Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

A Novel Method for the Synthesis of Dihydrofuranyl Alcohols through cascade reactions of 1,3-Diketones and α, β-Unsaturated Epoxides

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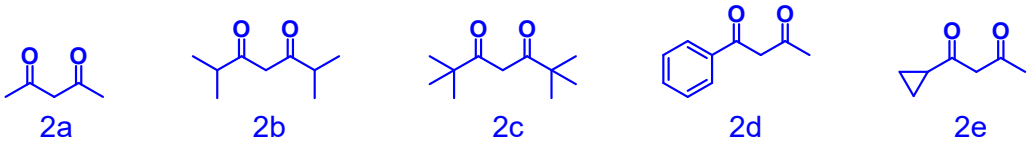
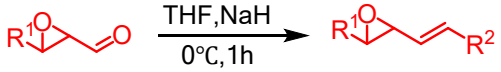
1.Data for Nucleophilic Reagents



All nucleophilic reagents, other chemicals and solvents were purchased from commercial company and used as received.

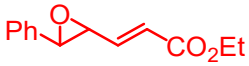
2.General Procedure for Synthesis of raw material



I II

Dry THF and NaH (0.5625 M, 1.2 equiv.) were added to a three-neck flask at 0 ° C, and phosphorus Yelide reagent (0.45 M, 1.2 equiv.) was dropped-added to the three-neck flask. The reaction was stirred for 5min and then the corresponding epoxy aldehyde Ⅰ (0.375 M, 1 equiv.) was added. The mixture was stirred at 0 °C for 1 hours. Then the reaction was quenched with water, extraction with EtOAc, washed with brine, drying over Na_2SO_4, evaporation, and purification by flash column chromatography provided α,β-unsaturated epoxides **II** as a clear, colorless oil. Compound Ⅰ was obtained from trans cinnamaldehyde, so compound **II** was trans α, β-Unsaturated Epoxides.

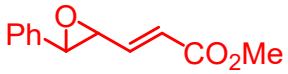
Ethyl (E)-3-(3-phenyloxiran-2-yl)acrylate



(1a): Colorless oil. R_f=0.25（petroleum ether/EtOAc = 30:1）

1H NMR (400 MHz, Chloroform-d) δ 7.38 – 7.33 (m, 3H), 7.29 (dd, J = 7.7, 1.9 Hz, 2H), 6.82 (dd, J = 15.7, 6.9 Hz, 1H), 6.20 (dd, J = 15.7, 0.8 Hz, 1H), 4.23 (q, J = 7.1 Hz, 2H), 3.84 (d, J = 1.8 Hz, 1H), 3.48 (ddd, J = 7.0, 1.8, 0.8 Hz, 1H), 1.31 (t, J = 7.1 Hz, 3H).13C NMR (101 MHz, Chloroform-d) δ 165.56, 143.59, 136.13, 128.63, 125.53, 124.06, 61.01, 60.64, 60.54, 14.22. HRMS calcd for $C_{13}H_{14}O_3$ [M + Na]$^+$: 241.0835, found: 241.0854.

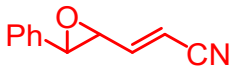
Methyl (E)-3-(3-phenyloxiran-2-yl)acrylate



(1b): Colorless oil. R_f=0.25（petroleum ether/EtOAc = 30:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.39 – 7.33 (m, 3H), 7.29 (dd, J = 7.8, 1.8 Hz, 2H), 6.84 (dd, J = 15.7, 6.8 Hz, 1H), 6.21 (dd, J = 15.7, 0.8 Hz, 1H), 3.83 (d, J = 1.9 Hz, 1H), 3.77 (s, 3H), 3.48 (ddd, J = 6.9, 1.8, 0.8 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 166.00, 143.91, 136.10, 128.64, 125.55, 123.57, 61.05, 60.49, 51.74. HRMS calcd for $C_{12}H_{12}O_3$ [M + Na]$^+$: 227.0679, found: 227.0694.

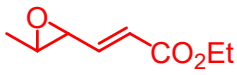
(E)-3-(3-phenyloxiran-2-yl)acrylonitrile



(1c): Colorless oil. R_f=0.2（petroleum ether/EtOAc = 30:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.40 (ddd, J = 5.3, 4.3, 2.4 Hz, 3H), 7.34 – 7.29 (m, 2H), 6.72 (dd, J = 16.2, 5.6 Hz, 1H), 5.74 (dd, J = 16.2, 1.0 Hz, 1H), 3.82 (d, J = 1.9 Hz, 1H), 3.50 (ddd, J = 5.7, 1.9, 0.9 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-d) δ 149.67, 135.30, 129.01, 128.77, 125.56, 116.52, 101.91, 61.77, 60.08. HRMS calcd for $C_{11}H_9NO$ [M + Na]$^+$: 194.0576, found: 194.0592.

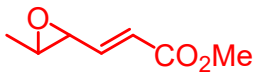
Ethyl (E)-3-(3-methyloxiran-2-yl)acrylate



(1d): Colorless oil. R_f=0.25（petroleum ether/EtOAc = 30:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 6.65 (ddd, J = 15.6, 7.1, 1.2 Hz, 1H), 6.10 (dd, J = 15.7, 0.9 Hz, 1H), 4.21 – 4.15 (m, 2H), 3.16 (dt, J = 7.2, 1.4 Hz, 1H), 2.95 (qt, J = 5.2, 1.5 Hz, 1H), 1.37 (dd, J = 5.2, 1.4 Hz, 3H), 1.28 – 1.25 (m, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 165.59, 144.58, 123.64, 60.49, 57.31, 57.15, 17.46, 14.15. HRMS calcd for $C_8H_{12}O_3$ [M + Na]$^+$: 179.0679, found: 179.0700.

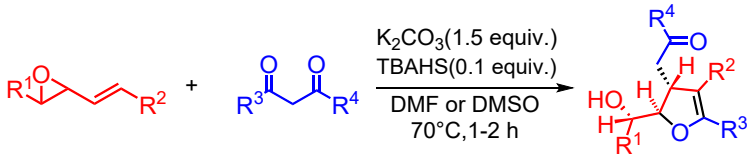
Methyl (E)-3-(3-methyloxiran-2-yl)acrylate



(1e): Colorless oil. R_f=0.25（petroleum ether/EtOAc = 30:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 6.69 (dd, J = 15.7, 7.0 Hz, 1H), 6.13 (dd, J = 15.7, 0.9 Hz, 1H), 3.74 (d, J = 0.8 Hz, 3H), 3.18 (dd, J = 7.1, 1.9 Hz, 1H), 2.97 (tdd, J = 5.2, 4.3, 2.1 Hz, 1H), 1.39 (d, J = 5.2 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 166.08, 144.92, 123.14, 57.39, 57.14, 51.65, 17.47. HRMS calcd for $C_7H_{10}O_3$ [M + Na]$^+$: 165.0522, found: 165.0543.

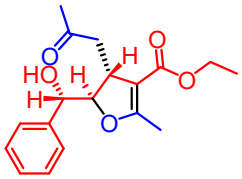
3.General procedure for the reaction of α,β-unsaturated epoxides with β-dicarbonyl compounds



1 2 6

1 (0.458mmol, 1 equiv.)**,** **2** (0.687mmol, 1.5 equiv.)**,** **K_2CO_3** (0.687mmol, 1.5 equiv.) and tetrabutylammonium hydrogen sulfate (**TBAHS**, 0.0458mmol, 0.1 equiv.) were added to 4 ml of DMSO or DMF, and product **6** was obtained by stirring at 70 ° C until the reaction was completed (monitored by TLC). Then the reaction was extracted with EtOAc, washed with brine, drying over Na_2SO_4, evaporation, the product was obtained after purification by column chromatography.

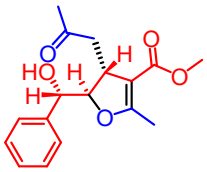
Ethyl (4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-2-methyl-4-(2-oxopropyl)-4,5-dihydrofuran-3-carboxylate



(6aa): New compound. Pale yellow solid. m.p.58℃. R_f=0.2（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.29 (m, 5H), 4.69 (d, *J* = 7.4 Hz, 1H), 4.31 (dd, *J* = 7.4, 4.0 Hz, 1H), 4.16 (p, *J* = 6.2, 5.3 Hz, 3H), 3.67 – 3.59 (m, 1H), 3.13 (dd, *J* = 18.4, 2.9 Hz, 1H), 2.56 (dd, *J* = 18.4, 10.5 Hz, 1H), 2.19 – 2.12 (m, 6H), 1.29 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 209.92, 168.32, 165.41, 140.43, 128.16, 127.94, 127.01, 103.98, 90.32, 74.60, 59.61, 47.61, 40.35, 30.03, 14.39. HRMS calcd for $C_{18}H_{22}O_5$ [M + Na]$^+$: 341.1359, found: 341.1360.

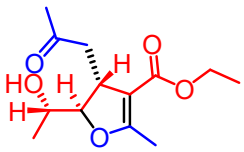
Methyl (4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-2-methyl-4-(2-oxopropyl)-4,5-dihydrofuran-3-carboxylate



(6ba): New compound. Pale yellow oil. R_f=0.18（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.40 – 7.28 (m, 5H), 4.69 (d, J = 7.2 Hz, 1H), 4.32 (dd, J = 7.2, 4.1 Hz, 1H), 3.69 (s, 3H), 3.64 – 3.59 (m, 1H), 3.10 (dd, J = 18.3, 3.0 Hz, 1H), 2.54 (dd, J = 18.3, 10.4 Hz, 1H), 2.17 – 2.11 (m, 6H).^{13}C NMR (101 MHz, Chloroform-d) δ 209.72, 168.65, 165.78, 140.33, 128.15, 127.94, 127.00, 103.80, 90.42, 74.58, 50.81, 47.63, 40.25, 29.99, 14.32. HRMS calcd for $C_{17}H_{20}O_5$ [M + Na]$^+$: 327.1203, found: 327.1203.

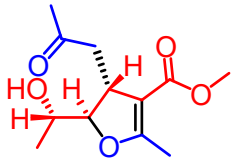
Ethyl (4R*,5R*)-5-((S*)-1-hydroxyethyl)-2-methyl-4-(2-oxopropyl)-4,5-dihydrofuran-3-carboxylate



(6da): New compound. Pale yellow oil. R_f=0.1（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 4.18 (qd, J = 7.1, 2.4 Hz, 2H), 4.03 (dd, J = 6.8, 4.2 Hz, 1H), 3.82 (p, J = 6.5 Hz, 1H), 3.49 – 3.43 (m, 1H), 3.24 (s, 1H), 3.18 (dd, J = 18.5, 2.8 Hz, 1H), 2.58 (dd, J = 18.5, 10.5 Hz, 1H), 2.21 – 2.17 (m, 6H), 1.28 (d, J = 7.2 Hz, 3H), 1.22 (d, J = 6.2 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 209.34, 168.46, 165.49, 103.90, 91.47, 68.87, 59.56, 47.91, 40.20, 30.11, 18.59, 14.36, 14.34. HRMS calcd for $C_{13}H_{20}O_5$ [M + Na]$^+$: 279.1203, found: 279.1207.

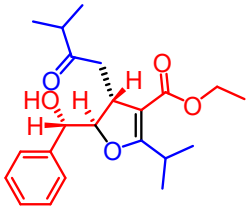
Methyl (4R*,5R*)-5-((S*)-1-hydroxyethyl)-2-methyl-4-(2-oxopropyl)-4,5-dihydrofuran-3-carboxylate



(6ea): New compound. Pale yellow oil. R_f=0.08（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 4.03 (dd, J = 6.8, 4.2 Hz, 1H), 3.86 – 3.80 (m, 1H), 3.72 (s, 3H), 3.49 – 3.43 (m, 1H), 3.18 (dd, J = 18.5, 2.8 Hz, 1H), 2.59 (dd, J = 18.5, 10.5 Hz, 1H), 2.22 – 2.17 (m, 6H), 1.23 (d, J = 6.2 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 209.29, 168.81, 165.89, 103.72, 91.57, 68.88, 50.81, 47.93, 40.13, 30.11, 18.59, 14.32. HRMS calcd for $C_{12}H_{18}O_5$ [M + Na]$^+$: 265.1046, found: 265.1049.

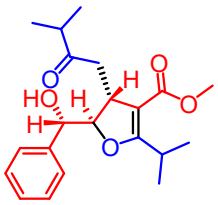
Ethyl (4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-2-isopropyl-4-(3-methyl-2-oxobutyl)-4,5-dihydrofuran-3-carboxylate



(6ab): New compound. Pale yellow oil. R_f=0.55（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.41 – 7.29 (m, 5H), 4.60 (dd, J = 8.3, 3.8 Hz, 1H), 4.54 (d, J = 3.9 Hz, 1H), 4.24 – 4.14 (m, 3H), 3.67 (ddd, J = 10.8, 3.8, 2.6 Hz, 1H), 3.58 (p, J = 6.9 Hz, 1H), 3.23 (dd, J = 18.8, 2.6 Hz, 1H), 2.66 – 2.53 (m, 2H), 1.30 (t, J = 7.1 Hz, 3H), 1.15 (d, J = 6.9 Hz, 6H), 1.10 (d, J = 6.9 Hz, 3H), 1.03 (d, J = 7.0 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 216.63, 176.08, 165.31, 141.11, 128.03, 127.79, 127.17, 101.67, 90.26, 74.64, 59.51, 44.39, 40.97, 40.57, 26.98, 19.71, 19.45, 18.24, 18.19, 14.39. HRMS calcd for $C_{22}H_{30}O_5$ [M + Na]$^+$: 397.1985, found: 397.1985.

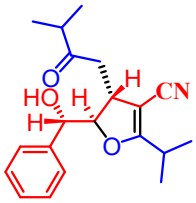
Methyl (4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-2-isopropyl-4-(3-methyl-2-oxobutyl)-4,5-dihydrofuran-3-carboxylate



(6bb): New compound. Pale yellow oil. R_f=0.5（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.41 – 7.30 (m, 5H), 4.60 (dd, J = 8.2, 3.7 Hz, 1H), 4.48 (d, J = 3.8 Hz, 1H), 4.22 (dd, J = 8.2, 3.7 Hz, 1H), 3.72 (s, 3H), 3.67 (ddd, J = 10.8, 3.8, 2.7 Hz, 1H), 3.57 (p, J = 6.9 Hz, 1H), 3.19 (dd, J = 18.7, 2.7 Hz, 1H), 2.65 – 2.55 (m, 2H), 1.14 (d, J = 6.9 Hz, 6H), 1.10 (d, J = 6.9 Hz, 3H), 1.03 (d, J = 6.9 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 216.51, 176.34, 165.74, 141.01, 128.04, 127.81, 127.17, 101.50, 90.36, 74.62, 50.83, 44.48, 40.96, 40.48, 26.96, 19.72, 19.49, 18.30, 18.12. HRMS calcd for $C_{21}H_{28}O_5$ [M + Na]$^+$: 383.1829, found: 383.1828.

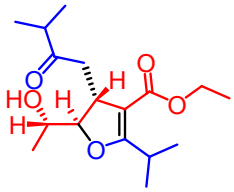
(4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-2-isopropyl-4-(3-methyl-2-oxobutyl)-4,5-dihydrofuran-3-carbonitrile



(6cb): New compound. Pale yellow oil. R_f=0.45（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.39 – 7.31 (m, 5H), 4.78 (d, J = 6.4 Hz, 1H), 4.44 (dd, J = 6.4, 5.4 Hz, 1H), 3.80 (s, 1H), 3.55 (ddd, J = 9.2, 5.3, 3.7 Hz, 1H), 2.85 (dd, J = 18.5, 3.8 Hz, 1H), 2.79 – 2.73 (m, 1H), 2.64 – 2.56 (m, 2H), 1.12 (d, J = 6.9 Hz, 12H).^{13}C NMR (101 MHz, Chloroform-d) δ 213.94, 178.31, 139.54, 128.27, 128.20, 127.09, 115.90, 91.67, 82.47, 74.42, 44.03, 41.04, 40.37, 28.28, 19.64, 19.59, 18.16, 18.08. HRMS calcd for $C_{20}H_{25}NO_3$ [M + Na]$^+$: 350.1727, found: 350.1736.

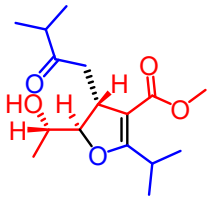
Ethyl (4R*,5R*)-5-((S*)-1-hydroxyethyl)-2-isopropyl-4-(3-methyl-2-oxobutyl)-4,5-dihydrofuran-3-carboxylate



(6db): New compound. Pale yellow oil. R_f=0.4（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 4.23 – 4.13 (m, 2H), 3.96 (dd, J = 7.3, 3.7 Hz, 1H), 3.78 (td, J = 6.9, 4.1 Hz, 1H), 3.61 (p, J = 6.9 Hz, 1H), 3.44 (ddd, J = 10.9, 3.8, 2.5 Hz, 1H), 3.39 (d, J = 4.4 Hz, 1H), 3.22 (dd, J = 18.6, 2.5 Hz, 1H), 2.64 – 2.53 (m, 2H), 1.29 (t, J = 7.1 Hz, 3H), 1.23 (d, J = 6.2 Hz, 3H), 1.15 – 1.11 (m, 12H).^{13}C NMR (101 MHz, Chloroform-d) δ 215.79, 176.21, 165.36, 101.74, 91.17, 68.84, 59.44, 44.58, 40.94, 40.35, 27.00, 19.67, 19.37, 18.83, 18.18, 18.15, 14.35. HRMS calcd for $C_{17}H_{28}O_5$ [M + Na]$^+$: 335.1829, found: 335.1833.

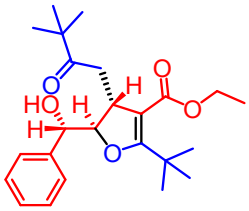
Methyl (4R*,5R*)-5-((S*)-1-hydroxyethyl)-2-isopropyl-4-(3-methyl-2-oxobutyl)-4,5-dihydrofuran-3-carboxylate



(6eb): New compound. Pale yellow oil. R_f=0.36（petroleum ether/EtOAc = 4:1）

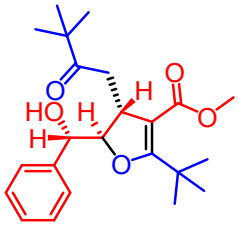
^{1}H NMR (400 MHz, Chloroform-d) δ 3.96 (dd, J = 7.2, 3.8 Hz, 1H), 3.82 – 3.75 (m, 1H), 3.71 (s, 3H), 3.60 (p, J = 6.9 Hz, 1H), 3.44 (ddd, J = 10.8, 3.8, 2.5 Hz, 1H), 3.34 (d, J = 4.4 Hz, 1H), 3.18 (dd, J = 18.6, 2.6 Hz, 1H), 2.64 – 2.54 (m, 2H), 1.23 (d, J = 6.2 Hz, 3H), 1.16 – 1.11 (m, 12H).^{13}C NMR (101 MHz, Chloroform-d) δ 215.66, 176.48, 165.78, 101.59, 91.28, 68.83, 50.74, 44.66, 40.94, 40.28, 26.98, 19.67, 19.39, 18.75, 18.21, 18.07. HRMS calcd for $C_{16}H_{26}O_5$ [M + Na]$^+$: 321.1672, found: 321.1676.

Ethyl (4R*,5R*)-2-(tert-butyl)-4-(3,3-dimethyl-2-oxobutyl)-5-((S*)-hydroxy(phenyl)methyl)-4,5-dihydrofuran-3-carboxylate



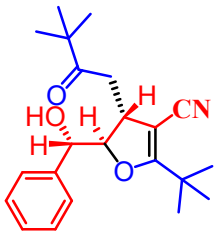
(6ac): New compound. Pale yellow solid. m.p.96℃. R_f=0.7（petroleum ether/EtOAc = 4:1）
^{1}H NMR (400 MHz, Chloroform-d) δ 7.41 – 7.30 (m, 5H), 4.62 (dd, J = 8.4, 3.5 Hz, 1H), 4.51 (d, J = 3.6 Hz, 1H), 4.21 – 4.08 (m, 3H), 3.67 (dt, J = 11.0, 2.7 Hz, 1H), 3.28 (dd, J = 18.9, 2.4 Hz, 1H), 2.60 (dd, J = 18.9, 11.0 Hz, 1H), 1.29 (t, J = 7.1 Hz, 3H), 1.24 (s, 9H), 1.20 (s, 9H).^{13}C NMR (101 MHz, Chloroform-d) δ 218.31, 177.83, 164.66, 141.13, 128.00, 127.79, 127.15, 101.72, 89.24, 74.54, 59.57, 44.26, 42.70, 41.40, 34.50, 27.49, 26.48, 14.34. HRMS calcd for $C_{24}H_{34}O_5$ [M + Na]$^+$: 425.2298, found: 425.2296.

Methyl (4R*,5R*)-2-(tert-butyl)-4-(3,3-dimethyl-2-oxobutyl)-5-((S*)-hydroxy(phenyl)methyl)-4,5-dihydrofuran-3-carboxylate



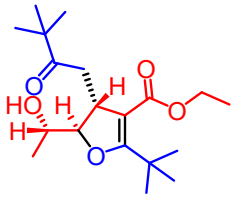
(6bc): New compound. Pale yellow oil. R_f=0.65（petroleum ether/EtOAc = 4:1）
^{1}H NMR (400 MHz, Chloroform-d) δ 7.41 – 7.30 (m, 5H), 4.61 (dd, J = 8.3, 3.0 Hz, 1H), 4.42 (d, J = 3.5 Hz, 1H), 4.09 (dd, J = 8.3, 3.3 Hz, 1H), 3.71 (s, 3H), 3.67 (dt, J = 10.9, 2.8 Hz, 1H), 3.21 (dd, J = 18.9, 2.5 Hz, 1H), 2.61 (dd, J = 18.9, 11.0 Hz, 1H), 1.24 (s, 9H), 1.20 (s, 9H).^{13}C NMR (101 MHz, Chloroform-d) δ 218.18, 178.18, 165.08, 141.01, 128.02, 127.82, 127.14, 101.53, 89.38, 74.51, 50.81, 44.28, 42.57, 41.51, 34.53, 27.45, 26.46. HRMS calcd for $C_{23}H_{32}O_5$ [M + Na]$^+$: 411.2142, found: 411.2142.

(4R*,5R*)-2-(tert-butyl)-4-(3,3-dimethyl-2-oxobutyl)-5-((S*)-hydroxy(phenyl)methyl)-4,5-dihydrofuran-3-carbonitrile



(6cc): New compound. Pale yellow solid. m.p.99℃. R_f=0.6（petroleum ether/EtOAc = 4:1）
^{1}H NMR (400 MHz, Chloroform-d) δ 7.42 – 7.31 (m, 5H), 4.75 (d, J = 7.0 Hz, 1H), 4.35 (dd, J = 7.0, 5.1 Hz, 1H), 3.89 (s, 1H), 3.58 (ddd, J = 10.1, 5.1, 3.3 Hz, 1H), 2.98 (dd, J = 18.7, 3.2 Hz, 1H), 2.66 (dd, J = 18.7, 10.0 Hz, 1H), 1.21 (d, J = 16.4 Hz, 18H).^{13}C NMR (101 MHz, Chloroform-d) δ 215.96, 179.16, 139.87, 128.23, 128.17, 127.15, 116.52, 90.95, 74.61, 44.31, 41.94, 40.72, 34.55, 28.00, 26.44. HRMS calcd for $C_{22}H_{29}NO_3$ [M + Na]$^+$: 378.2040, found: 378.2042.

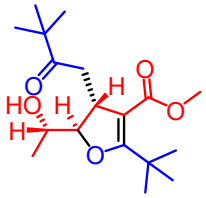
Ethyl (4R*,5R*)-2-(tert-butyl)-4-(3,3-dimethyl-2-oxobutyl)-5-((S*)-1-hydroxyethyl)-4,5-dihydrofuran-3-carboxylate



(6dc): New compound. Pale yellow oil. R_f=0.5（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 4.21 – 4.10 (m, 3H), 3.85 (dd, J = 7.6, 3.4 Hz, 1H), 3.76 (ddd, J = 7.5, 6.0, 4.1 Hz, 1H), 3.47 – 3.43 (m, 1H), 3.22 (dd, J = 18.7, 2.3 Hz, 1H), 2.59 (dd, J = 18.7, 10.9 Hz, 1H), 1.31 (s, 9H), 1.27 – 1.25 (m, 3H), 1.23 (d, J = 6.1 Hz, 3H), 1.17 (s, 9H).^{13}C NMR (101 MHz, Chloroform-d) δ 217.40, 177.66, 164.78, 101.89, 90.03, 68.63, 59.50, 44.12, 42.27, 41.62, 34.57, 27.59, 26.42, 19.00, 14.28. HRMS calcd for $C_{19}H_{32}O_5$ [M + Na]$^+$: 363.2142, found: 363.2146.

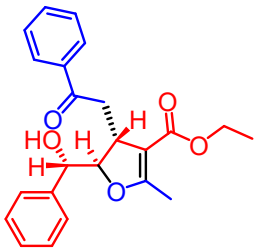
Methyl (4R*,5R*)-2-(tert-butyl)-4-(3,3-dimethyl-2-oxobutyl)-5-((S*)-1-hydroxyethyl)-4,5-dihydrofuran-3-carboxylate



(6ec): New compound. Pale yellow oil. R_f=0.45（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 3.84 (dd, J = 7.5, 3.4 Hz, 1H), 3.76 (ddd, J = 7.4, 6.0, 4.1 Hz, 1H), 3.70 (s, 3H), 3.47 (ddd, J = 10.8, 3.4, 2.4 Hz, 1H), 3.37 (d, J = 4.2 Hz, 1H), 3.16 (dd, J = 18.7, 2.4 Hz, 1H), 2.61 (dd, J = 18.7, 10.8 Hz, 1H), 1.32 (s, 9H), 1.24 (d, J = 6.1 Hz, 3H), 1.18 (s, 9H).^{13}C NMR (101 MHz, Chloroform-d) δ 165.20, 101.71, 90.18, 68.64, 50.73, 44.16, 42.19, 41.73, 34.61, 27.56, 26.41, 18.97. HRMS calcd for $C_{18}H_{30}O_5$ [M + Na]$^+$: 349.1985, found: 349.1989.

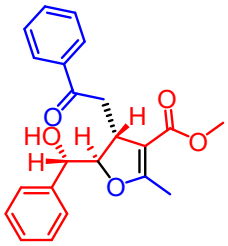
Ethyl (4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-2-methyl-4-(2-oxo-2-phenylethyl)-4,5-dihydrofuran-3-carboxylate



(6ad): New compound. Pale yellow solid. m.p.131℃. R_f=0.3（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 8.00 (d, J = 7.6 Hz, 2H), 7.65 – 7.60 (m, 1H), 7.50 (t, J = 7.5 Hz, 2H), 7.41 (d, J = 8.2 Hz, 2H), 7.37 – 7.29 (m, 3H), 4.79 – 4.74 (m, 1H), 4.44 (dd, J = 7.7, 3.7 Hz, 1H), 4.31 (d, J = 3.7 Hz, 1H), 4.23 – 4.17 (m, 2H), 3.85 (dd, J = 11.7, 3.6 Hz, 1H), 3.74 (dd, J = 18.1, 2.6 Hz, 1H), 3.09 (dd, J = 18.1, 10.8 Hz, 1H), 2.20 (s, 3H), 1.30 (td, J = 7.1, 1.1 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 200.66, 168.53, 165.47, 140.48, 136.29, 133.70, 128.69, 128.28, 128.12, 127.94, 127.05, 104.12, 90.34, 74.78, 59.63, 42.68, 40.89, 14.41. HRMS calcd for $C_{23}H_{24}O_5$ [M + Na]$^+$: 403.1516, found: 403.1519.

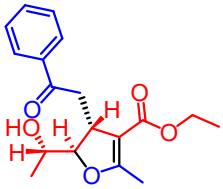
Methyl (4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-2-methyl-4-(2-oxo-2-phenylethyl)-4,5-dihydrofuran-3-carboxylate



(6bd): New compound. Pale yellow oil. R_f=0.27（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 8.01 – 7.96 (m, 2H), 7.64 – 7.59 (m, 1H), 7.52 – 7.47 (m, 2H), 7.42 – 7.39 (m, 2H), 7.37 – 7.29 (m, 3H), 4.78 (dd, J = 7.3, 3.7 Hz, 1H), 4.45 (dd, J = 7.3, 3.8 Hz, 1H), 4.22 (d, J = 3.7 Hz, 1H), 3.83 (dddd, J = 10.7, 4.1, 2.8, 1.5 Hz, 1H), 3.72 (m, 4H), 3.09 (dd, J = 18.1, 10.7 Hz, 1H), 2.19 (d, J = 1.3 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 200.54, 168.82, 165.85, 140.39, 136.35, 133.65, 128.67, 128.26, 128.11, 127.94, 127.06, 103.96, 90.50, 74.77, 50.84, 42.73, 40.81, 14.35. HRMS calcd for $C_{22}H_{22}O_5$ [M + Na]$^+$: 389.1359, found: 389.1370.

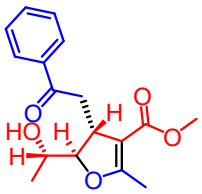
Ethyl (4R*,5R*)-5-((S*)-1-hydroxyethyl)-2-methyl-4-(2-oxo-2-phenylethyl)-4,5-dihydrofuran-3-carboxylate



(6dd): New compound. Pale yellow oil. R_f=0.2（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 8.03 – 7.98 (m, 2H), 7.51 – 7.41 (m, 3H), 4.23 – 4.16 (m, 3H), 3.91 (td, J = 6.5, 4.3 Hz, 1H), 3.77 (dd, J = 17.7, 2.6 Hz, 1H), 3.67 (dddd, J = 10.7, 4.0, 2.6, 1.3 Hz, 1H), 3.31 (d, J = 4.5 Hz, 1H), 3.06 (dd, J = 17.7, 10.7 Hz, 1H), 2.26 (d, J = 1.3 Hz, 3H), 1.30 (t, J = 7.1 Hz, 3H), 1.23 (d, J = 6.2 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 200.30, 168.70, 165.58, 136.47, 133.57, 128.68, 128.21, 104.16, 91.43, 68.91, 59.61, 43.08, 40.66, 18.59, 14.40, 14.39. HRMS calcd for $C_{18}H_{22}O_5$ [M + Na]$^+$: 341.1359, found: 341.1363.

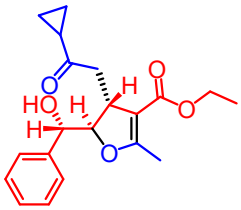
Methyl (4R*,5R*)-5-((S*)-1-hydroxyethyl)-2-methyl-4-(2-oxo-2-phenylethyl)-4,5-dihydrofuran-3-carboxylate



(6ed): New compound. Pale yellow oil. R_f=0.18（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 8.01 – 7.97 (m, 2H), 7.51 – 7.40 (m, 3H), 4.17 (dd, J = 6.6, 3.9 Hz, 1H), 3.91 (ddd, J = 9.2, 6.6, 3.6 Hz, 1H), 3.76 – 3.70 (m, 4H), 3.65 (dtd, J = 4.0, 3.3, 2.6, 1.2 Hz, 1H), 3.35 (d, J = 4.5 Hz, 1H), 3.07 (dd, J = 17.8, 10.5 Hz, 1H), 2.25 (d, J = 1.3 Hz, 3H), 1.23 (d, J = 6.3 Hz, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 200.21, 169.01, 165.97, 136.48, 133.56, 128.67, 128.20, 103.98, 91.58, 68.90, 50.83, 43.10, 40.58, 18.51, 14.35. HRMS calcd for $C_{17}H_{20}O_5$ [M + Na]$^+$: 327.1203, found: 327.1207.

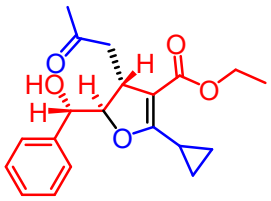
Ethyl (4R*,5R*)-4-(2-cyclopropyl-2-oxoethyl)-5-((S*)-hydroxy(phenyl)methyl)-2-methyl-4,5-dihydrofuran-3-carboxylate



(6ae$_1$): New compound. Pale yellow solid. m.p.83℃. R_f=0.25（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.40 – 7.30 (m, 5H), 4.65 (dd, J = 7.9, 3.7 Hz, 1H), 4.45 (d, J = 3.8 Hz, 1H), 4.29 (dd, J = 7.9, 3.8 Hz, 1H), 4.20 (q, J = 7.1 Hz, 2H), 3.70 – 3.63 (m, 1H), 3.32 (dd, J = 18.6, 2.7 Hz, 1H), 2.74 (dd, J = 18.6, 10.8 Hz, 1H), 2.16 (d, J = 1.3 Hz, 3H), 1.94 (td, J = 7.8, 3.9 Hz, 1H), 1.30 (t, J = 7.1 Hz, 3H), 1.16 – 1.09 (m, 2H), 0.96 (ddd, J = 7.5, 3.4, 2.1 Hz, 2H).^{13}C NMR (101 MHz, Chloroform-d) δ 212.11, 168.24, 165.44, 140.84, 128.08, 127.84, 127.06, 103.94, 90.38, 74.74, 59.56, 47.00, 40.63, 21.00, 14.40, 14.34, 11.40, 11.37. HRMS calcd for $C_{20}H_{24}O_5$ [M + Na]$^+$: 367.1516, found: 367.1512.

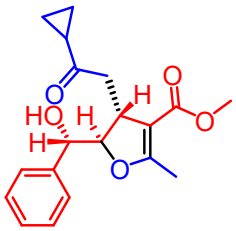
Ethyl (4R*,5R*)-2-cyclopropyl-5-((S*)-hydroxy(phenyl)methyl)-4-(2-oxopropyl)-4,5-dihydrofuran-3-carboxylate



(6ae$_2$): New compound. Pale yellow oil. R_f=0.22（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.36 – 7.29 (m, 5H), 4.58 (dd, J = 8.2, 3.3 Hz, 1H), 4.25 – 4.17 (m, 4H), 3.70 (dt, J = 10.7, 3.2 Hz, 1H), 3.18 (dd, J = 18.5, 2.8 Hz, 1H), 2.68 – 2.62 (m, 1H), 2.57 (dd, J = 18.5, 10.7 Hz, 1H), 2.18 (s, 3H), 1.31 (t, J = 7.1 Hz, 3H), 0.90 – 0.79 (m, 4H).^{13}C NMR (101 MHz, Chloroform-d) δ 210.28, 171.82, 165.90, 140.84, 128.11, 127.88, 127.00, 103.06, 89.80, 74.62, 59.51, 47.65, 41.09, 30.00, 14.46, 9.23, 7.97, 7.47. HRMS calcd for $C_{20}H_{24}O_5$ [M + Na]$^+$: 367.1516, found: 367.1511.

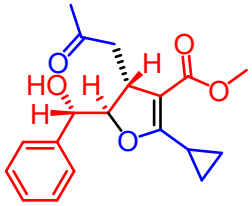
Methyl (4R*,5R*)-4-(2-cyclopropyl-2-oxoethyl)-5-((S*)-hydroxy(phenyl)methyl)-2-methyl-4,5-dihydrofuran-3-carboxylate



(6be$_1$): New compound. Pale yellow oil. R_f=0.23（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.39 – 7.30 (m, 5H), 4.65 (dd, J = 7.7, 3.3 Hz, 1H), 4.44 (d, J = 3.8 Hz, 1H), 4.29 (dd, J = 7.7, 3.9 Hz, 1H), 3.72 (s, 3H), 3.67 – 3.63 (m, 1H), 3.30 (dd, J = 18.6, 2.8 Hz, 1H), 2.74 (dd, J = 18.6, 10.8 Hz, 1H), 2.15 (d, J = 1.3 Hz, 3H), 1.97 – 1.91 (m, 1H), 1.12 (dd, J = 4.4, 2.9 Hz, 2H), 0.98 – 0.93 (m, 2H).^{13}C NMR (101 MHz, Chloroform-d) δ 212.02, 168.59, 165.86, 140.73, 128.08, 127.86, 127.06, 103.74, 90.47, 74.72, 50.82, 47.09, 40.53, 20.99, 14.31, 11.44. HRMS calcd for $C_{19}H_{22}O_5$ [M + Na]$^+$: 353.1359, found: 353.1360.

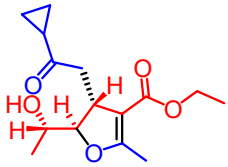
Methyl (4R*,5R*)-2-cyclopropyl-5-((S*)-hydroxy(phenyl)methyl)-4-(2-oxopropyl)-4,5-dihydrofuran-3-carboxylate



(6be$_2$): New compound. Pale yellow solid. m.p.89℃. R_f=0.2（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.36 – 7.29 (m, 5H), 4.58 (dd, J = 8.1, 2.9 Hz, 1H), 4.26 (d, J = 3.5 Hz, 1H), 4.19 (dd, J = 8.1, 3.6 Hz, 1H), 3.74 (s, 3H), 3.72 – 3.66 (m, 1H), 3.16 (dd, J = 18.5, 2.9 Hz, 1H), 2.64 (ddd, J = 8.0, 4.3, 2.0 Hz, 1H), 2.56 (dd, J = 18.5, 10.6 Hz, 1H), 2.18 (s, 3H), 0.89 – 0.80 (m, 4H).^{13}C NMR (101 MHz, Chloroform-d) δ 210.22, 172.14, 166.30, 140.76, 128.11, 127.89, 127.01, 102.86, 89.88, 74.61, 50.78, 47.65, 41.01, 29.98, 9.25, 8.04, 7.54. HRMS calcd for $C_{19}H_{22}O_5$ [M + Na]$^+$: 353.1359, found: 353.1362.

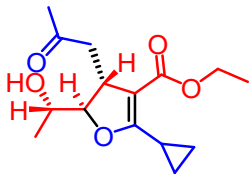
Ethyl (4R*,5R*)-4-(2-cyclopropyl-2-oxoethyl)-5-((S*)-1-hydroxyethyl)-2-methyl-4,5-dihydrofuran-3-carboxylate



(6de$_1$): New compound. Pale yellow oil. R_f=0.17（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 4.23 – 4.17 (m, 2H), 4.01 (dd, J = 7.2, 4.1 Hz, 1H), 3.80 (td, J = 6.6, 3.7 Hz, 1H), 3.49 (dddt, J = 6.8, 4.1, 2.7, 1.5 Hz, 2H), 3.37 – 3.32 (m, 1H), 2.72 (dd, J = 18.4, 10.8 Hz, 1H), 2.21 (d, J = 1.3 Hz, 3H), 1.96 – 1.92 (m, 1H), 1.31 (t, J = 7.1 Hz, 3H), 1.22 (d, J = 6.2 Hz, 3H), 1.08 (dtd, J = 6.9, 3.5, 1.5 Hz, 2H), 0.95 – 0.92 (m, 2H).^{13}C NMR (101 MHz, Chloroform-d) δ 211.53, 168.39, 165.55, 103.96, 91.48, 68.90, 59.54, 47.43, 40.38, 20.91, 18.80, 14.39, 14.35, 11.21, 11.16. HRMS calcd for $C_{15}H_{22}O_5$ [M + Na]$^+$: 305.1359, found: 305.1367.

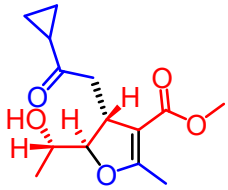
Ethyl (4R*,5R*)-2-cyclopropyl-5-((S*)-1-hydroxyethyl)-4-(2-oxopropyl)-4,5-dihydrofuran-3-carboxylate



(6de$_2$): New compound. Pale yellow oil. R_f=0.14（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 4.24 – 4.19 (m, 2H), 3.93 (dd, J = 7.2, 3.8 Hz, 1H), 3.79 – 3.72 (m, 1H), 3.48 (ddd, J = 10.6, 3.8, 2.7 Hz, 1H), 3.20 (dd, J = 18.5, 2.7 Hz, 2H), 2.70 (ddd, J = 8.3, 5.8, 3.1 Hz, 1H), 2.59 (dd, J = 18.5, 10.6 Hz, 1H), 2.19 (s, 3H), 1.31 (t, J = 7.1 Hz, 3H), 1.17 (d, J = 6.2 Hz, 3H), 0.97 – 0.88 (m, 4H).^{13}C NMR (101 MHz, Chloroform-d) δ 209.59, 171.87, 165.95, 103.08, 90.89, 68.76, 59.46, 47.86, 40.70, 30.09, 18.85, 14.44, 9.20, 8.10, 7.41. HRMS calcd for $C_{15}H_{22}O_5$ [M + Na]$^+$: 305.1359, found: 305.1366.

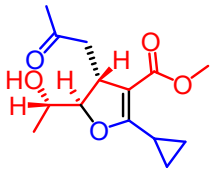
Methyl (4R*,5R*)-4-(2-cyclopropyl-2-oxoethyl)-5-((S*)-1-hydroxyethyl)-2-methyl-4,5-dihydrofuran-3-carboxylate



(6ee$_1$): New compound. Pale yellow oil. R_f=0.15（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.00 (dd, *J* = 7.0, 4.1 Hz, 1H), 3.78 (tt, *J* = 6.6, 3.4 Hz, 1H), 3.71 (s, 3H), 3.50 (d, *J* = 4.3 Hz, 1H), 3.48 – 3.42 (m, 1H), 3.30 (dd, *J* = 18.3, 2.6 Hz, 1H), 2.70 (dd, *J* = 18.3, 10.7 Hz, 1H), 2.19 (d, *J* = 1.3 Hz, 3H), 1.92 (ddd, *J* = 7.8, 4.5, 3.2 Hz, 1H), 1.19 (d, *J* = 6.3 Hz, 3H), 1.08 – 1.03 (m, 2H), 0.93 – 0.89 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-d) δ 211.40, 168.76, 165.93, 103.76, 91.54, 68.84, 50.76, 47.48, 40.25, 20.88, 18.64, 14.28, 11.21, 11.17. HRMS calcd for $C_{14}H_{20}O_5$ [M + Na]$^+$: 291.1203, found: 291.1203.

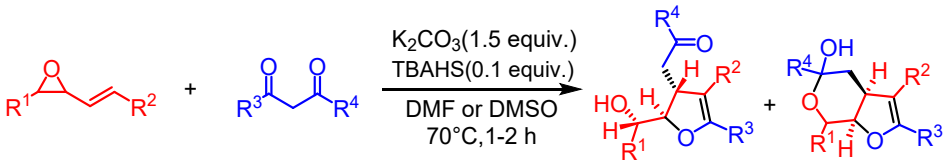
Methyl (4R*,5R*)-2-cyclopropyl-5-((S*)-1-hydroxyethyl)-4-(2-oxopropyl)-4,5-dihydrofuran-3-carboxylate



(6ee$_2$): New compound. Pale yellow oil. R_f=0.11（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-*d*) δ 3.96 – 3.91 (m, 1H), 3.77 – 3.74 (m, 1H), 3.73 (s, 3H), 3.46 (ddd, *J* = 10.6, 3.8, 2.7 Hz, 1H), 3.24 (d, *J* = 4.2 Hz, 1H), 3.17 (dd, *J* = 18.5, 2.7 Hz, 1H), 2.72 – 2.65 (m, 1H), 2.58 (dd, *J* = 18.5, 10.6 Hz, 1H), 2.18 (s, 3H), 1.16 (d, *J* = 6.2 Hz, 3H), 0.98 – 0.88 (m, 4H). ^{13}C NMR (101 MHz, Chloroform-d) δ 209.53, 172.20, 166.35, 102.87, 90.97, 68.74, 50.73, 47.85, 40.62, 30.08, 18.76, 9.21, 8.16, 7.46. HRMS calcd for $C_{14}H_{20}O_5$ [M + Na]$^+$: 291.1203, found: 291.1204.

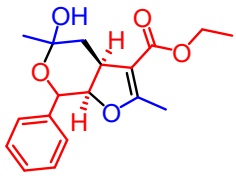
4.Preparation method of 7



1 2 6 7

After the reaction of α,β-unsaturated epoxides with β-dicarbonyl compounds is completed, the product **6** will partially undergo hemiketal reaction to obtain **7**. Because the hemiketal is a six-membered ring structure, product 10 is relatively stable, like fructose, it is stable as a six-ring hemiketal.

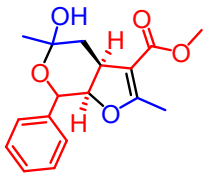
Ethyl (3aS*,7aR*)-5-hydroxy-2,5-dimethyl-7-phenyl-3a,4,7,7a-tetrahydro-5H-furo[2,3-c]pyran-3-carboxylate



(7aa): New compound. Pale yellow oil. Rf=0.28（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.48 – 7.45 (m, 2H), 7.42 – 7.31 (m, 5H), 4.91 (d, J = 9.3 Hz, 1H), 4.63 (t, J = 9.5 Hz, 1H), 4.21 (dddd, J = 16.8, 10.8, 7.1, 3.4 Hz, 3H), 3.34 – 3.24 (m, 1H), 2.43 (dd, J = 14.2, 5.2 Hz, 1H), 2.22 (d, J = 1.2 Hz, 3H), 1.93 – 1.86 (m, 1H), 1.53 (s, 3H), 1.30 (d, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 169.28, 165.78, 139.88, 128.46, 128.04, 126.64, 106.07, 97.26, 84.81, 71.34, 59.58, 39.01, 36.30, 28.45, 14.39, 14.37. HRMS calcd for $C_{18}H_{22}O_5$ [M + Na]$^+$: 341.1359, found: 341.1359.

Methyl (3aS*,7aR*)-5-hydroxy-2,5-dimethyl-7-phenyl-3a,4,7,7a-tetrahydro-5H-furo[2,3-c]pyran-3-carboxylate

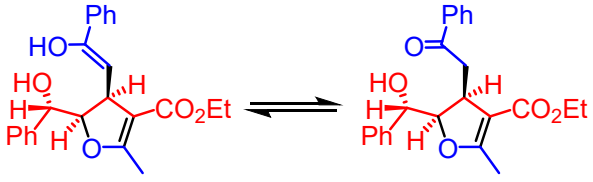


(7ba): New compound. Pale yellow oil. Rf=0.25（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.48 – 7.45 (m, 2H), 7.42 – 7.37 (m, 3H), 4.91 (d, J = 9.3 Hz, 1H), 4.64 (t, J = 9.5 Hz, 1H), 3.75 (s, 3H), 3.34 – 3.24 (m, 1H), 2.42 (dd, J = 14.2, 5.1 Hz, 1H), 2.22 (d, J = 1.2 Hz, 3H), 1.88 (t, J = 13.5 Hz, 1H), 1.53 (s, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 169.66, 166.21, 139.81, 128.49, 128.09, 126.64, 105.86, 97.27, 84.88, 77.39, 71.33, 50.92, 38.93, 36.27, 28.51, 14.37. HRMS calcd for $C_{17}H_{20}O_5$ [M + Na]$^+$: 327.1203, found: 327.1203.

Ethyl (4S*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-4-((Z)-2-hydroxy-2-phenylvinyl)-2-methyl-4,5-dihydrofuran-3-carboxylate and **Ethyl (4S*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-2-methyl-4-(2-oxo-2-phenylethyl)-4,5-dihydrofuran-3-carboxylate**

We took the HSQC spectrum and also took IR spectra of the compound both by tablet method of the crystals and by solution method in $CHCl_3$. The tablet method showed absorption by stretches of phenyl ketone functionality (1650 cm^{-1}) and alkene functionality (1650cm^{-1}) and ester functionality (1690 cm^{-1}), the solution method only indicated ester functionality (1690 cm^{-1}) and alkene functionality (1640 cm^{-1}).



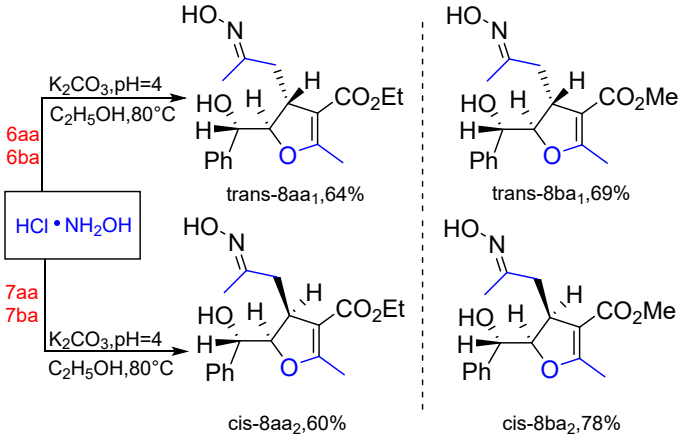
nmr structure　　crystal structure

(cis-6ad): New compound. yellow solid. m.p.147℃. Rf=0.28（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (dd, *J* = 8.1, 1.7 Hz, 2H), 7.51 (dt, *J* = 6.5, 1.5 Hz, 2H), 7.47 – 7.42 (m, 3H), 7.36 – 7.31 (m, 3H), 6.04 (d, *J* = 4.0 Hz, 1H), 4.89 (dd, *J* = 9.3, 8.2 Hz, 1H), 4.79 (d, *J* = 8.2 Hz, 1H), 4.33 – 4.23 (m, 2H), 4.06 (ddd, *J* = 9.3, 3.9, 1.7 Hz, 1H), 2.26 (d, *J* = 1.6 Hz, 3H), 1.38 (t, *J* = 7.1

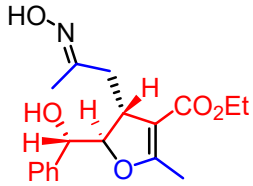
Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 167.35, 165.70, 152.19, 138.53, 134.79, 128.51, 128.40, 128.37, 128.22, 127.15, 124.80, 107.40, 98.61, 81.54, 76.38, 59.74, 39.90, 14.51, 14.39. HRMS calcd for $C_{23}H_{24}O_5$ [M + Na]+: 403.1516, found: 403.1519.

5.General procedure for the 8 derivatization reaction



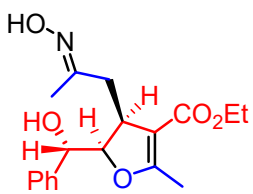
6 or **7** (0.329mmol, 1 equiv.) and hydroxylamine hydrochloride (0.658mmol, 2 equiv.) were added to 4ml of ethanol, adjusted to pH=4 by K_2CO_3 (2 M in H_2O), and reacted for 2h at 80 degrees. The product was obtained after purification by column chromatography.

Ethyl (4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-4-((E)-2-(hydroxyimino)propyl)-2-methyl-4,5-dihydrofuran-3-carboxylate



(8aa$_1$): New compound. white solid. m.p.186℃. Rf=0.16（petroleum ether/EtOAc = 4:1）
^{1}H NMR (400 MHz, Chloroform-d) δ 9.67 (s, 1H), 7.42 – 7.31 (m, 5H), 6.53 (s, 1H), 4.63 (d, *J* = 8.9 Hz, 1H), 4.41 (dd, *J* = 8.9, 3.4 Hz, 1H), 4.23 (qd, *J* = 7.1, 2.9 Hz, 2H), 3.77 – 3.70 (m, 1H), 2.88 (dd, *J* = 17.7, 2.6 Hz, 1H), 2.25 – 2.17 (m, 4H), 1.81 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 168.09, 165.62, 157.18, 141.06, 128.16, 127.84, 127.05, 104.72, 89.57, 74.86, 59.59, 41.43, 39.67, 14.86, 14.42, 14.33. HRMS calcd for $C_{18}H_{23}NO_5$ [M + Na]$^+$: 356.1468, found: 356.1468.

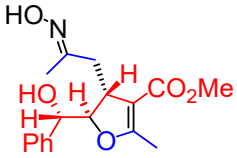
Ethyl (4S*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-4-((E)-2-(hydroxyimino)propyl)-2-methyl-4,5-dihydrofuran-3-carboxylate



(8aa$_2$): New compound. white solid. m.p.177℃. Rf=0.16（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.33 (m, 5H), 4.87 (d, *J* = 9.7 Hz, 1H), 4.48 (dd, *J* = 9.7, 7.4 Hz, 1H), 4.21 (q, *J* = 7.1 Hz, 2H), 3.53 (t, *J* = 8.1 Hz, 1H), 2.70 (dd, *J* = 16.7, 8.9 Hz, 1H), 2.39 (dd, *J* = 16.8, 2.6 Hz, 1H), 2.09 (d, *J* = 1.0 Hz, 3H), 2.00 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 168.80, 165.51, 159.50, 140.73, 128.22, 127.96, 127.13, 108.68, 88.09, 70.50, 59.61, 40.57, 35.11, 14.70, 14.41. HRMS calcd for $C_{18}H_{23}NO_5$ [M + Na]$^+$: 356.1468, found: 356.1468.

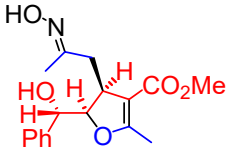
Methyl (4R*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-4-((E)-2-(hydroxyimino)propyl)-2-methyl-4,5-dihydrofuran-3-carboxylate



(8ba$_1$): New compound. white solid. m.p.189℃. Rf=0.13（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.31 (m, 5H), 4.63 (d, *J* = 8.6 Hz, 1H), 4.42 (dd, *J* = 8.6, 3.3 Hz, 1H), 3.75 (s, 3H), 3.71 (d, *J* = 11.7 Hz, 1H), 2.85 (dd, *J* = 17.5, 2.6 Hz, 1H), 2.26 – 2.17 (m, 4H), 1.82 (s, 3H). 13C NMR (101 MHz, Chloroform-d) δ 168.43, 166.00, 157.47, 140.92, 128.19, 127.86, 126.99, 104.59, 89.70, 50.83, 41.28, 39.75, 14.75, 14.30. HRMS calcd for $C_{17}H_{21}NO_5$ [M + Na]$^+$: 342.1312, found: 342.1312.

Methyl (4S*,5R*)-5-((S*)-hydroxy(phenyl)methyl)-4-((E)-2-(hydroxyimino)propyl)-2-methyl-4,5-dihydrofuran-3-carboxylate

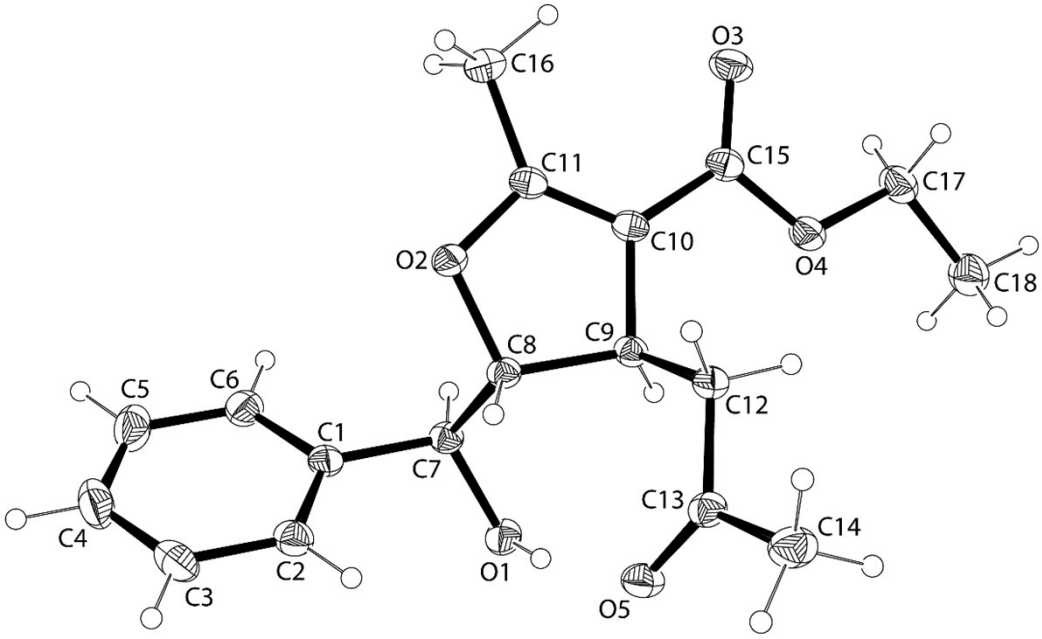


(8ba$_2$): New compound. white solid. m.p.179℃. Rf=0.13（petroleum ether/EtOAc = 4:1）

^{1}H NMR (400 MHz, Chloroform-d) δ 7.41 – 7.33 (m, 5H), 4.81 (d, J = 9.8 Hz, 1H), 4.46 (dd, J = 9.8, 7.2 Hz, 1H), 3.73 (s, 3H), 3.52 (dddd, J = 8.2, 7.2, 2.7, 1.4 Hz, 1H), 2.65 (dd, J = 17.1, 9.2 Hz, 1H), 2.35 (dd, J = 17.1, 2.3 Hz, 1H), 2.08 (d, J = 1.0 Hz, 3H), 1.97 (s, 3H).^{13}C NMR (101 MHz, Chloroform-d) δ 169.14, 165.95, 159.25, 140.52, 128.25, 128.02, 127.15, 108.54, 88.14, 70.48, 50.94, 40.43, 35.15, 14.85, 14.42. HRMS calcd for $C_{17}H_{21}NO_5$ [M + Na]$^+$: 342.1312, found: 342.1313.

6.X-Ray crystallography data

Crystal Structure of 6aa



Bond precision: C-C = 0.0021 A Wavelength=1.54178

Cell: a=9.2088(4) b=9.7622(4) c=21.0942(8)
alpha=78.302(2) beta=89.303(2) gamma=64.975(1)
Temperature: 173 K

	Calculated	Reported
Volume	1676.82(12)	1676.82(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H22 O5	C18 H22 O5
Sum formula	C18 H22 O5	C18 H22 O5
Mr	318.36	318.35
Dx,g cm-3	1.261	1.261
Z	4	4
Mu (mm-1)	0.752	0.752
F000	680.0	680.0
F000'	682.21	
h,k,lmax	11,11,25	11,11,25
Nref	6130	6072
Tmin,Tmax	0.900,0.921	0.704,0.753
Tmin'	0.900	

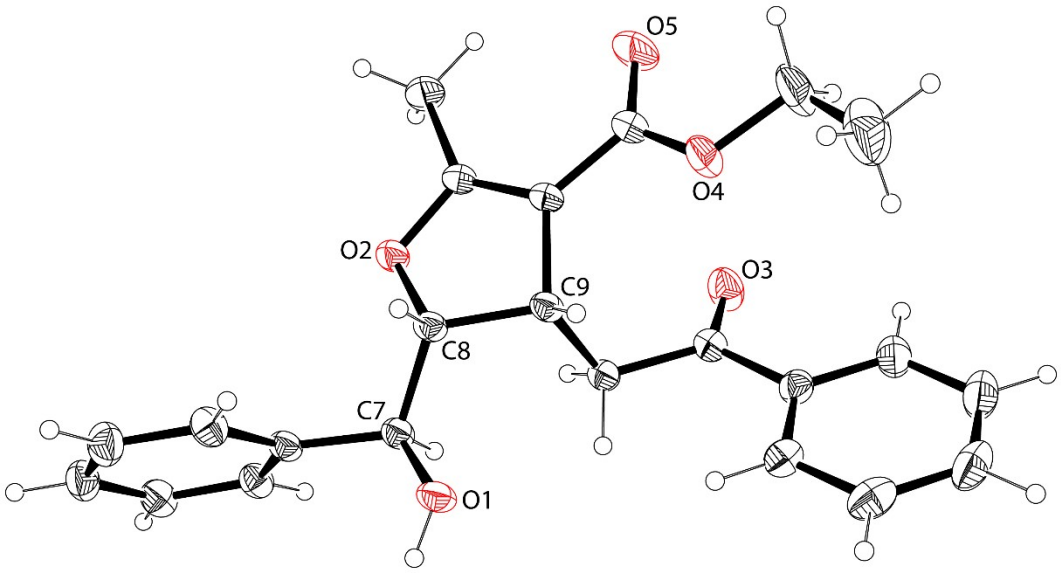
Correction method= # Reported T Limits: Tmin=0.704 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 68.200

R(reflections)= 0.0380(5571) wR2(reflections)= 0.0961(6072)

S = 1.031 Npar= 423

Crystal Structure of cis-6ad



Bond precision: C-C = 0.0027 A Wavelength=1.54178

Cell: a=9.2814(3) b=10.4848(3) c=11.7654(3)
alpha=64.177(1) beta=78.373(1) gamma=76.259(1)
Temperature: 173 K

	Calculated	Reported
Volume	994.79(5)	994.79(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C23 H24 O5	C23 H24 O5
Sum formula	C23 H24 O5	C23 H24 O5
Mr	380.42	380.42
Dx,g cm-3	1.270	1.270
Z	2	2
Mu (mm-1)	0.724	0.724
F000	404.0	404.0
F000'	405.28	
h,k,lmax	11,12,14	11,12,14
Nref	3640	3608
Tmin,Tmax	0.885,0.910	0.673,0.753
Tmin'	0.859	

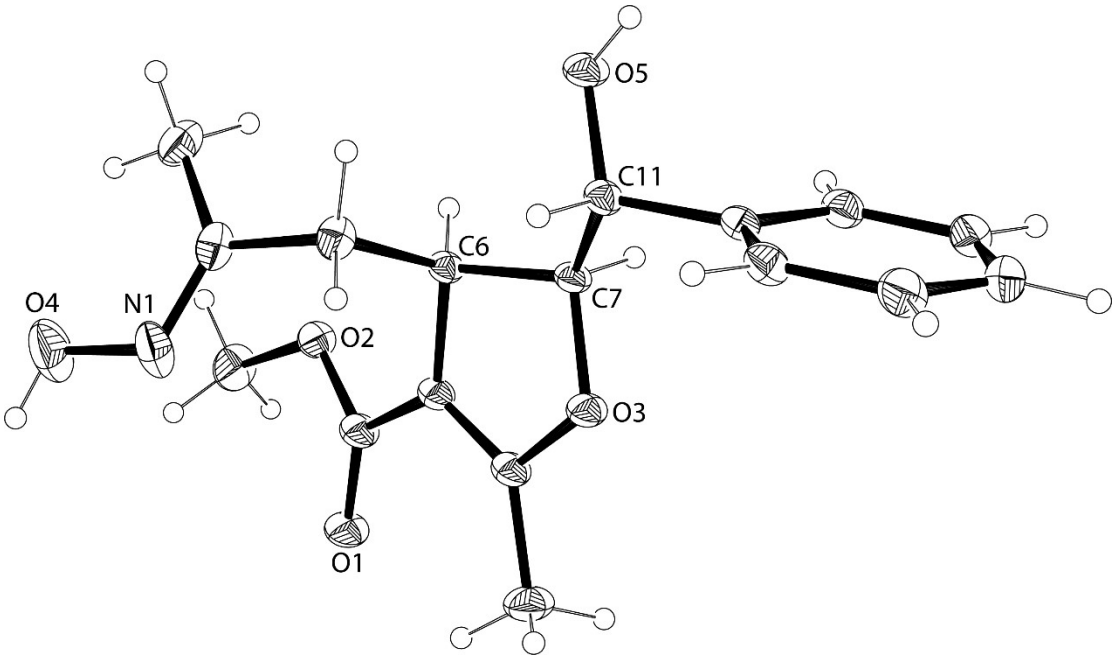
Correction method= # Reported T Limits: Tmin=0.673 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 68.265

R(reflections)= 0.0460(3150) wR2(reflections)= 0.1252(3608)

S = 1.052 Npar= 256

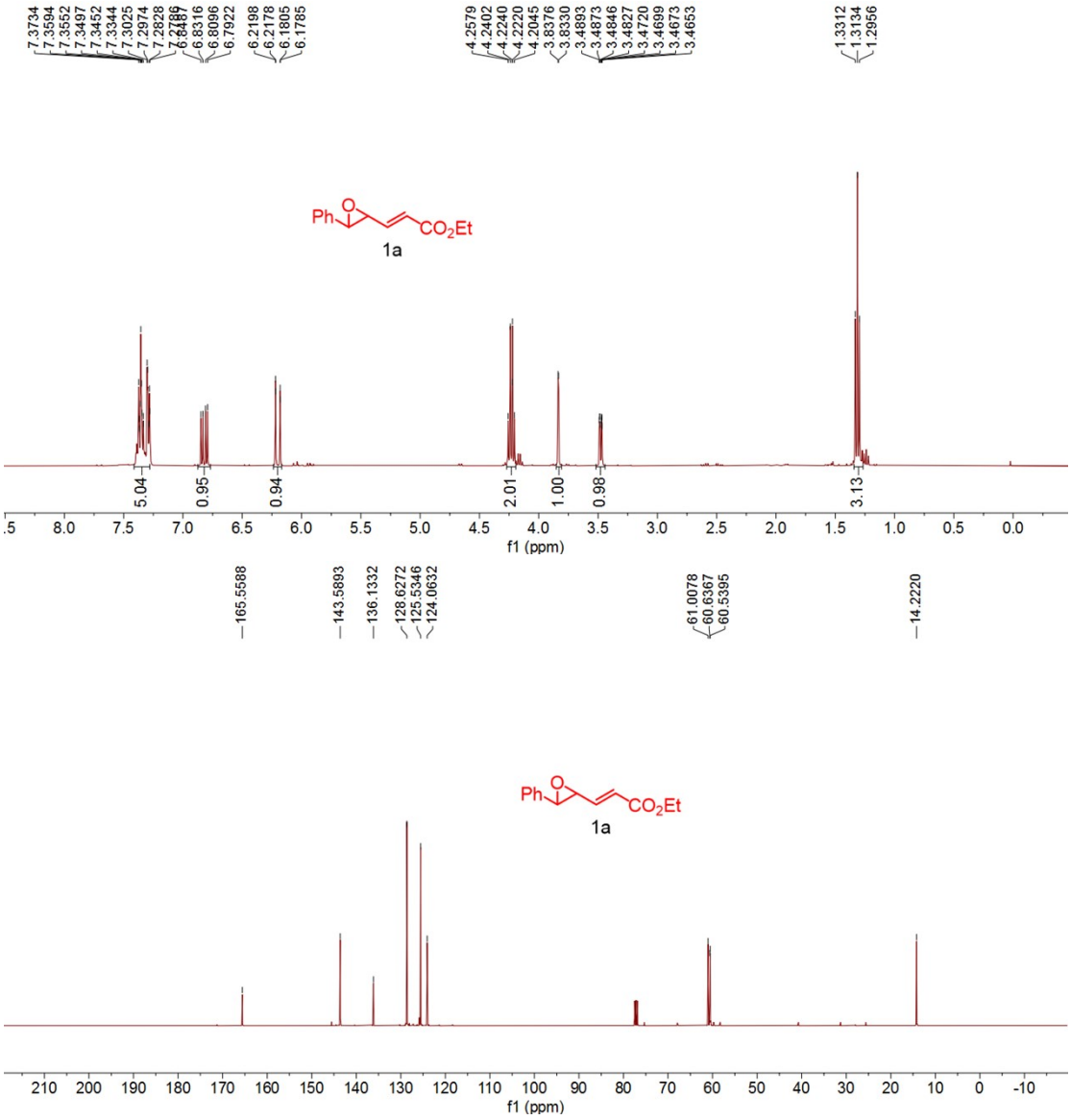
Crystal Structure of 8ba$_2$



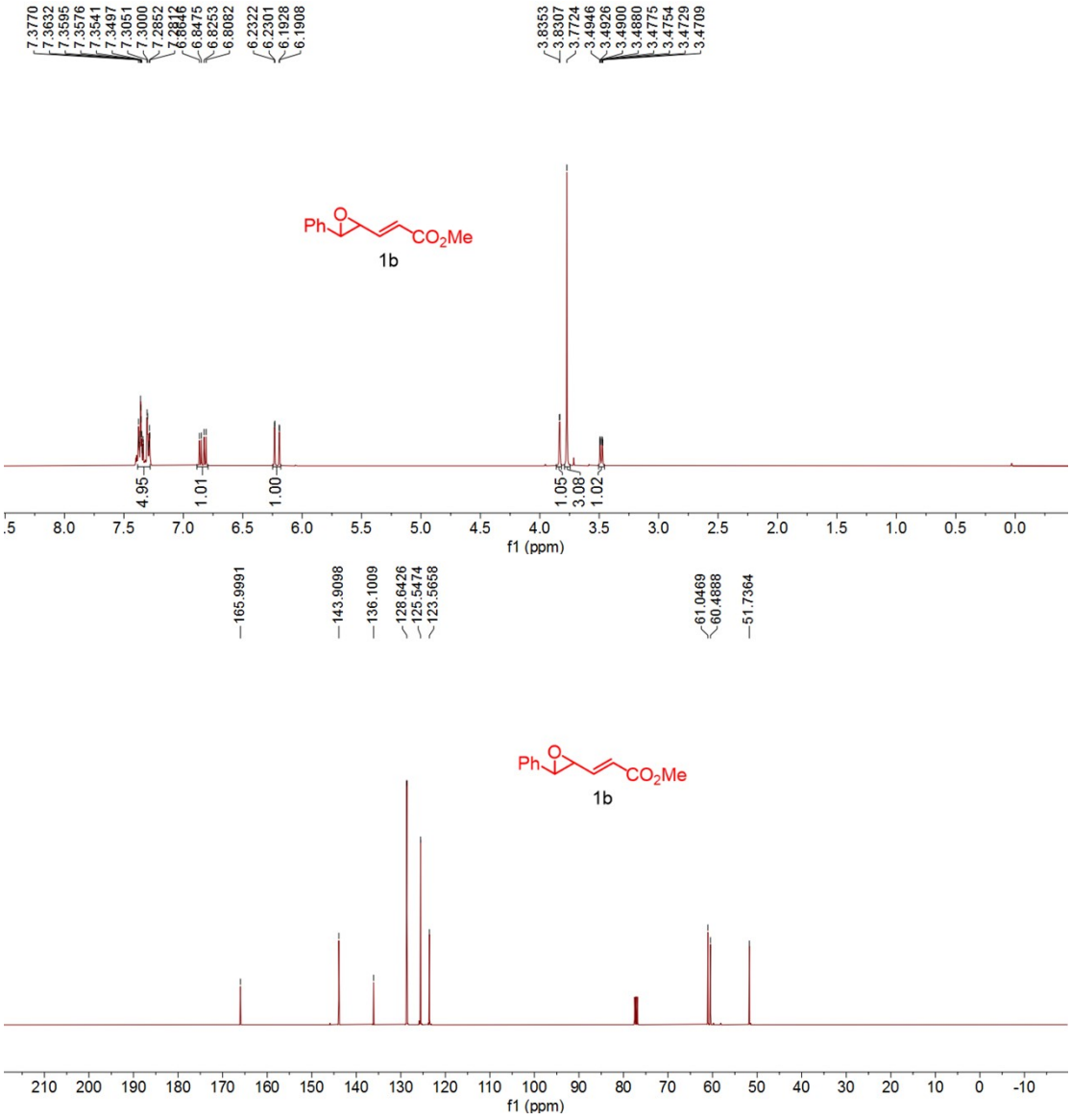
```
Bond precision:   C-C = 0.0035 A          Wavelength=1.54178

Cell:          a=9.2667(3)       b=9.3632(3)       c=10.5150(3)
               alpha=99.574(1)   beta=114.052(1)   gamma=97.069(1)
Temperature:   173 K

                Calculated                Reported
Volume          802.86(4)                 802.86(4)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C17 H21 N O5              C17 H21 N O5
Sum formula     C17 H21 N O5              C17 H21 N O5
Mr              319.35                    319.35
Dx,g cm-3       1.321                     1.321
Z               2                         2
Mu (mm-1)       0.806                     0.806
F000            340.0                     340.0
F000'           341.12
h,k,lmax        11,11,12                  11,11,12
Nref            3162                      3124
Tmin,Tmax       0.886,0.908               0.688,0.754
Tmin'           0.886

Correction method= # Reported T Limits: Tmin=0.688 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.988          Theta(max)= 72.044

R(reflections)= 0.0597( 2754)                wR2(reflections)=
                                             0.1608( 3124)
S = 1.079                 Npar= 242
```

7.^{1}H and ^{13}C NMR Spectrogram

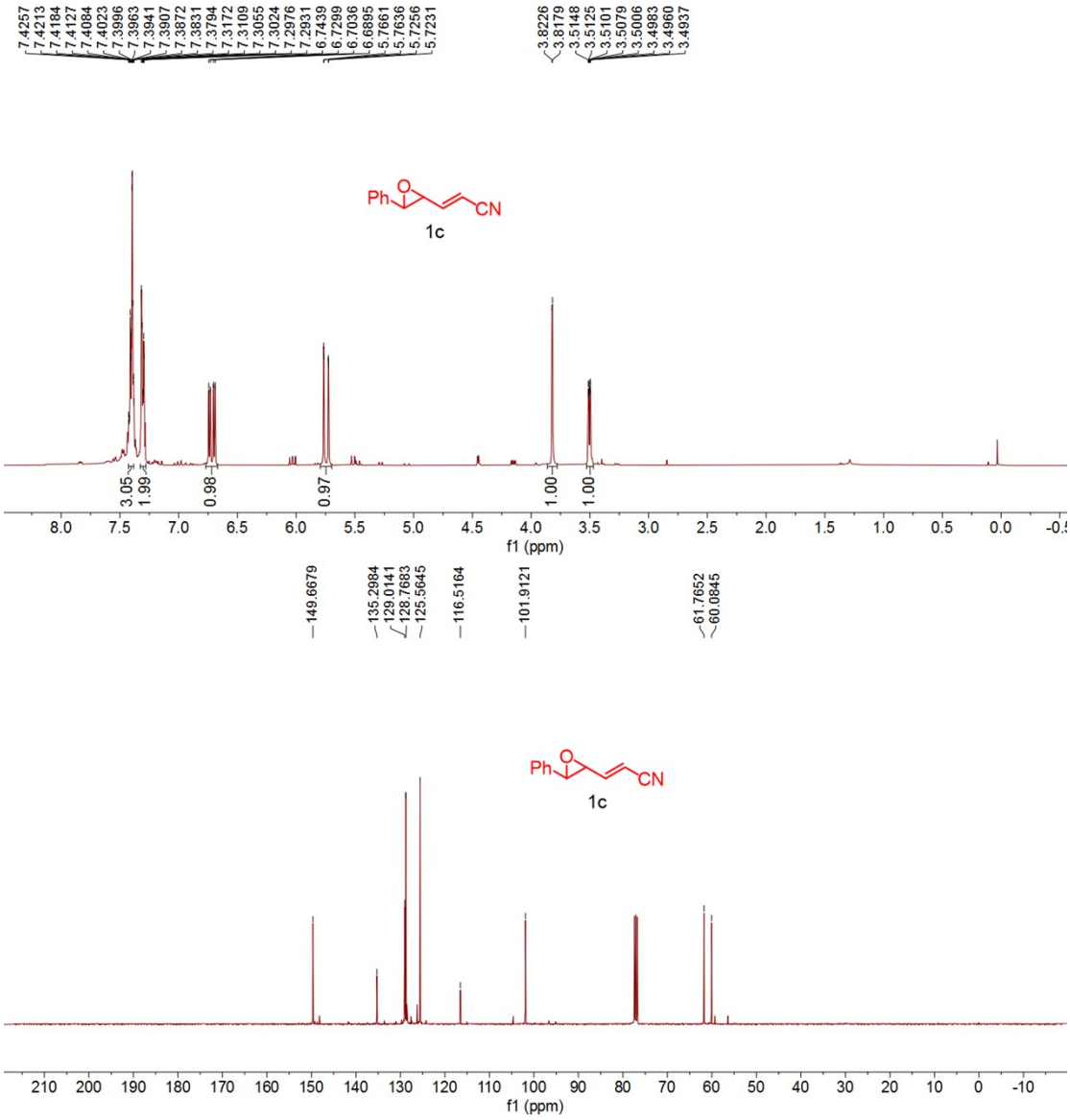
^{1}H and ^{13}C NMR Spectra for 1a



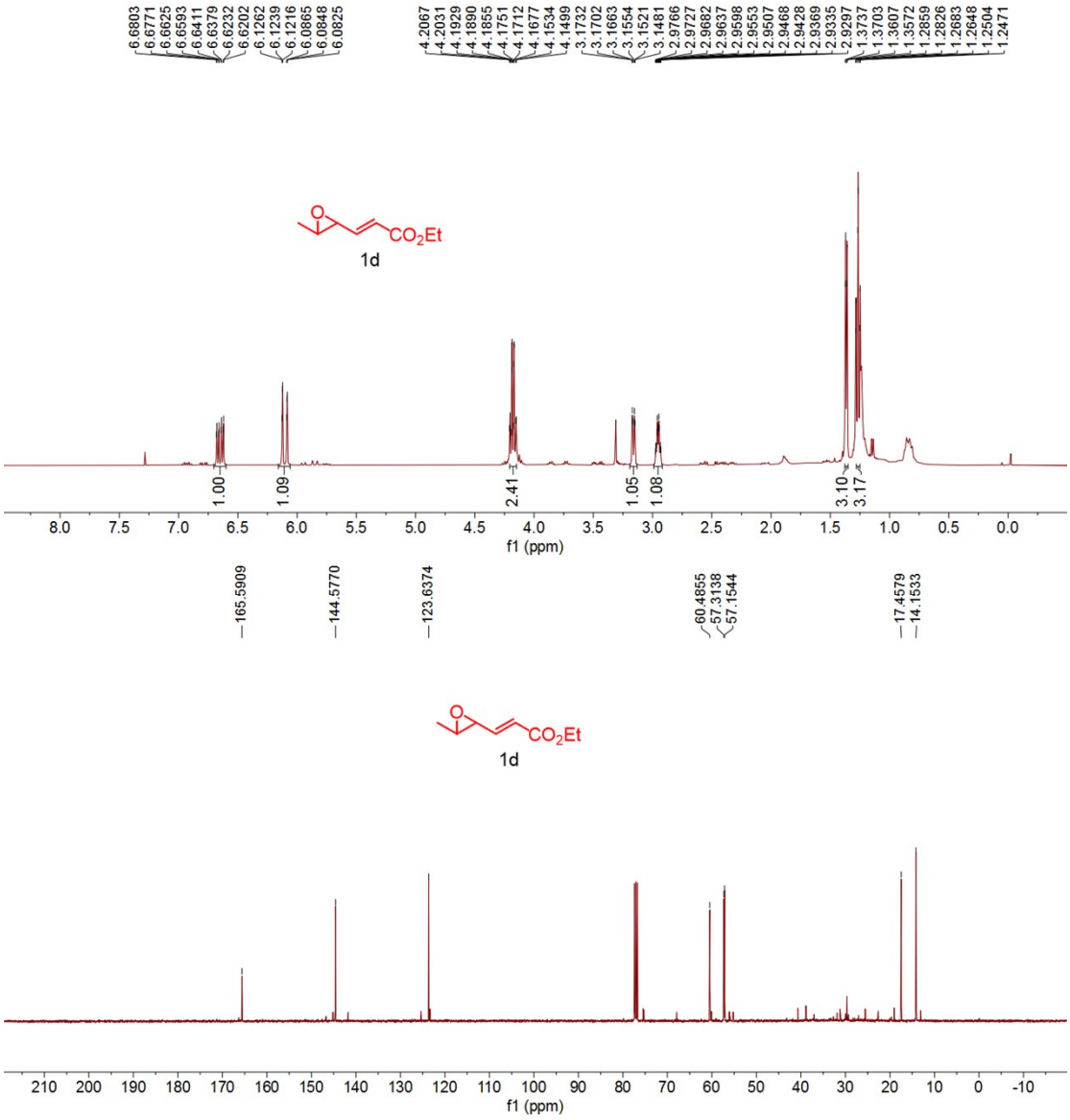
^{1}H and ^{13}C NMR Spectra for 1b



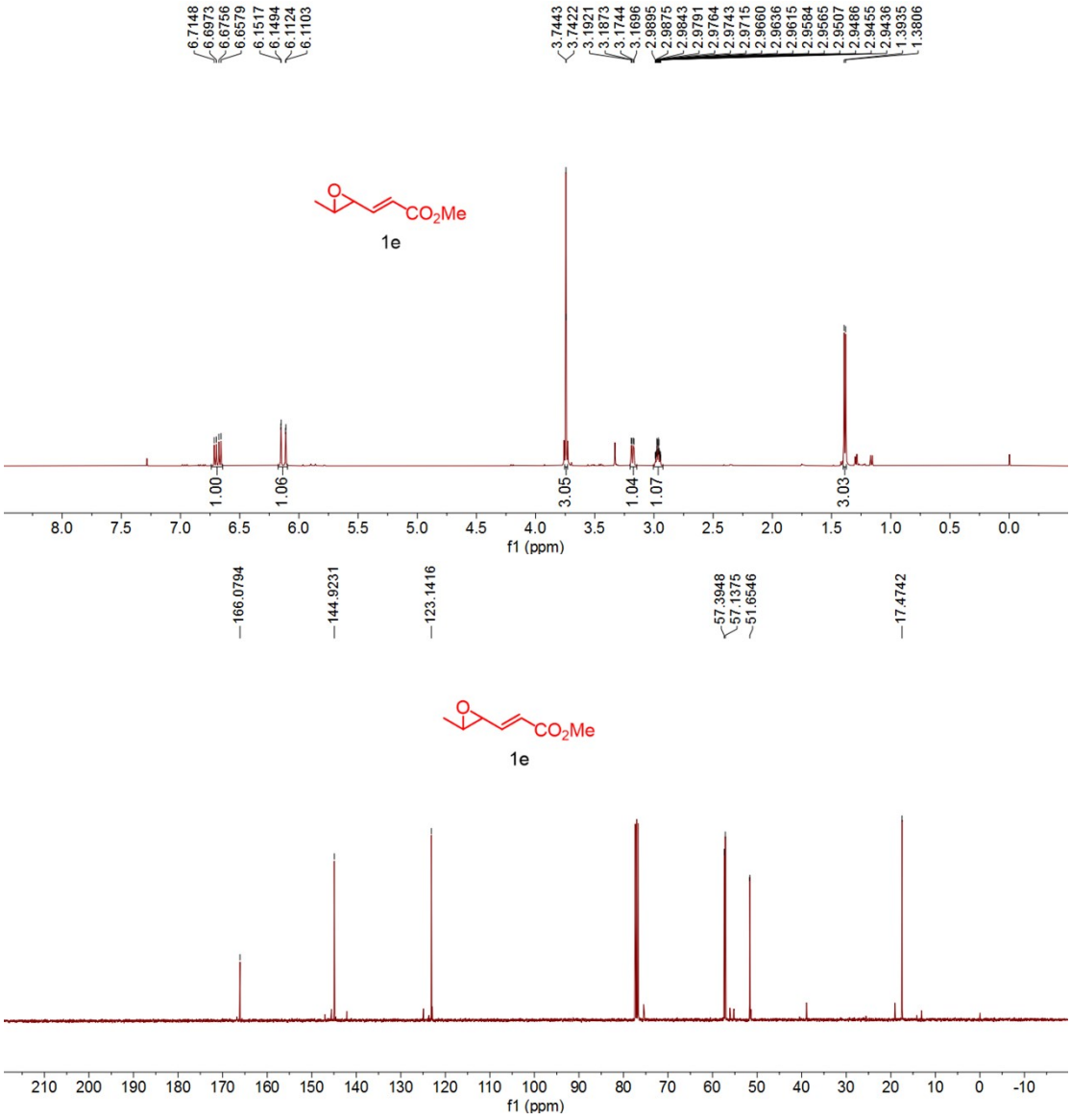
^{1}H and ^{13}C NMR Spectra for 1c



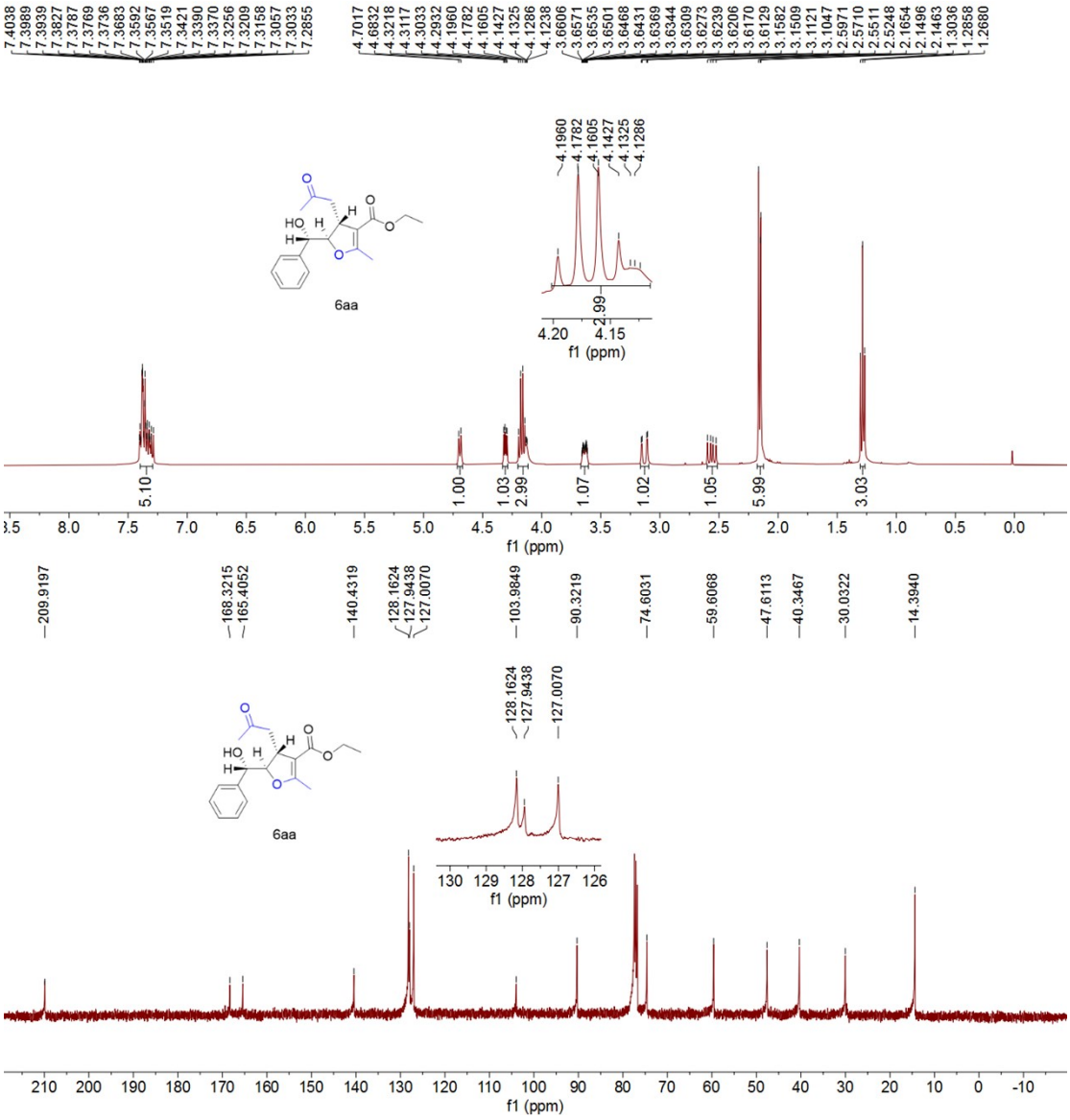
^{1}H and ^{13}C NMR Spectra for 1d



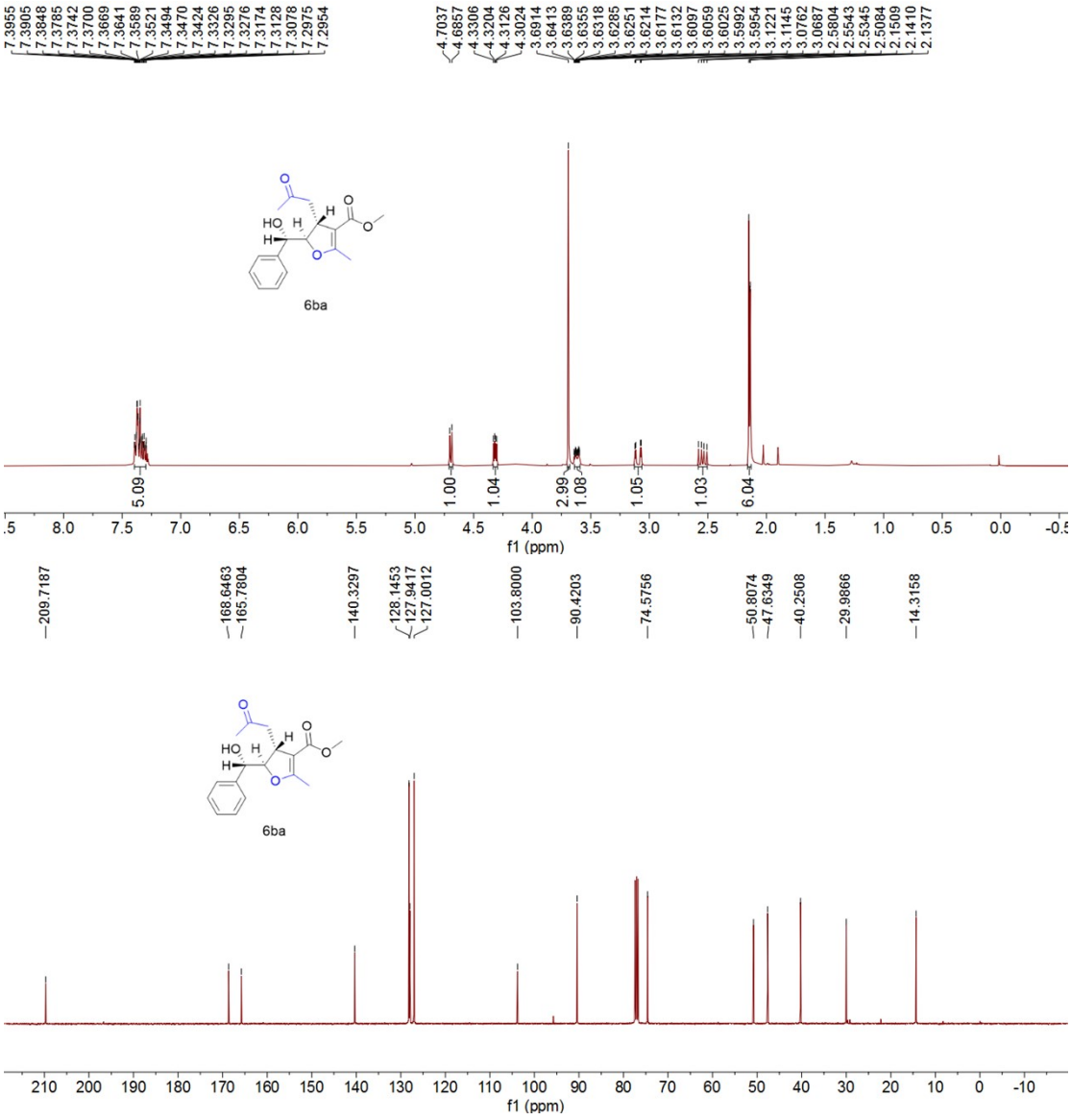
^{1}H and ^{13}C NMR Spectra for 1e



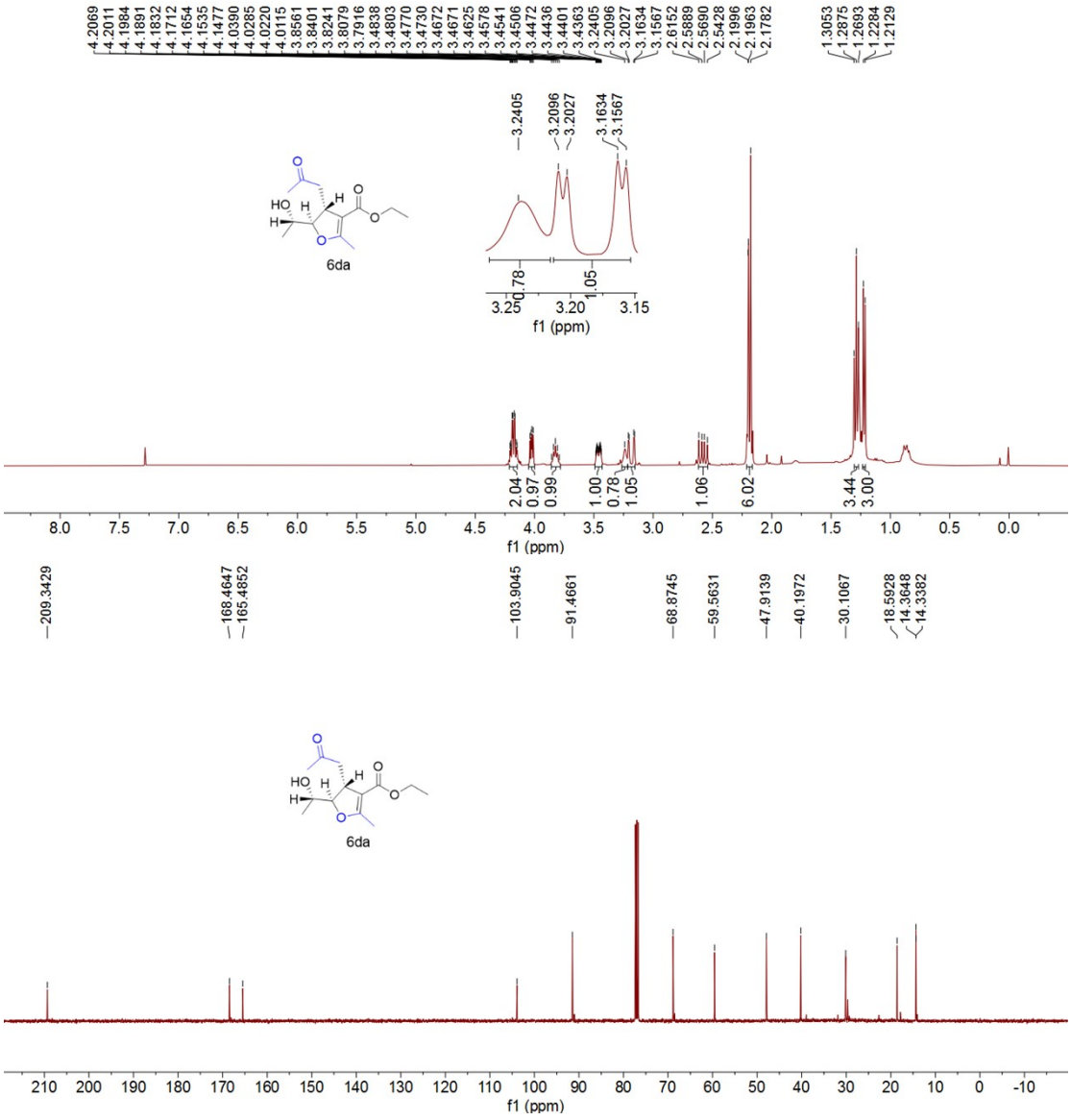
^{1}H and ^{13}C NMR Spectra for 6aa



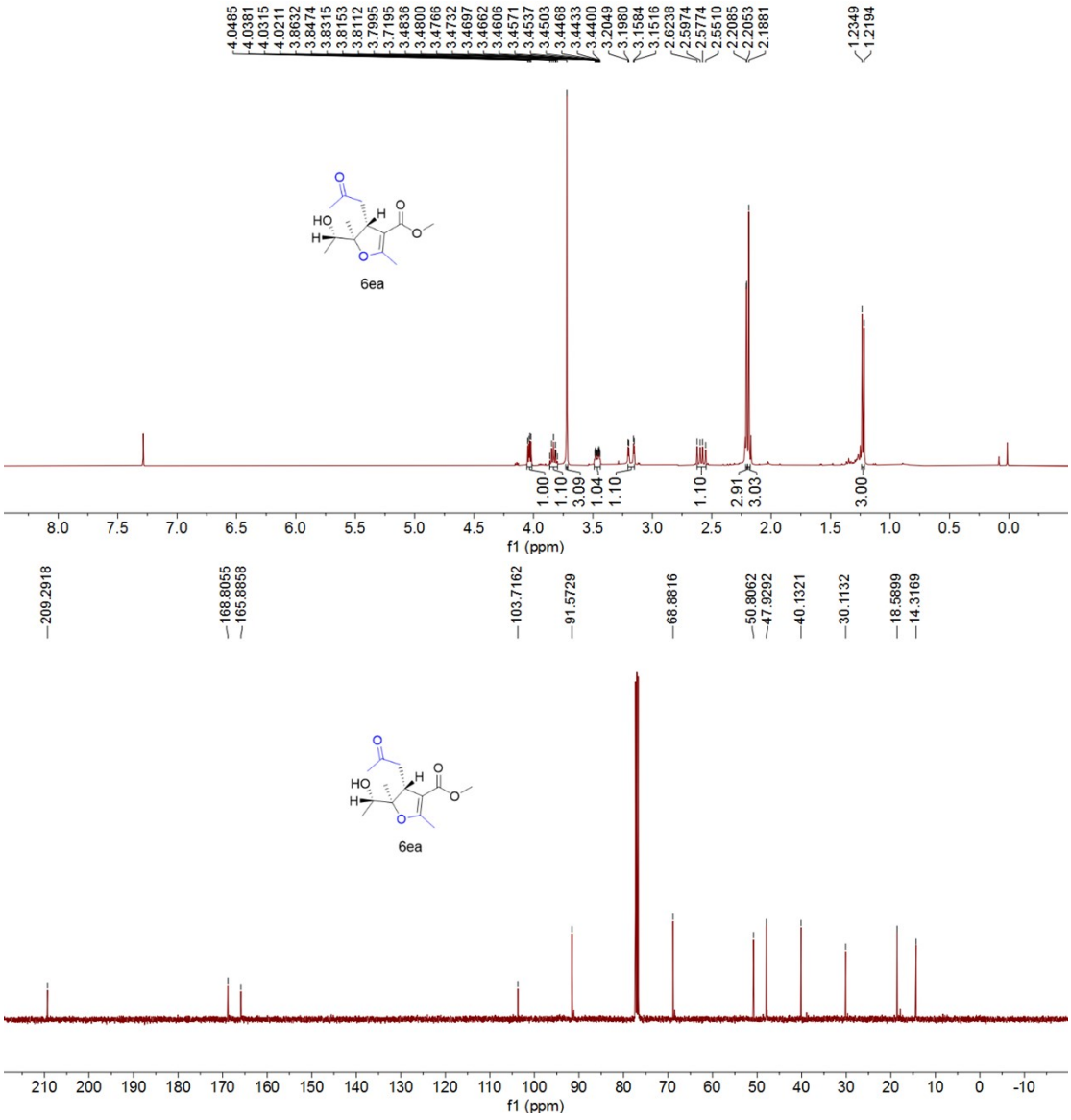
^{1}H and ^{13}C NMR Spectra for 6ba



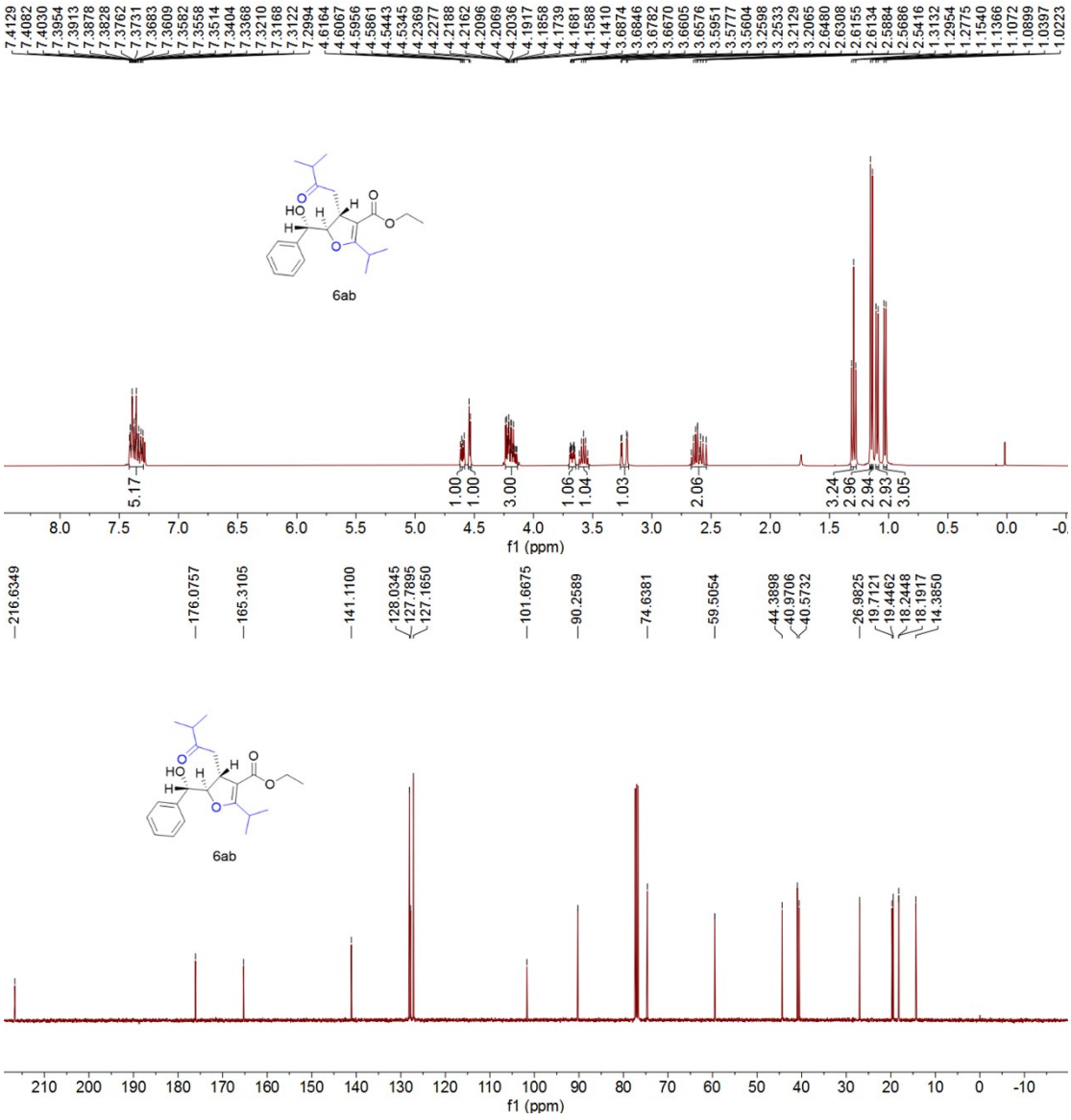
^{1}H and ^{13}C NMR Spectra for 6da



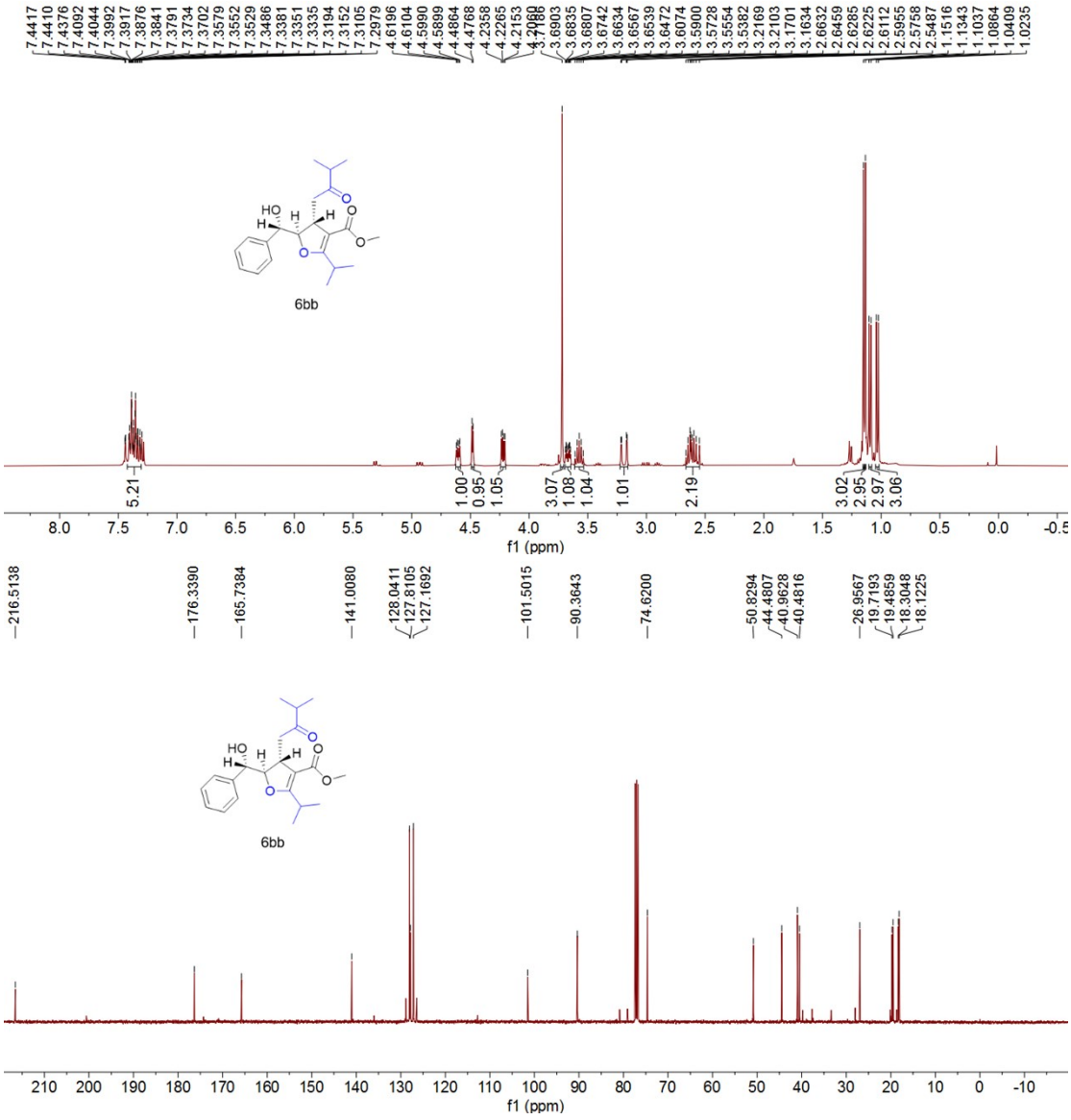
^{1}H and ^{13}C NMR Spectra for 6ea



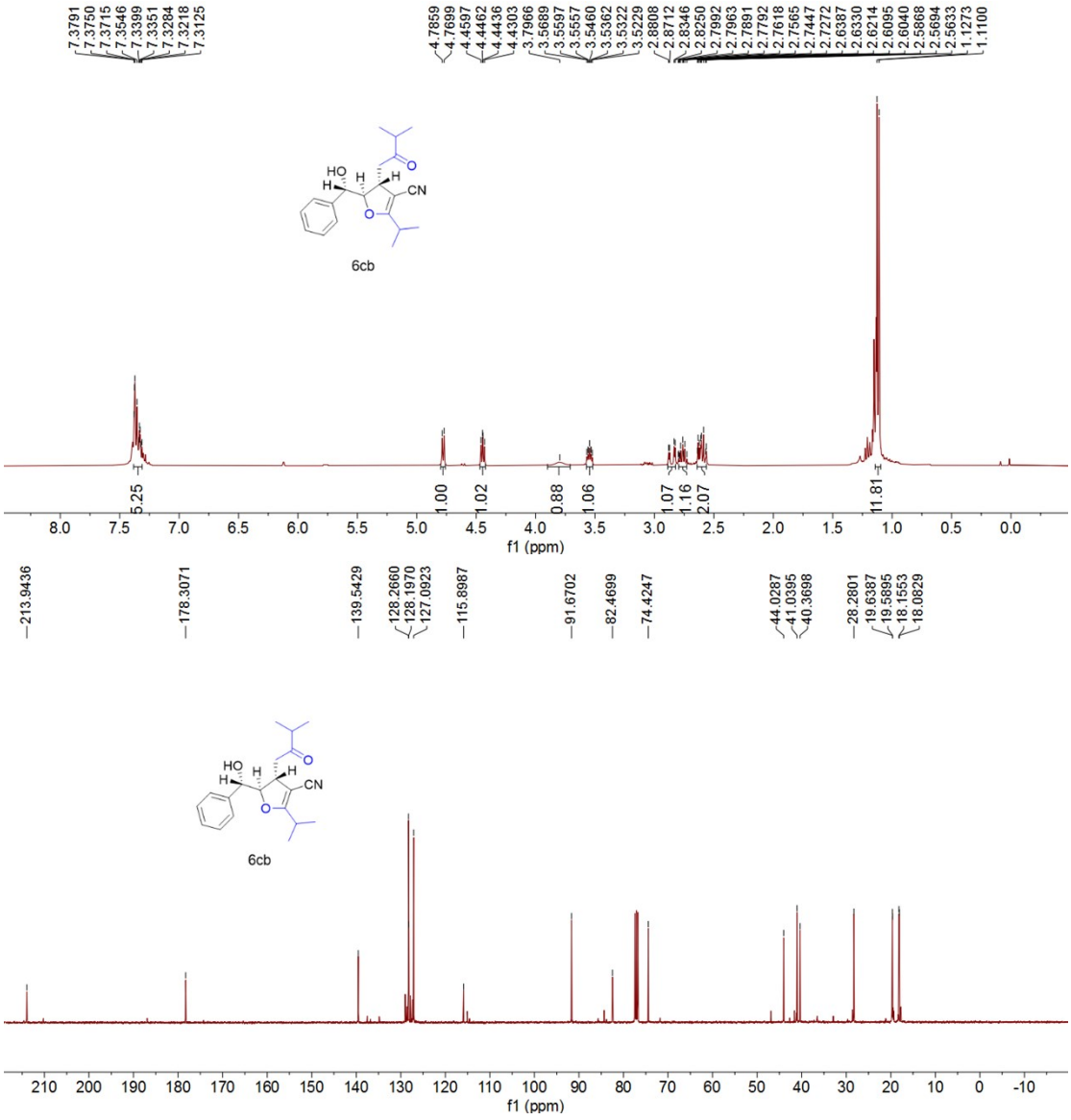
^{1}H and ^{13}C NMR Spectra for 6ab



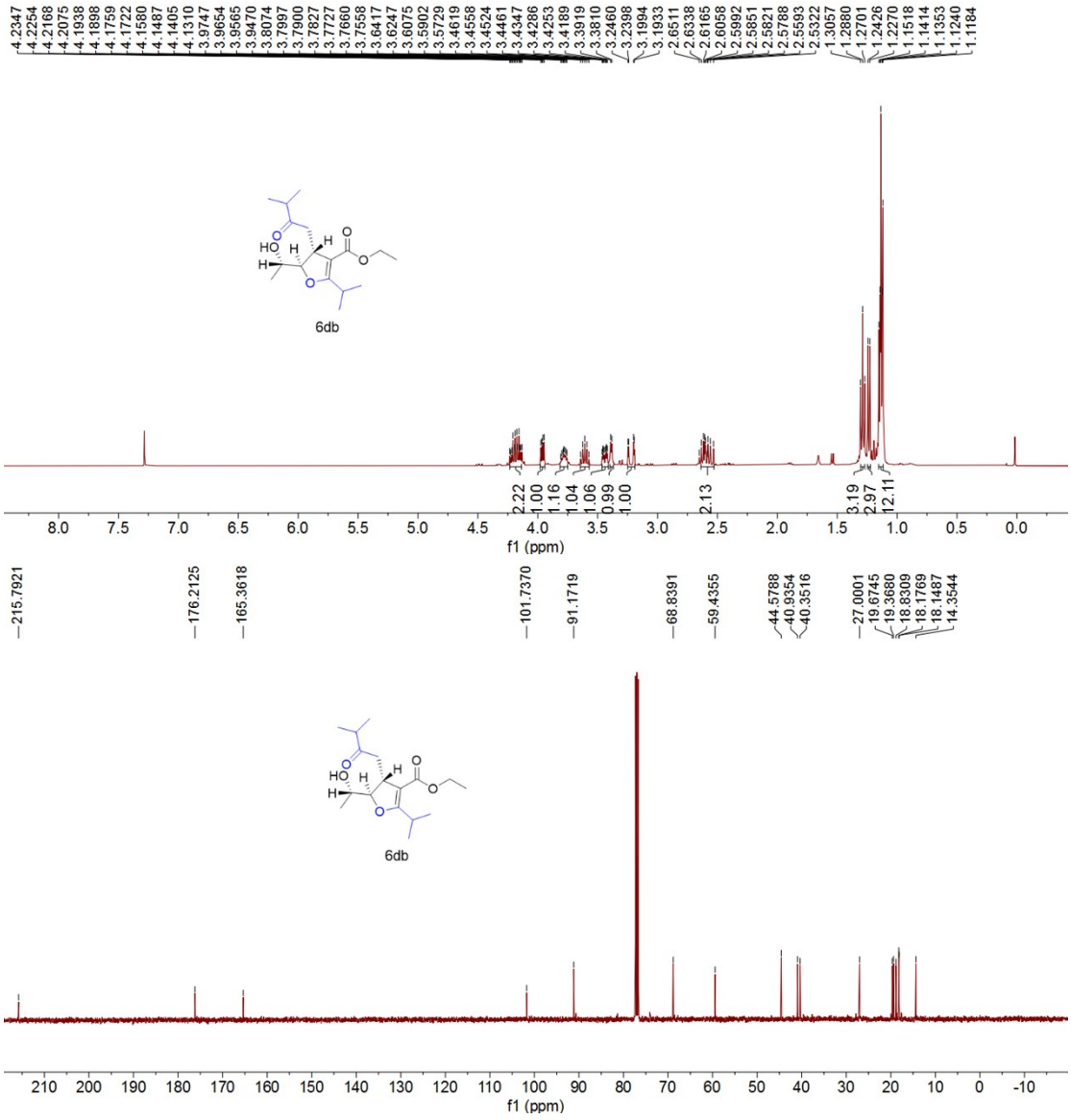
^{1}H and ^{13}C NMR Spectra for 6bb



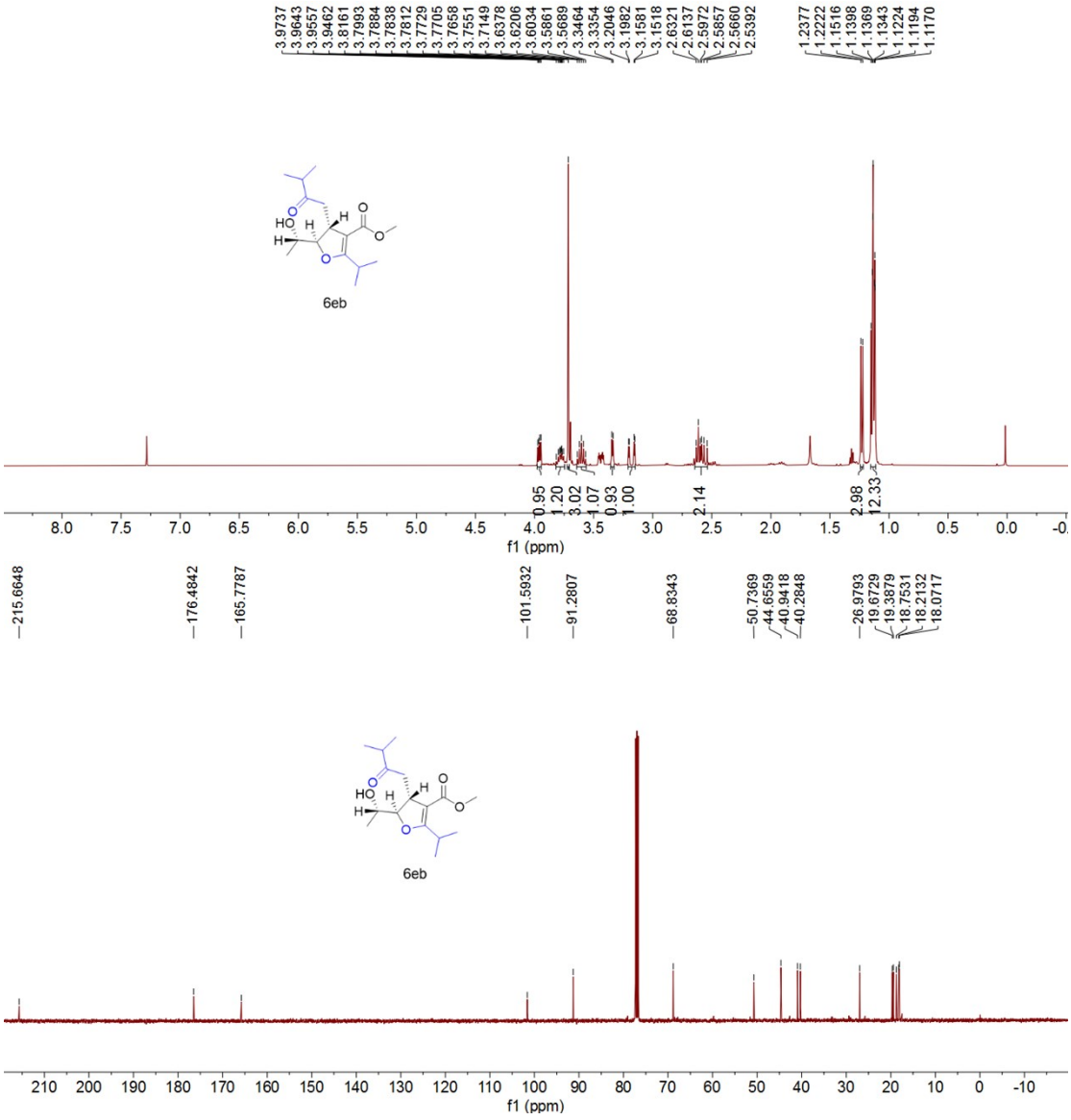
^{1}H and ^{13}C NMR Spectra for 6cb



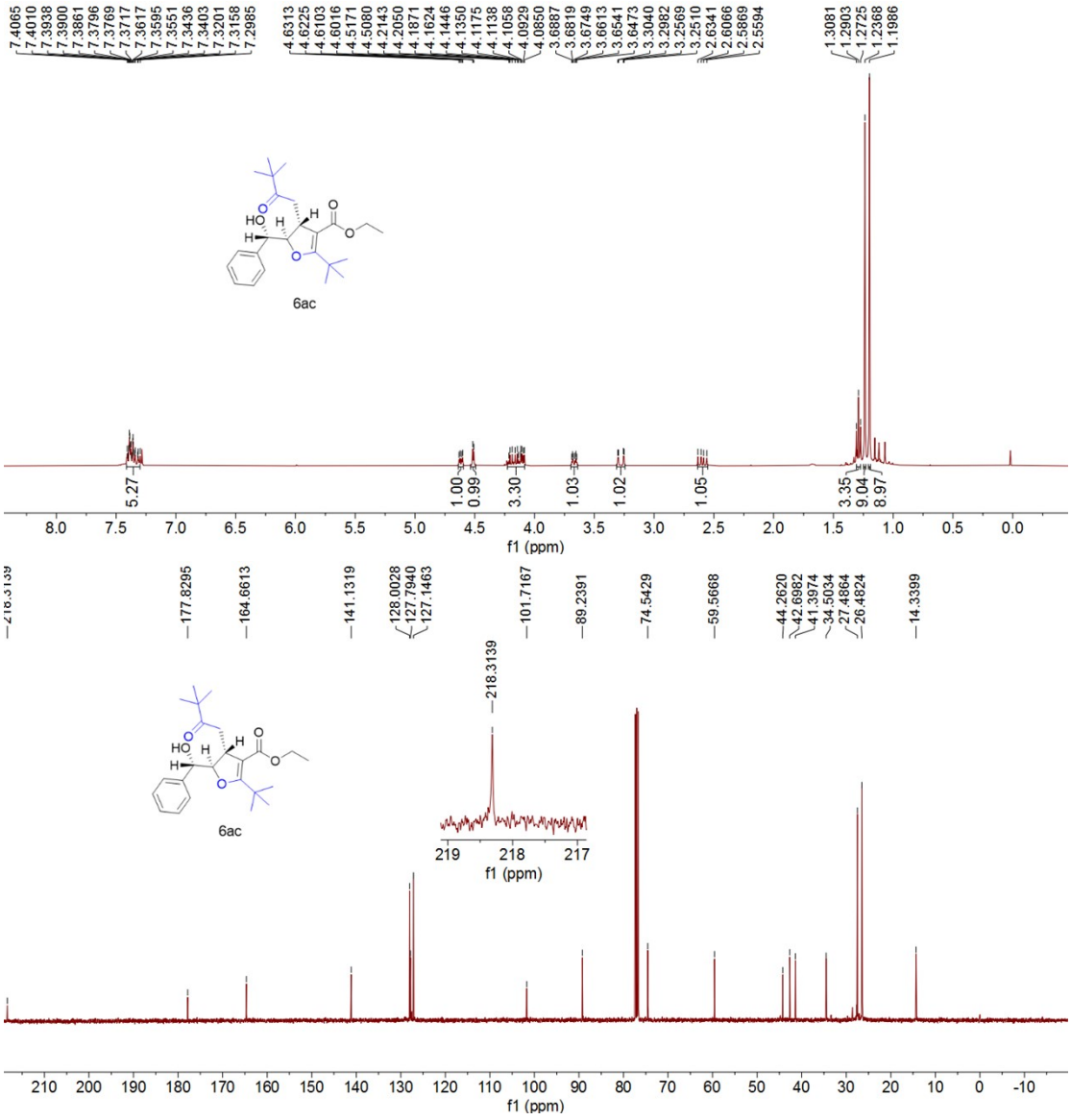
^{1}H and ^{13}C NMR Spectra for 6db



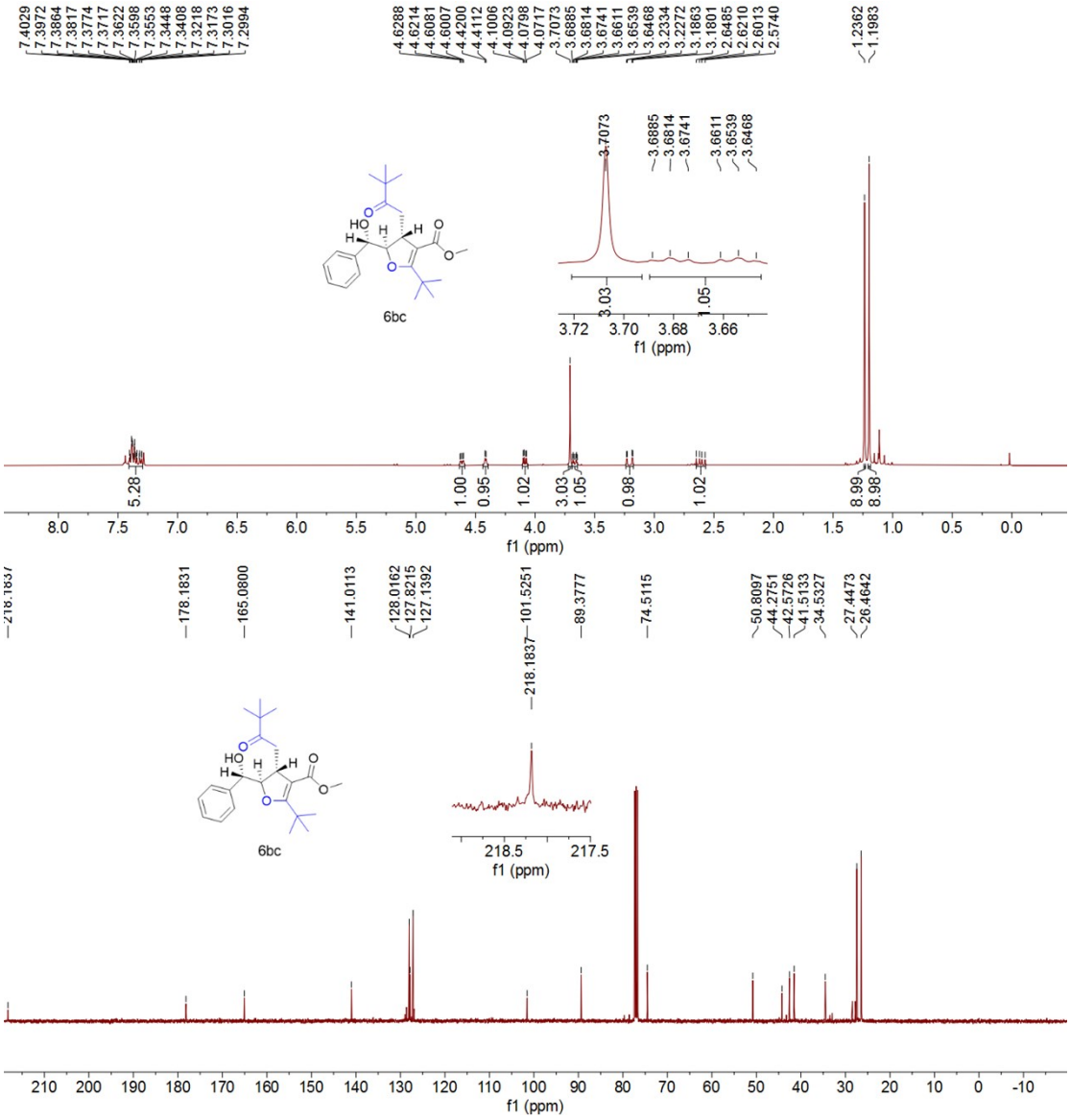
^{1}H and ^{13}C NMR Spectra for 6eb



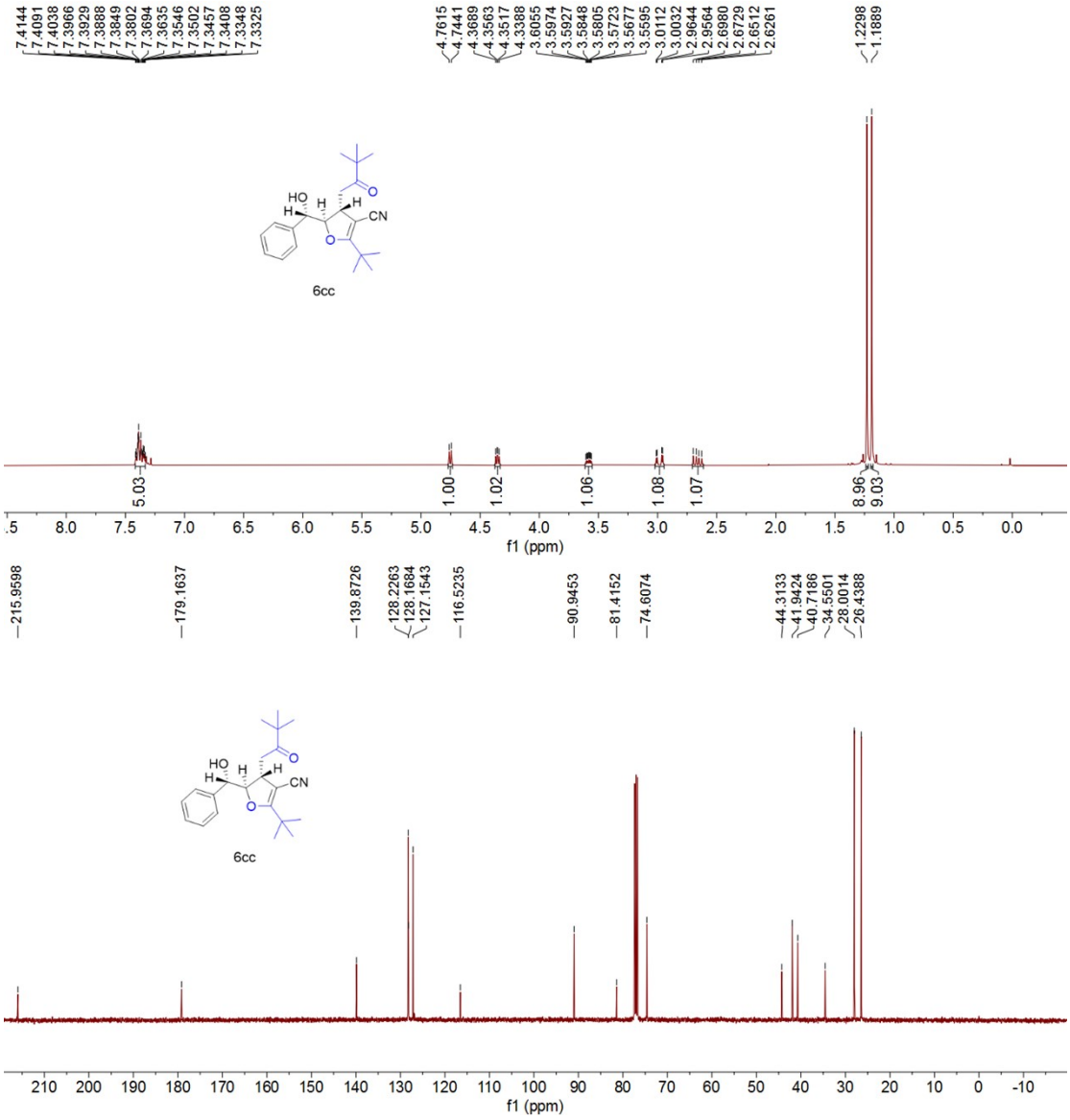
^{1}H and ^{13}C NMR Spectra for 6ac



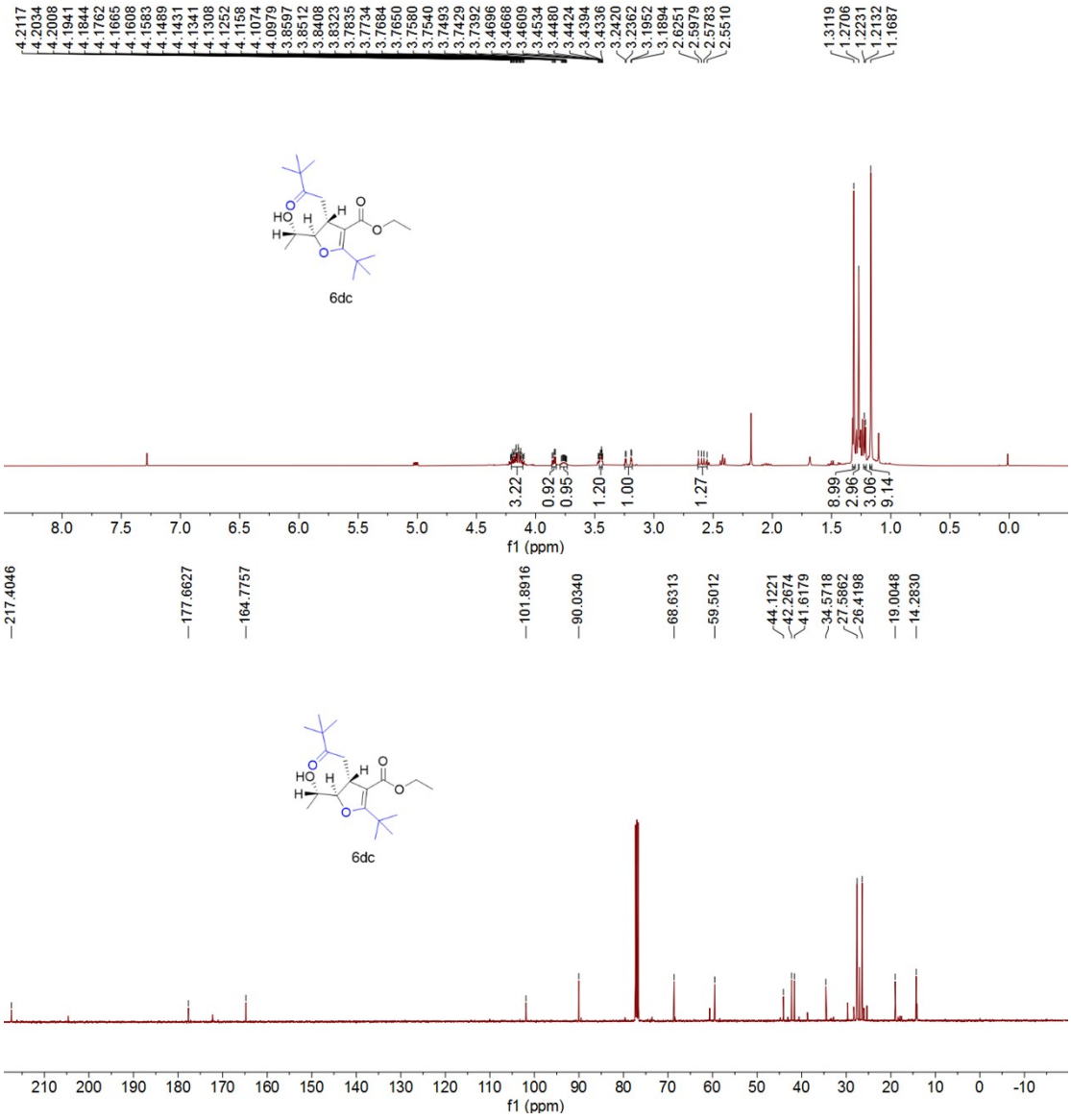
^{1}H and ^{13}C NMR Spectra for 6bc



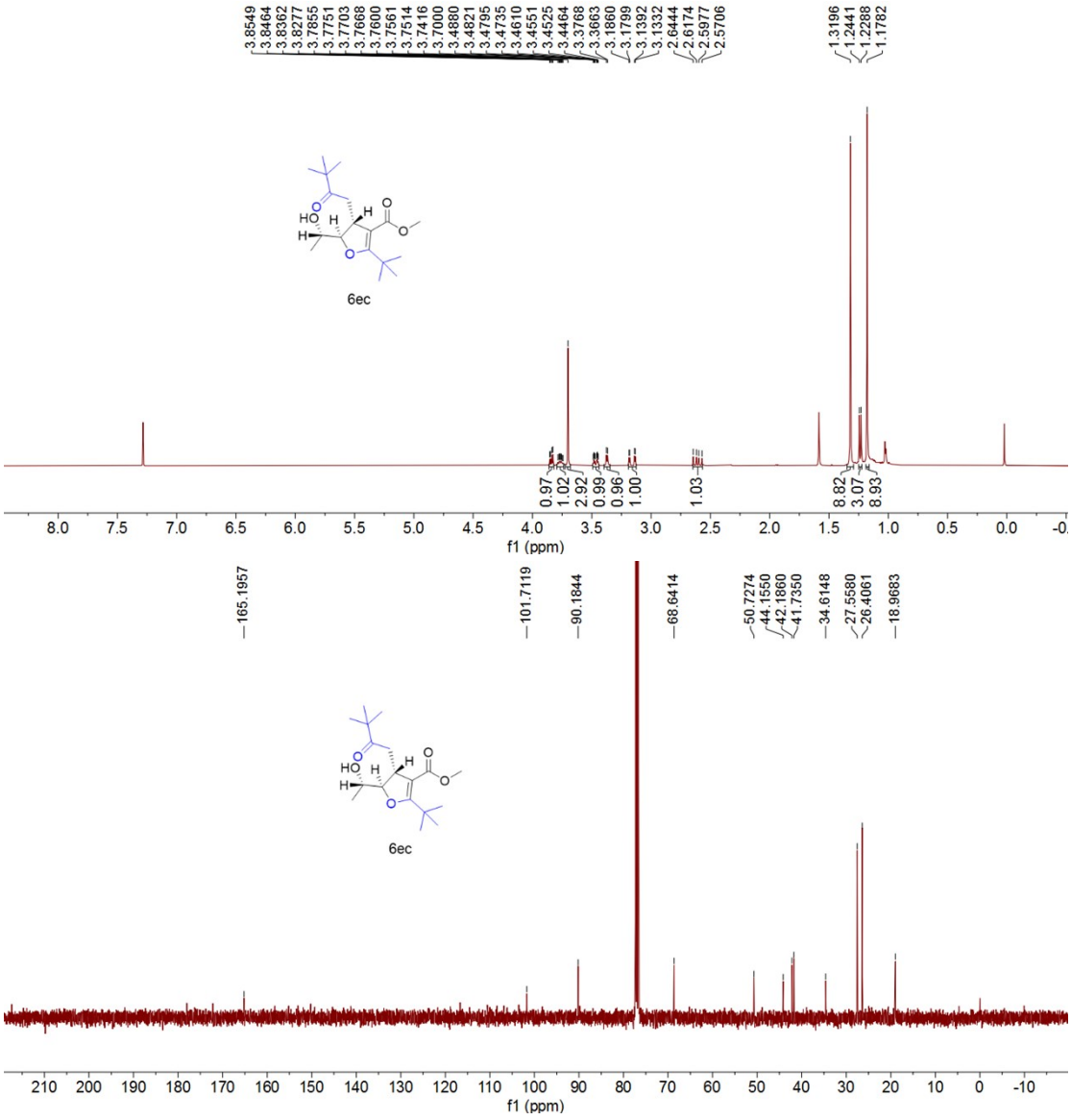
^{1}H and ^{13}C NMR Spectra for 6cc



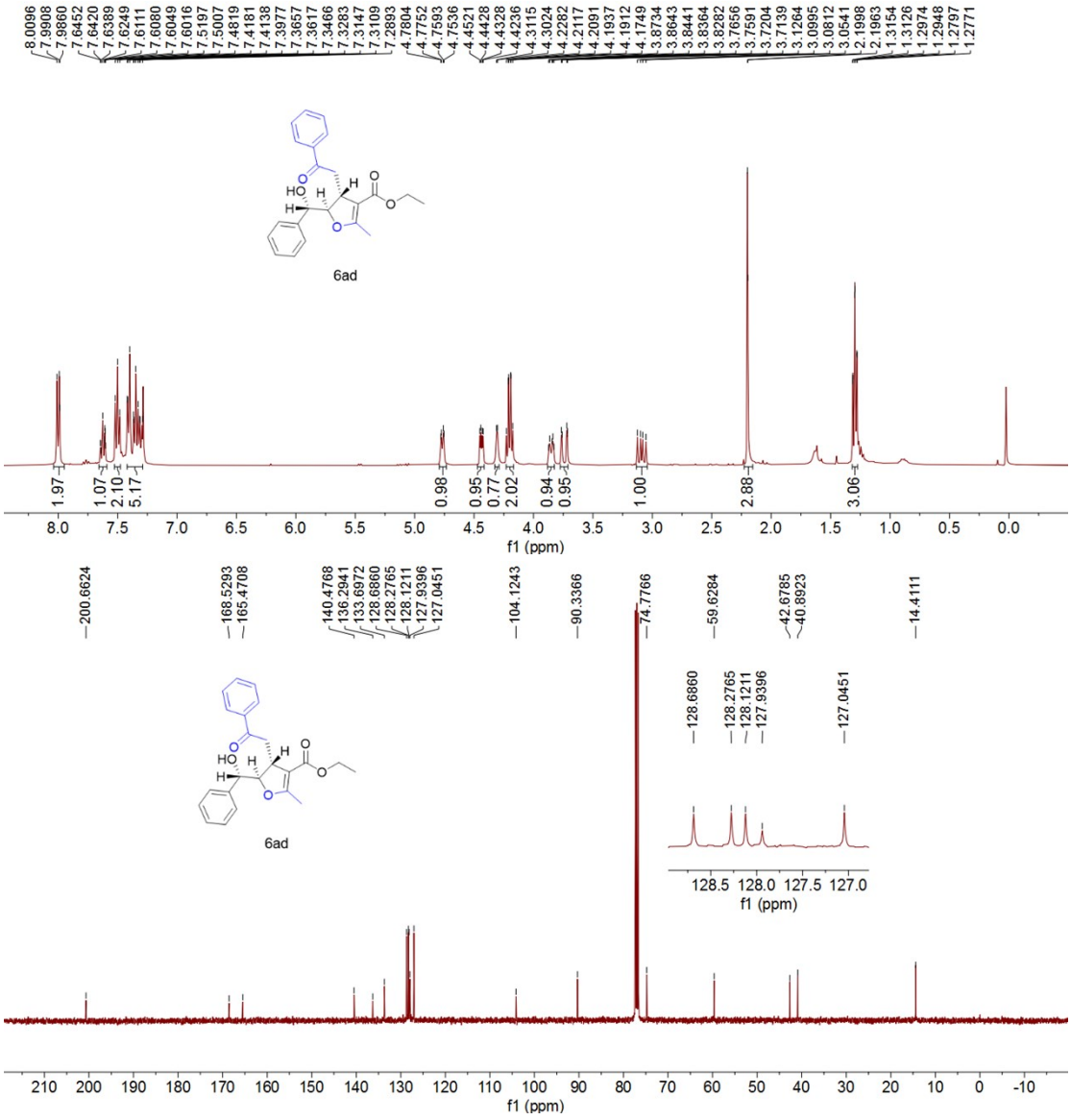
^{1}H and ^{13}C NMR Spectra for 6dc



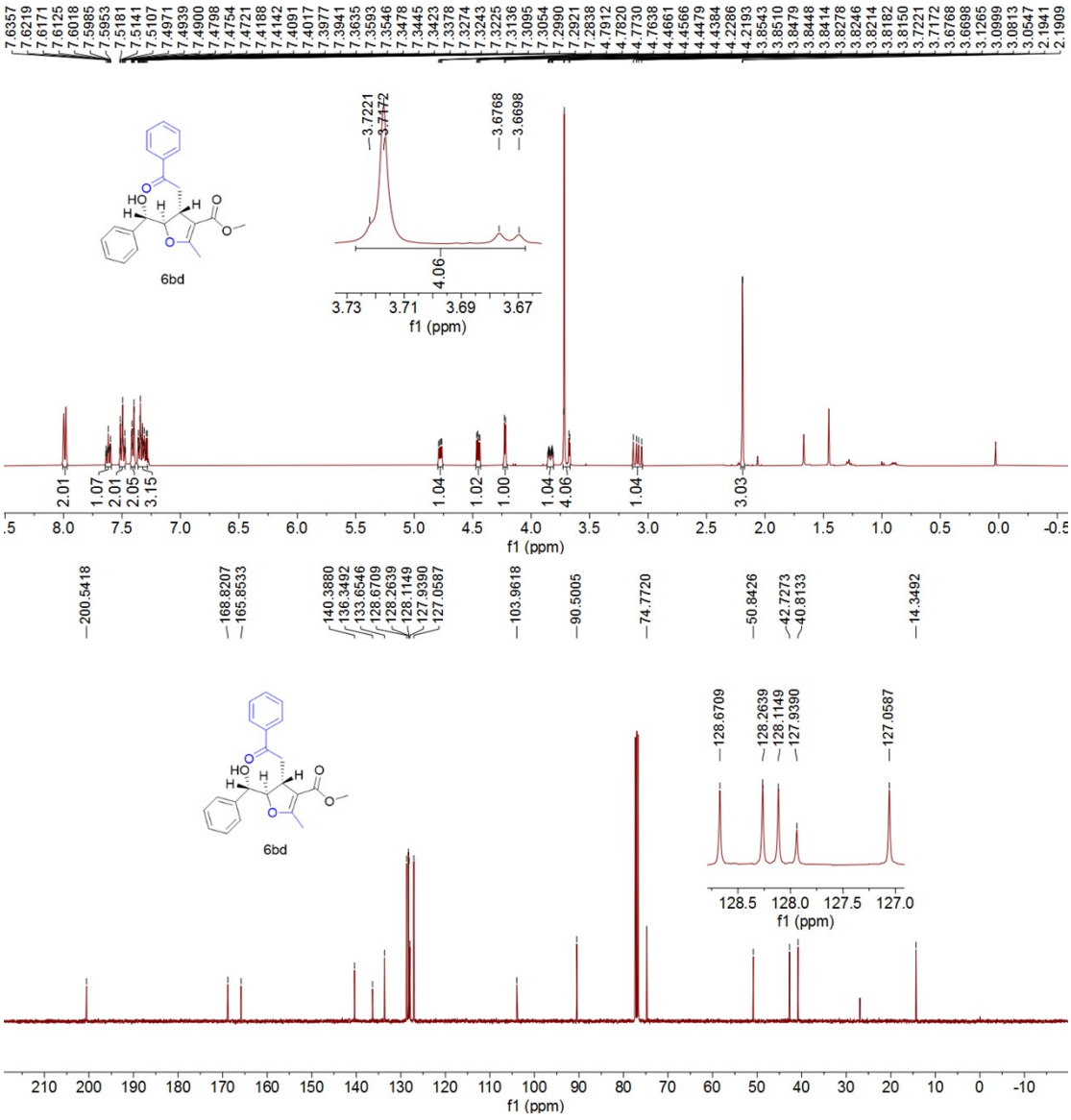
^{1}H and ^{13}C NMR Spectra for 6ec



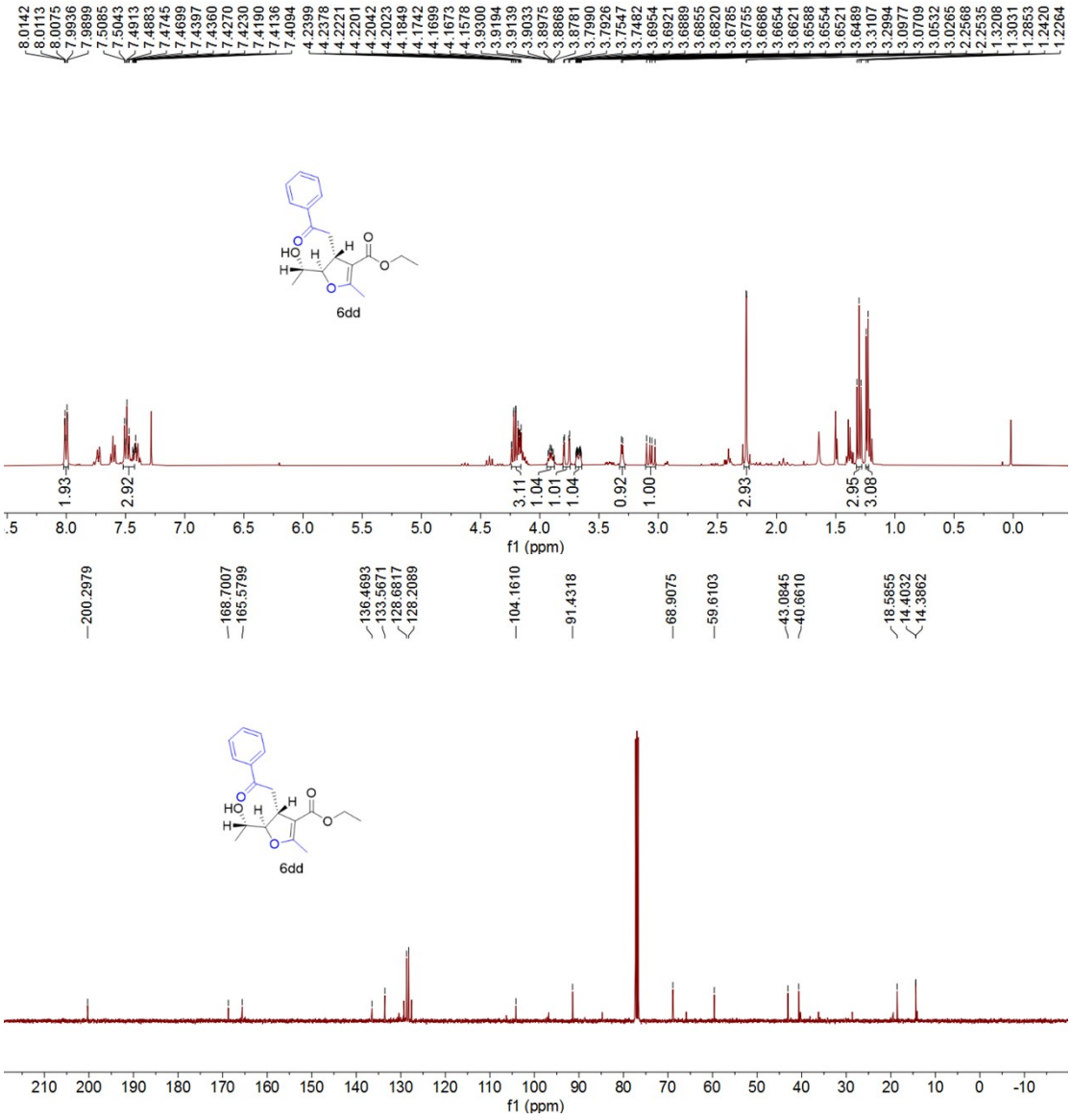
^{1}H and ^{13}C NMR Spectra for 6ad



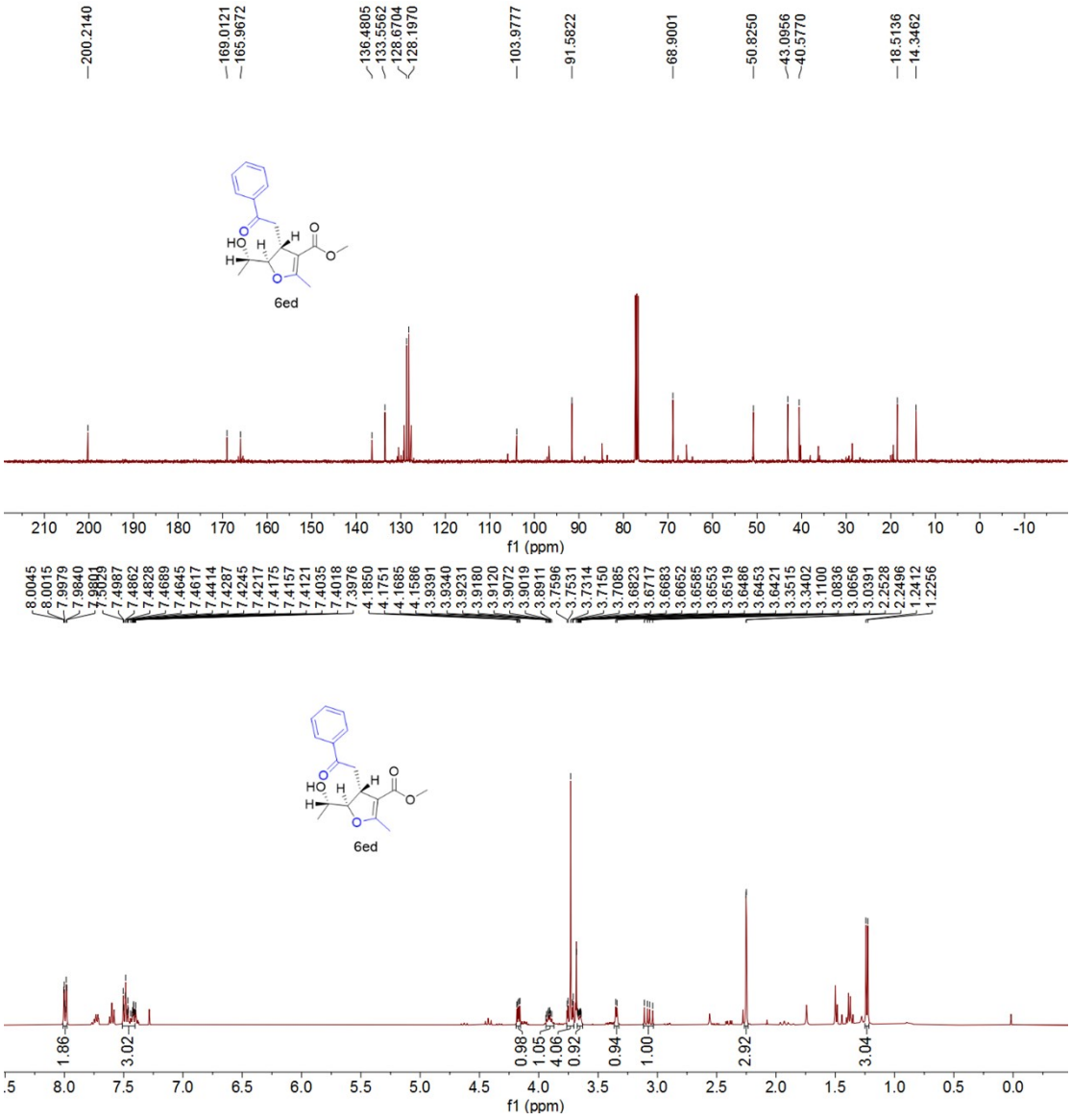
^{1}H and ^{13}C NMR Spectra for 6bd



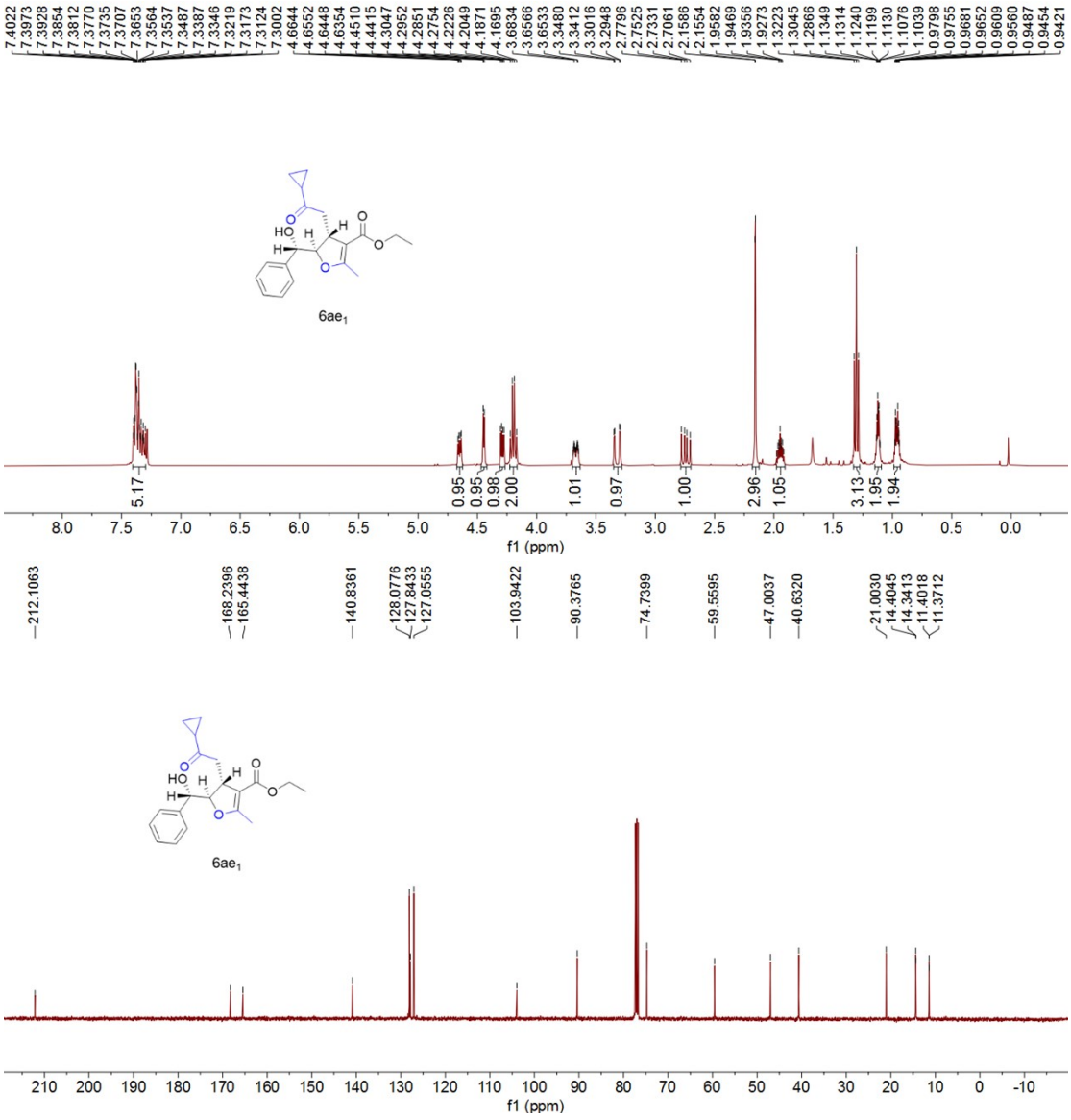
^{1}H and ^{13}C NMR Spectra for 6dd



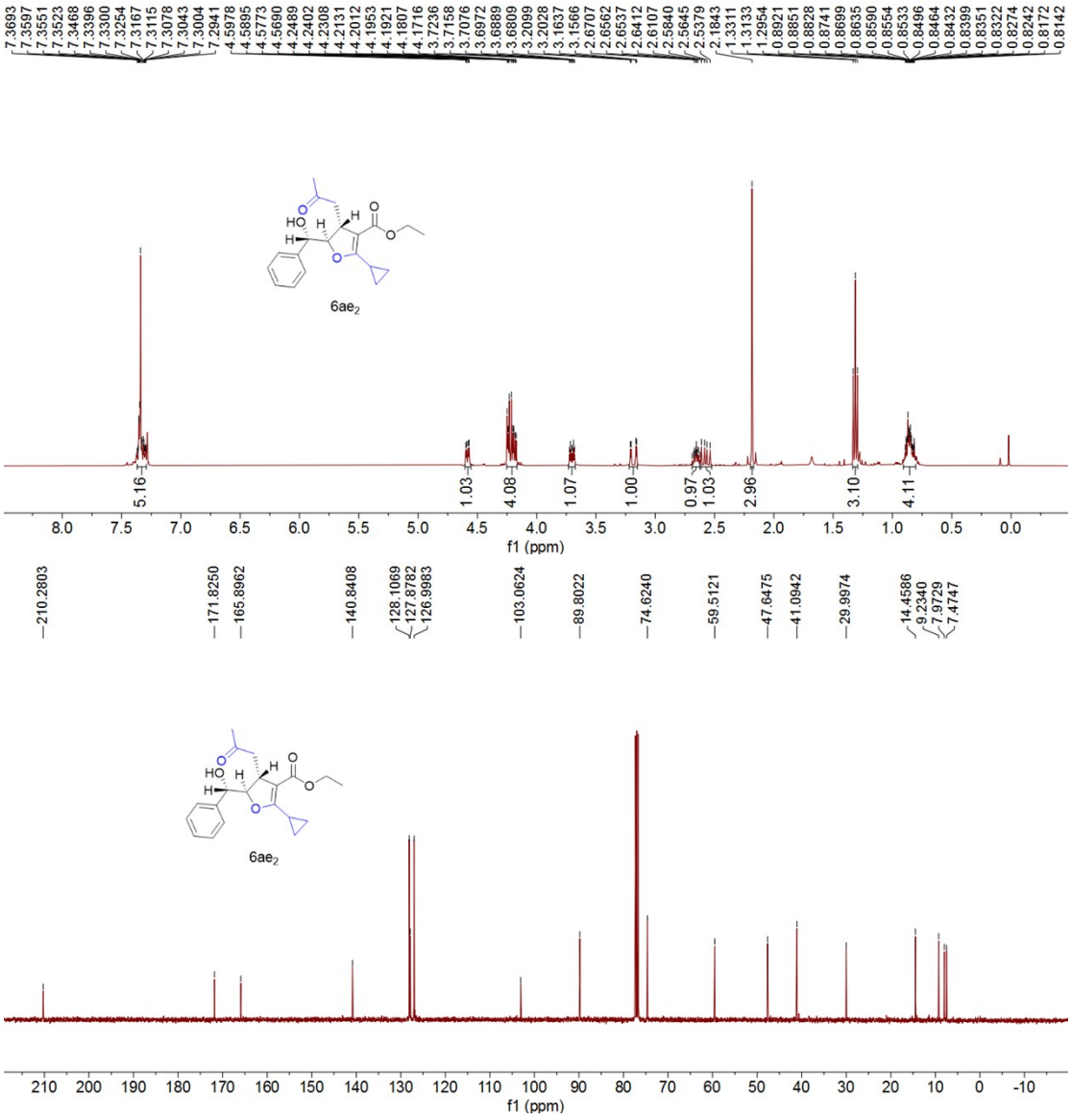
^{1}H and ^{13}C NMR Spectra for 6ed



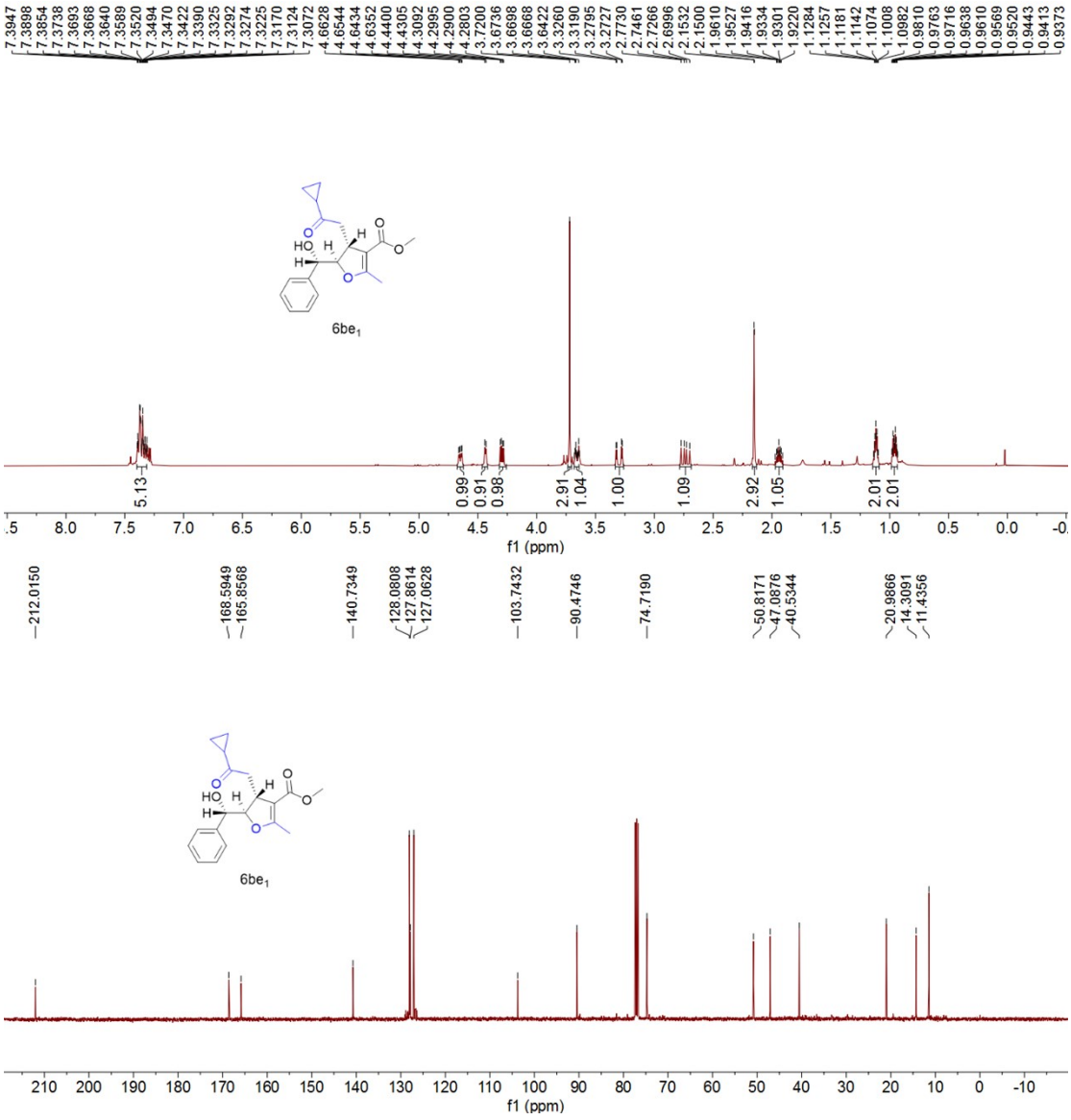
^{1}H and ^{13}C NMR Spectra for $6ae_1$



^{1}H and ^{13}C NMR Spectra for $6ae_2$



^{1}H and ^{13}C NMR Spectra for $6be_1$



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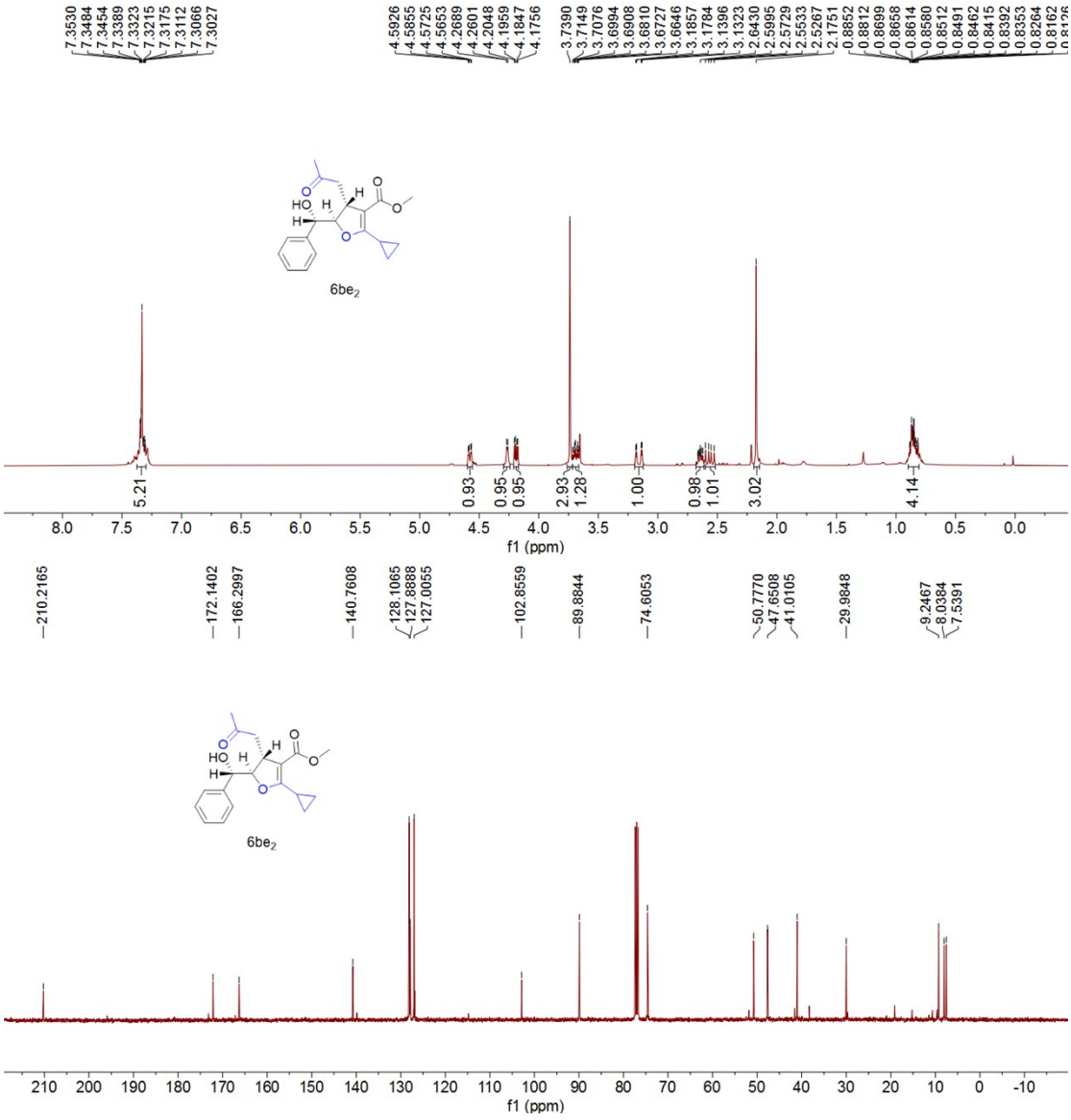

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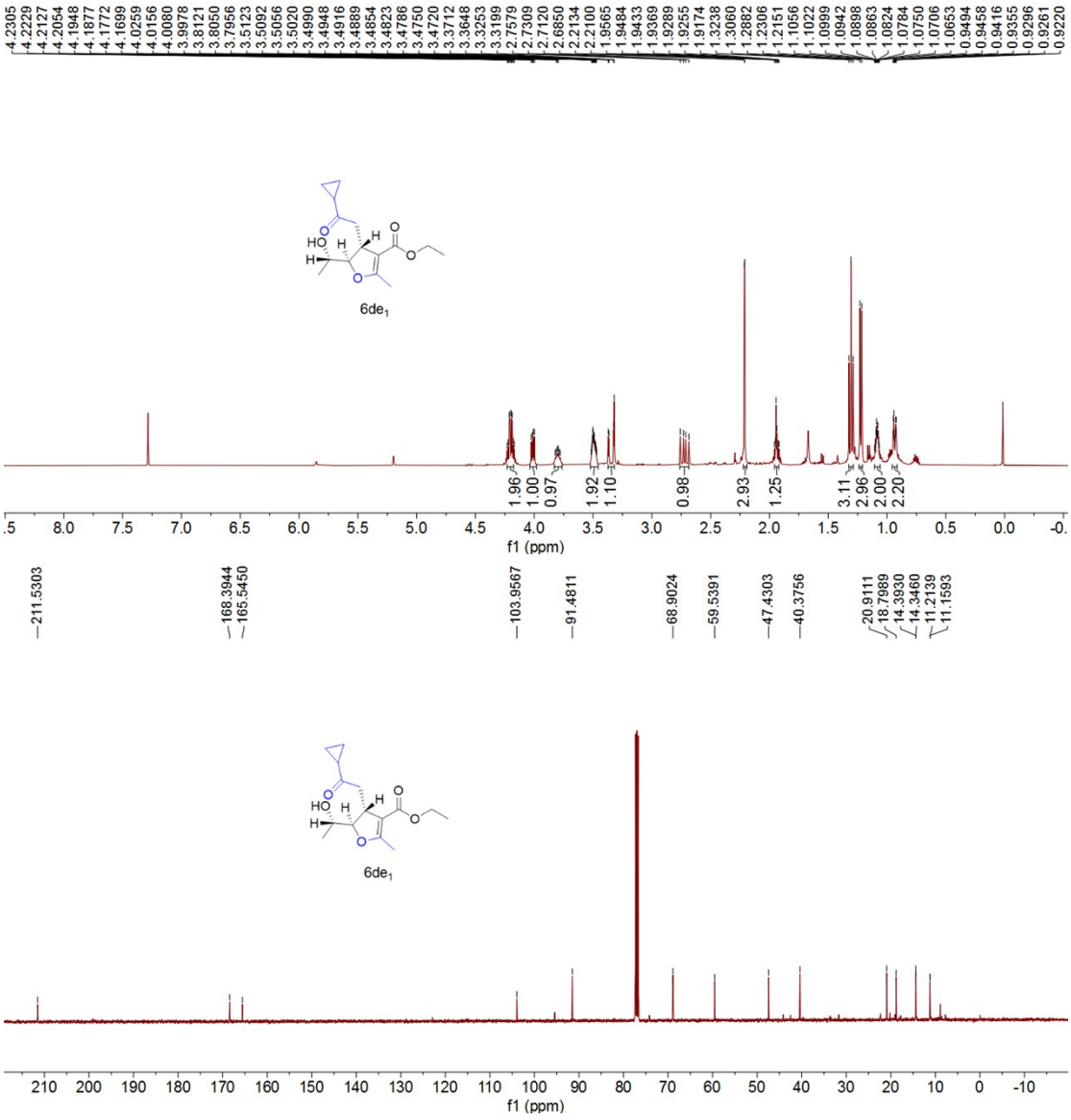

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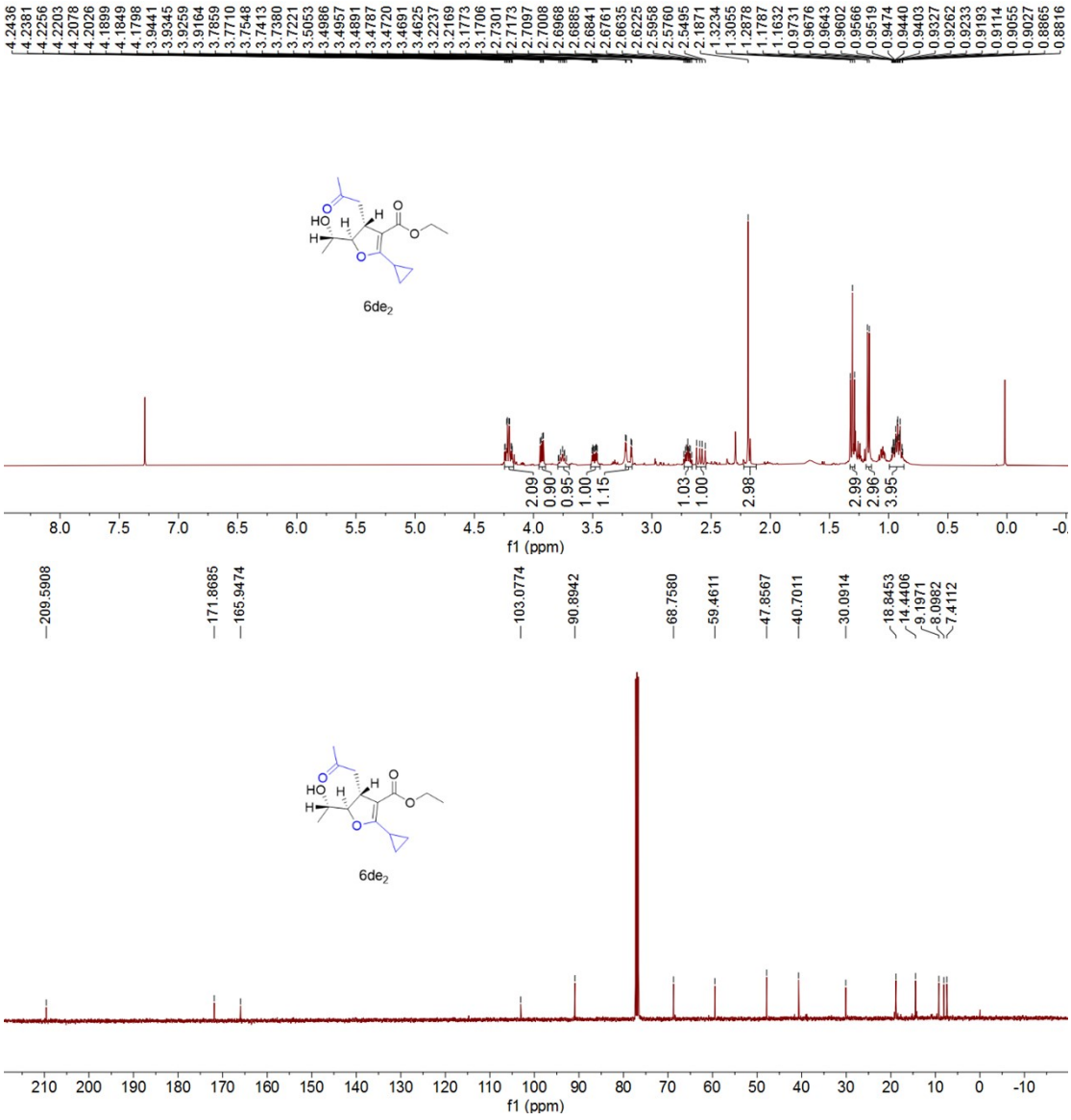
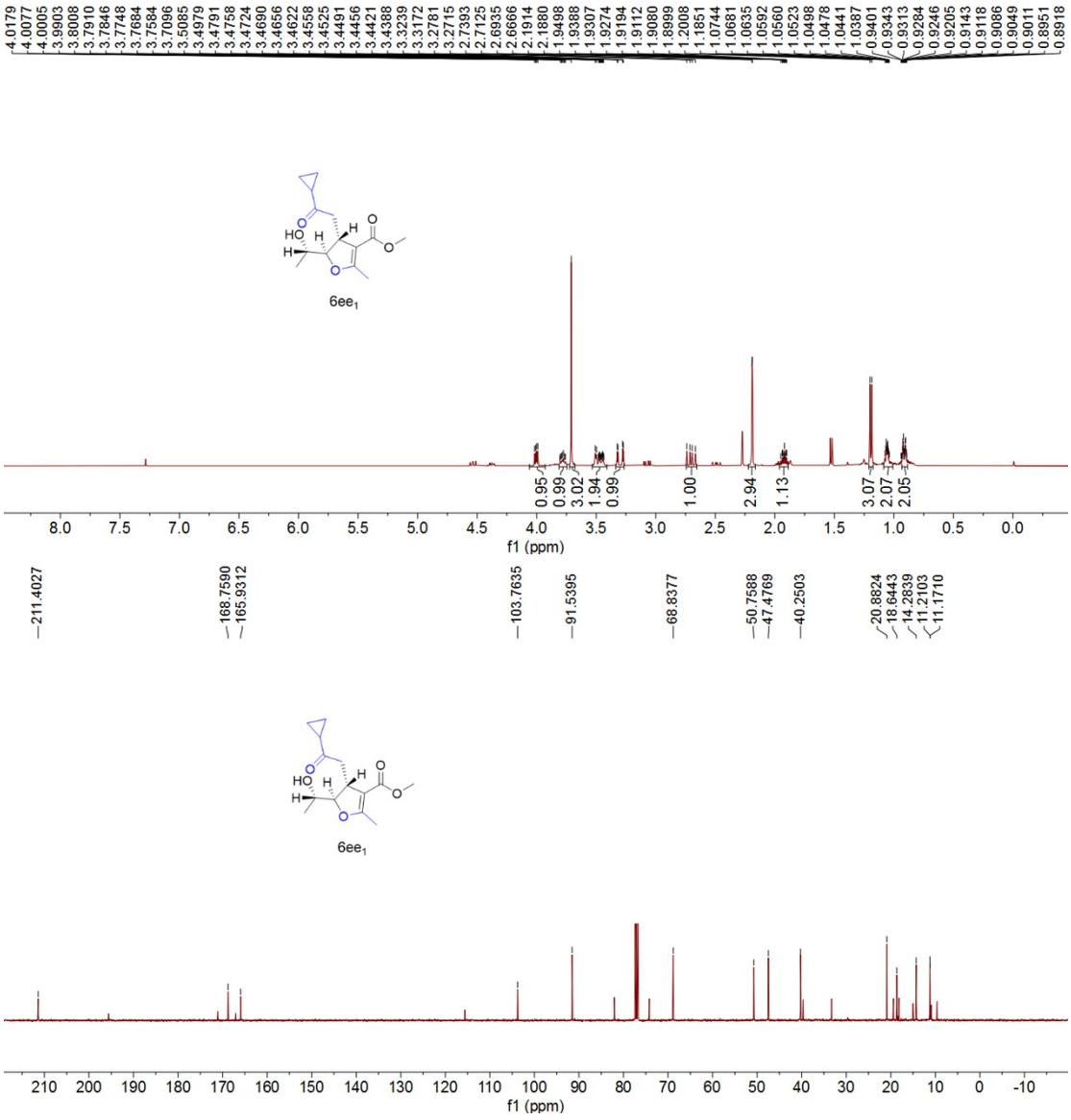


^{1}H and ^{13}C NMR Spectra for $6ee_1$



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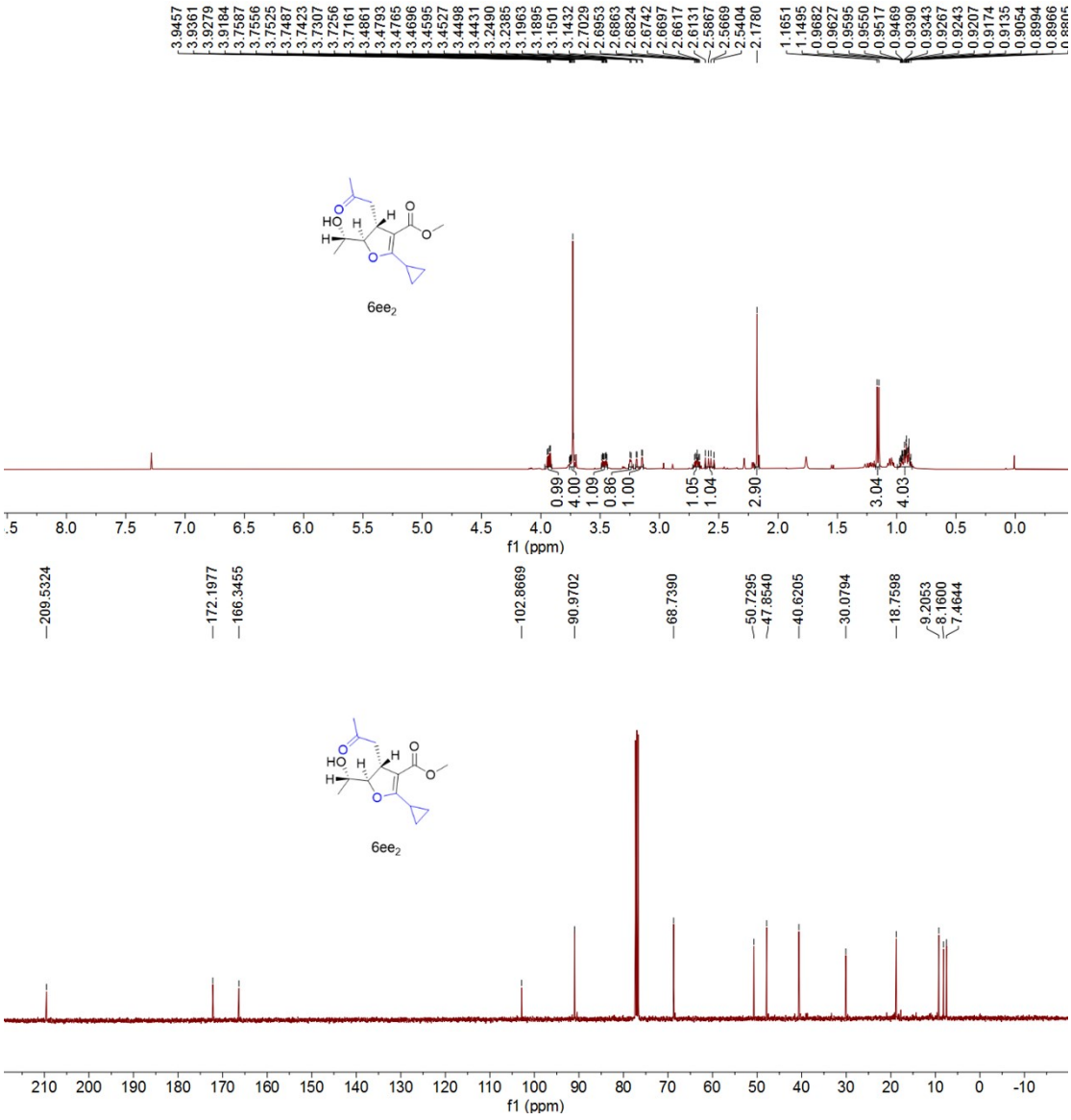
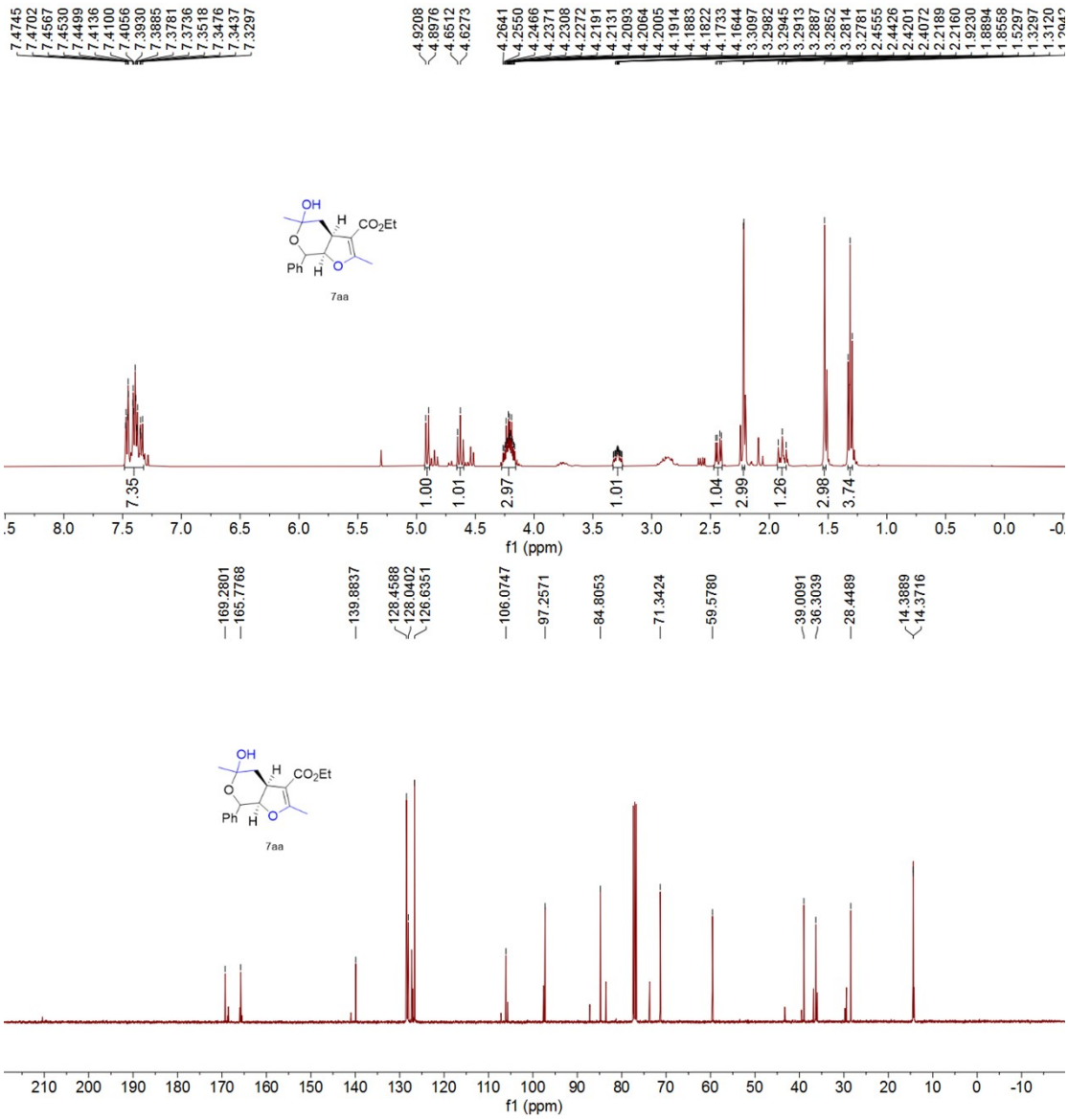
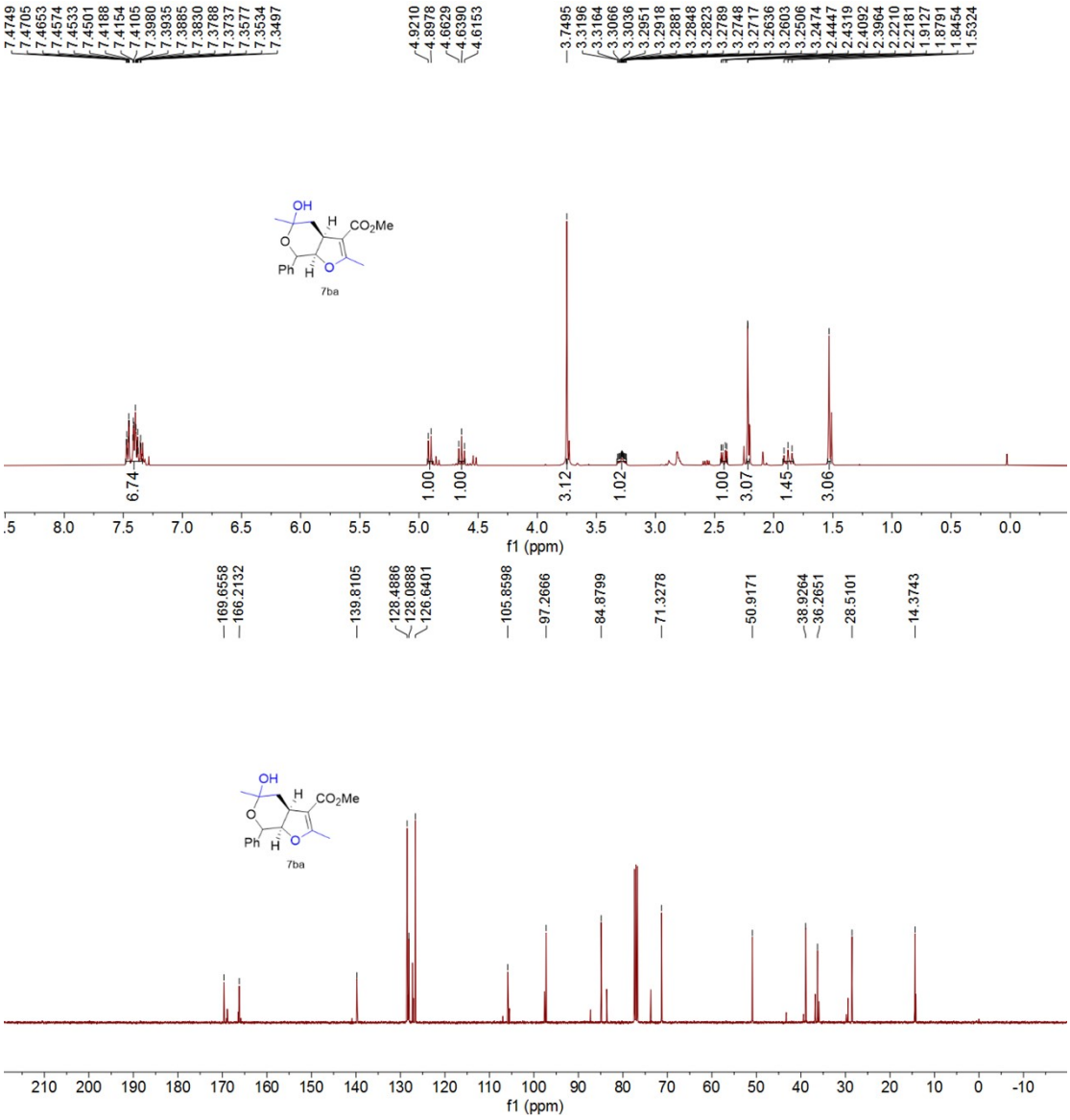


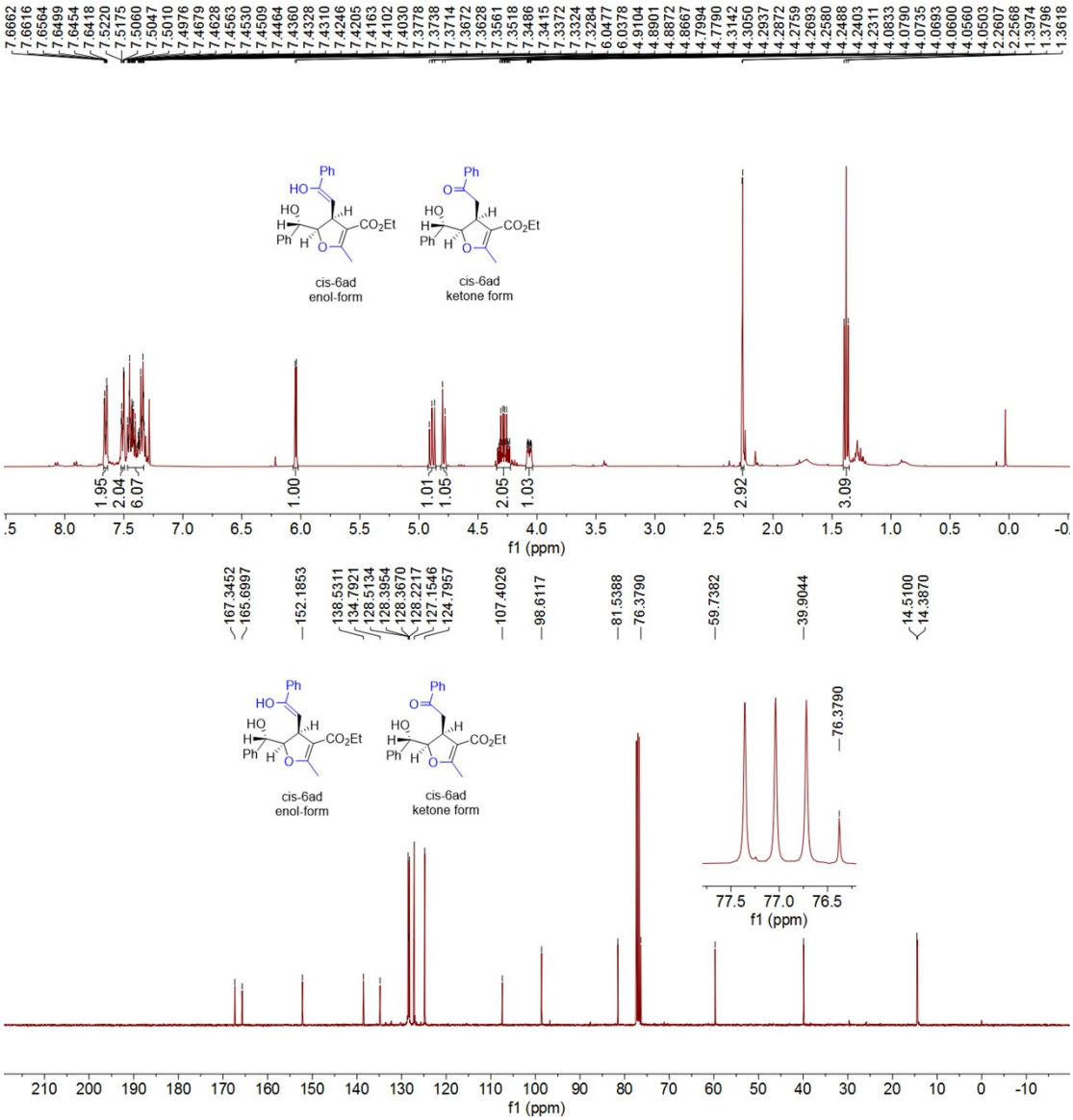
^{1}H and ^{13}C NMR Spectra for 7aa



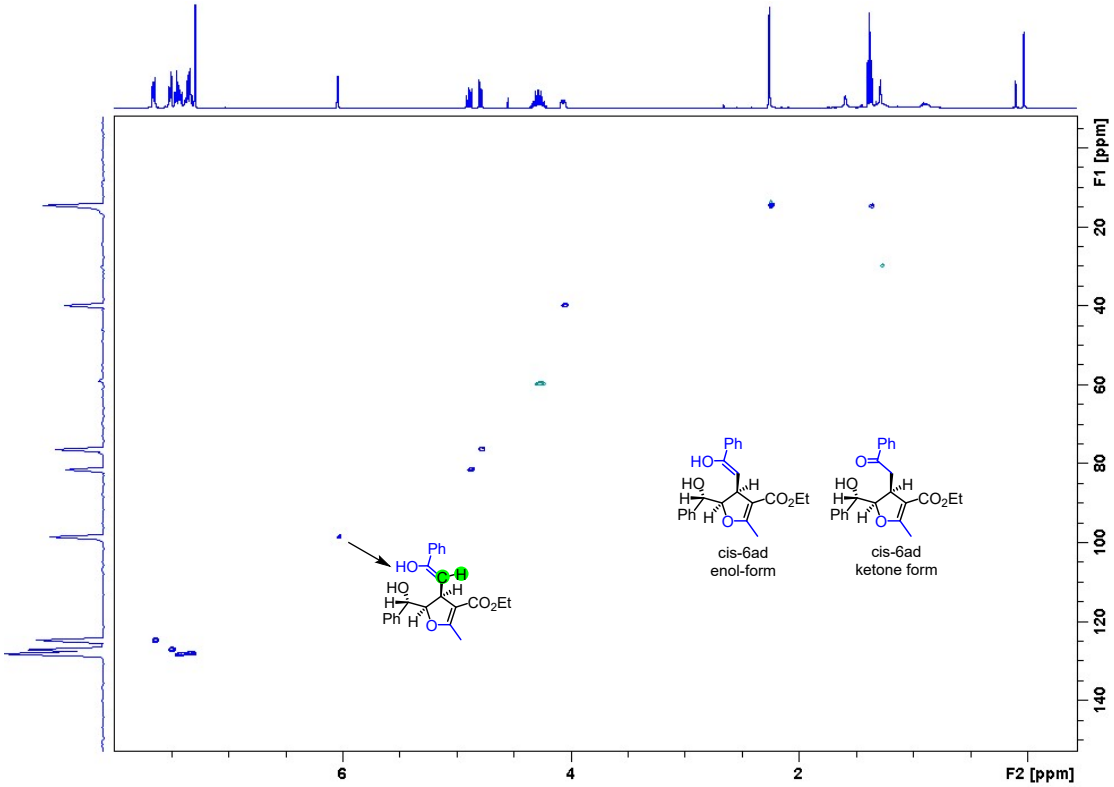
^{1}H and ^{13}C NMR Spectra for 7ba



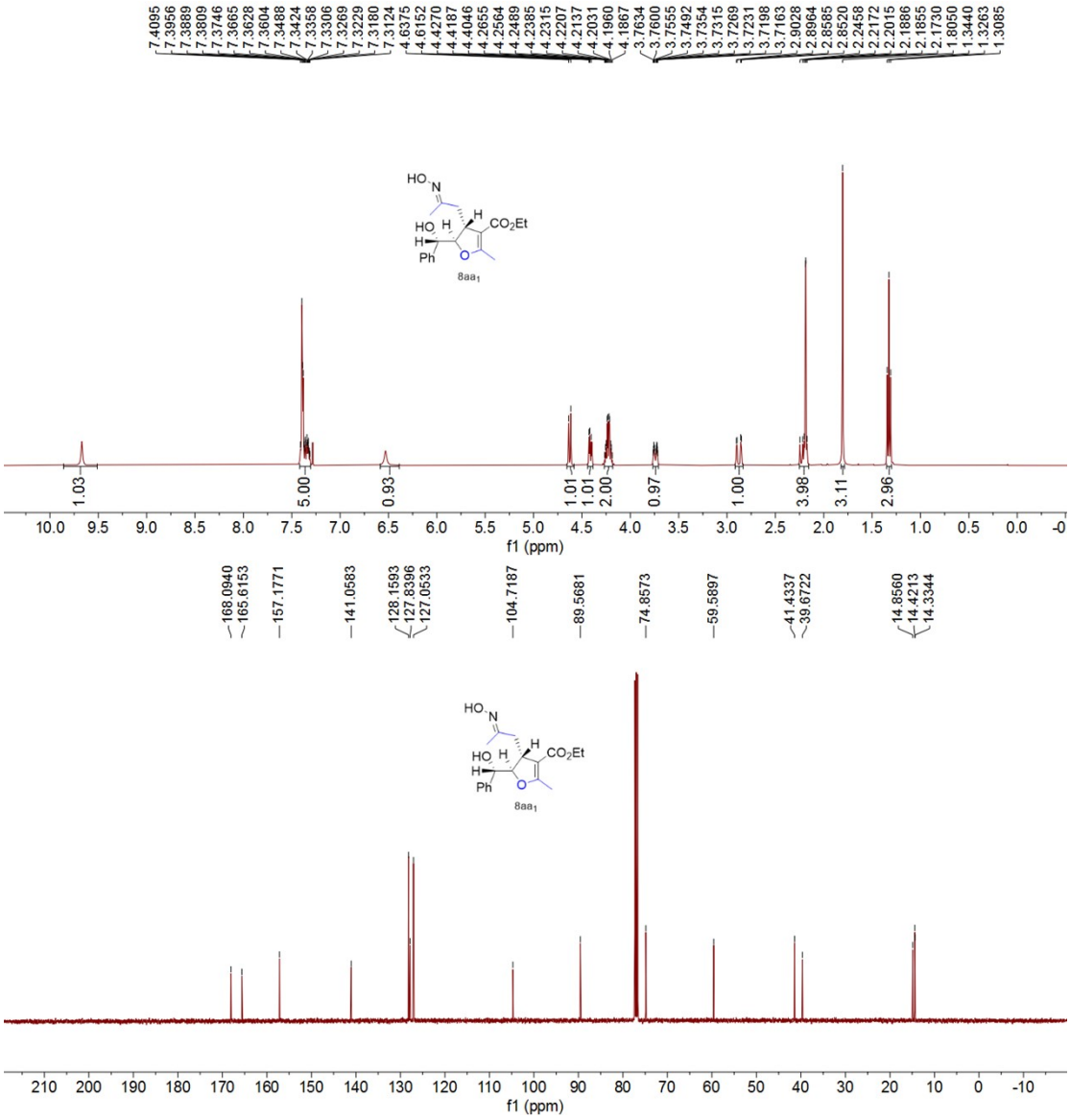
^{1}H and ^{13}C NMR Spectra for cis-6ad



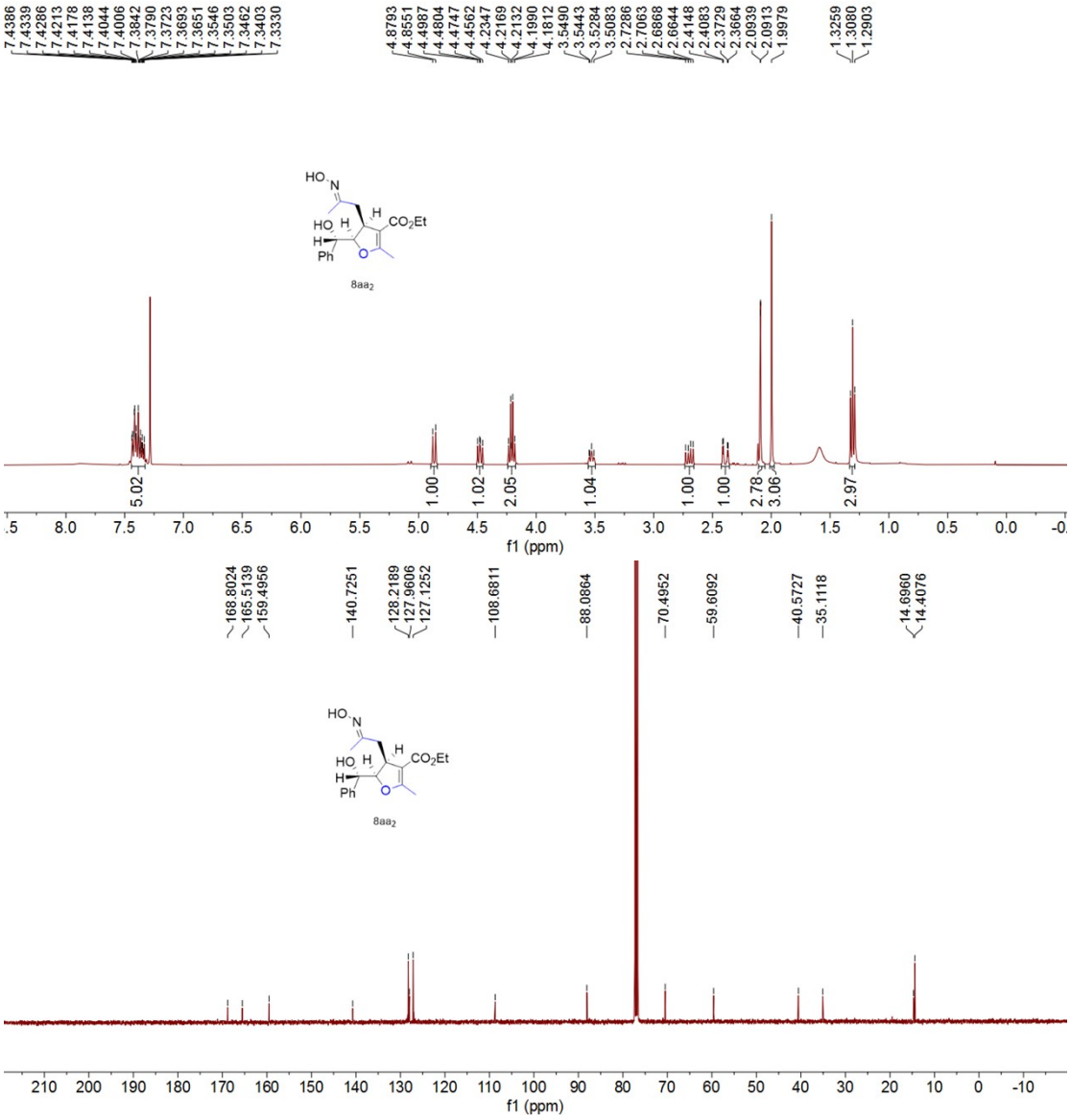
^{1}H- ^{13}C-HSQC NMR for cis-6ad



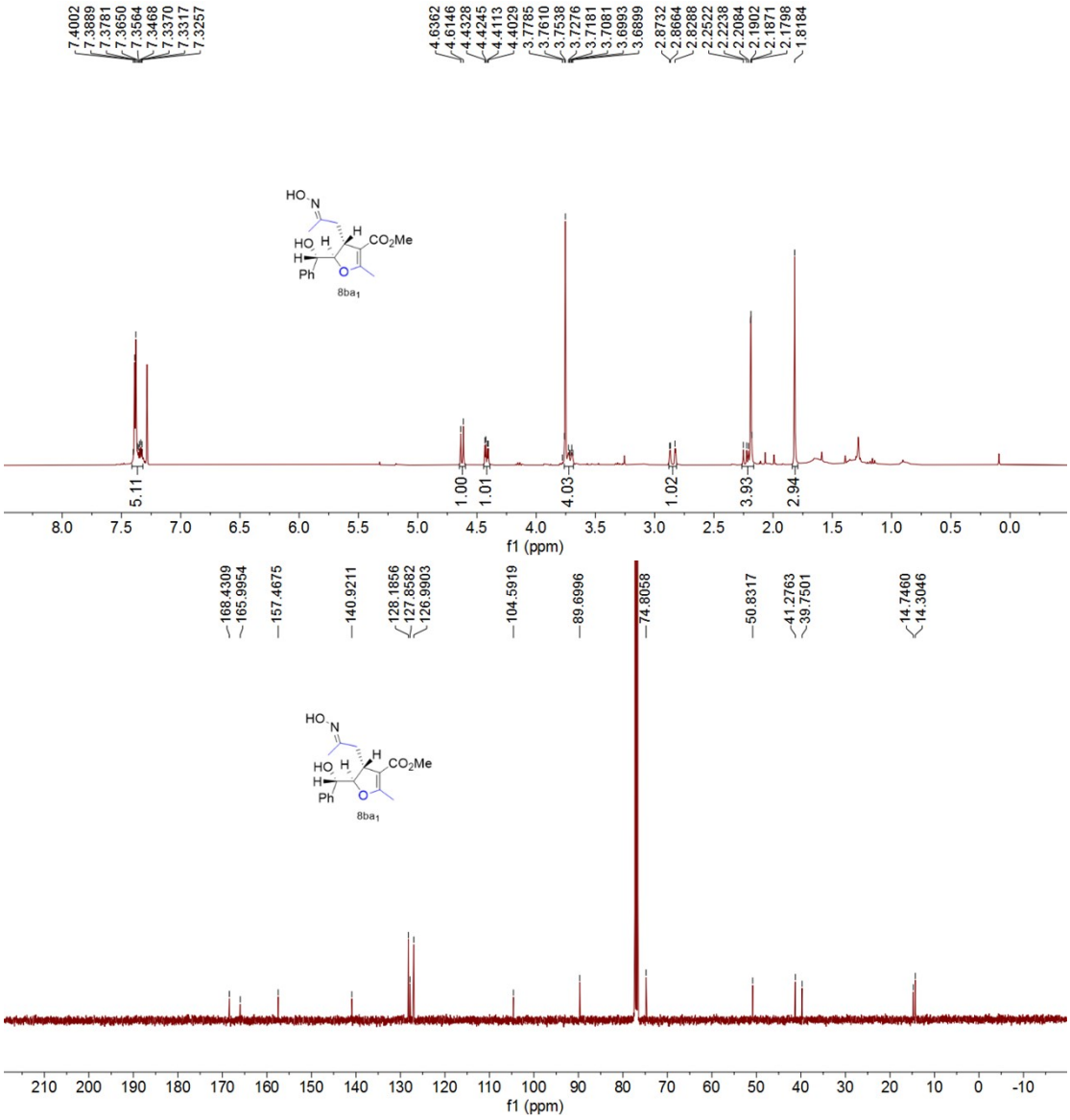
^{1}H and ^{13}C NMR Spectra for $8aa_1$



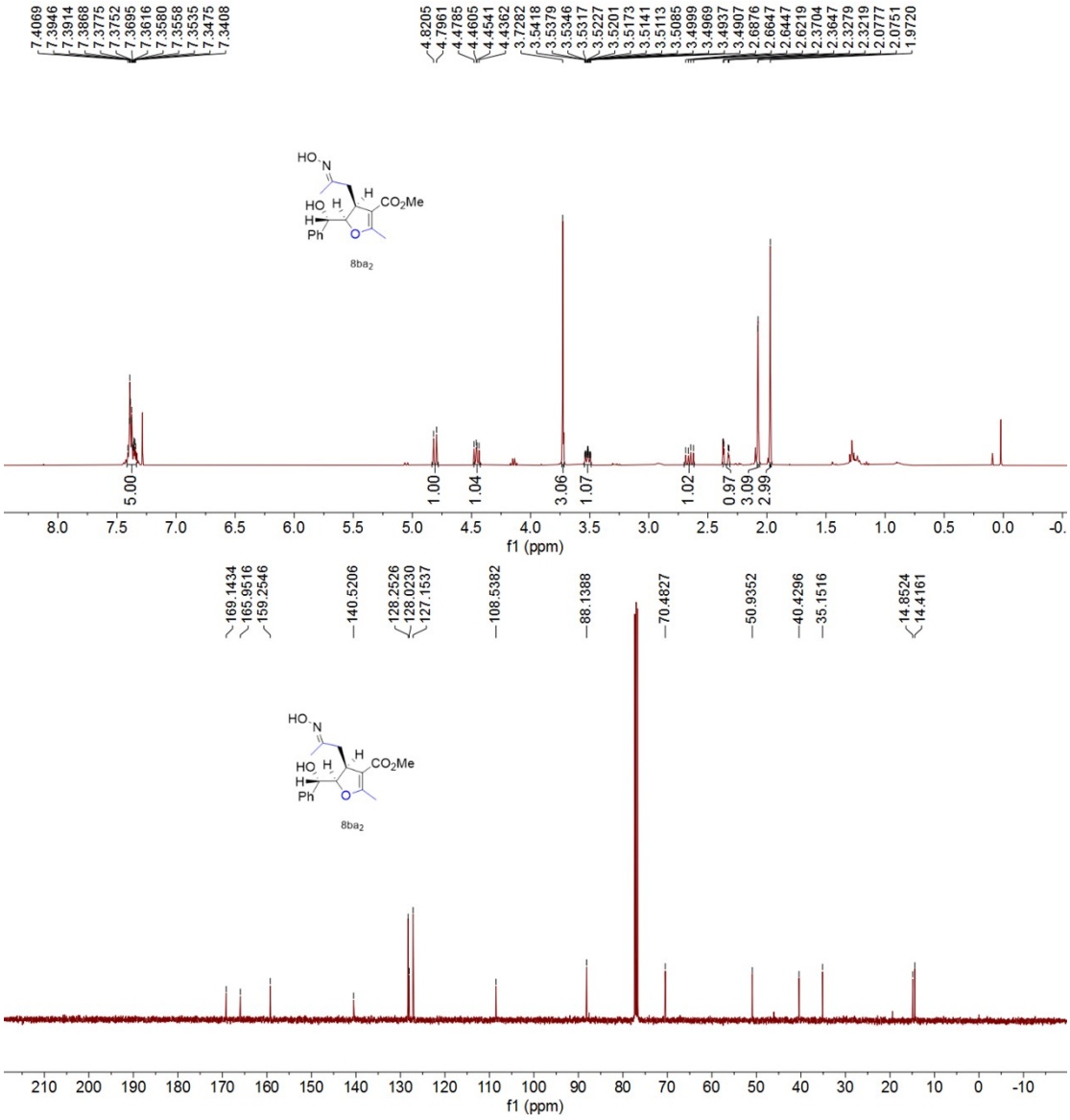
^{1}H and ^{13}C NMR Spectra for $8aa_2$



^{1}H and ^{13}C NMR Spectra for $8ba_1$

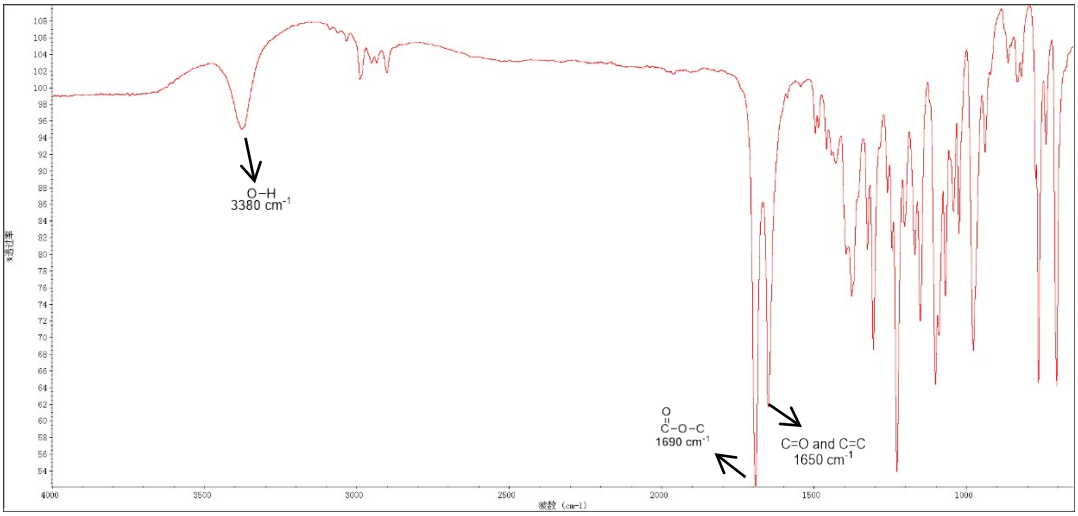


^{1}H and ^{13}C NMR Spectra for $8ba_2$

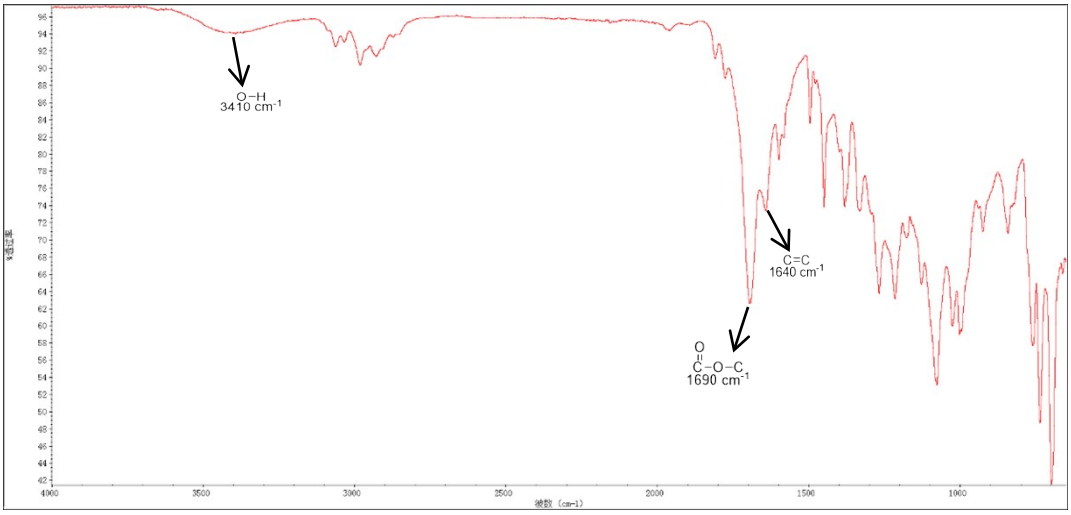


8.Infrared Spectroscopy for cis-6ad

tablet method of the crystals



solution method in CHCl3



9.Density Functional Theory (DFT) calculations results

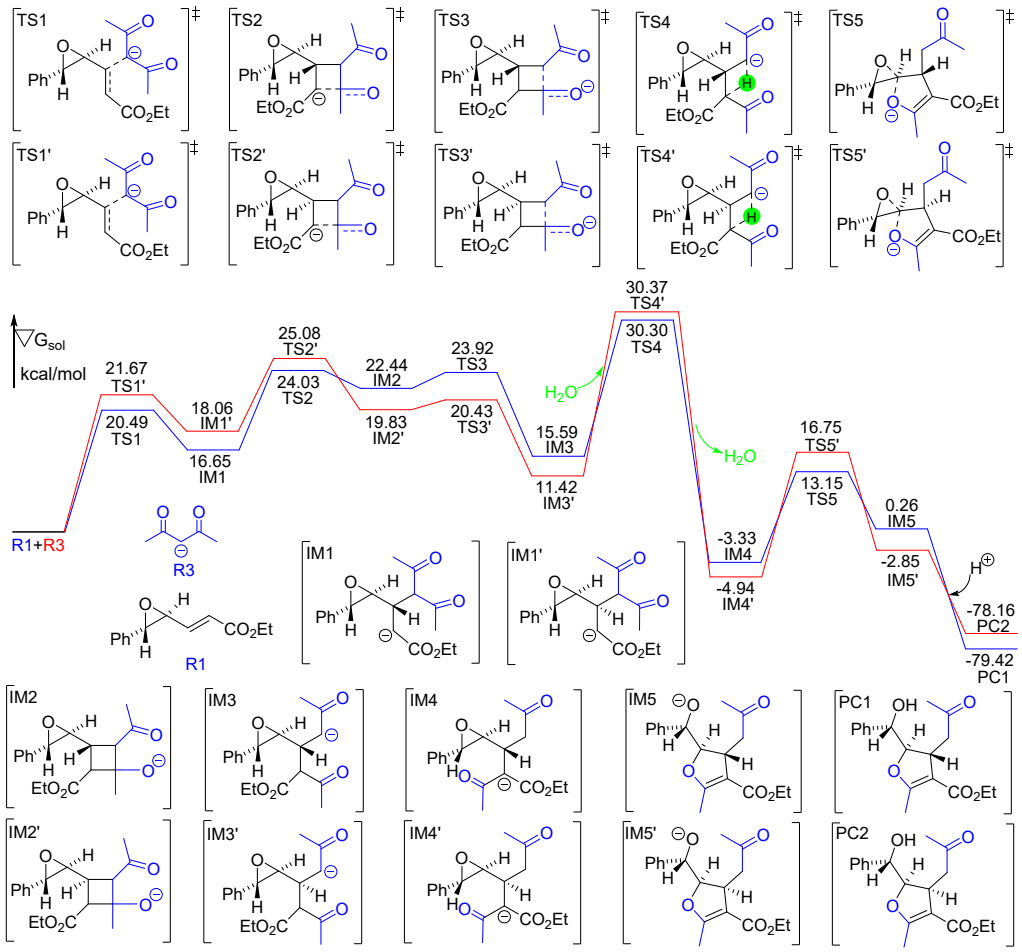


Figure 1. DFT-computed free energy surface fore the conversion of R1+R2 into PC1/PC2 intermediate at the M062X(D3)/6-31G(d) level with the SMD solvation model and DMF as the solvent.

In order to prove the **Scheme 5** inferred mechanism from R1+R3 to PC1/PC2, DFT calculations at the M062X(D3)/6-31G(d) level with the SMD solvation model and DMF as the solvent were carried out to study the mechanism by Gaussian 09. The intrinsic reaction coordinate (IRC)[19] calculations haD confirmed that all stationary points were smoothly connected to each other. The calculated distribution of free energy (△Gsol) is shown in **Figure 1**, and the intermediate and transition states collected in this reaction process are shown in **Figure 2**. Taking the trans synthesis route as an example, the reaction begins with R1 and R3. Under Michael's induction, R1 and R3 undergo an addition reaction to form the transition state TS1, which absorbs 20.49 kcal/mol. Then, the intermediate IM1 was obtained after 3.84 kcal/mol exothermal heat of TS1. The intermediate IM1 with bond length of 1.64 A was generated from the transition state TS1 with bond length of 2.04 A. The intermediate IM2 underwent intramolecular aldol reaction, and the intermediate IM2 was obtained through TS2.The heat was first absorbed by 7.38 kcal/mol and then released by 1.59 kcal/mol. The length of the bond involved in the reaction was shortened from 1.99 A to 1.72 A.IM2 breaks the C-C bond through the inverse aldol reaction and generates the intermediate IM3. The heat release of the reaction is 6.85 kcal/mol. The transformation of IM3 to IM4 is a proton transfer process. It has been shown that the energy barrier can be reduced by the water-assisted proton displacement process. Therefore, the way is through the water catalyzed

proton shift process. Finally, IM4 endothermic 3.59 kcal/mol, first through enolization transition and then attack the epoxy group to obtain IM5, IM5 acidized to form the final product PC1. This reaction has multiple endothermic processes, which means that the reaction is more difficult at room temperature. This conclusion is in good agreement with the reaction temperature of 70℃.

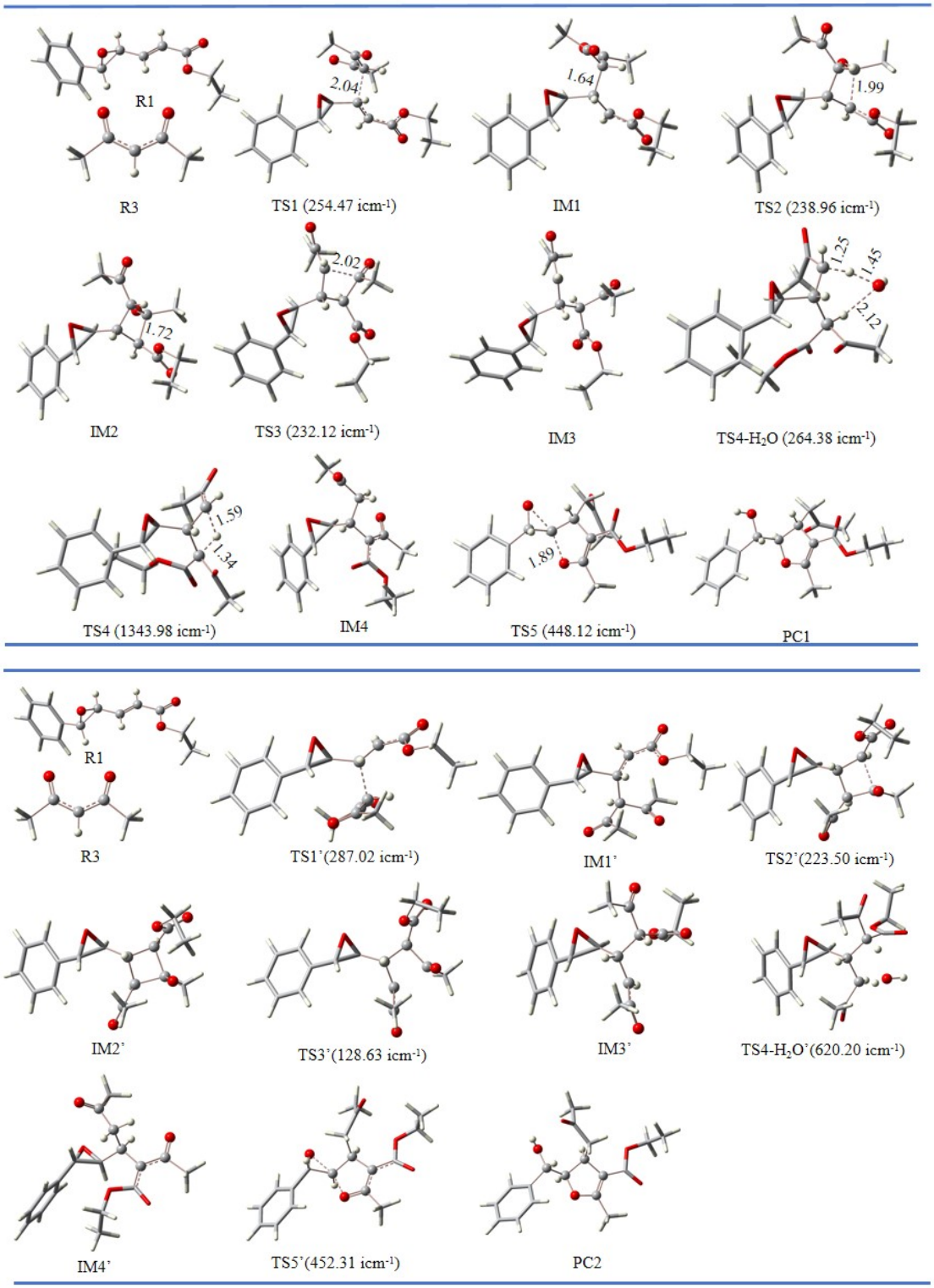


Figure 2. Optimized corresponding structures of intermediates and transition states along different pathways of Figure S1 from R1 and R3 conversion to generate PC1/PC2 at the M062X(D3)/6-31G(d) level with the SMD solvation

model and DMF as the solvent (distances in Å). Parameters in parentheses are the unique imaginary frequencies of the transition state.

Table 1. The gibbs energies of all optimized stationary points in solvent[a]

Structure	Gsol (Hartree)	△Gsol (Hartree)	△Gsol (kcal/mol) =△Gsol(Hartree)*627.51
R3	-344.9881913		
R1	-728.7197335		
TS1	-1073.675276	0.032648677	20.49
IM1	-1073.681388	0.026537007	16.65
TS2	-1073.669633	0.038291537	24.03
IM2	-1073.672165	0.035760267	22.44
TS3	-1073.669811	0.038113807	23.92
IM3	-1073.683084	0.024841207	15.59
H_2O	-76.38159247		0.00
TS4-H_2O	-1150.041229	0.048288467	30.30
IM4	-1073.713224	-0.005299423	-3.33
TS5	-1073.686966	0.020959037	13.15
IM5	-1073.707509	0.000415877	0.26
PC1	-1074.21257	-0.126566849	-79.42

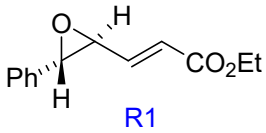
[a]Gibbs free energies for the conversion of R1 and R3 into PC1 at the M06-2X(D3)/6-31G(d) level with the SMD solvation model and DMF as the solvent.

Structure	Gsol (Hartree)	△Gsol (Hartree)	△Gsol (kcal/mol) =△Gsol(Hartree)*627.51
R1	-728.7197335		
R3	-344.9881913		
TS1’	-1073.673392	0.034532687	21.67
IM1’	-1073.679152	0.028772967	18.06
TS2’	-1073.667961	0.039963947	25.08
IM2’	-1073.676322	0.031602617	19.83
TS3’	-1073.675375	0.032550177	20.43
IM3’	-1073.689721	0.018203817	11.42
H_2O	-76.38159247		0.00
TS4’-H_2O	-1150.041123	0.048394087	30.37

IM4’	-1073.71583	-0.007905373	-4.96
TS5’	-1073.681228	0.026696987	16.75
IM5’	-1073.712459	-0.004534013	-2.85
PC2	-1074.210552	-0.124549709	-78.16

[a]Gibbs free energies for the conversion of R1 and R3 into PC2 at the M06-2X(D3)/6-31G(d) level with the SMD solvation model and DMF as the solvent.

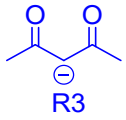
10.DFT-calculated Cartesian Coordinates



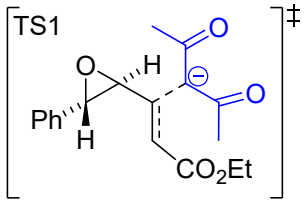
R1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.515189	1.695399	-0.361883
2	6	0	3.247610	1.471386	0.164755
3	6	0	2.792227	0.168605	0.372405
4	6	0	3.623546	-0.908795	0.061696
5	6	0	4.891692	-0.682784	-0.461455
6	6	0	5.339555	0.618470	-0.677803
7	1	0	4.861574	2.712720	-0.521557
8	1	0	2.605673	2.312996	0.415943
9	1	0	3.270182	-1.917830	0.254077
10	1	0	5.536084	-1.525698	-0.695790
11	1	0	6.331336	0.793128	-1.085383
12	6	0	1.423437	-0.059699	0.897909
13	1	0	1.016220	0.738676	1.521781
14	6	0	0.445431	-0.885392	0.145578
15	1	0	0.804145	-1.338879	-0.779513
16	6	0	-0.994189	-0.624247	0.243526
17	1	0	-1.367153	-0.314762	1.217512
18	6	0	-1.833196	-0.728961	-0.792867
19	1	0	-1.491469	-1.046352	-1.774359
20	6	0	-3.275568	-0.432938	-0.726054
21	8	0	-4.019470	-0.530522	-1.678414
22	8	0	-3.671696	-0.050466	0.501708
23	6	0	-5.064764	0.259304	0.640172
24	1	0	-5.646332	-0.462759	0.060691
25	1	0	-5.270599	0.119061	1.704153
26	6	0	-5.359929	1.676436	0.197802

27	1	0	-5.165880	1.789714	-0.872058
28	1	0	-6.412879	1.914347	0.383286
29	1	0	-4.742515	2.391987	0.749671
30	8	0	1.086836	-1.364895	1.326564



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.271374	-0.089109	-0.000029
2	8	0	-1.540315	-1.299946	-0.000000
3	6	0	0.000000	0.542868	-0.000092
4	1	0	0.000020	1.631587	-0.000110
5	6	0	1.271346	-0.089124	-0.000028
6	8	0	1.540280	-1.299954	0.000024
7	6	0	-2.480542	0.871358	0.000040
8	1	0	-3.102146	0.663678	0.880529
9	1	0	-2.213289	1.935011	-0.000326
10	1	0	-3.102638	0.663176	-0.879978
11	6	0	2.480589	0.871349	0.000029
12	1	0	3.102341	0.663365	0.880340
13	1	0	2.213385	1.935010	-0.000003
14	1	0	3.102487	0.663316	-0.880164



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.056709	-2.156937	0.059827
2	6	0	3.776842	-1.960833	-0.449101
3	6	0	3.207488	-0.685852	-0.466620
4	6	0	3.946203	0.394588	0.022269
5	6	0	5.225904	0.198451	0.528390
6	6	0	5.786488	-1.077304	0.550997
7	1	0	5.486064	-3.155918	0.070939

8	1	0	3.205891	-2.804172	-0.831748
9	1	0	3.501052	1.384789	-0.012787
10	1	0	5.790757	1.047216	0.906391
11	1	0	6.787551	-1.228736	0.947176
12	6	0	1.829124	-0.488731	-0.974582
13	1	0	1.475455	-1.237252	-1.685949
14	6	0	0.796240	0.194038	-0.170893
15	1	0	1.104354	0.585377	0.800433
16	6	0	-0.639999	-0.172166	-0.305714
17	1	0	-1.021451	-0.100929	-1.323884
18	6	0	-1.071192	-1.258196	0.477447
19	1	0	-0.496041	-1.569537	1.344932
20	6	0	-2.298525	-1.941955	0.284067
21	8	0	-2.738373	-2.891942	0.931263
22	8	0	-3.027653	-1.416341	-0.774268
23	6	0	-4.300053	-1.995772	-0.977091
24	1	0	-4.548078	-1.794531	-2.025314
25	1	0	-4.241448	-3.078171	-0.820575
26	6	0	-5.338119	-1.389950	-0.049568
27	1	0	-5.370183	-0.301854	-0.171466
28	1	0	-6.336135	-1.795142	-0.259517
29	1	0	-5.076409	-1.621831	0.986453
30	8	0	1.430854	0.842556	-1.272003
31	6	0	-1.176135	2.505898	-0.955940
32	8	0	-1.718529	2.415638	-2.057795
33	6	0	-1.557190	1.596224	0.128265
34	1	0	-2.541600	1.165214	-0.046782
35	6	0	-1.212498	1.815007	1.520142
36	8	0	-0.210184	2.420819	1.919629
37	6	0	-0.098726	3.546202	-0.733016
38	1	0	-0.075167	4.203726	-1.606523
39	1	0	-0.269370	4.111077	0.187442
40	1	0	0.874532	3.059351	-0.617617
41	6	0	-2.118114	1.112064	2.506939
42	1	0	-3.164995	1.408652	2.374123
43	1	0	-2.066550	0.029862	2.304422
44	1	0	-1.793829	1.318316	3.530334

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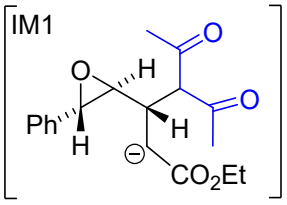
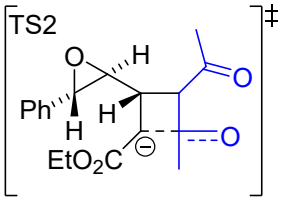


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.238025	-1.793489	0.271467
2	6	0	3.933680	-1.648365	-0.189455
3	6	0	3.413957	-0.380190	-0.457583
4	6	0	4.224427	0.740948	-0.267661
5	6	0	5.529490	0.595000	0.189981
6	6	0	6.041650	-0.671785	0.462332
7	1	0	5.628331	-2.786188	0.482486
8	1	0	3.303121	-2.523025	-0.332893
9	1	0	3.811461	1.719447	-0.495309
10	1	0	6.151691	1.475304	0.333474
11	1	0	7.061904	-0.784761	0.820713
12	6	0	2.011272	-0.230051	-0.916555
13	1	0	1.612873	-1.069374	-1.490404
14	6	0	1.030804	0.570327	-0.176814
15	1	0	1.387198	1.093571	0.712237
16	6	0	-0.430151	0.209503	-0.207016
17	1	0	-0.609269	-0.276626	-1.173538
18	6	0	-0.752239	-0.719492	0.896842
19	1	0	-0.179931	-0.665373	1.818545
20	6	0	-1.708730	-1.724298	0.817383
21	8	0	-2.036672	-2.581818	1.647909
22	8	0	-2.380337	-1.711518	-0.442789
23	6	0	-3.522570	-2.533320	-0.503562
24	1	0	-3.702398	-2.717342	-1.571637
25	1	0	-3.314871	-3.487494	-0.006600
26	6	0	-4.728121	-1.866307	0.137956
27	1	0	-4.893480	-0.870875	-0.287322
28	1	0	-5.634342	-2.471264	-0.000116
29	1	0	-4.539659	-1.755895	1.209479
30	8	0	1.619687	1.056442	-1.390879
31	6	0	-1.147448	2.399058	0.947100
32	8	0	-0.313430	3.289805	1.040646
33	6	0	-1.245856	1.605398	-0.332513
34	1	0	-0.690173	2.170875	-1.092666
35	6	0	-2.626840	1.362458	-0.890845
36	8	0	-3.667033	1.569382	-0.290287
37	6	0	-2.007480	1.982706	2.097226
38	1	0	-1.742770	2.553758	2.990776
39	1	0	-3.061256	2.108056	1.832419
40	1	0	-1.860093	0.899367	2.240412
41	6	0	-2.664577	0.831479	-2.308465

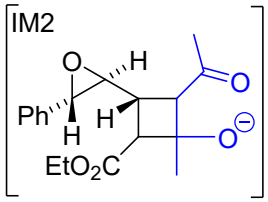
42	1	0	-1.842857	1.212645	-2.922968
43	1	0	-2.570170	-0.258479	-2.242711
44	1	0	-3.628790	1.077833	-2.760079



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.839286	-0.362738	1.353037
2	6	0	3.450120	-0.406861	1.298400
3	6	0	2.800346	-0.877092	0.155152
4	6	0	3.564303	-1.318880	-0.926780
5	6	0	4.953053	-1.278465	-0.870571
6	6	0	5.596418	-0.798060	0.268069
7	1	0	5.332106	0.011905	2.246786
8	1	0	2.859180	-0.067603	2.146375
9	1	0	3.045762	-1.703596	-1.800335
10	1	0	5.537671	-1.625990	-1.719183
11	1	0	6.682246	-0.765429	0.310939
12	6	0	1.317980	-0.885712	0.089977
13	1	0	0.799374	-1.008824	1.041930
14	6	0	0.584980	-0.165318	-0.965923
15	1	0	1.202960	0.333136	-1.718960
16	6	0	-0.802008	0.396225	-0.786119
17	1	0	-1.411365	-0.039498	-1.585398
18	6	0	-1.530697	0.198062	0.526229
19	1	0	-0.941427	0.378789	1.423095
20	6	0	-2.456468	-0.890723	0.731987
21	8	0	-2.866361	-1.315059	1.804488
22	8	0	-2.945553	-1.400043	-0.455386
23	6	0	-3.902565	-2.434196	-0.323159
24	1	0	-4.571693	-2.208960	0.513561
25	1	0	-4.476045	-2.419055	-1.256893
26	6	0	-3.235153	-3.781542	-0.116906
27	1	0	-2.702928	-3.781231	0.837837
28	1	0	-3.979018	-4.588027	-0.105517
29	1	0	-2.515440	-3.977901	-0.918586
30	8	0	0.718106	-1.589149	-0.988823
31	6	0	0.236145	2.765610	-0.486231

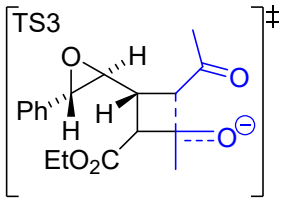
32	8	0	0.714207	3.572021	-1.272540
33	6	0	-0.955856	1.933335	-0.865634
34	1	0	-1.270069	2.293912	-1.852553
35	6	0	-2.150504	1.924029	0.219242
36	8	0	-2.140912	2.698232	1.216139
37	6	0	0.761868	2.632444	0.914558
38	1	0	1.602961	3.312858	1.067952
39	1	0	-0.099085	2.859371	1.565837
40	1	0	1.068847	1.603421	1.130165
41	6	0	-3.489278	1.758092	-0.506510
42	1	0	-3.475005	1.002054	-1.298836
43	1	0	-4.252531	1.484794	0.229464
44	1	0	-3.764224	2.728606	-0.941610

IM2



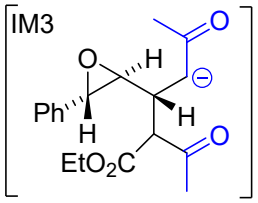
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.872514	-2.106814	0.364921
2	6	0	3.623474	-1.900539	-0.212237
3	6	0	3.162597	-0.607303	-0.465769
4	6	0	3.980029	0.478848	-0.144574
5	6	0	5.228919	0.272936	0.429681
6	6	0	5.680528	-1.019898	0.688349
7	1	0	5.215978	-3.119649	0.561440
8	1	0	2.991978	-2.750178	-0.463795
9	1	0	3.618976	1.479605	-0.362817
10	1	0	5.854971	1.126913	0.676947
11	1	0	6.657259	-1.179176	1.138466
12	6	0	1.816800	-0.392058	-1.050920
13	1	0	1.427511	-1.226853	-1.639293
14	6	0	0.829084	0.503032	-0.425948
15	1	0	1.116248	1.023292	0.488273
16	6	0	-0.638363	0.236329	-0.559271
17	1	0	-0.820441	-0.298402	-1.499854
18	6	0	-1.123215	-0.475374	0.716747
19	1	0	-0.355570	-0.843833	1.397899
20	6	0	-2.186820	-1.471505	0.606981
21	8	0	-2.463250	-2.322844	1.437028

22	8	0	-2.947190	-1.317040	-0.525595
23	6	0	-4.077597	-2.168991	-0.626297
24	1	0	-4.533593	-2.283199	0.362113
25	1	0	-4.774112	-1.642394	-1.286877
26	6	0	-3.702851	-3.523979	-1.195702
27	1	0	-3.027787	-4.037728	-0.506280
28	1	0	-4.596197	-4.144008	-1.339220
29	1	0	-3.201661	-3.408785	-2.162800
30	8	0	1.548474	0.891137	-1.603762
31	6	0	-1.330886	2.852411	-0.719090
32	8	0	-2.196860	3.517065	-1.279738
33	6	0	-1.587061	1.433055	-0.337606
34	1	0	-2.559862	1.159726	-0.754620
35	6	0	-1.577855	1.086047	1.258947
36	8	0	-0.637689	1.617680	1.960505
37	6	0	-0.044321	3.477068	-0.256344
38	1	0	-0.088420	4.560710	-0.396898
39	1	0	0.070665	3.186455	0.802146
40	1	0	0.811118	3.069653	-0.807333
41	6	0	-2.974514	1.125035	1.882376
42	1	0	-3.739826	0.635777	1.267676
43	1	0	-2.938802	0.639933	2.864249
44	1	0	-3.259096	2.174344	2.027602



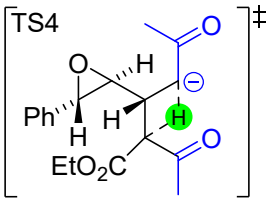
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.701271	0.321768	0.890300
2	6	0	-3.471730	0.530074	0.274406
3	6	0	-2.813854	-0.520960	-0.369414
4	6	0	-3.414000	-1.781796	-0.397626
5	6	0	-4.644592	-1.988580	0.215944
6	6	0	-5.293056	-0.939033	0.863612
7	1	0	-5.199364	1.147318	1.392983
8	1	0	-3.008073	1.513964	0.299221
9	1	0	-2.900668	-2.585078	-0.918375
10	1	0	-5.102339	-2.974580	0.186417
11	1	0	-6.254841	-1.102029	1.343510

12	6	0	-1.486113	-0.299626	-0.989838
13	1	0	-1.299677	0.711038	-1.358026
14	6	0	-0.296264	-1.071486	-0.584429
15	1	0	-0.462519	-1.849326	0.162381
16	6	0	1.073600	-0.457205	-0.651626
17	1	0	1.068513	0.175947	-1.545271
18	6	0	1.463281	0.408356	0.538948
19	1	0	1.225429	-0.059343	1.495992
20	6	0	1.013570	1.821905	0.618146
21	8	0	0.930746	2.492703	1.627264
22	8	0	0.746605	2.354273	-0.613095
23	6	0	0.403508	3.734087	-0.623560
24	1	0	1.016234	4.262687	0.112718
25	1	0	0.661821	4.084122	-1.627798
26	6	0	-1.070529	3.941243	-0.333295
27	1	0	-1.330140	5.004609	-0.395905
28	1	0	-1.688566	3.393849	-1.053550
29	1	0	-1.300944	3.586866	0.675295
30	8	0	-0.969952	-1.332965	-1.818806
31	6	0	2.553944	-2.549262	0.020088
32	8	0	3.296381	-3.447203	-0.396551
33	6	0	2.312932	-1.342031	-0.737975
34	1	0	2.740895	-1.434658	-1.737838
35	6	0	3.049782	0.176571	0.372609
36	8	0	3.724891	-0.051556	1.394877
37	6	0	2.057251	-2.632714	1.452057
38	1	0	1.004044	-2.358828	1.581265
39	1	0	2.221173	-3.645134	1.830325
40	1	0	2.660813	-1.910569	2.024446
41	6	0	3.684260	1.018061	-0.732953
42	1	0	3.896299	2.021546	-0.334553
43	1	0	4.636575	0.556325	-1.008314
44	1	0	3.061663	1.123022	-1.626793



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.019275	-0.694744	-0.710374

2	6	0	-2.806384	-1.047723	-0.130426
3	6	0	-2.296546	-0.307150	0.940651
4	6	0	-3.017594	0.785835	1.421344
5	6	0	-4.233533	1.135586	0.840155
6	6	0	-4.739665	0.397470	-0.226897
7	1	0	-4.402642	-1.269817	-1.550422
8	1	0	-2.217794	-1.875089	-0.519328
9	1	0	-2.601454	1.352014	2.249826
10	1	0	-4.787561	1.991040	1.220719
11	1	0	-5.687174	0.673742	-0.683694
12	6	0	-0.970990	-0.660818	1.497817
13	1	0	-0.766799	-1.729003	1.567357
14	6	0	0.171458	0.234571	1.290031
15	1	0	-0.017205	1.181535	0.792653
16	6	0	1.599586	-0.251048	1.180861
17	1	0	1.715327	-1.010723	1.969427
18	6	0	1.887485	-0.988900	-0.194833
19	1	0	2.971924	-0.939745	-0.317728
20	6	0	1.331359	-0.404285	-1.474550
21	8	0	1.959368	-0.399796	-2.512053
22	8	0	0.023574	-0.113287	-1.381650
23	6	0	-0.564688	0.599478	-2.465760
24	1	0	0.140625	0.606523	-3.300766
25	1	0	-1.460598	0.037619	-2.754332
26	6	0	-0.908717	2.000331	-2.002849
27	1	0	-0.000974	2.477612	-1.619284
28	1	0	-1.321903	2.585336	-2.834734
29	1	0	-1.655291	1.964277	-1.201689
30	8	0	-0.459118	0.113437	2.576907
31	6	0	2.631038	1.879199	0.495180
32	8	0	1.944560	1.911663	-0.579520
33	6	0	2.562458	0.864777	1.424170
34	1	0	3.164505	0.863047	2.328043
35	6	0	1.499697	-2.443844	-0.057935
36	8	0	0.400597	-2.899979	-0.319705
37	6	0	3.585504	3.041481	0.737551
38	1	0	3.021639	3.983415	0.749458
39	1	0	4.143556	2.952893	1.677532
40	1	0	4.298198	3.112227	-0.094385
41	6	0	2.599011	-3.338861	0.479196
42	1	0	3.346741	-3.490324	-0.309680
43	1	0	3.115795	-2.864940	1.321237
44	1	0	2.188018	-4.306066	0.777962



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.514636	0.385329	-0.222873
2	6	0	-3.241913	0.297401	-0.777933
3	6	0	-2.518077	-0.895774	-0.710196
4	6	0	-3.099190	-2.007706	-0.096680
5	6	0	-4.372883	-1.920835	0.453473
6	6	0	-5.085224	-0.724063	0.396703
7	1	0	-5.064814	1.321876	-0.278840
8	1	0	-2.792985	1.160076	-1.265847
9	1	0	-2.535878	-2.936192	-0.070956
10	1	0	-4.814588	-2.793262	0.929356
11	1	0	-6.080726	-0.658057	0.828753
12	6	0	-1.144644	-0.952663	-1.257217
13	1	0	-0.912956	-0.225481	-2.039259
14	6	0	0.003055	-1.395339	-0.443286
15	1	0	-0.208660	-1.734599	0.570486
16	6	0	1.363217	-0.804341	-0.727502
17	1	0	1.379402	-0.716051	-1.819478
18	6	0	1.470440	0.676305	-0.226844
19	1	0	2.374327	0.735414	0.403484
20	6	0	0.313206	1.144395	0.613178
21	8	0	-0.080590	0.621967	1.633754
22	8	0	-0.256195	2.273879	0.128056
23	6	0	-1.320930	2.818475	0.910761
24	1	0	-1.890998	3.433340	0.208278
25	1	0	-1.953490	2.001609	1.268358
26	6	0	-0.788010	3.645823	2.062295
27	1	0	-0.236973	3.007998	2.758142
28	1	0	-0.118963	4.431436	1.695842
29	1	0	-1.614767	4.118664	2.604804
30	8	0	-0.556041	-2.235075	-1.452110
31	6	0	2.693339	-2.312508	0.949251
32	8	0	3.145597	-3.448682	1.110225
33	6	0	2.559748	-1.684102	-0.362871
34	1	0	2.726605	-2.436757	-1.138911
35	6	0	1.716472	1.628760	-1.401903

36	8	0	1.167223	1.481995	-2.477585
37	6	0	2.456370	-1.436433	2.170807
38	1	0	3.195835	-0.624771	2.140266
39	1	0	1.468970	-0.963635	2.180424
40	1	0	2.598064	-2.032491	3.076476
41	6	0	2.739678	2.689302	-1.138922
42	1	0	2.844898	3.353918	-1.999880
43	1	0	2.469744	3.262706	-0.243484
44	1	0	3.671523	2.138533	-0.904203
45	8	0	4.271523	0.312280	-0.189832
46	1	0	5.041910	-0.028799	0.284062
47	1	0	3.542276	-0.778537	-0.349376

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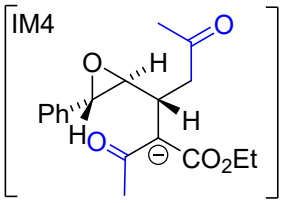
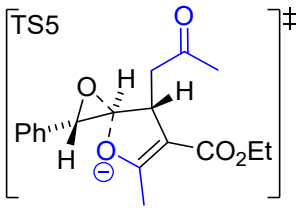


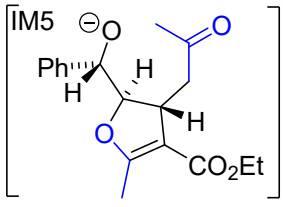
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.366021	0.404569	0.088682
2	6	0	3.079885	0.217669	-0.405773
3	6	0	2.159797	1.269328	-0.402645
4	6	0	2.552380	2.513224	0.093994
5	6	0	3.840499	2.700920	0.584498
6	6	0	4.752627	1.648031	0.584930
7	1	0	5.070048	-0.424310	0.086932
8	1	0	2.773039	-0.753793	-0.787402
9	1	0	1.829884	3.324097	0.078196
10	1	0	4.135300	3.675369	0.967607
11	1	0	5.759103	1.794901	0.969467
12	6	0	0.783436	1.042528	-0.903295
13	1	0	0.686351	0.317703	-1.713273
14	6	0	-0.389048	1.171167	-0.030574
15	1	0	-0.222777	1.484639	0.999536
16	6	0	-1.562568	0.259231	-0.273199
17	1	0	-1.612232	0.090675	-1.354104
18	6	0	-1.249628	-1.075990	0.377295
19	1	0	-2.886244	0.913488	1.275354
20	6	0	-0.797559	-2.068325	-0.533745
21	8	0	-0.640681	-1.927675	-1.754343
22	8	0	-0.493177	-3.297576	0.032984

23	6	0	0.075530	-4.241272	-0.851422
24	1	0	-0.082532	-5.214394	-0.371468
25	1	0	-0.455348	-4.221739	-1.808537
26	6	0	1.556247	-3.985504	-1.073243
27	1	0	2.087329	-3.948874	-0.115558
28	1	0	2.003311	-4.774645	-1.690960
29	1	0	1.680962	-3.027548	-1.585262
30	8	0	-0.071749	2.177933	-1.014296
31	6	0	-3.341778	2.129481	-0.442034
32	8	0	-4.157513	2.185664	-1.346161
33	6	0	-2.929000	0.821757	0.184423
34	1	0	-3.687806	0.080216	-0.083494
35	6	0	-1.238622	-1.138191	1.800640
36	8	0	-1.449325	-0.130126	2.514961
37	6	0	-2.724383	3.398931	0.109501
38	1	0	-2.677124	3.374520	1.203554
39	1	0	-1.696715	3.489188	-0.259426
40	1	0	-3.302456	4.262270	-0.230045
41	6	0	-0.969160	-2.439961	2.548341
42	1	0	-1.616571	-3.254031	2.209982
43	1	0	0.060089	-2.780378	2.394963
44	1	0	-1.134105	-2.238675	3.610540



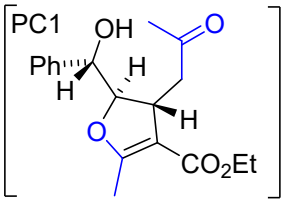
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.497543	-2.109250	0.652410
2	6	0	3.293832	-1.665879	0.114368
3	6	0	3.225467	-0.438099	-0.548221
4	6	0	4.377031	0.337022	-0.660568
5	6	0	5.585655	-0.107823	-0.130036
6	6	0	5.650923	-1.333785	0.527735
7	1	0	4.538989	-3.062870	1.175756
8	1	0	2.386800	-2.253912	0.230686
9	1	0	4.271743	1.289120	-1.174374
10	1	0	6.480888	0.504296	-0.226605
11	1	0	6.592578	-1.683218	0.946795

12	6	0	1.943227	0.083672	-1.162327
13	1	0	1.515081	-0.716425	-1.809386
14	6	0	0.949651	0.638152	-0.229821
15	1	0	1.370874	1.297494	0.519168
16	6	0	-0.440955	0.922219	-0.762960
17	1	0	-0.379096	0.843204	-1.853206
18	6	0	-1.390098	-0.121704	-0.225580
19	1	0	-1.816216	2.547538	-1.011905
20	6	0	-2.711948	-0.194178	-0.753729
21	8	0	-3.186308	0.543518	-1.613398
22	8	0	-3.490744	-1.189304	-0.200617
23	6	0	-4.811894	-1.253002	-0.703636
24	1	0	-5.321409	-0.295053	-0.541601
25	1	0	-4.793672	-1.418789	-1.787753
26	6	0	-5.511964	-2.383253	0.018955
27	1	0	-4.994353	-3.332286	-0.155861
28	1	0	-5.526852	-2.200664	1.098630
29	1	0	-6.545891	-2.482036	-0.330805
30	8	0	1.994060	1.331803	-1.706055
31	6	0	-0.985223	2.754755	0.956189
32	8	0	-0.087211	3.302665	1.570864
33	6	0	-0.859014	2.393374	-0.501995
34	1	0	-0.083823	3.022573	-0.948095
35	6	0	-0.795388	-0.918732	0.742453
36	8	0	0.421818	-0.667980	1.049971
37	6	0	-2.283114	2.391329	1.641817
38	1	0	-3.140661	2.788600	1.086546
39	1	0	-2.388921	1.299460	1.636083
40	1	0	-2.283017	2.767428	2.667691
41	6	0	-1.444550	-2.065388	1.475361
42	1	0	-2.328521	-1.731919	2.027133
43	1	0	-1.788248	-2.832728	0.775366
44	1	0	-0.714263	-2.492000	2.167124



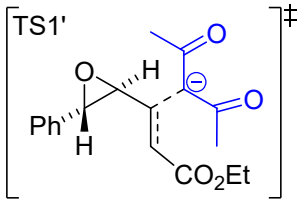
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.841852	-1.839826	-0.390770

2	6	0	-3.617601	-1.502653	0.181821
3	6	0	-3.328142	-0.177735	0.517888
4	6	0	-4.292360	0.799096	0.277976
5	6	0	-5.517992	0.469173	-0.293944
6	6	0	-5.798748	-0.853832	-0.632294
7	1	0	-5.054172	-2.876511	-0.649590
8	1	0	-2.870995	-2.272414	0.366212
9	1	0	-4.011323	1.805856	0.582034
10	1	0	-6.263284	1.243135	-0.475127
11	1	0	-6.757042	-1.117845	-1.076715
12	6	0	-2.005949	0.287425	1.159154
13	1	0	-1.803280	-0.469702	1.980433
14	6	0	-0.848815	0.092943	0.161131
15	1	0	-1.073640	0.641065	-0.759407
16	6	0	0.485767	0.549237	0.756969
17	1	0	0.429288	0.413070	1.848120
18	6	0	1.452561	-0.452842	0.168614
19	1	0	1.457385	2.418774	1.266075
20	6	0	2.877800	-0.276551	0.214117
21	8	0	3.447721	0.691489	0.698304
22	8	0	3.593409	-1.294788	-0.361989
23	6	0	5.005078	-1.132795	-0.342321
24	1	0	5.371605	-1.755250	-1.165152
25	1	0	5.251591	-0.086508	-0.545568
26	6	0	5.599699	-1.570888	0.982122
27	1	0	5.235773	-0.921615	1.782489
28	1	0	5.316872	-2.604357	1.209084
29	1	0	6.694118	-1.509161	0.951539
30	6	0	1.175677	2.442628	-0.833497
31	8	0	0.962522	1.798673	-1.845076
32	6	0	0.735460	2.034037	0.538249
33	1	0	-0.252995	2.481288	0.775136
34	6	0	0.719795	-1.484443	-0.332842
35	8	0	-0.597248	-1.297154	-0.265689
36	6	0	1.940927	3.750914	-0.900730
37	1	0	1.452437	4.527133	-0.300517
38	1	0	2.937854	3.585937	-0.473021
39	1	0	2.038954	4.078432	-1.938537
40	6	0	1.108206	-2.788777	-0.932094
41	1	0	0.834734	-2.798466	-1.993992
42	1	0	2.176656	-2.969589	-0.833185
43	1	0	0.539893	-3.589919	-0.446055
44	8	0	-1.999840	1.565028	1.536758



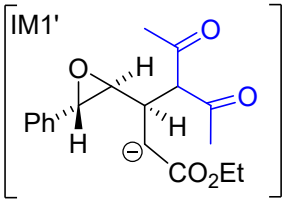
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.732198	-1.920043	0.383511
2	6	0	3.516793	-1.614341	-0.219157
3	6	0	3.213853	-0.299621	-0.573424
4	6	0	4.145625	0.707414	-0.315924
5	6	0	5.363973	0.402464	0.282809
6	6	0	5.659937	-0.911842	0.634103
7	1	0	4.958296	-2.947756	0.654579
8	1	0	2.790519	-2.399863	-0.413214
9	1	0	3.906104	1.730759	-0.592167
10	1	0	6.083325	1.193418	0.477391
11	1	0	6.611581	-1.150689	1.100923
12	6	0	1.881958	0.040866	-1.195278
13	1	0	1.488246	-0.849199	-1.715617
14	6	0	0.845200	0.457458	-0.155827
15	1	0	1.219951	1.314049	0.408960
16	6	0	-0.544825	0.727737	-0.767317
17	1	0	-0.514748	0.521764	-1.845269
18	6	0	-1.391273	-0.302266	-0.054743
19	1	0	-1.914895	2.316308	-1.243960
20	6	0	-2.815681	-0.400603	-0.301936
21	8	0	-3.425360	0.362388	-1.034491
22	8	0	-3.426339	-1.411520	0.357757
23	6	0	-4.836667	-1.533826	0.143027
24	1	0	-5.202034	-2.065230	1.025758
25	1	0	-5.280158	-0.534979	0.113653
26	6	0	-5.137490	-2.298632	-1.128430
27	1	0	-4.782591	-1.740337	-1.998525
28	1	0	-4.653269	-3.280235	-1.113584
29	1	0	-6.217806	-2.448554	-1.230713
30	6	0	-1.339698	2.578230	0.807070
31	8	0	-0.692228	2.169149	1.750266
32	6	0	-1.029518	2.171507	-0.619964
33	1	0	-0.250031	2.847484	-1.001233
34	6	0	-0.606385	-1.002163	0.797972
35	8	0	0.683371	-0.625162	0.778691

36	6	0	-2.511542	3.508421	0.986605
37	1	0	-2.421145	4.380614	0.328132
38	1	0	-3.424860	2.979546	0.685519
39	1	0	-2.590984	3.827650	2.027338
40	6	0	-0.886914	-2.091566	1.762984
41	1	0	-0.675633	-1.733284	2.776884
42	1	0	-1.922470	-2.417220	1.696601
43	1	0	-0.214506	-2.934979	1.571355
44	8	0	1.958874	1.144850	-2.076888
45	1	0	2.663289	0.957921	-2.711979



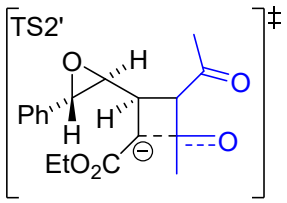
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.966319	0.800813	-0.348994
2	6	0	-3.625645	0.663383	-0.692142
3	6	0	-3.003436	-0.585608	-0.598994
4	6	0	-3.738597	-1.688324	-0.162761
5	6	0	-5.080694	-1.546700	0.177311
6	6	0	-5.699608	-0.302532	0.084701
7	1	0	-5.441030	1.776953	-0.416178
8	1	0	-3.033036	1.519414	-1.005118
9	1	0	-3.239317	-2.651356	-0.105608
10	1	0	-5.646629	-2.412296	0.514337
11	1	0	-6.748057	-0.191869	0.351477
12	6	0	-1.566387	-0.720563	-0.948193
13	1	0	-1.232740	-0.100603	-1.779432
14	6	0	-0.548450	-1.079645	0.051076
15	1	0	-0.898923	-1.296983	1.062226
16	6	0	0.875025	-0.646641	-0.063720
17	1	0	1.150494	-0.480393	-1.105786
18	6	0	1.815794	-1.412472	0.669903
19	1	0	1.526588	-1.892396	1.598499
20	6	0	3.192476	-1.416971	0.369229
21	8	0	4.103182	-2.025950	0.930491
22	8	0	3.491177	-0.596463	-0.735739
23	6	0	4.859310	-0.529758	-1.073905
24	1	0	5.321335	-1.512407	-0.931954

25	1	0	4.891081	-0.266811	-2.138635
26	6	0	5.586531	0.509083	-0.238512
27	1	0	5.106566	1.489109	-0.339969
28	1	0	5.553436	0.209245	0.812297
29	1	0	6.635821	0.600461	-0.547572
30	8	0	-1.008197	-2.027939	-0.920529
31	6	0	0.226202	1.264795	1.787907
32	8	0	0.844654	0.965270	2.804616
33	6	0	0.889795	1.183933	0.473378
34	1	0	1.970139	1.220957	0.596019
35	6	0	0.437181	1.960856	-0.676207
36	8	0	-0.730072	2.276027	-0.929900
37	6	0	-1.227178	1.677502	1.885423
38	1	0	-1.486650	1.770541	2.943211
39	1	0	-1.409692	2.613640	1.350082
40	1	0	-1.882008	0.937835	1.413914
41	6	0	1.539257	2.318006	-1.660543
42	1	0	2.206057	1.463709	-1.825475
43	1	0	1.102285	2.656163	-2.603695
44	1	0	2.156792	3.124600	-1.243900



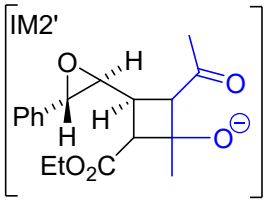
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.294893	0.813519	0.086455
2	6	0	-3.961993	0.756322	-0.305499
3	6	0	-3.302313	-0.474659	-0.369289
4	6	0	-3.992918	-1.639678	-0.033451
5	6	0	-5.327878	-1.578762	0.355577
6	6	0	-5.984871	-0.352518	0.414288
7	1	0	-5.796809	1.776604	0.143202
8	1	0	-3.409895	1.667004	-0.522772
9	1	0	-3.462554	-2.585886	-0.088648
10	1	0	-5.857749	-2.493487	0.611819
11	1	0	-7.027830	-0.303842	0.718514
12	6	0	-1.874501	-0.541267	-0.778448
13	1	0	-1.606264	0.077601	-1.636623
14	6	0	-0.808297	-0.866372	0.184856

15	1	0	-1.143613	-1.083619	1.202884
16	6	0	0.624015	-0.398946	0.083609
17	1	0	0.898217	-0.312997	-0.973661
18	6	0	1.498781	-1.374479	0.762107
19	1	0	1.108752	-1.937593	1.604910
20	6	0	2.779714	-1.699629	0.318804
21	8	0	3.584450	-2.532910	0.756033
22	8	0	3.152124	-0.895161	-0.786043
23	6	0	4.485543	-1.038544	-1.210062
24	1	0	4.797908	-2.081976	-1.092101
25	1	0	4.495452	-0.775795	-2.275938
26	6	0	5.412567	-0.124194	-0.426532
27	1	0	5.421267	-0.440973	0.620974
28	1	0	6.439094	-0.168915	-0.814289
29	1	0	5.055954	0.910153	-0.479504
30	8	0	-1.259482	-1.821744	-0.771649
31	6	0	-0.312522	2.017780	-0.083749
32	8	0	-1.327595	2.436630	0.456790
33	6	0	0.650224	1.132529	0.660580
34	1	0	0.278682	1.061544	1.689483
35	6	0	2.066385	1.670797	0.694422
36	8	0	2.554169	2.365748	-0.183355
37	6	0	-0.009849	2.351086	-1.522026
38	1	0	-0.875725	2.840215	-1.975638
39	1	0	0.870854	3.000597	-1.547529
40	1	0	0.269698	1.456599	-2.089165
41	6	0	2.837113	1.267491	1.915596
42	1	0	2.362065	1.677192	2.815618
43	1	0	2.774813	0.167876	1.984992
44	1	0	3.872542	1.606344	1.845833



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.282261	0.755593	0.066159
2	6	0	-3.947286	0.669977	-0.312325
3	6	0	-3.306162	-0.572396	-0.341540
4	6	0	-4.013003	-1.720111	0.015477

5	6	0	-5.350358	-1.630429	0.391664
6	6	0	-5.989992	-0.393853	0.415867
7	1	0	-5.771805	1.726082	0.094612
8	1	0	-3.381109	1.566505	-0.557875
9	1	0	-3.494974	-2.674516	-0.010232
10	1	0	-5.895856	-2.530696	0.665536
11	1	0	-7.034466	-0.323894	0.710167
12	6	0	-1.874880	-0.641882	-0.726349
13	1	0	-1.601357	-0.045262	-1.599870
14	6	0	-0.816630	-0.870043	0.267522
15	1	0	-1.149423	-1.057307	1.291818
16	6	0	0.522719	-0.206173	0.127300
17	1	0	0.875217	-0.312980	-0.902655
18	6	0	1.635714	-0.616915	1.063710
19	1	0	1.360979	-0.760953	2.107769
20	6	0	2.791575	-1.349179	0.667941
21	8	0	3.655757	-1.817914	1.406502
22	8	0	2.936643	-1.386135	-0.702140
23	6	0	4.222060	-1.754128	-1.164216
24	1	0	4.594450	-2.602127	-0.578759
25	1	0	4.073582	-2.073783	-2.202467
26	6	0	5.186020	-0.584533	-1.085274
27	1	0	5.353700	-0.322398	-0.037915
28	1	0	6.147520	-0.838436	-1.551133
29	1	0	4.754987	0.291425	-1.577292
30	8	0	-1.213119	-1.896458	-0.648300
31	6	0	-0.101480	2.231033	-0.511742
32	8	0	-1.066723	2.944373	-0.263940
33	6	0	0.464785	1.284318	0.504409
34	1	0	-0.118104	1.411145	1.425769
35	6	0	2.018518	1.362585	0.838906
36	8	0	2.828054	1.646952	-0.072304
37	6	0	0.572967	2.256901	-1.857571
38	1	0	0.239918	3.128749	-2.426417
39	1	0	1.659003	2.235144	-1.687413
40	1	0	0.327320	1.347005	-2.420337
41	6	0	2.359069	1.802471	2.256609
42	1	0	1.639043	1.452374	3.002773
43	1	0	3.351421	1.416341	2.507871
44	1	0	2.396817	2.901626	2.288220



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.235826	0.802359	0.048648
2	6	0	-3.900103	0.677129	-0.315350
3	6	0	-3.299455	-0.585354	-0.348089
4	6	0	-4.045293	-1.712816	-0.008379
5	6	0	-5.383769	-1.583408	0.352951
6	6	0	-5.983615	-0.327247	0.379867
7	1	0	-5.694277	1.787692	0.080677
8	1	0	-3.301826	1.557128	-0.546117
9	1	0	-3.557263	-2.682959	-0.033480
10	1	0	-5.960970	-2.467696	0.613554
11	1	0	-7.028662	-0.226376	0.662853
12	6	0	-1.866865	-0.689796	-0.718891
13	1	0	-1.575320	-0.120577	-1.605088
14	6	0	-0.821154	-0.887347	0.290817
15	1	0	-1.161759	-1.037255	1.318523
16	6	0	0.495137	-0.197135	0.123829
17	1	0	0.868933	-0.341319	-0.892680
18	6	0	1.633473	-0.427811	1.110033
19	1	0	1.293835	-0.604647	2.134717
20	6	0	2.791376	-1.278356	0.802040
21	8	0	3.640147	-1.610024	1.609481
22	8	0	2.883798	-1.558815	-0.520967
23	6	0	4.179743	-1.900077	-1.000150
24	1	0	4.763791	-2.314222	-0.173111
25	1	0	4.031228	-2.678281	-1.757615
26	6	0	4.832426	-0.659568	-1.579212
27	1	0	4.795453	0.145045	-0.838537
28	1	0	5.868923	-0.867250	-1.874991
29	1	0	4.278060	-0.307464	-2.454974
30	8	0	-1.215212	-1.946293	-0.593095
31	6	0	0.014323	2.280201	-0.573901
32	8	0	-0.850168	3.131769	-0.373863
33	6	0	0.421058	1.300200	0.464382
34	1	0	-0.200215	1.457913	1.355193
35	6	0	2.019838	1.186851	0.901405

36	8	0	2.891260	1.430682	-0.019719
37	6	0	0.794670	2.218124	-1.856290
38	1	0	0.593460	3.102326	-2.467052
39	1	0	1.856431	2.110017	-1.555911
40	1	0	0.542559	1.315990	-2.428905
41	6	0	2.293772	1.863489	2.248217
42	1	0	1.526613	1.661287	3.007254
43	1	0	3.262304	1.508992	2.619976
44	1	0	2.361677	2.946462	2.089451

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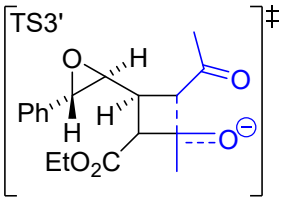
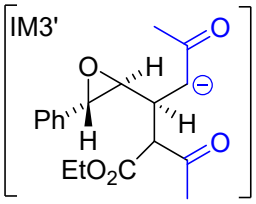


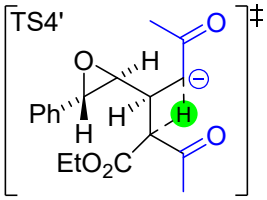
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.491252	0.494040	-0.508863
2	6	0	-4.135453	0.454192	-0.815797
3	6	0	-3.322927	-0.559693	-0.302988
4	6	0	-3.891376	-1.539031	0.513446
5	6	0	-5.248202	-1.500478	0.817460
6	6	0	-6.053541	-0.484044	0.308739
7	1	0	-6.111135	1.292833	-0.908636
8	1	0	-3.694160	1.222210	-1.447169
9	1	0	-3.249354	-2.329863	0.890603
10	1	0	-5.680677	-2.270177	1.452598
11	1	0	-7.113931	-0.454058	0.546934
12	6	0	-1.870937	-0.577329	-0.608817
13	1	0	-1.596941	-0.197948	-1.596039
14	6	0	-0.852611	-0.452917	0.442481
15	1	0	-1.225623	-0.395860	1.469143
16	6	0	0.458249	0.225805	0.184046
17	1	0	0.741179	0.069793	-0.860592
18	6	0	1.641635	-0.196565	1.043174
19	1	0	1.374308	-0.271859	2.102950
20	6	0	2.468588	-1.383033	0.681809
21	8	0	3.217687	-1.966310	1.441784
22	8	0	2.370342	-1.687092	-0.626803
23	6	0	3.362137	-2.571114	-1.135684
24	1	0	3.540513	-3.373701	-0.413014
25	1	0	2.923412	-2.994816	-2.044226

26	6	0	4.636683	-1.807386	-1.436394
27	1	0	5.064624	-1.418476	-0.509115
28	1	0	5.371995	-2.459101	-1.924132
29	1	0	4.418685	-0.953148	-2.082909
30	8	0	-1.129035	-1.714166	-0.185904
31	6	0	0.362477	2.775250	-0.433387
32	8	0	0.083448	3.945179	-0.124955
33	6	0	0.463247	1.706673	0.511829
34	1	0	0.092625	1.958356	1.508330
35	6	0	2.453562	1.148654	0.791171
36	8	0	3.162047	1.209848	-0.233756
37	6	0	0.791499	2.457001	-1.858343
38	1	0	0.766787	3.375060	-2.451596
39	1	0	1.811294	2.043295	-1.828049
40	1	0	0.145958	1.705131	-2.332228
41	6	0	2.865391	1.934933	2.023636
42	1	0	2.121573	1.894797	2.824649
43	1	0	3.816450	1.530464	2.400785
44	1	0	3.023498	2.977658	1.733680



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.991509	0.232610	-0.969590
2	6	0	3.821033	0.720183	-0.398961
3	6	0	3.003556	-0.119495	0.361567
4	6	0	3.376144	-1.451431	0.545442
5	6	0	4.549779	-1.937076	-0.023053
6	6	0	5.362031	-1.097803	-0.781706
7	1	0	5.615707	0.893114	-1.566563
8	1	0	3.519615	1.753227	-0.556523
9	1	0	2.730693	-2.088313	1.143317
10	1	0	4.832566	-2.976396	0.128253
11	1	0	6.278523	-1.477906	-1.226564
12	6	0	1.742492	0.405916	0.941068
13	1	0	1.789483	1.434201	1.306576
14	6	0	0.431653	-0.044868	0.479100
15	1	0	0.411122	-0.835177	-0.268303

16	6	0	-0.719146	0.931451	0.474720
17	1	0	-0.578596	1.555436	1.365678
18	6	0	-2.120874	0.227765	0.693399
19	1	0	-2.809446	1.044745	0.931345
20	6	0	-2.677731	-0.422370	-0.547576
21	8	0	-3.824189	-0.320580	-0.920401
22	8	0	-1.763791	-1.185348	-1.173123
23	6	0	-2.232437	-1.917679	-2.302781
24	1	0	-2.919083	-1.288790	-2.876357
25	1	0	-1.337470	-2.111306	-2.900564
26	6	0	-2.900709	-3.205622	-1.865767
27	1	0	-3.797903	-2.981165	-1.283664
28	1	0	-3.185683	-3.804278	-2.739105
29	1	0	-2.222916	-3.792686	-1.238752
30	8	0	0.976755	-0.483062	1.750369
31	6	0	-0.750704	3.157647	-0.838175
32	8	0	-0.640462	3.837679	-1.889346
33	6	0	-0.666235	1.767546	-0.756116
34	1	0	-0.517400	1.238766	-1.697000
35	6	0	-2.140788	-0.760155	1.842591
36	8	0	-2.332123	-1.953272	1.686828
37	6	0	-1.003278	3.983664	0.438180
38	1	0	-1.882375	4.614352	0.259828
39	1	0	-1.171002	3.420453	1.365247
40	1	0	-0.157304	4.665212	0.596369
41	6	0	-1.845232	-0.184552	3.208573
42	1	0	-0.760923	-0.039876	3.284026
43	1	0	-2.326396	0.788553	3.354201
44	1	0	-2.167109	-0.889886	3.978444



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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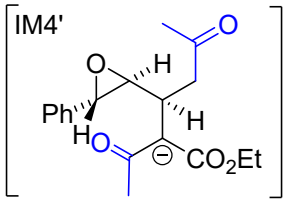
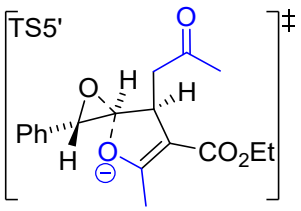
2	6	0	-3.711452	-0.291262	-0.462829
3	6	0	-2.963215	0.369549	0.516672
4	6	0	-3.390090	1.606772	0.995260
5	6	0	-4.563798	2.177707	0.509684

6	6	0	-5.314325	1.516850	-0.458848
7	1	0	-5.453733	-0.229169	-1.714943
8	1	0	-3.348283	-1.235819	-0.864877
9	1	0	-2.785866	2.108304	1.745787
10	1	0	-4.892834	3.142463	0.889300
11	1	0	-6.230197	1.963076	-0.839245
12	6	0	-1.710893	-0.257248	1.010929
13	1	0	-1.810951	-1.297603	1.326640
14	6	0	-0.400163	0.153613	0.506027
15	1	0	-0.382348	0.996336	-0.181126
16	6	0	0.693256	-0.868654	0.338810
17	1	0	0.607786	-1.575154	1.173459
18	6	0	2.145307	-0.340294	0.402481
19	1	0	2.712229	-1.317632	0.283716
20	6	0	2.586410	0.531979	-0.741497
21	8	0	3.606992	0.388435	-1.373471
22	8	0	1.719893	1.544791	-0.983474
23	6	0	2.141544	2.502477	-1.951958
24	1	0	2.641722	1.984052	-2.775028
25	1	0	1.217994	2.958857	-2.320242
26	6	0	3.056987	3.529343	-1.316515
27	1	0	3.957471	3.039558	-0.937768
28	1	0	3.346938	4.291313	-2.049816
29	1	0	2.556364	4.019377	-0.475942
30	8	0	-0.843224	0.517453	1.831266
31	6	0	-0.588079	-2.649186	-0.968023
32	8	0	-1.433984	-2.758701	-1.858426
33	6	0	0.484688	-1.652719	-0.961025
34	1	0	0.393384	-0.985651	-1.826112
35	6	0	2.548510	0.302277	1.697135
36	8	0	3.204638	1.330587	1.745746
37	6	0	-0.518883	-3.701368	0.134500
38	1	0	-1.165507	-4.540737	-0.134653
39	1	0	0.523671	-4.025639	0.246036
40	1	0	-0.850402	-3.308378	1.104096
41	6	0	2.148014	-0.428450	2.958441
42	1	0	1.075197	-0.283845	3.131600
43	1	0	2.329054	-1.504669	2.857530
44	1	0	2.711929	-0.023010	3.801813
45	8	0	2.669973	-2.984239	-0.366560
46	1	0	1.553127	-2.356148	-0.912891
47	1	0	3.322839	-2.838868	-1.066324



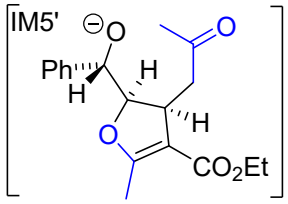
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.419622	0.122509	0.812919
2	6	0	3.130736	-0.378559	0.963214
3	6	0	2.402113	-0.810666	-0.146832
4	6	0	2.996428	-0.756565	-1.409351
5	6	0	4.286567	-0.259988	-1.559984
6	6	0	5.002292	0.186335	-0.450610
7	1	0	4.970798	0.465277	1.685336
8	1	0	2.671495	-0.425231	1.947891
9	1	0	2.429148	-1.119122	-2.262090
10	1	0	4.737357	-0.220654	-2.548976
11	1	0	6.009152	0.578791	-0.569877
12	6	0	1.003773	-1.270378	0.019451
13	1	0	0.757490	-1.670520	1.002450
14	6	0	-0.078199	-0.666220	-0.764272
15	1	0	0.227366	0.077040	-1.503235
16	6	0	-1.512143	-0.532908	-0.317626
17	1	0	-2.121886	-0.980499	-1.114883
18	6	0	-1.998422	0.892872	-0.249575
19	6	0	-1.235021	1.937643	0.326710
20	8	0	-1.485156	3.142455	0.410028
21	8	0	-0.032431	1.461210	0.865347
22	6	0	0.875551	2.456891	1.289481
23	1	0	0.326860	3.267676	1.779846
24	1	0	1.527274	1.965766	2.021370
25	6	0	1.691051	2.999836	0.129653
26	1	0	1.023254	3.495882	-0.580684
27	1	0	2.431003	3.730115	0.481469
28	1	0	2.221182	2.189422	-0.381568
29	8	0	0.412089	-1.985790	-1.065496
30	6	0	-1.676354	-2.805985	0.902103
31	8	0	-1.019340	-3.436151	1.713702
32	6	0	-3.348659	1.069624	-0.675350
33	8	0	-4.055480	0.111122	-1.058677
34	6	0	-2.395717	-3.501382	-0.233294
35	1	0	-2.607157	-4.538501	0.040143

36	1	0	-3.309500	-2.971545	-0.521392
37	1	0	-1.723144	-3.496150	-1.098580
38	6	0	-3.981387	2.452360	-0.661384
39	1	0	-3.989516	2.875530	0.348190
40	1	0	-3.410061	3.160991	-1.268637
41	1	0	-5.002737	2.356872	-1.042121
42	6	0	-1.840004	-1.310344	0.973616
43	1	0	-2.906997	-1.117632	1.150791
44	1	0	-1.272216	-0.916717	1.822119



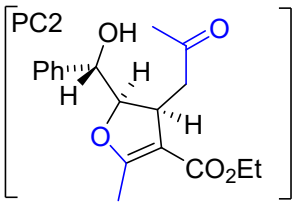
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.179561	-1.086424	-0.655521
2	6	0	3.846601	-0.712624	-0.790811
3	6	0	3.369789	0.434876	-0.152027
4	6	0	4.240683	1.193640	0.625926
5	6	0	5.578112	0.825693	0.754308
6	6	0	6.052877	-0.315315	0.112431
7	1	0	5.541109	-1.987614	-1.147055
8	1	0	3.152212	-1.324153	-1.360928
9	1	0	3.823278	2.067091	1.119932
10	1	0	6.252561	1.428238	1.360284
11	1	0	7.095753	-0.608781	0.214433
12	6	0	1.933989	0.887246	-0.283222
13	1	0	1.700163	1.004833	-1.362026
14	6	0	0.932654	0.125942	0.456467
15	1	0	1.268152	-0.198526	1.435049
16	6	0	-0.565998	0.317872	0.299835
17	1	0	-0.887035	0.839990	1.206246
18	6	0	-1.200399	-1.055702	0.250433
19	6	0	-2.596904	-1.261684	0.470596
20	8	0	-3.254725	-2.298563	0.423468
21	8	0	-3.218623	-0.069846	0.788348
22	6	0	-4.631637	-0.124206	0.914221
23	1	0	-4.911217	-1.030624	1.460661
24	1	0	-4.893838	0.753316	1.515483

25	6	0	-5.314664	-0.076599	-0.439247
26	1	0	-5.071837	-0.981258	-1.003178
27	1	0	-6.403714	-0.023040	-0.316427
28	1	0	-4.973200	0.794737	-1.005380
29	8	0	1.541221	1.916440	0.538336
30	6	0	-2.138962	2.076877	-0.751554
31	8	0	-2.992483	2.183717	-1.614938
32	6	0	-0.285462	-2.045743	-0.086368
33	8	0	0.943738	-1.718456	-0.206888
34	6	0	-2.190419	2.914255	0.509206
35	1	0	-2.838288	3.779403	0.346938
36	1	0	-2.609049	2.302337	1.315583
37	1	0	-1.185271	3.224732	0.814771
38	6	0	-0.625774	-3.491272	-0.323749
39	1	0	-0.050101	-4.112062	0.372864
40	1	0	-1.692641	-3.677391	-0.201066
41	1	0	-0.304146	-3.765967	-1.335374
42	6	0	-0.924182	1.205017	-0.912390
43	1	0	-1.026294	0.613106	-1.825821
44	1	0	-0.098805	1.924197	-1.022811



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.724504	1.819650	-0.070869
2	6	0	-3.414504	1.405293	-0.295078
3	6	0	-3.026849	0.089388	-0.022377
4	6	0	-3.978743	-0.800680	0.475233
5	6	0	-5.290042	-0.388682	0.695601
6	6	0	-5.669837	0.924121	0.425550
7	1	0	-5.009742	2.847807	-0.286183
8	1	0	-2.679237	2.107294	-0.679705
9	1	0	-3.644817	-1.814109	0.674729
10	1	0	-6.021281	-1.096473	1.081850
11	1	0	-6.694000	1.248021	0.599410
12	6	0	-1.610824	-0.399284	-0.253065
13	1	0	-1.426340	-0.390138	-1.347212
14	6	0	-0.559635	0.484764	0.422986

15	1	0	-0.893884	0.759504	1.431529
16	6	0	0.809196	-0.215998	0.457097
17	1	0	0.967446	-0.673187	1.438343
18	6	0	1.727343	0.962844	0.218437
19	6	0	3.167222	0.968290	0.340721
20	8	0	3.938872	1.878964	0.069405
21	8	0	3.612106	-0.215505	0.842765
22	6	0	5.023399	-0.354821	0.945562
23	1	0	5.457121	0.587283	1.294986
24	1	0	5.173263	-1.126458	1.706665
25	6	0	5.631788	-0.767491	-0.380271
26	1	0	5.490581	0.026791	-1.118059
27	1	0	6.706561	-0.953211	-0.268197
28	1	0	5.155646	-1.680495	-0.751414
29	8	0	-1.411556	-1.656248	0.264893
30	6	0	-0.188002	-2.397873	-0.622373
31	8	0	-0.579224	-2.756185	-1.766007
32	6	0	0.987863	1.992664	-0.265517
33	8	0	-0.330657	1.754776	-0.275023
34	6	0	0.117133	-3.503202	0.400918
35	1	0	-0.777926	-4.122223	0.514753
36	1	0	0.928846	-4.132202	0.013255
37	1	0	0.405702	-3.113708	1.385671
38	6	0	1.392481	3.316185	-0.800420
39	1	0	2.477551	3.413752	-0.767905
40	1	0	1.035446	3.418849	-1.832249
41	1	0	0.924769	4.117057	-0.215334
42	6	0	0.913656	-1.285413	-0.632848
43	1	0	1.902057	-1.760665	-0.580966
44	1	0	0.843057	-0.808452	-1.617964



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.763257	-1.331430	0.957213
2	6	0	-3.512623	-0.728150	1.031994
3	6	0	-3.083162	0.135039	0.023426
4	6	0	-3.923098	0.390595	-1.059813

5	6	0	-5.176257	-0.210318	-1.134017
6	6	0	-5.598823	-1.073540	-0.126972
7	1	0	-5.089044	-2.000110	1.749419
8	1	0	-2.858710	-0.932270	1.876113
9	1	0	-3.588843	1.076847	-1.832134
10	1	0	-5.825950	-0.001171	-1.979784
11	1	0	-6.578272	-1.540683	-0.183586
12	6	0	-1.710197	0.764198	0.089073
13	1	0	-1.454444	0.959092	1.138709
14	6	0	-0.634541	-0.131374	-0.510888
15	1	0	-0.876031	-0.297500	-1.569132
16	6	0	0.826145	0.344967	-0.389712
17	1	0	1.125615	0.861444	-1.305328
18	6	0	1.510725	-0.995118	-0.242238
19	6	0	2.940969	-1.229004	-0.341601
20	8	0	3.520261	-2.286425	-0.175101
21	8	0	3.587780	-0.082002	-0.668260
22	6	0	5.013123	-0.178225	-0.772438
23	1	0	5.269592	-1.125904	-1.253178
24	1	0	5.296607	0.648656	-1.428747
25	6	0	5.672485	-0.062014	0.585393
26	1	0	5.385827	-0.905192	1.219339
27	1	0	6.762331	-0.067829	0.476464
28	1	0	5.382388	0.870538	1.080503
29	6	0	0.696491	2.680086	0.700081
30	8	0	-0.075675	3.186330	1.493256
31	6	0	0.584349	-1.912841	0.122265
32	8	0	-0.672175	-1.425253	0.128699
33	6	0	1.264401	3.462974	-0.458834
34	1	0	1.222433	4.531794	-0.238919
35	1	0	2.287686	3.159455	-0.701299
36	1	0	0.638859	3.264883	-1.337354
37	6	0	0.714175	-3.331498	0.522195
38	1	0	1.763782	-3.624136	0.522730
39	1	0	0.280526	-3.473878	1.518614
40	1	0	0.149801	-3.966539	-0.169782
41	6	0	1.138029	1.239301	0.827663
42	1	0	2.229543	1.240987	0.942247
43	1	0	0.707630	0.816069	1.740609
44	8	0	-1.626230	1.959004	-0.668937
45	1	0	-1.856627	2.690321	-0.079498