	-0.01823100	2.39109400	0.96386900
C	-0.54632600	3.65795700	0.72792100
C	-1.92040600	3.81056300	0.59051500
C	-2.73826200	2.68425200	0.66829000
H	1.04524200	2.34388900	1.11894100
H	0.14296900	4.49478800	0.70812200
H	-2.36049400	4.79065300	0.43166700
H	-3.81063200	2.81442600	0.57101600
C	0.88032700	-0.92105900	-0.02267100
C	-0.47312100	-1.82026700	2.21869300
C	-0.01031700	-2.15297500	-0.25641700
H	1.88378600	-1.26929100	0.26594100
C	-0.17401600	-2.85485100	1.09891300
H	-1.54845100	-1.69634200	2.29911700
H	-0.99181300	-1.83768400	-0.62200800
H	0.43794600	-2.81656100	-1.00484800
H	-0.97785000	-3.59564100	1.06833800
H	0.75624400	-3.38319800	1.34749500
P	0.18386400	-0.21385900	1.54438100
C	1.00306600	0.04495300	-1.19958900
C	0.10771100	-2.22293800	3.57603200
H	-0.09766800	-1.46753500	4.33518300
H	-0.36153400	-3.16460900	3.88410500
H	1.18829100	-2.39939900	3.53330000
H	1.64782400	0.89849700	-0.96828000
H	1.43338000	-0.47419500	-2.06296800
H	0.02325700	0.43394000	-1.49337500
C	-4.40641800	0.32567500	2.51496300
C	-4.86765600	0.35729700	-0.20142700

C	-5.87803400	0.24458500	2.05995300
H	-4.19153100	1.35911200	2.81596700
C	-5.98820200	0.93222900	0.68625900
H	-5.13267700	-0.68579800	-0.42779800
H	-6.17187600	-0.80949400	1.96519200
H	-6.54414700	0.69850100	2.80196400
H	-6.97048600	0.77278100	0.22702000
H	-5.86447200	2.01784100	0.80099700
P	-3.44213300	0.04642900	0.95125400
O	-2.84388800	-1.32300200	0.74016000
C	-4.60235000	1.06731900	-1.52813300
C	-4.00457600	-0.62176900	3.64416400
H	-2.97804400	-0.42217300	3.96514700
H	-4.66684500	-0.48722300	4.50762200
H	-4.07432400	-1.66547300	3.32029200
H	-3.78050500	0.58918700	-2.07150300
H	-5.49466000	1.02021500	-2.16274500
H	-4.34398400	2.12072300	-1.39525400
C	1.64326900	0.36422200	2.49805700
H	2.05682600	-0.55613800	2.92775400
C	1.40961300	1.44083200	3.52978300
C	0.09244300	1.49766200	4.09461900
O	-0.13236300	2.48938200	4.98713500
C	-1.47273300	2.58643500	5.47212800
H	-1.76616500	1.67502800	6.00102200
H	-1.47516300	3.43883300	6.15260700
H	-2.17123200	2.75668900	4.64699300
O	-0.81412700	0.69573900	3.79640700
C	2.36774500	2.39331000	3.80327900
H	2.09675300	3.14444900	4.53462400
C	4.34069400	0.74054200	5.55448600
C	4.33501300	0.88402900	4.15975500
C	4.72315600	-0.21247200	3.38282900
C	5.09566400	-1.41981200	3.97935900
C	5.08631500	-1.55091600	5.36697800
C	4.70847300	-0.46080500	6.15492500
H	4.04700900	1.58515100	6.17356300
H	4.72945800	-0.12132000	2.30171900
H	5.39750900	-2.25694100	3.35490100
H	5.37680600	-2.48896100	5.83196300
H	4.70259100	-0.54735600	7.23825400

C	3.87376800	2.20708000	3.55392300
C	4.15228400	2.39465400	2.08545300
H	5.00530600	1.95895900	1.58205400
C	3.26125500	3.24209100	1.48794400
O	2.30323800	3.80261100	2.17645100
C	3.20951100	3.39019900	0.05205900
C	2.96159100	3.44516400	-1.13851500
C	2.61247500	3.46017700	-2.51775200
C	1.25333700	3.46687600	-2.89428800
C	3.59515700	3.44245600	-3.52593900
C	0.89514900	3.45412300	-4.23865200
H	0.49439400	3.47814700	-2.11805100
C	3.22679200	3.43250200	-4.86824800
H	4.64213800	3.43683500	-3.23997700
C	1.87809800	3.43728400	-5.23129900
H	-0.15608900	3.45801400	-4.51429400
H	3.99600100	3.42034500	-5.63561300
H	1.59518600	3.42838400	-6.28007600
H	4.36434100	3.00723200	4.13289700
H	2.38111600	0.71368200	1.77004500

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C	-2.18798500	1.50216200	1.03196200
C	-0.83721300	1.44086200	1.44751100
C	-0.12767400	2.64317500	1.58829600
C	-0.74174400	3.88047800	1.40806100
C	-2.09443100	3.94582600	1.09059400
C	-2.79783900	2.75981200	0.89250600
H	0.91290100	2.66720900	1.87956900
H	-0.14028400	4.77358600	1.54248800
H	-2.59733700	4.90186000	0.97897900
H	-3.84362100	2.81429900	0.60482700
C	0.85266700	-0.83418200	0.32906500
C	-0.51823100	-1.58314200	2.65199000
C	0.41549300	-2.30976400	0.43094900
H	1.94001300	-0.77692800	0.46322000
C	0.30986600	-2.66827600	1.91642300
H	-1.54650300	-1.65799900	2.30091600
H	-0.56292000	-2.42200100	-0.03965500

H	1.13160200	-2.95465300	-0.09059100
H	-0.16846700	-3.64199300	2.06798600
H	1.31060100	-2.72975800	2.36776500
P	0.17375100	-0.03340100	1.87540800
C	0.48359200	-0.14448300	-0.98234000
C	-0.44627900	-1.73112600	4.17035600
H	-1.15141200	-1.07973100	4.68337000
H	-0.68812600	-2.77159700	4.41931500
H	0.54901800	-1.51509000	4.56850900
H	0.79694200	0.90190600	-0.99748500
H	0.97953600	-0.65287900	-1.81686300
H	-0.59490900	-0.19704900	-1.15012600
C	-4.75855500	0.09349900	1.47502100
C	-3.97637100	0.45935000	-1.15085000
C	-5.85583100	-0.05585500	0.40041500
H	-4.84413900	1.08881300	1.92920300
C	-5.44374300	0.79554400	-0.81431500
H	-3.95243800	-0.53754700	-1.61336000
H	-5.92837600	-1.11018700	0.10178800
H	-6.83581200	0.23570800	0.79344000
H	-6.09332100	0.61551900	-1.67809500
H	-5.53395400	1.86259600	-0.56857500
P	-3.18701800	0.08055500	0.49083400
O	-2.42607500	-1.22303800	0.48403900
C	-3.26362300	1.44246400	-2.07933900
C	-4.76382300	-0.97280400	2.56954800
H	-3.98484300	-0.77979100	3.31561600
H	-5.72918100	-0.98939600	3.08745900
H	-4.57967300	-1.96463800	2.14576500
H	-2.21986300	1.15975900	-2.24668200
H	-3.76427400	1.46742600	-3.05395500
H	-3.26693800	2.45814100	-1.67429500
C	1.69556000	0.42932800	2.81344600
H	1.97058800	-0.54116700	3.25465900
C	1.74470300	1.57227100	3.79309800
C	0.61061900	1.98840200	4.54846500
O	-0.50046100	1.15725000	4.30223200
C	-1.74402100	1.67698500	4.75674500
H	-2.03715900	2.55092900	4.16394200
H	-2.47814800	0.87745500	4.62144900
H	-1.68403800	1.96784000	5.80755700

O	0.49192700	2.94432200	5.30573500
C	2.84669400	2.45334900	3.74809800
H	2.81194700	3.21915900	4.51505200
C	4.58191600	0.42536800	5.30058200
C	4.58755700	0.60265200	3.90949000
C	4.85148800	-0.51018000	3.10496500
C	5.09702500	-1.76503200	3.66909500
C	5.08083900	-1.92758300	5.05281400
C	4.82285100	-0.82257400	5.86871600
H	4.37035000	1.27718600	5.94156800
H	4.85120800	-0.40268000	2.02516100
H	5.30124800	-2.61441700	3.02198100
H	5.27029800	-2.90240300	5.49382200
H	4.80689500	-0.93500300	6.94947900
C	4.27226200	1.98128600	3.34242600
C	4.34761100	2.12158900	1.84211600
H	5.05475800	1.60618800	1.20691700
C	3.39504000	2.98193100	1.39912800
O	2.63282900	3.57930600	2.31418200
C	2.98763900	3.14107800	0.03679600
C	2.43531400	3.21915500	-1.04497500
C	1.72360300	3.25034600	-2.27642700
C	0.32742300	3.45421100	-2.27062300
C	2.37381700	3.03983400	-3.50735900
C	-0.38929100	3.44337000	-3.46308600
H	-0.17694800	3.61250600	-1.32320600
C	1.64739500	3.03300700	-4.69482500
H	3.44744100	2.88127800	-3.51563100
C	0.26514200	3.23248200	-4.67944400
H	-1.46400000	3.60283200	-3.44367200
H	2.16233400	2.86984200	-5.63748400
H	-0.29745900	3.22537300	-5.60859800
H	4.97173900	2.69009200	3.81536900
H	2.43833600	0.60960900	2.03431400

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C	-4.37699000	4.47024600	2.04503400
C	-3.14840100	3.99382600	1.53848400
C	-2.73000900	4.45207200	0.28029700

C	-3.47420900	5.39268000	-0.42938100
C	-4.65847300	5.89883100	0.10199200
C	-5.11042300	5.42068500	1.32898900
H	-1.82438300	4.07048300	-0.16986700
H	-3.12160300	5.72816500	-1.40011600
H	-5.23316300	6.64318500	-0.44091400
H	-6.05227900	5.78183300	1.73172300
C	-1.15212600	3.88454500	3.85261200
C	-0.43068500	2.77371300	1.47429800
C	0.37272100	3.72772000	3.60703100
H	-1.44912500	3.37037900	4.76814200
C	0.62965000	2.61392800	2.58215200
H	-0.26249100	3.76382100	1.03200700
H	0.76727300	4.67174000	3.21035400
H	0.88852400	3.53225000	4.55259600
H	1.63818200	2.67593900	2.15762500
H	0.54339900	1.62842300	3.05576100
P	-1.98975700	2.91424300	2.48802000
C	-1.57758900	5.34920000	3.95026100
C	-0.38152600	1.71314300	0.37546700
H	-1.19757800	1.82639400	-0.34058800
H	0.57714400	1.77746200	-0.15319400
H	-0.46942800	0.70487500	0.78865000
H	-2.63307200	5.43399400	4.20925700
H	-0.99250500	5.84687800	4.73268100
H	-1.40311000	5.88635700	3.01081700
C	-6.04578800	4.76540500	4.60975900
C	-6.42309200	2.56388600	3.00999400
C	-7.04730700	3.72750500	5.16417000
H	-6.59438200	5.47344000	3.97131500
C	-7.58990500	2.92519200	3.96873200
H	-6.07405800	1.56237400	3.25629700
H	-6.52765700	3.04685400	5.84876300
H	-7.84771800	4.21905500	5.72926900
H	-8.08757300	2.01237700	4.30897300
H	-8.32886900	3.53225100	3.42782100
P	-5.03199800	3.66786000	3.53455600
O	-3.82250400	3.10144600	4.25322300
C	-6.79326200	2.63044700	1.52703700
C	-5.23261900	5.51202300	5.66325100
H	-4.58491000	6.26961200	5.20852000

H	-5.89582600	6.01791700	6.37403500
H	-4.59839300	4.81340500	6.21659200
H	-5.92859600	2.43695200	0.88821200
H	-7.55167800	1.86977700	1.31176200
H	-7.21050600	3.60473500	1.24716700
C	-2.23221000	1.18348200	3.12396300
C	-3.50524300	0.43116200	2.90052400
C	-3.98009300	0.51421900	1.56452100
O	-5.10676200	-0.21704200	1.27699900
C	-5.45510800	-0.28444200	-0.10314600
H	-5.67039400	0.70570500	-0.51358600
H	-4.64806800	-0.73491500	-0.69042400
H	-6.34777600	-0.91142800	-0.14923200
O	-3.44300500	1.20830900	0.67717500
C	-4.16731300	-0.33740200	3.88050600
H	-4.93007100	-0.98069900	3.45079600
C	-1.05337100	-0.79984300	5.53276300
C	-2.35089200	-0.31717900	5.72853700
C	-2.52387000	0.87679600	6.44468900
C	-1.41959600	1.58692900	6.91102900
C	-0.12331900	1.11056900	6.68559500
C	0.05624300	-0.09194200	6.00142900
H	-0.90979500	-1.72605000	4.98072700
H	-3.52353500	1.27376300	6.57140900
H	-1.56966200	2.52082300	7.44676100
H	0.73610900	1.66557600	7.05265600
H	1.05747200	-0.48076700	5.83399300
C	-3.54543300	-1.03047100	5.11095400
C	-4.68280700	-1.18125300	6.09488400
H	-4.67375600	-1.88267100	6.91826100
C	-5.61671500	-0.21603000	5.89915000
O	-5.44489300	0.60972900	4.87209200
C	-6.76466300	0.02546300	6.71462400
C	-7.75197600	0.35335600	7.34517100
C	-8.90598600	0.74449100	8.07785000
C	-9.73270000	1.78047000	7.59804400
C	-9.24416300	0.11489400	9.29173000
C	-10.85983700	2.17167100	8.31356900
H	-9.47565500	2.26527700	6.66140600
C	-10.37398200	0.51228300	10.00039800
H	-8.60988700	-0.68304400	9.66431400

C	-11.18591000	1.54071600	9.51656900
H	-11.48825700	2.97159900	7.93137500
H	-10.62275600	0.01743600	10.93518200
H	-12.06690500	1.84805400	10.07281100
H	-3.19747700	-2.01080800	4.75408100
H	-1.37895800	0.66155600	2.67503900
H	-2.02787000	1.30545100	4.17936800

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C	-3.18061900	-1.36425400	0.42539600
C	-2.32777300	-0.98404800	1.49480300
C	-2.89567800	-0.88569900	2.77814500
C	-4.23470000	-1.18276900	3.01487300
C	-5.05920600	-1.57844600	1.96444300
C	-4.52739300	-1.65559300	0.68042100
H	-2.29136300	-0.56184600	3.61478200
H	-4.63063000	-1.09983400	4.02272500
H	-6.10536500	-1.81148100	2.13729600
H	-5.18195200	-1.93354300	-0.13974100
C	0.57403500	-1.90817600	0.99091400
C	0.09300900	-0.03833900	2.93863000
C	1.57041400	-1.85650200	2.17800000
H	1.09538200	-1.66489900	0.06273700
C	1.56813300	-0.45709200	2.80318100
H	-0.37016800	-0.77598500	3.60772200
H	1.25619500	-2.58990500	2.93268600
H	2.56861500	-2.14976000	1.83611300
H	2.05302400	-0.45127400	3.78662400
H	2.10271000	0.24534200	2.15942600
P	-0.58197400	-0.45380700	1.25176000
C	-0.09527600	-3.27464900	0.85522400
C	-0.14276100	1.36466800	3.50499600
H	-1.16444400	1.71599000	3.33749200
H	0.05464100	1.35747700	4.58361200
H	0.52542700	2.09289600	3.04405500
H	-0.74168100	-3.30928500	-0.02110200
H	0.67646700	-4.04424600	0.73683000
H	-0.68596200	-3.51875900	1.74575700
C	-3.48783500	-2.64739800	-2.29024600

C	-3.41502700	0.12597300	-2.15135600
C	-3.87660700	-1.88721900	-3.57501500
H	-4.40628000	-2.93873100	-1.76698500
C	-4.41173900	-0.51169200	-3.14767800
H	-2.57659500	0.56445800	-2.70892600
H	-2.98544500	-1.76292700	-4.20460500
H	-4.61044400	-2.45130100	-4.16127600
H	-4.58128900	0.14904600	-4.00458800
H	-5.38193200	-0.63927800	-2.64757300
P	-2.62089400	-1.33463200	-1.30938900
O	-1.11565700	-1.41388800	-1.42577400
C	-4.04840900	1.19416100	-1.25334200
C	-2.60854500	-3.87844200	-2.50749400
H	-2.38045400	-4.37868000	-1.56033200
H	-3.11476100	-4.59954800	-3.15923000
H	-1.66035800	-3.59583800	-2.97348300
H	-3.34207600	1.65446800	-0.55518000
H	-4.46359700	1.99324100	-1.87841600
H	-4.86977100	0.77289200	-0.66418000
C	-0.34488600	1.06989200	-0.12056600
H	0.22166600	0.51694800	-0.86281800
C	0.19724600	2.29684300	0.37506100
C	-0.71782300	3.18900600	0.96871400
O	-0.11939800	4.37163600	1.39260000
C	-0.99210300	5.28151900	2.05261100
H	-1.81130800	5.59342600	1.39681300
H	-1.42718800	4.83420500	2.95246300
H	-0.37598700	6.14263300	2.32206300
O	-1.93197600	2.99725700	1.15828700
C	1.67393100	2.56344800	0.37022700
H	2.02407000	3.00629100	1.30632600
C	2.88028800	5.65598200	0.06714800
C	3.26296000	4.41724800	-0.46533000
C	4.62536600	4.11955100	-0.56420100
C	5.58717500	5.04381300	-0.15259800
C	5.19766000	6.27738400	0.36910500
C	3.83832500	6.57939900	0.48066300
H	1.82137500	5.87750700	0.17087900
H	4.92927500	3.15891700	-0.96980900
H	6.64258100	4.79855300	-0.24002800
H	5.94609600	6.99784300	0.68809600

H	3.52516300	7.53654600	0.88989800
C	2.18639700	3.41857900	-0.85023700
C	2.62324700	2.32203000	-1.78928100
H	2.82624600	2.43868200	-2.84509400
C	2.69415400	1.16507000	-1.11106300
O	2.37182600	1.28277000	0.22719200
C	2.89910200	-0.16165300	-1.56382300
C	2.91768300	-1.33560100	-1.87661700
C	2.80127700	-2.71341100	-2.22533600
C	3.93334200	-3.51325800	-2.45953400
C	1.51570900	-3.28621800	-2.31077800
C	3.78300800	-4.86246000	-2.76950100
H	4.92082600	-3.06792100	-2.39186000
C	1.38042900	-4.63803500	-2.61422900
H	0.64429300	-2.66284400	-2.13252600
C	2.50871600	-5.42900600	-2.84475300
H	4.66237900	-5.47443800	-2.94919800
H	0.38770000	-5.07616100	-2.67097000
H	2.39625700	-6.48318000	-3.08227100
H	1.32864600	3.96800900	-1.25098800
H	-1.38270600	1.15937700	-0.42559700

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C	-1.54538500	1.09777300	0.75655900
C	-0.80955100	1.11204700	1.96855400
C	-0.61590500	2.34952600	2.61189200
C	-1.04035000	3.54783200	2.04153600
C	-1.67647900	3.53793700	0.80640100
C	-1.95222200	2.31699100	0.19475100
H	-0.11204300	2.38132400	3.56663700
H	-0.83829400	4.48194800	2.55398300
H	-1.97285000	4.46565700	0.32817800
H	-2.50910600	2.31724100	-0.73804200
C	1.01728500	-1.55749600	1.93815600
C	-1.13751300	-1.40208800	3.69977900
C	0.36964700	-2.88875400	2.39102300
H	2.00624900	-1.46489500	2.40606700
C	-0.29868300	-2.69399000	3.76109700
H	-1.95870400	-1.55589900	2.99336300

H	-0.39288300	-3.16181900	1.65891500
H	1.12583000	-3.68198100	2.42070000
H	-0.93384500	-3.54834300	4.02225100
H	0.45944600	-2.60454100	4.55223400
P	0.05004300	-0.23979200	2.86922100
C	1.22540600	-1.46717200	0.42873300
C	-1.66222600	-0.90189500	5.04375500
H	-2.18855900	0.05309800	4.93809500
H	-2.36651400	-1.62708100	5.46811700
H	-0.85287700	-0.75992200	5.76763700
H	1.61530500	-0.49345000	0.12392200
H	1.96540300	-2.21804300	0.12741400
H	0.29475300	-1.67616000	-0.09625700
C	-4.02176600	-0.13537900	-0.28316600
C	-1.75570600	-0.43224400	-1.84590800
C	-4.24522900	-0.60585000	-1.73363600
H	-4.21526700	0.94232400	-0.23101400
C	-3.07146200	-0.07592100	-2.57276300
H	-1.54266700	-1.49648400	-2.01555100
H	-4.25614200	-1.70367900	-1.76297500
H	-5.21266000	-0.26307200	-2.11701200
H	-3.07522200	-0.48144800	-3.59059200
H	-3.15086800	1.01621400	-2.66678500
P	-2.20053100	-0.40986300	-0.03362200
O	-1.89129500	-1.68307500	0.71458000
C	-0.54859100	0.39657900	-2.28613200
C	-4.85386100	-0.85885100	0.77389900
H	-4.67702900	-0.44058300	1.77064100
H	-5.92295500	-0.76459400	0.55180200
H	-4.59542500	-1.92100300	0.80892300
H	0.36553400	0.07257900	-1.78269100
H	-0.39426700	0.28935800	-3.36598400
H	-0.68616500	1.45993300	-2.06968100
C	1.58338200	0.50884600	4.28542400
H	1.00321600	0.48442800	5.20290800
C	2.24438300	1.73368300	4.02072900
C	1.94711400	2.92631200	4.74063500
O	0.85239800	2.78286700	5.59144200
C	0.54550100	3.94111900	6.36218000
H	0.33692900	4.80193700	5.71906100
H	-0.33959500	3.68175900	6.94757900

H	1.37364900	4.20484200	7.02725000
O	2.52530600	4.01449100	4.66670600
C	3.25365800	1.82042100	2.93045500
C	2.24724500	4.28726800	1.50154700
C	2.24126800	3.05365200	0.84180200
C	1.71739300	2.99108000	-0.45757400
C	1.21646600	4.12545700	-1.08998900
C	1.22852900	5.35472800	-0.42618500
C	1.74477700	5.42677100	0.86643900
H	2.60616900	4.36620400	2.52285200
H	1.69321000	2.03554600	-0.97573300
H	0.81729900	4.05109100	-2.09862000
H	0.84047100	6.24502300	-0.91415000
H	1.75584400	6.37580000	1.39622400
C	2.70775100	1.75912900	1.47661400
C	3.82163600	1.02271200	0.77145400
H	3.95368400	0.93587500	-0.29799600
C	4.56946400	0.40675500	1.70706300
O	4.18527600	0.67341900	2.99861000
C	5.65212000	-0.48515300	1.52935100
C	6.57378300	-1.26299600	1.38036100
C	7.65270600	-2.17220300	1.20478600
C	8.32777400	-2.70158000	2.32209500
C	8.06183300	-2.55802400	-0.08662900
C	9.38169800	-3.59274900	2.14690100
H	8.01418400	-2.40290100	3.31707200
C	9.11780100	-3.44885400	-0.25124100
H	7.54326400	-2.14970500	-0.94814600
C	9.78079100	-3.96962900	0.86241600
H	9.89524900	-3.99419900	3.01591300
H	9.42544800	-3.73822300	-1.25214500
H	10.60479000	-4.66482600	0.72996800
H	1.82000800	1.10511800	1.47875900
H	2.18748600	-0.38660900	4.14024200
H	3.86408200	2.71962000	3.05698500

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C	-4.61142800	4.00191800	2.95657600
C	-3.31093900	4.28809900	2.46798700

C	-3.19601500	5.25908200	1.44976700
C	-4.31241500	5.85920900	0.87172500
C	-5.59020600	5.49237100	1.28267400
C	-5.72493700	4.58857200	2.33170400
H	-2.21365300	5.57959700	1.12288400
H	-4.17452400	6.60440900	0.09384400
H	-6.47159600	5.92501000	0.81872600
H	-6.72355100	4.35348500	2.68884000
C	-1.44154800	1.77306500	3.36129000
C	-1.11396800	4.26035700	4.55086400
C	-0.96222100	1.77130400	4.83102600
H	-0.57528600	1.52343200	2.74108800
C	-0.26954300	3.11092500	5.13873600
H	-2.04864700	4.31724400	5.11834300
H	-1.82365000	1.63600700	5.48461900
H	-0.26434200	0.93873600	4.98034400
H	-0.15377800	3.25706700	6.21911600
H	0.72713300	3.12320400	4.69007000
P	-1.65204400	3.57647500	2.90954900
C	-2.54698900	0.77625900	3.02754800
C	-0.42584800	5.62592100	4.52505800
H	-1.02202700	6.36951000	3.98607100
H	-0.29051400	5.98315200	5.55269000
H	0.55522300	5.58055200	4.04991600
H	-2.90819600	0.89633700	1.99935000
H	-2.15723400	-0.24385200	3.11935400
H	-3.38270600	0.88404400	3.71846900
C	-6.13101300	4.14480400	5.49636500
C	-6.18842700	1.71605700	4.16542900
C	-7.19051700	3.12896000	5.96689800
H	-6.61185800	4.86673500	4.82643100
C	-7.51744000	2.21989200	4.77107600
H	-5.79921000	0.90858700	4.80033900
H	-6.77845100	2.52786500	6.78842500
H	-8.08145800	3.63611900	6.35336300
H	-8.15975500	1.37897800	5.05513000
H	-8.06663400	2.79557700	4.01269000
P	-4.97043100	3.08977900	4.49875800
O	-3.74301300	2.68113200	5.26947100
C	-6.30243600	1.21166400	2.72662000
C	-5.39938600	4.88846500	6.61241800

H	-4.69964600	5.62561000	6.20436500
H	-6.11411000	5.41787700	7.25276800
H	-4.82474000	4.19163700	7.22895700
H	-5.34328000	0.84882200	2.34816600
H	-7.01987500	0.38470600	2.67466400
H	-6.65091600	1.99868000	2.05087400
C	-0.26284500	3.82200200	1.28233600
H	-0.12818400	2.75698800	1.09860900
C	0.92635800	4.55175300	1.56112200
C	0.98165800	5.95971400	1.47356900
O	-0.25094200	6.53811700	1.13925300
C	-0.22716800	7.95834400	1.03705000
H	0.44712600	8.28824100	0.24031300
H	-1.25333100	8.25867500	0.80886000
H	0.10065800	8.41661100	1.97480900
O	1.96046900	6.68480600	1.68588300
C	2.16000100	3.88322100	2.09858800
H	2.62742300	4.48883500	2.87872000
C	4.99381200	5.23557700	1.47571700
C	4.65193000	3.87616700	1.41519400
C	5.61198900	2.92123900	1.75931600
C	6.89814600	3.31050100	2.14045900
C	7.23504500	4.66234000	2.18917800
C	6.27532800	5.62349100	1.86059700
H	4.23419600	5.98029600	1.25121600
H	5.34979200	1.86746100	1.73515600
H	7.63442500	2.55483700	2.40255400
H	8.23514100	4.96661900	2.48669100
H	6.52554400	6.68026700	1.90704600
C	3.23303000	3.50333900	1.01002000
C	2.97580000	2.02813300	0.85336400
H	3.37940500	1.39413300	0.07558100
C	2.19129000	1.60694400	1.86108000
O	1.79151300	2.60599300	2.72057200
C	1.68544800	0.31693800	2.14436700
C	1.19040200	-0.75969600	2.41571100
C	0.59709400	-2.01518200	2.72179700
C	-0.14580200	-2.18124300	3.90770500
C	0.73258200	-3.10640500	1.84199300
C	-0.73984800	-3.40562400	4.19745200
H	-0.24568800	-1.34403200	4.59040600

C	0.13651600	-4.32730400	2.14236900
H	1.30555400	-2.98021600	0.92909700
C	-0.60194800	-4.48188400	3.31787800
H	-1.31019900	-3.52112200	5.11468900
H	0.24811200	-5.16208600	1.45634000
H	-1.06600600	-5.43652000	3.54799700
H	2.98392000	4.05241300	0.09510800
H	-0.92365100	4.26115300	0.54117800

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C	2.79536000	-0.42727300	-0.81213600
C	1.68095900	0.32819100	-0.36927800
C	0.94320800	1.03629700	-1.34103600
C	1.26055000	0.99789200	-2.69728800
C	2.30622000	0.19483700	-3.13178200
C	3.06078300	-0.50053700	-2.18751000
H	0.07947900	1.61505800	-1.03958100
H	0.65745700	1.56431500	-3.40045500
H	2.54460900	0.10903800	-4.18791100
H	3.88101400	-1.11505600	-2.53867100
C	1.11415700	2.05502300	1.99277800
C	1.32915600	-0.62083300	2.65920900
C	2.20376000	1.69991200	3.02008500
H	0.19562900	2.31680600	2.53789700
C	1.75197200	0.41906500	3.72618200
H	2.22872100	-1.14438700	2.34665600
H	3.15068100	1.51135800	2.50148200
H	2.35677200	2.52640500	3.72644300
H	2.54580400	0.00132100	4.35362100
H	0.89725700	0.64315200	4.38031400
P	0.73911600	0.39166200	1.20494700
C	1.46523100	3.20075400	1.04958800
C	0.29038100	-1.62422000	3.16500800
H	0.02893500	-2.35267800	2.39265700
H	0.70258400	-2.16949700	4.02255000
H	-0.62906500	-1.13074000	3.50334300
H	0.64589800	3.42498400	0.35868200
H	1.67232600	4.10672300	1.63213600
H	2.35348200	2.96705300	0.45499300

C	3.53245800	-3.13975500	0.03088600
C	5.64275700	-1.46088400	-0.51923800
C	4.87120100	-3.80233300	-0.35749200
H	2.84753000	-3.17223600	-0.82439600
C	5.66858600	-2.82206000	-1.23660900
H	6.23516300	-1.57252300	0.40098900
H	5.44537200	-4.01654200	0.55422100
H	4.69998300	-4.76082400	-0.86027000
H	6.69908100	-3.16200400	-1.39382000
H	5.20608700	-2.74535300	-2.22989000
P	3.95819700	-1.34096200	0.26357800
O	4.05733500	-0.80616800	1.67238400
C	6.20216000	-0.25722900	-1.27584800
C	2.83285100	-3.76469100	1.23622300
H	1.82108800	-3.36670600	1.33439700
H	2.75439100	-4.85061400	1.10583200
H	3.38627700	-3.56879900	2.16076400
H	6.11906900	0.65340500	-0.67334900
H	7.26396900	-0.41565000	-1.49802400
H	5.68810800	-0.07693200	-2.22289400
C	-1.37354900	-0.27283000	0.57855300
H	-1.32348700	-1.07224300	1.30636700
C	-1.39711600	-0.63895100	-0.77456200
C	-0.60769200	-1.77625300	-1.11879400
O	-0.70687300	-2.14325400	-2.43933300
C	0.16962500	-3.19093200	-2.84216100
H	0.04251700	-4.07519700	-2.21184600
H	-0.09577700	-3.41920100	-3.87656700
H	1.21450400	-2.86550900	-2.78831300
O	0.15162500	-2.37612100	-0.34347900
C	-2.12829600	0.15702700	-1.81265500
H	-1.68148000	0.00128000	-2.79350500
C	-4.09726300	-2.53843700	-2.22344300
C	-4.11703100	-1.43354200	-1.36603400
C	-4.47481300	-1.62965900	-0.02826700
C	-4.80679600	-2.89925700	0.44247700
C	-4.78045100	-3.99571900	-0.42034500
C	-4.42250400	-3.81107700	-1.75651600
H	-3.80655100	-2.39953900	-3.26162100
H	-4.48187200	-0.77958500	0.64784100
H	-5.08193300	-3.03309300	1.48533900

H	-5.03672600	-4.98617400	-0.05450900
H	-4.39717300	-4.65856700	-2.43631000
C	-3.69221000	-0.07785200	-1.88351700
C	-4.20299000	1.12395400	-1.12927600
H	-5.21662500	1.26044700	-0.77857000
C	-3.20062100	2.00700000	-0.97748200
O	-2.00239700	1.59114700	-1.51499300
C	-3.16072000	3.25529500	-0.31588000
C	-3.03353000	4.30736700	0.27922800
C	-2.87420600	5.52934200	0.98850300
C	-1.58439300	6.04308500	1.22837200
C	-3.99333800	6.23728500	1.46708500
C	-1.42411000	7.23407500	1.92901600
H	-0.72157100	5.49705500	0.86073300
C	-3.82196400	7.42761300	2.16694600
H	-4.98698300	5.84201700	1.28249300
C	-2.53980000	7.93007600	2.40043400
H	-0.42517100	7.62128400	2.10854200
H	-4.69199500	7.96609500	2.53161600
H	-2.41063300	8.85961900	2.94716200
H	-4.00111800	-0.00840200	-2.93795300
H	-1.96984700	0.57657500	0.89932500

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C	-1.82314300	0.12287100	-0.56153300
C	-0.78720000	0.60543500	0.27783600
C	0.37191700	1.10045600	-0.34650500
C	0.52250400	1.11894300	-1.73131800
C	-0.49581600	0.63871900	-2.54678800
C	-1.65584900	0.15060700	-1.95363300
H	1.19433700	1.47188000	0.24622500
H	1.43984400	1.50755200	-2.16325600
H	-0.39367900	0.64274700	-3.62767400
H	-2.44984700	-0.22083900	-2.59331800
C	-1.94270400	1.73029200	2.94197900
C	0.74819200	1.47578400	2.65057900
C	-1.05837500	2.64468000	3.83957200
H	-2.58301700	1.11857000	3.57510100
C	0.34774900	2.06361200	4.01227500

H	0.69399000	2.32064100	1.94843700
H	-0.98267800	3.63013400	3.36108300
H	-1.54720300	2.76726600	4.80746300
H	1.06831900	2.83671100	4.30535000
H	0.33357600	1.29770700	4.78793600
P	-0.76631500	0.51385300	2.13895400
C	-2.76902600	2.55815500	1.95751500
C	2.15501100	0.87625200	2.57610400
H	2.29744500	0.22070600	1.71218300
H	2.88632700	1.69092300	2.51282400
H	2.37994800	0.28597100	3.46326300
H	-3.50098100	1.93869900	1.44624900
H	-3.30550700	3.33461700	2.51527200
H	-2.13761100	3.06282800	1.21598400
C	-4.77924200	0.15245500	-0.96775600
C	-3.58028200	-2.30480200	-0.57732300
C	-5.52124000	-1.08570200	-1.51630200
H	-4.32227400	0.69118300	-1.80613700
C	-4.48308200	-2.17662000	-1.81729200
H	-4.16434800	-2.77521800	0.22174700
H	-6.21800800	-1.45213900	-0.75057400
H	-6.11973000	-0.82470000	-2.39597500
H	-4.95586700	-3.13791900	-2.04811700
H	-3.88539600	-1.90144300	-2.69723800
P	-3.39776500	-0.57256100	0.06038200
O	-3.52587300	-0.38678700	1.55142200
C	-2.30390900	-3.11771700	-0.76738500
C	-5.67154200	1.10804000	-0.17480800
H	-5.14929900	2.03604300	0.07299200
H	-6.55980800	1.36773300	-0.76218600
H	-5.99823300	0.64979900	0.76347200
H	-1.75949400	-3.22947100	0.17198900
H	-2.55735500	-4.12250800	-1.12339200
H	-1.63356200	-2.65372900	-1.49886400
C	-0.78791000	-1.24474400	2.54078100
H	-1.19168300	-1.71737200	1.65379300
C	0.46953700	-1.86879700	2.97527700
C	1.06068300	-2.96424500	2.16212900
O	0.58075300	-2.98092500	0.88627000
C	1.05515700	-4.06483200	0.08125800
H	0.71742400	-5.02023400	0.49330200

H	0.62615300	-3.90571200	-0.90858800
H	2.14691100	-4.06436200	0.03613300
O	1.89622700	-3.76223900	2.54412900
C	1.03374800	-1.64101100	4.18454400
H	1.90247100	-2.21177900	4.49363900
H	0.69386500	-0.84521700	4.82833600
C	-1.74475100	-4.27518100	3.16504500
C	-2.60534600	-3.16624400	3.23722600
C	-3.90215800	-3.29933800	2.72194200
C	-4.32468500	-4.49797100	2.14525200
C	-3.44975500	-5.58163500	2.04951300
C	-2.15722300	-5.46405500	2.56549100
H	-0.74716300	-4.20464400	3.58488200
H	-4.57216500	-2.44759200	2.77239700
H	-5.34114900	-4.58520100	1.76792500
H	-3.77609200	-6.51197700	1.59261800
H	-1.47000100	-6.30454200	2.51289000
C	-2.17090100	-1.88985000	3.87275000
C	-1.63146500	-2.00039800	5.18322000
H	-1.37097000	-2.96999900	5.59090400
C	-1.43305900	-0.84735100	5.97122200
O	-1.60070800	0.33336200	5.55691700
C	-0.93588100	-1.05527600	7.32352200
C	-0.49982900	-1.18698500	8.45101800
C	0.01053500	-1.35056500	9.76947300
C	0.21006300	-0.23397100	10.60484500
C	0.32745300	-2.63184200	10.26181600
C	0.71112300	-0.39820100	11.89263900
H	-0.03447800	0.75362500	10.22714000
C	0.82881000	-2.78735400	11.55053400
H	0.17416200	-3.49328300	9.61972700
C	1.02258400	-1.67327200	12.37056700
H	0.85950300	0.47151100	12.52686300
H	1.06924400	-3.78136200	11.91756500
H	1.41374900	-1.79806700	13.37638300
H	-2.85912600	-1.06846900	3.70903500

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C	-2.79555200	0.50178300	1.18153900
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C	-1.68549900	1.38106800	1.31581900
C	-1.92564600	2.76000000	1.26997100
C	-3.21167300	3.29073400	1.17541000
C	-4.30397600	2.43423600	1.14079200
C	-4.08391700	1.05723100	1.13197300
H	-1.13152600	3.49145000	1.34917800
H	-3.31137300	4.37053900	1.16837100
H	-5.31846500	2.82054000	1.10606000
H	-4.94381200	0.39755800	1.06708900
C	0.94635600	0.38546800	0.07561300
C	0.40149300	-0.54767600	2.64668800
C	1.57319300	-0.97266700	0.48670300
H	1.73263700	1.13216000	-0.06771100
C	1.73086900	-1.02449900	2.01608500
H	-0.36325600	-1.26506300	2.35131600
H	0.89690300	-1.77095200	0.17401400
H	2.53373300	-1.11055800	-0.02140000
H	1.95302500	-2.04114200	2.35945200
H	2.55333700	-0.37766500	2.34566100
P	0.07998800	0.95954900	1.62527500
C	0.08959300	0.33230800	-1.18906100
C	0.41796800	-0.39157100	4.16393800
H	-0.53194000	-0.00994000	4.54775000
H	0.59113600	-1.37568100	4.61478200
H	1.20524100	0.27750900	4.52042900
H	-0.36158300	1.30445400	-1.41251700
H	0.71887000	0.05003800	-2.04092600
H	-0.69897200	-0.41602300	-1.08749000
C	-3.79563600	-2.08299500	2.23622500
C	-3.88232700	-1.75503100	-0.50596400
C	-4.73170500	-3.02884800	1.45435100
H	-4.39820200	-1.28264300	2.68346900
C	-5.15643100	-2.31250800	0.15955000
H	-3.32298100	-2.60330000	-0.92528000
H	-4.18690200	-3.94829000	1.20190300
H	-5.59332900	-3.32220700	2.06380200
H	-5.68897500	-2.98504100	-0.52211800
H	-5.84725400	-1.49167600	0.39555500
P	-2.75628500	-1.30775100	0.90700800
O	-1.37753100	-1.89627600	0.73148400
C	-4.09577700	-0.72523600	-1.61377500

C	-2.94837000	-2.75353700	3.31708100
H	-2.34887300	-2.01923700	3.86611000
H	-3.58735100	-3.27346300	4.03957000
H	-2.26115100	-3.48117300	2.87481300
H	-3.14091000	-0.37453300	-2.01899000
H	-4.66543900	-1.17206900	-2.43634700
H	-4.64704100	0.14990100	-1.25993700
C	1.02457800	2.29817300	2.40207800
H	1.58256000	1.75469800	3.15639300
C	1.97169700	3.01881100	1.52284100
C	3.43432700	2.74300500	1.65107800
O	3.72189200	1.90827000	2.69264000
C	5.11598200	1.63602200	2.88257400
H	5.16957300	0.98349600	3.75463700
H	5.53405500	1.14031900	2.00243400
H	5.66720600	2.56315000	3.05875600
O	4.30576700	3.18643600	0.92990900
C	1.63403400	4.01682300	0.68170100
H	2.40628000	4.51800400	0.10834100
H	0.61058400	4.34537700	0.54820400
C	1.74741400	2.95090600	5.45318200
C	0.43488500	3.02262900	4.96038200
C	-0.60167700	2.51902100	5.75636800
C	-0.34072800	1.95640400	7.00651200
C	0.96857400	1.88235100	7.48105600
C	2.01167800	2.38500200	6.69808000
H	2.56502500	3.31872900	4.84029100
H	-1.62362600	2.57457200	5.38857800
H	-1.16115200	1.57430500	7.60842600
H	1.17623500	1.44017800	8.45138600
H	3.03552700	2.33298800	7.05920700
C	0.12537200	3.60719900	3.62259600
C	0.56942600	4.94012000	3.37202100
H	1.43114200	5.32629500	3.90652800
C	-0.09688800	5.79724800	2.47098800
O	-1.06469300	5.48200300	1.71811500
C	0.40479000	7.16452000	2.41479100
C	0.79702400	8.31248100	2.33188400
C	1.25886300	9.65525500	2.23585500
C	0.62639300	10.57079400	1.37180000
C	2.35678600	10.09420900	3.00167000

C	1.08062900	11.88292800	1.27988800
H	-0.21946200	10.23451100	0.78086000
C	2.80534600	11.40785000	2.90356300
H	2.84585600	9.39087700	3.66807500
C	2.17046400	12.30716300	2.04377600
H	0.58304300	12.57829600	0.60933000
H	3.65365900	11.73230900	3.50009100
H	2.52286500	13.33215200	1.96944100
H	-0.91142600	3.44840300	3.34206900

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C	-2.41317200	-0.21603300	0.19349300
C	-1.28257500	0.57973200	0.53242500
C	-1.05720500	1.74897400	-0.21228600
C	-1.89250300	2.15277600	-1.25187200
C	-3.00853100	1.38907800	-1.56663100
C	-3.25115300	0.22165400	-0.84600200
H	-0.19312500	2.36885300	-0.01582100
H	-1.65497600	3.06874300	-1.78462500
H	-3.68724800	1.68852000	-2.35967200
H	-4.12221800	-0.36996600	-1.10923100
C	0.94485300	-1.22289500	1.84104500
C	-0.94377400	-0.02790000	3.50764500
C	0.68463000	-1.92193500	3.20838300
H	1.96869200	-0.84726400	1.78031100
C	0.05477700	-0.95405500	4.23246800
H	-1.79775400	-0.64226300	3.21983500
H	-0.01249900	-2.74177000	3.03184400
H	1.61999200	-2.34345900	3.59218600
H	-0.47106800	-1.51645800	5.01219100
H	0.81973000	-0.34808200	4.72462400
P	-0.07963000	0.32829700	1.90602800
C	0.71154800	-2.15073300	0.64372200
C	-1.41224800	1.19233200	4.29418900
H	-2.10567600	1.80456600	3.70702400
H	-1.94076200	0.85893000	5.19490100
H	-0.58636600	1.83572800	4.59917000
H	0.71118900	-1.60627800	-0.30210000
H	1.52432900	-2.88276800	0.59715700

H	-0.23101500	-2.68377700	0.76301900
C	-4.74282000	-1.64953400	1.35166200
C	-3.17391100	-3.06300600	-0.44199600
C	-5.36207500	-2.92702700	0.74617300
H	-5.14370600	-0.77746900	0.82251700
C	-4.70300400	-3.16758200	-0.62332500
H	-2.82502600	-3.97646900	0.05928400
H	-5.15413700	-3.77789400	1.40842000
H	-6.45103500	-2.83809200	0.66821700
H	-4.97874300	-4.14079100	-1.04427400
H	-5.04377200	-2.40697300	-1.33916500
P	-2.94333000	-1.81467100	0.92155900
O	-2.09238900	-2.33075900	2.05459700
C	-2.37229600	-2.87147400	-1.72858200
C	-4.95099900	-1.47609700	2.85577600
H	-4.52570700	-0.53027900	3.20889600
H	-6.01972100	-1.47612400	3.09747800
H	-4.46729800	-2.28577600	3.40969700
H	-1.29926900	-2.80566700	-1.52456500
H	-2.53568600	-3.72015700	-2.40228600
H	-2.66679600	-1.96108500	-2.25845900
C	0.94968400	1.81804000	1.99583100
H	0.28267100	2.67246600	1.89649200
C	1.74054300	1.98747200	3.24620500
C	1.68983600	3.36479100	3.86718300
O	0.45459600	3.89163200	3.79939400
C	0.35254800	5.29816700	4.08580800
H	0.75575100	5.84422400	3.23153100
H	-0.71417200	5.49483900	4.19997600
H	0.89441500	5.54189400	5.00169400
O	2.63911900	3.90988600	4.38928800
C	2.62903100	1.13632300	3.78735500
H	3.22111500	1.45093700	4.63974000
H	2.80146300	0.13881500	3.40451600
C	2.53007800	0.29494300	-0.86132200
C	2.97402300	1.08169800	0.21268100
C	4.13623700	0.68128500	0.89116100
C	4.81590200	-0.48150000	0.52663900
C	4.35941800	-1.25590400	-0.54071000
C	3.21937000	-0.85462600	-1.24041000
H	1.63413300	0.58914600	-1.40024600

H	4.50794100	1.29698500	1.70352700
H	5.71207600	-0.77332400	1.06756800
H	4.89316200	-2.15571100	-0.83344400
H	2.86092600	-1.44582200	-2.07904300
C	2.25289900	2.31411300	0.62898100
C	1.69325000	3.15123300	-0.39508400
H	1.59671200	2.80355300	-1.41718100
C	1.16597300	4.40627300	-0.03488500
O	1.16304000	4.88049800	1.13305700
C	0.47878900	5.12543200	-1.10813500
C	-0.17496000	5.67930700	-1.97246800
C	-0.94501200	6.31986800	-2.98398600
C	-1.64127100	7.51397500	-2.71124800
C	-1.03567200	5.76351400	-4.27558000
C	-2.40316900	8.12755100	-3.70098700
H	-1.57175400	7.94558700	-1.71800600
C	-1.79994400	6.38330700	-5.25974700
H	-0.49484700	4.84706800	-4.49087300
C	-2.48699200	7.56624900	-4.97751200
H	-2.93357900	9.04892000	-3.47657200
H	-1.85808800	5.94401600	-6.25197200
H	-3.08172100	8.04894000	-5.74786500
H	2.81361300	2.88691800	1.36464700

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C	-3.06840900	0.77561100	0.49430300
C	-2.09019300	1.50470700	1.22065600
C	-2.39972900	2.81776300	1.61404000
C	-3.61461200	3.42164100	1.29831800
C	-4.56700300	2.71128200	0.57828200
C	-4.28776800	1.40308800	0.19121100
H	-1.68076500	3.38275500	2.18563300
H	-3.79966900	4.43504200	1.63596600
H	-5.52201600	3.16048700	0.32246000
H	-5.04415600	0.85673100	-0.36341500
C	0.83288700	0.29920200	0.60903600
C	-0.56701100	-0.60091900	2.82548200
C	1.22538200	-1.08487200	1.19105500
H	1.65399500	0.99989900	0.78629000

C	0.87495700	-1.13872300	2.69328900
H	-1.19362900	-1.23850000	2.19636500
H	0.65949500	-1.85597300	0.66388200
H	2.29361900	-1.25922200	1.02379700
H	0.91646800	-2.16667500	3.06998900
H	1.57197300	-0.54268400	3.29619700
P	-0.44643800	0.93483000	1.82680500
C	0.51037600	0.31920700	-0.88212700
C	-1.17124900	-0.50763800	4.21955100
H	-2.18974900	-0.10217800	4.17751400
H	-1.22917300	-1.51220900	4.65386700
H	-0.58086900	0.12433100	4.88287300
H	0.21658400	1.32169500	-1.21137400
H	1.40738200	0.03660300	-1.44599400
H	-0.27800100	-0.39472200	-1.11992300
C	-4.47136100	-1.83653200	0.44418000
C	-3.33595800	-0.98531700	-1.93503000
C	-4.96115000	-2.52986300	-0.84486400
H	-5.21171300	-1.08550700	0.74352900
C	-4.77268700	-1.54379700	-2.01133200
H	-2.64512300	-1.76722200	-2.27975800
H	-4.35708300	-3.42933400	-1.02309200
H	-6.00227000	-2.85550800	-0.74594500
H	-4.95445000	-2.01862000	-2.98178900
H	-5.49509000	-0.72053100	-1.92313700
P	-2.94026600	-0.94804300	-0.11654800
O	-1.65507700	-1.65469100	0.23093200
C	-3.07994000	0.28756300	-2.74079300
C	-4.18458900	-2.77104700	1.61912800
H	-3.88149500	-2.20890700	2.50910700
H	-5.07829200	-3.35145900	1.87401700
H	-3.37558900	-3.46504200	1.37386700
H	-2.04401600	0.62468900	-2.63553700
H	-3.26741500	0.10358900	-3.80458900
H	-3.73107100	1.10687500	-2.42230000
C	0.45109600	2.25022100	2.66318200
H	1.28636900	1.70433700	3.12916800
C	1.00617900	3.28926300	1.76369400
C	2.36256700	3.77450200	2.21028900
O	3.25868200	2.77934200	2.12312100
C	4.49178400	2.95381700	2.85033400

H	4.29019400	2.72155400	3.89824000
H	5.18849900	2.23096700	2.42500900
H	4.86399600	3.97261200	2.73130300
O	2.60238300	4.89626400	2.61045900
C	0.49450800	3.86521000	0.66009600
H	1.04278700	4.65271800	0.15350300
H	-0.45771400	3.58198100	0.22805500
C	-2.28271900	3.56062800	4.85752700
C	-1.03144300	3.98215800	4.38016400
C	-0.93166500	5.25470900	3.79343000
C	-2.05210900	6.07967000	3.68779000
C	-3.28911500	5.65187100	4.17439200
C	-3.39878500	4.38736400	4.76001900
H	-2.37923500	2.57227000	5.29592300
H	0.03217500	5.58561700	3.41738300
H	-1.95491700	7.06273500	3.23492800
H	-4.15939000	6.29900800	4.10334400
H	-4.35819900	4.04524800	5.13911900
C	0.17228600	3.11889700	4.44686900
C	0.32507400	2.17328300	5.51218000
H	-0.48030100	1.98217300	6.21150500
C	1.50991000	1.42847500	5.60194100
O	2.45343500	1.47222100	4.74880200
C	1.60545100	0.48105400	6.70276400
C	1.70128400	-0.34564600	7.58981300
C	1.81327900	-1.31393000	8.62653900
C	2.94792400	-2.14493800	8.71208100
C	0.79128200	-1.46310300	9.58481500
C	3.05274500	-3.09332100	9.72500500
H	3.73710600	-2.03094800	7.97589000
C	0.90363200	-2.41414300	10.59447400
H	-0.08300300	-0.82284000	9.52288300
C	2.03292700	-3.23280800	10.66941300
H	3.93416300	-3.72650700	9.77912700
H	0.10786800	-2.51692700	11.32729800
H	2.11825900	-3.97378600	11.45930100
H	1.08211100	3.68384200	4.26204200

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C	-2.99435300	-1.00880100	-0.16977100
C	-1.89497500	-1.42512600	0.62745700
C	-2.22250200	-2.01340800	1.86211300
C	-3.53340000	-2.25561800	2.27289600
C	-4.59375700	-1.91669200	1.43959200
C	-4.31223000	-1.28597900	0.23246200
H	-1.43621700	-2.28398200	2.55441500
H	-3.71544100	-2.71548200	3.24041700
H	-5.62115100	-2.11942600	1.72740600
H	-5.14195800	-0.99108400	-0.40381500
C	0.28482200	-1.97660200	-1.37417300
C	0.64558500	-2.61881300	1.25644700
C	1.56492100	-2.82100800	-1.15808100
H	0.41597400	-1.21327400	-2.14075200
C	1.66825900	-3.31149300	0.31118700
H	-0.22719700	-3.27000400	1.32979900
H	1.53324400	-3.67383800	-1.84691500
H	2.44766500	-2.23537400	-1.40875000
H	1.50010600	-4.39373400	0.37435900
H	2.67658300	-3.11437100	0.67930800
P	0.02720500	-1.12458400	0.28124200
C	-0.86273100	-2.91690500	-1.75859200
C	1.22214700	-2.38756200	2.65244700
H	0.51549300	-1.91328100	3.34031700
H	1.52391300	-3.35023500	3.08347100
H	2.10317400	-1.74727000	2.58363700
H	-1.81458700	-2.41503200	-1.89958200
H	-0.60313700	-3.41392500	-2.70037900
H	-1.01184000	-3.69700900	-1.00342200
C	-3.93770100	-0.71234900	-3.02020100
C	-3.91274300	1.54696200	-1.42134800
C	-4.83028700	0.46777200	-3.46124900
H	-4.56786700	-1.48441000	-2.56192000
C	-5.20444500	1.28573200	-2.21863900
H	-3.32742700	2.30172300	-1.96504800
H	-4.26308600	1.10088800	-4.15677400
H	-5.71266600	0.10871500	-4.00263600
H	-5.69706900	2.22883600	-2.48189700
H	-5.91478500	0.72286300	-1.59781400
P	-2.86277200	0.02216500	-1.67893000
O	-1.44715200	0.32087200	-2.10954100

C	-4.13944300	2.02734000	0.01053900
C	-3.13014900	-1.31337600	-4.17247200
H	-2.63665300	-2.24446500	-3.88530500
H	-3.79122200	-1.52968400	-5.01990500
H	-2.35594500	-0.61545200	-4.50490100
H	-3.20261600	2.18459600	0.54869600
H	-4.68535000	2.97832000	0.00017300
H	-4.73304200	1.30420800	0.57727800
C	-0.20950100	0.72032600	0.72546900
H	-1.27274900	0.89748800	0.59832300
C	0.08132500	0.82850800	2.20734200
C	-1.06179300	0.76736100	3.16912700
O	-2.22068700	1.21095600	2.63009200
C	-3.35295200	1.17160600	3.50796300
H	-3.16023200	1.76298100	4.40616100
H	-4.17937800	1.59233700	2.93634000
H	-3.57133300	0.14015200	3.79324500
O	-0.98184800	0.37944700	4.31952100
C	1.29874600	0.94185400	2.75442400
H	1.40007600	0.98921000	3.83357300
H	2.19351800	0.99402800	2.15055600
C	0.97565700	3.85113600	1.13361300
C	0.16416000	3.15367900	0.23122800
C	-0.99654800	3.77746500	-0.24002100
C	-1.35833400	5.05128300	0.19624600
C	-0.55057600	5.72936000	1.11014600
C	0.62154900	5.12723200	1.57090400
H	1.89222000	3.38976200	1.48582800
H	-1.60853400	3.25645500	-0.97003700
H	-2.26360100	5.51744900	-0.18418300
H	-0.82574400	6.72334800	1.45209400
H	1.26352300	5.65349800	2.27237700
C	0.48908800	1.74262800	-0.23104900
C	1.94469800	1.51103300	-0.47949000
H	2.51453500	2.30148500	-0.95514000
C	2.52911600	0.31586700	-0.24919400
O	1.91029900	-0.71870300	0.33640300
C	3.90276300	0.07071700	-0.56914200
C	5.05851100	-0.20578000	-0.82710600
C	6.41217400	-0.51900700	-1.13051000
C	6.92317800	-1.80511700	-0.86623300

C	7.26495000	0.44708200	-1.69964400
C	8.24755900	-2.11105700	-1.16323400
H	6.26763900	-2.55089900	-0.42790000
C	8.58806000	0.13199200	-1.99344200
H	6.87399800	1.43854800	-1.90466900
C	9.08517000	-1.14590300	-1.72725700
H	8.62868400	-3.10677300	-0.95394800
H	9.23493400	0.88667400	-2.43216300
H	10.11865600	-1.38811600	-1.95787700
H	-0.03817800	1.59444000	-1.18015500

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C	8.31191400	1.46769000	-1.22241600
C	7.73269600	1.40000700	0.07358200
C	8.57516500	1.64493000	1.17140500
C	9.90888400	2.01921900	1.03218600
C	10.44337000	2.18313300	-0.24025000
C	9.64679900	1.89360800	-1.34411900
H	8.18422400	1.55916000	2.17358600
H	10.50582300	2.20618300	1.91956300
H	11.46821500	2.51384100	-0.37988100
H	10.08718700	1.98516000	-2.33212300
C	5.45874300	-0.63625800	0.45666900
C	4.78647500	1.82046600	-0.66031200
C	4.29437100	-0.63867000	-0.56640300
H	5.07177800	-0.89452600	1.44533400
C	3.66661000	0.76129100	-0.65952100
H	5.30675200	1.71886200	-1.61151200
H	4.69565800	-0.90709900	-1.54448400
H	3.54750900	-1.38396800	-0.27209400
H	3.06598200	0.86309300	-1.57092700
H	2.99637200	0.93723600	0.18734900
P	5.97194300	1.16385300	0.62340900
C	6.59119800	-1.60193700	0.10616900
C	4.30072200	3.25790300	-0.49258400
H	5.13165400	3.96559000	-0.40755000
H	3.70338600	3.54372400	-1.36675100
H	3.66451100	3.37929300	0.38900000
H	7.41422600	-1.54713700	0.82703200

H	6.21008000	-2.62995800	0.11126200
H	6.98123300	-1.39121200	-0.89274100
C	7.71250000	2.33445000	-3.99704100
C	8.81339800	-0.18322000	-3.69616400
C	8.34783200	1.70129500	-5.25301000
H	8.41944000	3.05669800	-3.57065000
C	9.43143600	0.71094000	-4.78972100
H	8.11870800	-0.88122500	-4.18398100
H	7.57433900	1.16045500	-5.81429700
H	8.75169800	2.47018600	-5.92065900
H	9.81052100	0.10458500	-5.62004600
H	10.29175900	1.26073900	-4.38399300
P	7.58715800	0.90718700	-2.81359900
O	6.22850000	0.26155800	-2.72889500
C	9.79814300	-0.99445600	-2.85642100
C	6.36155000	3.01154100	-4.22586200
H	5.99601000	3.48897300	-3.31019700
H	6.44367200	3.78422400	-4.99851700
H	5.61144100	2.28057500	-4.54230300
H	9.27783500	-1.58721100	-2.09676700
H	10.35676400	-1.68622400	-3.49707600
H	10.52121000	-0.35612100	-2.34154100
C	5.61787100	1.88500600	2.95724100
C	4.37348100	2.72328700	5.21684800
C	3.54168400	2.59726800	4.14199100
C	4.08859900	1.73018400	3.02299300
H	2.52445400	2.96589900	4.10503200
O	5.57318500	2.20422000	5.17297400
C	3.98551000	3.47244100	6.38037000
C	3.68671500	4.08985700	7.38397000
C	3.33287000	4.81770700	8.55368800
C	2.02321500	5.30705800	8.72839900
C	4.28721700	5.06343800	9.56078500
C	1.68286600	6.01847100	9.87488400
H	1.28532500	5.11944100	7.95485200
C	3.93840400	5.77601900	10.70392400
H	5.29706900	4.68879400	9.42827700
C	2.63688000	6.25635700	10.86700100
H	0.66860000	6.38936800	9.99561500
H	4.68537800	5.95820900	11.47182000
H	2.36803000	6.81227800	11.76082300

H	3.64422900	2.07156900	2.08266900
C	3.67297500	0.27896200	3.23460200
C	4.36558100	-0.55719400	4.12442200
C	2.54990100	-0.23344900	2.57581400
C	3.97547100	-1.88429600	4.29493300
H	5.18536100	-0.14595300	4.70394300
C	2.15738200	-1.56151200	2.74683600
H	1.97153600	0.41502600	1.92343600
C	2.88023100	-2.39842900	3.59642900
H	4.52676400	-2.51937600	4.98331400
H	1.28825800	-1.93961600	2.21511000
H	2.58469100	-3.43576800	3.72597800
C	6.23250700	3.22134400	3.02789200
C	5.60100900	4.32977700	2.60389200
H	4.65944300	4.28465700	2.07564700
H	6.02823800	5.30454000	2.80885000
C	7.47315800	3.40879800	3.83926900
O	8.10363500	2.23926500	4.12825800
C	9.12861100	2.33755700	5.12201300
H	8.68757900	2.65563800	6.07003600
H	9.54597900	1.33403200	5.21429900
H	9.89798300	3.05352800	4.82122500
O	7.90866900	4.48620600	4.18796700
H	6.22067400	1.05238400	3.27535900