Supplementary Information (SI) for Green Chemistry.
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Supporting Information for:

$B(C_6F_5)_3$ Catalysed Cyclic Carbonate Editing

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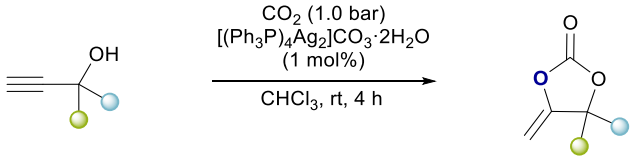
Contents:

1. General comments

Commercially available reagents and solvents were purchased from Energy, J&K, TCI, aladdin or Sinopharm, and used without further purification. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded at room temperature on a Bruker AV-400 spectrometer and referenced to the residual deuterated solvent signals ($CDCl_3$ ^{1}H NMR, δ = 7.26; ^{13}C NMR, δ = 77.16). All reported NMR values are given in parts per million (ppm). FT-IR measurements were carried out on a Bruker ALPHA II. High resolution mass spectra (HRMS) were obtained on a WATERS I-Class VION IMS Qtof Spectrometer. The X-ray analysis of **P13** was collected at 100 K on a Rigaku Oxford Diffraction Supernova Dual Source, Cu at Zero equipped with an AtlasS2 CCD using Cu Kα radiation. All the cyclic carbonates **1-32** were prepared according to reported procedures.[1-2]

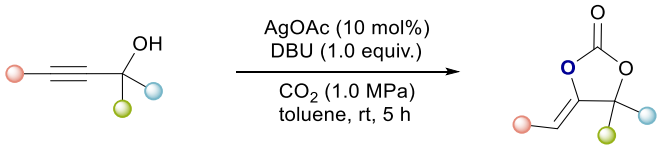
2. Typical procedure for the preparation of starting cyclic carbonates

Cyclic carbonates **1-3** were prepared according to our previously reported method.[1]



S1-S3 **1-3**

Preparation of cyclic carbonates **4-32**: The cyclic carbonates **4-32** were prepared according to previously reported method.[2]

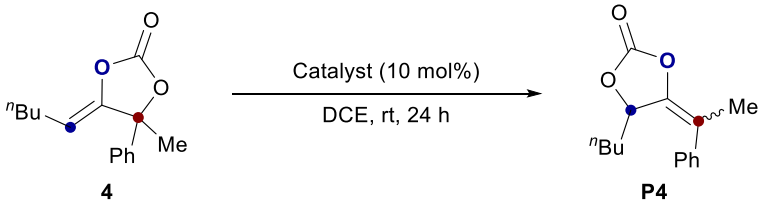


S4-S32 **4-32**

To a 20 mL of stainless steel autoclave added a solution of propargyl alcohol (2.5 mmol, 1.0 equiv.), AgOAc (0.25 mmol, 10 mol%) and DBU (2.5 mmol, 1.0 equiv.) in toluene (10 mL). The autoclave was then subjected to three cycles of pressurization and depressurization with carbon dioxide (0.5 MPa), before final stabilization of the pressure to 1.0 MPa. The autoclave was sealed and stirred at room temperature for 5 h. Afterward, the mixture was purified by flash column chromatography (Eluent: PE:EA = 50:1). Then, the eluent was concentrated to obtain the corresponding carbonates. Cyclic carbonates **4-32** could be prepared with yield >90% according to this procedure.

3. Additional condition screening data

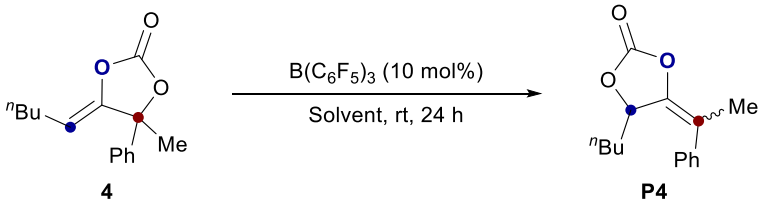
Table S1. Experimental results of Lewis acid catalysts.[a]



Entry	Catalyst	Yield of P4[b](%)	*E/Z* Ratio[c]	Entry	Catalyst	Yield of P4[b](%)	*E/Z* Ratio[c]
1	BBr_3	0	-	8	$Rh_2(OAc)_4$	0	-
2	BEt_3	0	-	9	$Y(OTf)_3$	0	-
3	$AlCl_3$	18	-	10	$Yb(OTf)_3$	0	-
4	$Ti(^iPrO)_4$	0	-	11	$La(OTf)_3$	0	-
5	$TiCl_4$	0	-	12	$Eu(OTf)_3$	0	-
6	AgCl	0	-	13	$Bi(OTf)_3$	0	-
7	$In(OTf)_2$	0	-	14	$AuCl_3$	12	-

[a] Reactions were performed with cyclic carbonate **4** (0.1 mmol) and Lewis acid catalyst (10 mol%) in dry DCE (0.3 mL) at room temperature for 24 h under nitrogen atmosphere. [b]Isolated yield including *E* and *Z* stereoisomers. [c]The *E/Z* ratio was determined by ^{1}H NMR analysis.

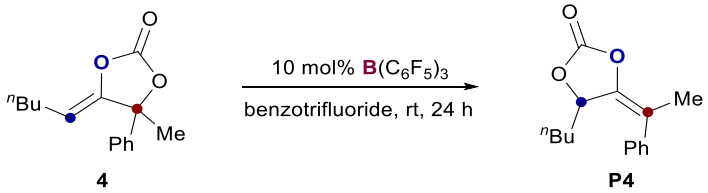
Table S2. Experimental results of different slovents.[a]



Entry	Solvent	Yield of P4[b](%)	*E/Z* Ratio[c]	Entry	Solvent	Yield of P4[b](%)	*E/Z* Ratio[c]
1	$CHCl_3$	0	-	8	EA	trace	-
2	$CHBr_2CHBr_2$	0	-	9	Acetone	0	-
3	Chlorobenzene	18	-	10	Benzene	87	5:1
4	HFIP	50	>20:1	11	Pentane	87	10:1
5	H_2O	0	-	12	Heptane	88	13:1
6	1,4-Dioxane	56	>20:1	13	Octane	90	7:1
7	DME	58	9:1				

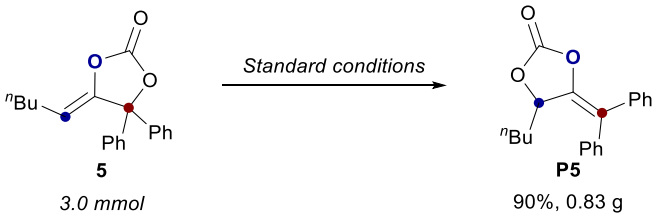
[a] Reactions were performed with cyclic carbonate **4** (0.1 mmol) and $B(C_6F_5)_3$ (10 mol%) in solvent (0.3 mL) at room temperature for 24 h under nitrogen atmosphere. [b]Isolated yield including *E* and *Z* stereoisomers. [c]The *E/Z* ratio was determined by ^{1}H NMR analysis.

4. Typical procedure for the cyclic carbonate editing reactions



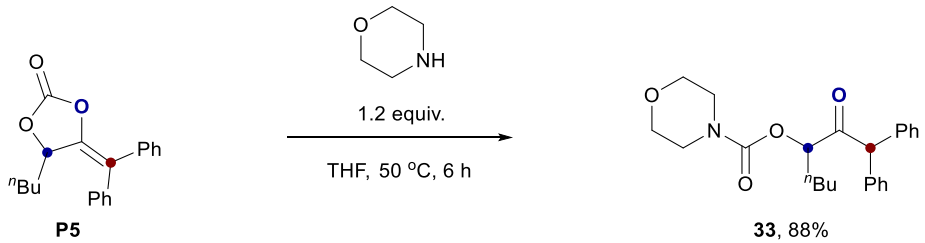
In a N_2-filled glovebox, a screw-capped vial equipped with a magnetic stir bar was charged with cyclic carbonate **4** (24.6 mg, 0.1 mmol, 1.0 equiv.), benzotrifluoride (0.3 mL) and $B(C_6F_5)_3$ (5.1 mg, 0.01 mmol, 10 mol%). The resulting solution was stirred for 24 h at room temperature in glovebox. Then, the crude product was purified by column chromatography (PE:EA = 50:1 to 20:1) to afford the desired product **P4** as a collorless oil (21.2 mg, 86%).

5. Scale-up reaction

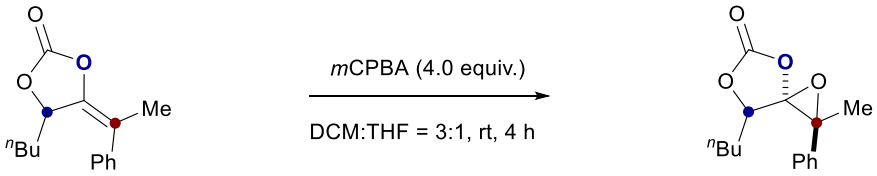


In a N_2-filled glovebox, an oven-dried round-bottomed flask equipped with a magnetic stir bar was charged with cyclic carbonate **5** (924.0 mg, 3.0 mmol, 1.0 equiv.), benzotrifluoride (9.0 mL) and $B(C_6F_5)_3$ (153.0 mg, 0.3 mmol, 10 mol%). The resulting solution was stirred for 24 h at room temperature in glovebox. Then, the crude product was purified by column chromatography (PE:EA = 50:1 to 20:1) to afford the desired product **P5** as a yellow oil (832.0 mg, 90%).

6. Synthetic transformation of P5, P4 and P4'

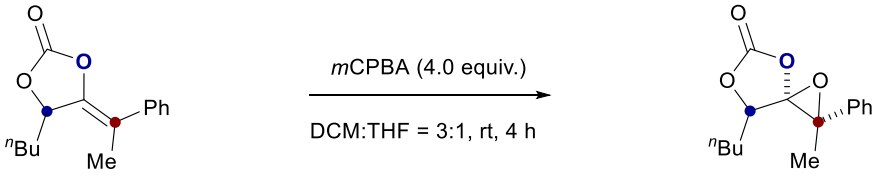


In a nitrogen-filled glove box, a GC vial equipped with a stirring bar was charged with **P5** (30.8 mg, 0.1 mmol, 1.0 equiv.) and morpholine (0.12 mmol, 1.2 equiv.) in THF (0.5 mL). The reaction mixture was stirred for 6 h at at 50 °C. After the completion of the reaction (monitored by TLC), the mixture was concentrated under reduced pressure. The resultant crude product was purified by column chromatography (PE:EA = 20:1) to afford the desired product **33** as a colourless oil (34.8 mg, 88% yield).



P4 (*E* isomer) *trans*-**34**, 79%

In a nitrogen-filled glove box, a GC vial equipped with a stirring bar was charged with **P4** (24.6 mg, 0.1 mmol, 1.0 equiv.) and *m*CPBA (3-chloroperoxybenzoic acid) (0.4 mmol, 4.0 equiv.) in a mixture solvent of DCM:THF = 3:1 (0.6 mL). The reaction mixture was stirred for 4 h at room temperature. After the completion of the reaction, the mixture was concentrated under reduced pressure. The resultant crude product was purified by column chromatography (PE:EA = 50:1 to 20:1) to afford the desired product *trans*-**34** as a colourless oil (20.7 mg, 79% yield).

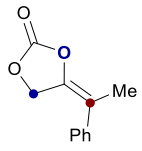


P4' (*Z* isomer) *cis*-**34**, 76%

In a nitrogen-filled glove box, a GC vial equipped with a stirring bar was charged with **P4'** (30.8 mg, 0.1 mmol, 1.0 equiv.) and *m*CPBA (3-chloroperoxybenzoic acid) (0.3 mmol, 3.0 equiv.) in a mixture solvent of DCM:THF = 3:1 (0.6 mL). The reaction mixture was stirred for 4 h at room temperature. After the completion of the reaction, the mixture was concentrated under reduced pressure. The resultant crude product was purified by column chromatography (PE:EA = 50:1 to 20:1) to afford the desired product *cis*-**34** as a colourless oil (20.0 mg, 76% yield).

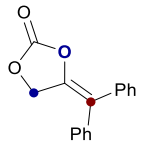
7. Characterization data of all the new compounds

Cyclic carbonates **1-3**, **6** and **7** were previously reported.[2a-c]



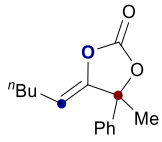
P1

(*E*)-4-(1-phenylethylidene)-1,3-dioxolan-2-one (P1): colourless oil; 8.6 mg, 45% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (t, *J* = 7.4 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 7.20-7.11 (m, 2H), 5.11-4.95 (m, 2H), 2.13 (t, *J* = 2.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 138.6, 137.5, 129.0, 128.0, 127.1, 113.7, 67.8, 16.7; IR (neat, cm^{-1}) 1826, 1812, 1716, 1599, 1494, 1446, 1367, 1267, 1223, 1127, 1071, 1039, 762, 729, 698, 591; HRMS (ESI): m/z: $[M+Na]^+$ calcd for $C_{11}H_{10}O_3Na$: 213.0522, found: 213.0527.



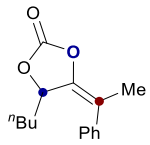
P3

4-(diphenylmethylene)-1,3-dioxolan-2-one (P3): white solid; 8.8 mg, 35% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.27 (m, 8H), 7.21-7.17 (m, 2H), 5.01 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 139.0, 136.4, 135.9, 129.6, 129.3, 129.1, 128.5, 128.4, 128.0, 117.9, 68.3; IR (neat, cm^{-1}) 1826, 1786, 1752, 1598, 1494, 1447, 1364, 1228, 1191, 1116, 1051, 973, 763, 695, 632; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{12}O_3Na$: 275.0679, found: 275.0689.



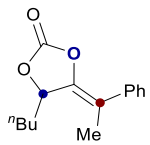
4

(*Z*)-4-methyl-5-pentylidene-4-phenyl-1,3-dioxolan-2-one (4): colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.34 (m, 5H), 4.74 (t, *J* = 7.6 Hz, 1H), 2.26-2.14 (m, 2H), 1.92 (s, 3H), 1.43-1.26 (m, 4H), 0.90 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 150.0, 140.1, 129.1, 128.9, 124.9, 105.0, 87.0, 31.4, 27.8, 24.9, 22.3, 13.9; IR (neat, cm^{-1}) 1816, 1713, 1448, 1222, 1041, 996, 764, 697; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{18}O_3Na$: 269.1149, found: 269.1149.



P4

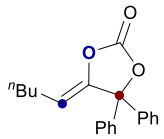
(*E*)-4-butyl-5-(1-phenylethylidene)-1,3-dioxolan-2-one (P4): colourless oil; 21.2 mg, 86% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.27 (m, 3H), 7.18 (d, *J* = 7.3 Hz, 2H), 5.50-5.32 (m, 1H), 2.09 (s, 3H), 1.46-1.35 (m, 1H), 1.31-1.02 (m, 5H), 0.74 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.2, 138.1, 129.1, 128.0, 127.7, 113.6, 80.0, 32.1, 25.6, 21.9, 18.0, 13.7; IR (neat, cm^{-1}) 1816, 1710, 1496, 1446, 1344, 1224, 1145, 1049, 765, 700, 648; HRMS (ESI): m/z: $[M+Na]^+$ calcd for $C_{15}H_{18}O_3Na$: 269.1149, found: 269.1150.



P4'

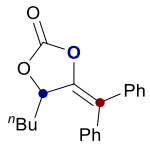
(*Z*)-4-butyl-5-(1-phenylethylidene)-1,3-dioxolan-2-one (P4′): colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 5.49-5.32 (m, 1H), 2.03-1.93 (m, 4H), 1.90-1.80 (m, 1H), 1.54-1.35 (m, 4H),

0.95 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (one carbon signal was overloped) δ 152.8, 141.3, 136.8, 128.5, 127.8, 110.5, 79.9, 33.5, 26.0, 22.4, 16.6, 14.0; IR (neat, cm^{-1}) 1813, 1695, 1448, 1347, 1229, 1139, 1101, 1074, 1049, 765, 696; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{18}O_3Na$: 269.1149, found: 269.1150.



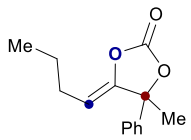
5

(*Z*)-5-pentylidene-4,4-diphenyl-1,3-dioxolan-2-one (5): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.34 (m, 10H), 4.76 (t, *J* = 7.7 Hz, 1H), 2.29 (dd, *J* = 14.8, 7.5 Hz, 2H), 1.49-1.30 (m, 4H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 148.3, 139.3, 129.3, 128.7, 127.2, 109.1, 91.4, 31.4, 25.2, 22.4, 14.0; IR (neat, cm^{-1}) 1816, 1711, 1493, 1449, 1309, 1210, 1199, 1151, 1036, 1018, 763, 697; HRMS (ESI): *m/z*: $[M+Na-CO_2]^+$ calcd for $C_{19}H_{20}ONa$:287.1406, found: 287.1409.



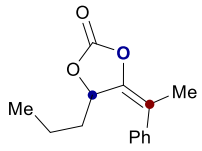
P5

4-butyl-5-(diphenylmethylene)-1,3-dioxolan-2-one (P5): yellow oil; 28.7 mg, 93% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.03 (m, 10H), 5.48-5.31 (dd, *J* = 5.9, 2.9 Hz, 1H), 1.45-1.32 (m, 1H), 1.32-1.01 (m, 5H), 0.69 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.6, 143.0, 136.6, 136.4, 129.9, 129.3, 129.2, 128.3, 118.0, 80.5, 31.8, 25.4, 21.9, 13.7; IR (neat, cm^{-1}) 1821, 1671, 1495, 1445, 1346, 1230, 1190, 1140, 1072, 1050, 1019, 767, 695, 658; HRMS (ESI): *m/z*: $[M+H]^+$ calcd for $C_{20}H_{21}O_3$: 309.1485, found: 309.1497.



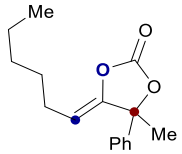
8

(*Z*)-5-butylidene-4-methyl-4-phenyl-1,3-dioxolan-2-one (8): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.31 (m, 5H), 4.75 (t, *J* = 7.6 Hz, 1H), 2.25-2.12 (m, 2H), 1.93 (s, 3H), 1.49-1.37 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 150.2, 140.1, 129.1, 128.9, 124.9, 104.8, 87.0, 27.7, 27.1, 22.5, 13.7; IR (neat, cm^{-1}) 1813, 1706, 1443, 1349, 1219, 1147, 1068, 1026, 764, 701; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{14}H_{16}O_3Na$: 255.0992, found: 255.1001.



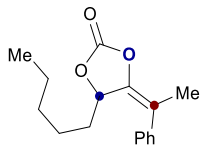
P8

(*E*)-4-(1-phenylethylidene)-5-propyl-1,3-dioxolan-2-one (P8): colourless oil; 19.3 mg, 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.27 (m, 3H), 7.22-7.08 (m, 2H), 5.50-5.32 (m, 1H), 2.08 (d, *J* = 1.8 Hz, 3H), 1.41-1.15 (m, 4H), 0.73 (t, *J* = 6.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.2, 138.0, 129.1, 128.0, 127.7, 113.5, 79.8, 34.6, 18.0, 17.0, 13.4; IR (neat, cm^{-1}) 1817, 1714, 1448, 1379, 1097, 1050, 1001, 764, 697; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{14}H_{16}O_3Na$: 255.0992, found: 255.1002.



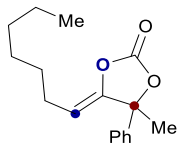
9

(*Z*)-5-hexylidene-4-methyl-4-phenyl-1,3-dioxolan-2-one (9): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.33 (m, 5H), 4.74 (t, *J* = 7.6 Hz, 1H), 2.25-2.13 (m, 2H), 1.92 (s, 3H), 1.45-1.36 (m, 2H), 1.34-1.23 (m, 4H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 150.0, 140.1, 129.1, 128.9, 124.9, 105.1, 87.0, 31.4, 28.9, 27.7, 25.2, 22.5, 14.1; IR (neat, cm^{-1}) 1817, 1714, 1448, 1379, 1097, 1050, 1001, 764, 697; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{20}O_3Na$: 283.1305, found: 283.1313.



P9

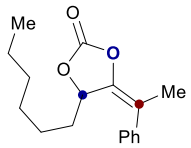
(*E*)-4-pentyl-5-(1-phenylethylidene)-1,3-dioxolan-2-one (P9): white solid; 23.9 mg, 92% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.27 (m, 3H), 7.18 (d, *J* = 7.0 Hz, 2H), 5.49-5.27 (m, 1H), 2.08 (d, *J* = 1.7 Hz, 3H), 1.40-0.98 (m, 8H), 0.79 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.2, 138.0, 129.1, 128.0, 127.7, 113.5, 80.0, 32.4, 30.9, 23.2, 22.3, 18.0, 14.0; IR (neat, cm^{-1}) 1816, 1706, 1347, 1222, 1145, 1068, 1026, 765, 701; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{20}O_3Na$: 283.1305, found: 283.1309.



10

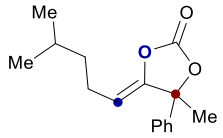
(*Z*)-5-heptylidene-4-methyl-4-phenyl-1,3-dioxolan-2-one (10): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.31 (m, 5H), 4.74 (t, *J* = 7.6 Hz, 1H), 2.26-2.11 (m, 2H), 1.92 (s, 3H),

1.44-1.36 (m, 2H), 1.34-1.22 (m, 6H), 0.93-0.81 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 150.0, 140.1, 129.1, 128.9, 124.9, 105.1, 87.1, 31.6, 29.2, 28.9, 27.8, 25.2, 22.7, 14.2; IR (neat, cm^{-1}) 1818, 1714, 1602, 1496, 1448, 1379, 1223, 1064, 1029, 764, 697; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{22}O_3Na$: 297.1461, found: 297.1467.



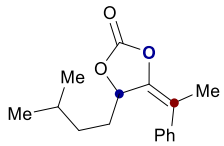
P10

(*E*)-4-hexyl-5-(1-phenylethylidene)-1,3-dioxolan-2-one (P10): white solid; 23.3 mg, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.27 (m, 3H), 7.23-7.08 (m, 2H), 5.53-5.26 (m, 1H), 2.08 (d, *J* = 1.8 Hz, 3H), 1.38-0.96 (m, 10H), 0.82 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.2, 138.0, 129.1, 128.0, 127.7, 113.5, 79.9, 32.4, 31.4, 28.4, 23.4, 22.5, 18.0, 14.1; IR (neat, cm^{-1}) 1817, 1706, 1443, 1347, 1222, 1144, 1068, 1028, 765, 701; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{22}O_3Na$: 297.1461, found: 297.1474.



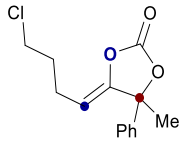
11

(*Z*)-4-methyl-5-(4-methylpentylidene)-4-phenyl-1,3-dioxolan-2-one (11): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.30 (m, 5H), 4.74 (t, *J* = 7.6 Hz, 1H), 2.29-2.11 (m, 2H), 1.92 (s, 3H), 1.61-1.46 (m, 1H), 1.35-1.19 (m, 2H), 0.89 (dd, *J* = 6.6, 1.1 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 149.8, 140.1, 129.0, 128.9, 124.8, 105.1, 87.0, 38.3, 27.71, 27.65, 23.2, 22.5, 22.4; IR (neat, cm^{-1}) 1817, 1714, 1449, 1222, 1057, 1010, 999, 765, 678; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{20}O_3Na$: 283.1305, found: 283.1318.



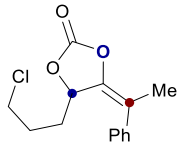
P11

(*E*)-4-isopentyl-5-(1-phenylethylidene)-1,3-dioxolan-2-one (P11): white solid; 22.1 mg, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.26 (m, 3H), 7.18 (d, *J* = 7.1 Hz, 2H), 5.51-5.25 (m, 1H), 2.09 (d, *J* = 1.6 Hz, 3H), 1.50-1.02 (m, 5H), 0.73-0.61 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.1, 138.0, 129.1, 128.0, 127.7, 113.6, 80.1, 32.2, 30.2, 27.4, 22.6, 22.0, 18.0; IR (neat, cm^{-1}) 1816, 1707, 1468, 1443, 1347, 1225, 1147, 1118, 1069, 1030, 765, 701; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{20}O_3Na$: 283.1305, found: 283.1314.



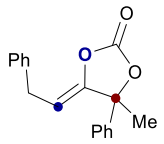
12

(*Z*)-5-(4-chlorobutylidene)-4-methyl-4-phenyl-1,3-dioxolan-2-one (12): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.32 (m, 5H), 4.75 (t, *J* = 7.6 Hz, 1H), 3.51 (t, *J* = 6.6 Hz, 2H), 2.42-2.28 (m, 2H), 1.93 (s, 3H), 1.89 (dt, *J* = 14.0, 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 151.2, 139.8, 129.2, 129.0, 124.8, 102.8, 87.0, 44.2, 31.9, 27.6, 22.7; IR (neat, cm-1) 1814, 1714, 1496, 1447, 1222, 1095, 1067, 1036, 995, 764, 697, 644; HRMS (ESI): m/z: $[M+H]^+$ calcd for $C_{14}H_{16}ClO_3$: 267.0783, found: 267.0796.



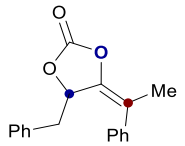
P12

(*E*)-4-(3-chloropropyl)-5-(1-phenylethylidene)-1,3-dioxolan-2-one (P12): white solid; 22.3 mg, 84% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.28 (m, 3H), 7.25-7.07 (m, 2H), 5.59-5.35 (m, 1H), 3.43-3.31 (m, 2H), 2.10 (d, *J* = 1.8 Hz, 3H), 1.81-1.66 (m, 2H), 1.64-1.54 (m, 1H), 1.48-1.38 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 141.5, 137.6, 129.2, 128.2, 127.6, 114.4, 79.1, 43.9, 30.0, 26.8, 18.1; IR (neat, cm^{-1}) 1815, 1707, 1493, 1443, 1346, 1222, 1134, 1070, 765, 701, 648; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{14}H_{15}ClO_3Na$: 289.0602, found: 289.0611.



13

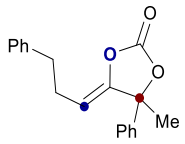
(*Z*)-4-methyl-4-phenyl-5-(2-phenylethylidene)-1,3-dioxolan-2-one (13): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.32 (m, 5H), 7.32-7.24 (m, 2H), 7.23-7.06 (m, 3H), 4.94 (t, *J* = 7.7 Hz, 1H), 3.64-3.39 (m, 2H), 1.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 150.6, 139.8, 139.3, 129.1, 128.9, 128.7, 128.3, 126.5, 124.8, 103.6, 87.1, 31.4, 27.6; IR (neat, cm^{-1}) 1816, 1713, 1603, 1495, 1451, 1222, 1065, 1027, 999, 761, 695; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{18}H_{16}O_3Na$: 303.0992, found: 303.1002.



P13

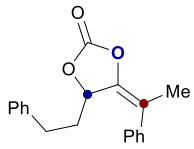
(*E*)-4-benzyl-5-(1-phenylethylidene)-1,3-dioxolan-2-one (P13): white solid; 23.9 mg, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52-7.17 (m, 8H), 7.04-6.86 (m, 2H), 5.78-5.50 (m, 1H), 2.73 (dd, *J* = 14.7, 3.0 Hz, 1H), 2.50 (dd, *J* = 14.7, 6.5 Hz, 1H), 2.06 (d, *J*

= 1.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 141.5, 138.0, 134.3, 129.5, 129.3, 128.6, 128.2, 127.7, 127.5, 114.1, 80.0, 38.3, 17.7; IR (neat, cm^{-1}) 1814, 1703, 1494, 1454, 1442, 1348, 1225, 1133, 1069, 1027, 765, 699; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{18}H_{16}O_3Na$: 303.0992, found: 303.0993.



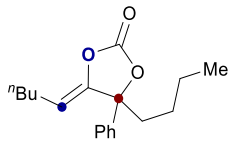
14

(*Z*)-4-methyl-4-phenyl-5-(3-phenylpropylidene)-1,3-dioxolan-2-one (14): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.30 (m, 5H), 7.26 (t, *J* = 7.4 Hz, 2H), 7.22-7.16 (m, 1H), 7.13 (d, *J* = 7.4 Hz, 2H), 4.70 (t, *J* = 7.6 Hz, 1H), 2.79-2.64 (m, 2H), 2.61-2.43 (m, 2H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 150.4, 140.8, 139.8, 129.0, 128.8, 128.6, 128.5, 126.2, 124.9, 103.8, 87.0, 35.2, 27.5, 26.7; IR (neat, cm^{-1}) 1813, 1714, 1496, 1451, 1222, 1093, 1065, 1030, 1017, 765, 748, 696; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{19}H_{18}O_3Na$: 317.1148, found: 317.1162.



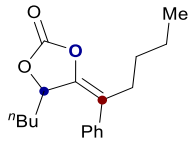
P14

(*E*)-4-phenethyl-5-(1-phenylethylidene)-1,3-dioxolan-2-one (P14): white solid; 25.0 mg, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.29 (m, 3H), 7.25-7.15 (m, 3H), 7.14-7.05 (m, 2H), 6.89 (d, *J* = 6.7 Hz, 2H), 5.45-5.27 (m, 1H), 2.70-2.44 (m, 2H), 2.09 (d, *J* = 1.8 Hz, 3H), 1.74-1.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.7, 141.9, 139.6, 137.8, 129.2, 128.6, 128.5, 128.0, 127.6, 126.4, 113.8, 78.8, 33.8, 30.0, 17.9; IR (neat, cm^{-1}) 1818, 1706, 1494, 1454, 1443, 1348, 1221, 1137, 1069, 1032, 765, 699; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{19}H_{18}O_3Na$: 317.1148, found: 317.1160.



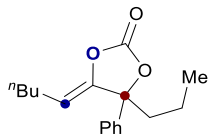
15

(*Z*)-4-butyl-5-pentylidene-4-phenyl-1,3-dioxolan-2-one (15): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.28 (m, 5H), 4.79 (t, *J* = 7.6 Hz, 1H), 2.30-2.12 (m, 3H), 2.10-1.99 (m, 1H), 1.45-1.28 (m, 8H), 0.96-0.83 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 148.9, 139.8, 128.8, 128.7, 124.6, 104.8, 89.6, 40.4, 31.3, 25.5, 24.8, 22.5, 22.2, 13.9, 13.8; IR (neat, cm^{-1}) 1816, 1713, 1449, 1313, 1241, 1199, 1122, 1071, 1059, 1012, 765, 698; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{18}H_{24}O_3Na$: 311.1618, found: 311.1615.



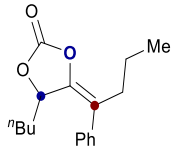
P15

(*E*)-4-butyl-5-(1-phenylpentylidene)-1,3-dioxolan-2-one (P15): white solid; 22.5 mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.27 (m, 3H), 7.22-7.06 (m, 2H), 5.31 (s, 1H), 2.78-2.51 (m, 1H), 2.48-2.25 (m, 1H), 1.42-1.02 (m, 10H), 0.86 (t, *J* = 6.9 Hz, 3H), 0.74 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 142.1, 136.9, 129.0, 128.3, 128.0, 118.5, 79.8, 32.1, 31.5, 29.6, 25.4, 22.5, 21.9, 14.0, 13.7; IR (neat, cm^{-1}) 1819, 1703, 1465, 1444, 1345, 1223, 1145, 1108, 1072, 1050, 1021, 766, 702; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{18}H_{24}O_3Na$: 311.1618, found: 311.1619.



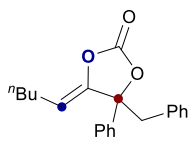
16

(*Z*)-5-pentylidene-4-phenyl-4-propyl-1,3-dioxolan-2-one (16): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.32 (m, 5H), 4.78 (t, *J* = 7.6 Hz, 1H), 2.26-2.10 (m, 3H), 2.09-1.96 (m, 1H), 1.49-1.27 (m, 6H), 0.98-0.86 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 148.9, 139.8, 128.8, 128.7, 124.6, 104.9, 89.6, 42.8, 31.4, 24.9, 22.3, 16.9, 13.91, 13.89; IR (neat, cm^{-1}) 1816, 1713, 1449, 1248, 1200, 1120, 1068, 1034, 1006, 764, 698; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{22}O_3Na$: 297.1461, found: 297.1469.



P16

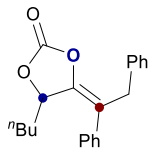
(*E*)-4-butyl-5-(1-phenylbutylidene)-1,3-dioxolan-2-one (P16): white solid; 22.2 mg, 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.27 (m, 3H), 7.19-7.05 (m, 2H), 5.32 (s, 1H), 2.74-2.46 (m, 1H), 2.42-2.25 (m, 1H), 1.42-1.04 (m, 8H), 0.89 (t, *J* = 7.4 Hz, 3H), 0.74 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 142.3, 136.8, 129.0, 128.3, 128.0, 118.2, 79.8, 33.6, 32.1, 25.4, 21.9, 20.6, 13.73, 13.70; IR (neat, cm^{-1}) 1818, 1702, 1464, 1444, 1345, 1224, 1145, 1105, 1072, 1051, 1022, 766, 702; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{22}O_3Na$: 297.1461, found: 297.1463.



17

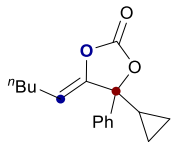
(*Z*)-4-benzyl-5-pentylidene-4-phenyl-1,3-dioxolan-2-one (17): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.4 Hz, 2H), 7.45-7.34 (m, 3H), 7.31-7.25 (m, 3H), 7.21-7.14 (m,

2H), 4.85 (t, *J* = 7.6 Hz, 1H), 3.50 (d, *J* = 14.2 Hz, 1H), 3.32 (d, *J* = 14.2 Hz, 1H), 2.22-2.00 (m, 2H), 1.43-1.20 (m, 4H), 0.88 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 147.6, 139.4, 133.3, 131.0, 129.0, 128.9, 128.4, 127.8, 125.1, 106.2, 89.0, 46.5, 31.4, 25.0, 22.4, 13.9; IR (neat, cm^{-1}) 1813, 1713, 1497, 1450, 1249, 1209, 1197, 1148, 1058, 1006, 761, 734, 697, 670, 645; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{21}H_{22}O_3Na$: 345.1461, found: 345.1469.



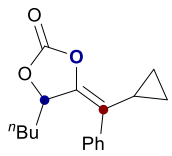
P17

(*E*)-4-butyl-5-(1,2-diphenylethylidene)-1,3-dioxolan-2-one (P17): white solid; 19.6 mg, 61% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.15 (m, 6H), 7.15-6.88 (m, 4H), 5.49-5.23 (m, 1H), 3.86 (d, *J* = 14.1 Hz, 1H), 3.74 (d, *J* = 14.1 Hz, 1H), 1.45-1.02 (m, 6H), 0.74 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.6, 142.8, 138.3, 136.3, 129.0, 128.9, 128.54, 128.51, 128.1, 126.5, 117.2, 79.9, 38.2, 32.1, 25.5, 21.9, 13.7; IR (neat, cm^{-1}) 1818, 1703, 1601, 1494, 1454, 1345, 1225, 1142, 1073, 1049, 1019, 765, 735, 699; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{21}H_{22}O_3Na$: 345.1461, found: 345.1472.



18

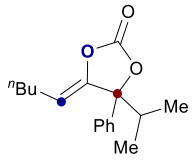
(*Z*)-4-cyclopropyl-5-pentylidene-4-phenyl-1,3-dioxolan-2-one (18): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.52 (m, 2H), 7.43-7.36 (m, 3H), 4.59 (t, *J* = 7.7 Hz, 1H), 2.25-2.10 (m, 2H), 1.62-1.55 (m, 1H), 1.38-1.26 (m, 4H), 0.89 (t, *J* = 7.1 Hz, 3H), 0.82-0.68 (m, 2H), 0.63-0.56 (m, 1H), 0.53-0.45 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 147.9, 139.1, 129.2, 128.6, 126.2, 106.7, 90.1, 31.4, 24.9, 22.3, 18.7, 13.9, 2.2, 1.8; IR (neat, cm^{-1}) 1816, 1712, 1449, 1310, 1228, 1200, 1037, 1017, 1003, 764, 699; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{20}O_3Na$: 295.1305, found: 295.1322.



P18

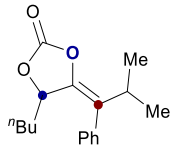
(*E*)-4-butyl-5-(cyclopropyl(phenyl)methylene)-1,3-dioxolan-2-one (P18): white solid; 11.2 mg, 41% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.29 (m, 3H), 7.09-6.98 (m, 2H), 5.19-4.92 (m, 1H), 2.10-1.99 (m, 1H), 1.37-1.08 (m, 6H), 0.81-0.64 (m, 5H), 0.41-0.32 (m, 1H), 0.21-0.13 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 142.4, 132.8, 130.0, 128.7, 128.3, 118.9, 80.0, 32.6, 25.3, 22.0, 13.7, 11.6, 4.1; IR (neat, cm^{-1}) 1818,

1697, 1492, 1443, 1339, 1232, 1145, 1103, 1073, 1051, 1022, 1001, 766, 705; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{20}O_3Na$: 295.1305, found: 295.1312.



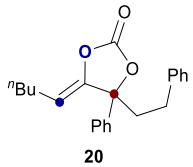
19

(*Z*)-4-isopropyl-5-pentylidene-4-phenyl-1,3-dioxolan-2-one (19): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.30 (m, 5H), 4.85 (t, *J* = 7.6 Hz, 1H), 2.48-2.35 (m, 1H), 2.29-2.17 (m, 1H), 2.16-2.04 (m, 1H), 1.42-1.24 (m, 4H), 1.07 (d, *J* = 6.8 Hz, 3H), 0.92-0.81 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 148.5, 139.5, 128.8, 128.4, 124.3, 104.6, 92.1, 37.6, 31.4, 24.9, 22.3, 16.5, 16.3, 13.8; IR (neat, cm^{-1}) 1810, 1710, 1467, 1448, 1223, 1201, 1173, 1124, 1036, 993, 763, 700; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{22}O_3Na$: 297.1461, found: 297.1460.



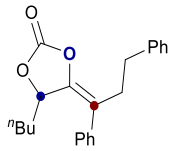
P19

(*E*)-4-butyl-5-(2-methyl-1-phenylpropylidene)-1,3-dioxolan-2-one (P19): white solid; 17.3 mg, 63% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.30 (m, 3H), 7.13-6.99 (m, 2H), 5.17-4.89 (m, 1H), 3.29-3.03 (m, 1H), 1.43-1.11 (m, 6H), 1.08 (d, *J* = 7.0 Hz, 3H), 0.92 (d, *J* = 6.9 Hz, 3H), 0.76 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 141.2, 134.2, 129.8, 128.7, 128.1, 123.5, 79.6, 32.4, 29.3, 25.2, 22.0, 21.2, 20.6, 13.7; IR (neat, cm^{-1}) 1821, 1698, 1464, 1340, 1300, 1225, 1144, 1099, 1073, 1051, 1021, 998, 766, 736, 704, 658; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{17}H_{22}O_3Na$: 297.1461, found: 297.1470.



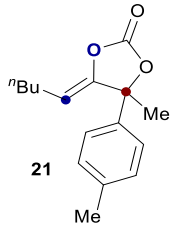
20

(*Z*)-5-pentylidene-4-phenethyl-4-phenyl-1,3-dioxolan-2-one (20): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.32 (m, 5H), 7.30-7.23 (m, 2H), 7.22-7.09 (m, 3H), 4.84 (t, *J* = 7.6 Hz, 1H), 2.84-2.43 (m, 3H), 2.40-2.08 (m, 3H), 1.47-1.25 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 148.6, 140.3, 139.4, 128.94, 128.87, 128.7, 128.3, 126.4, 124.5, 105.2, 89.1, 42.6, 31.3, 29.9, 24.9, 22.3, 13.9; IR (neat, cm^{-1}) 1817, 1712, 1603, 1497, 1449, 1228, 1200, 1160, 1150, 1070, 1046, 1001, 765, 670; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{22}H_{24}O_3Na$: 359.1618, found: 359.1618.



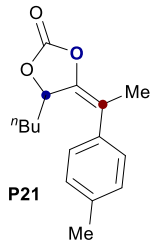
P20

(*E*)-4-butyl-5-(1,3-diphenylpropylidene)-1,3-dioxolan-2-one (P20): white solid; 26.2 mg, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.30 (m, 3H), 7.29-7.21 (m, 2H), 7.21-7.01 (m, 5H), 5.28 (d, *J* = 6.1 Hz, 1H), 3.09-2.88 (m, 1H), 2.80-2.57 (m, 3H), 1.41-1.02 (m, 6H), 0.73 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.7, 142.7, 141.0, 136.4, 129.1, 128.5, 128.41, 128.37, 128.1, 126.2, 117.3, 79.8, 33.6, 33.3, 32.1, 25.3, 21.9, 13.7; IR (neat, cm^{-1}) 1821, 1703, 1602, 1495, 1454, 1346, 1224, 1143, 1074, 1051, 1022, 766, 700; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{22}H_{24}O_3Na$: 359.1618, found: 359.1625.



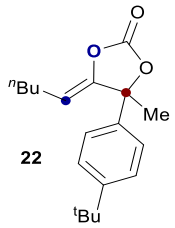
21

(*Z*)-4-methyl-5-pentylidene-4-(p-tolyl)-1,3-dioxolan-2-one (21): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.3 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 4.71 (t, *J* = 7.6 Hz, 1H), 2.36 (s, 3H), 2.24-2.14 (m, 2H), 1.91 (s, 3H), 1.43-1.28 (m, 4H), 0.90 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 150.2, 139.1, 137.1, 129.5, 124.9, 104.8, 87.1, 31.4, 27.6, 24.9, 22.3, 21.2, 13.9; IR (neat, cm^{-1}) 1818, 1714, 1513, 1454, 1379, 1221, 1080, 1044, 1000, 818, 766; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{20}O_3Na$: 283.1305, found: 283.1316.

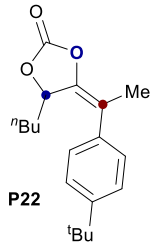


P21

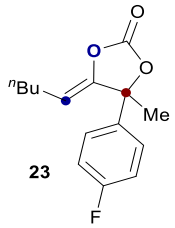
(*E*)-4-butyl-5-(1-(p-tolyl)ethylidene)-1,3-dioxolan-2-one (P21): colourless oil; 15.6 mg, 60% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (d, *J* = 7.6 Hz, 2H), 7.06 (d, *J* = 7.6 Hz, 2H), 5.40 (s, 1H), 2.36 (s, 3H), 2.06 (s, 3H), 1.46-1.39 (m, 1H), 1.30-1.04 (m, 5H), 0.76 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 141.9, 137.8, 135.0, 129.8, 127.5, 113.5, 80.0, 32.1, 25.6, 22.0, 21.3, 18.1, 13.8; IR (neat, cm^{-1}) 1820, 1706, 1513, 1457, 1346, 1225, 1146, 1074, 1019, 820, 766; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{20}O_3Na$: 283.1305, found: 283.1305.



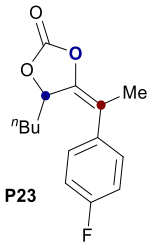
(*Z*)-4-(4-(tert-butyl)phenyl)-4-methyl-5-pentylidene-1,3-dioxolan-2-one (22): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.32 (m, 4H), 4.74 (t, *J* = 7.6 Hz, 1H), 2.27-2.15 (m, 2H), 1.92 (s, 3H), 1.43-1.29 (m, 13H), 0.91 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 151.9, 150.1, 137.0, 125.8, 124.8, 104.8, 87.1, 34.7, 31.4, 31.3, 27.7, 24.9, 22.3, 13.9; IR (neat, cm^{-1}) 1821, 1714, 1517, 1464, 1364, 1222, 1092, 1045, 1000, 835, 766; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{19}H_{26}O_3Na$: 325.1774, found: 325.1772.



(*E*)-4-butyl-5-(1-(4-(tert-butyl)phenyl)ethylidene)-1,3-dioxolan-2-one (P22): white solid; 13.9 mg, 46% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.31 (m, 2H), 7.18-7.01 (m, 2H), 5.50-5.32 (m, 1H), 2.08 (d, *J* = 1.7 Hz, 3H), 1.40-1.04 (m, 15H), 0.71 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 151.1, 142.0, 134.9, 127.3, 125.9, 113.4, 80.0, 34.7, 32.1, 31.4, 25.6, 21.8, 18.0, 13.6; IR (neat, cm^{-1}) 1822, 1705, 1512, 1463, 1345, 1226, 1146, 1077, 1017, 837, 766; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{19}H_{26}O_3Na$: 325.1774, found: 325.1772.

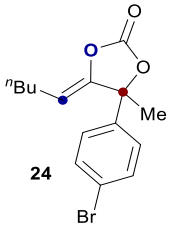


(*Z*)-4-(4-fluorophenyl)-4-methyl-5-pentylidene-1,3-dioxolan-2-one (23): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.38 (m, 2H), 7.16-7.01 (m, 2H), 4.72 (t, *J* = 7.6 Hz, 1H), 2.24-2.15 (m, 2H), 1.91 (s, 3H), 1.43-1.28 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1 (d, *J* = 267.0 Hz), 151.6, 149.9, 136.0 (d, *J* = 3.0 Hz), 127.1 (d, *J* = 9.0 Hz), 115.9 (d, *J* = 21.0 Hz), 105.3, 86.6, 31.4, 27.9, 24.9, 22.3, 13.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.53 (s); IR (neat, cm^{-1}) 1818, 1714, 1603, 1510, 1457, 1380, 1223, 1164, 1078, 1046, 1000, 836, 766, 732, 601; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}FO_3Na$: 287.1054, found: 287.1063.



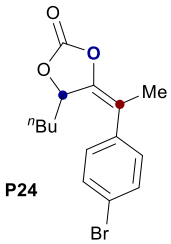
P23

(*E*)-4-butyl-5-(1-(4-fluorophenyl)ethylidene)-1,3-dioxolan-2-one (P23): white solid; 20.1 mg, 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.12 (m, 2H), 7.06 (t, *J* = 8.6 Hz, 2H), 5.44-5.27 (m, 1H), 2.06 (d, *J* = 1.8 Hz, 3H), 1.44-1.36 (m, 1H), 1.31-1.05 (m, 5H), 0.76 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3 (d, *J* = 246.0 Hz), 152.6, 142.4, 133.9 (d, *J* = 3.0 Hz), 129.4 (d, *J* = 8.0 Hz), 116.2 (d, *J* = 21.0 Hz), 112.6, 79.8, 32.2, 25.6, 21.9, 18.2, 13.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.52 (s); IR (neat, cm^{-1}) 1821, 1709, 1604, 1509, 1466, 1347, 1226, 1147, 1075, 1015, 839, 766; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}FO_3Na$: 287.1054, found: 287.1060.



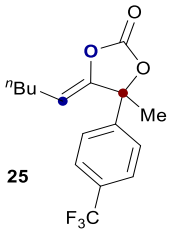
24

(*Z*)-4-(4-bromophenyl)-4-methyl-5-pentylidene-1,3-dioxolan-2-one (24): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 4.74 (t, *J* = 7.6 Hz, 1H), 2.24-2.12 (m, 2H), 1.89 (s, 3H), 1.42-1.26 (m, 4H), 0.89 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 149.5, 139.2, 132.0, 126.6, 123.3, 105.4, 86.4, 31.3, 27.6, 24.9, 22.3, 13.9; IR (neat, cm^{-1}) 1811, 1713, 1590, 1488, 1451, 1398, 1382, 1230, 1220, 1079, 1048, 1008, 829, 767, 730, 649; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}BrO_3Na$: 347.0253, found: 347.0267.



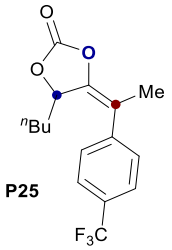
P24

(*E*)-4-(1-(4-bromophenyl)ethylidene)-5-butyl-1,3-dioxolan-2-one (P24): white solid; 26.6 mg, 82% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.2 Hz, 2H), 7.07 (d, *J* = 8.3 Hz, 2H), 5.49-5.24 (m, 1H), 2.06 (s, 3H), 1.45-1.38 (m, 1H), 1.32-1.06 (m, 5H), 0.77 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 142.6, 137.0, 132.3, 129.4, 122.0, 112.4, 79.8, 32.2, 25.6, 21.9, 17.9, 13.8; IR (neat, cm^{-1}) 1816, 1706, 1489, 1346, 1224, 1147, 1074, 1051, 1009, 827, 765; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}BrO_3Na$: 347.0253, found: 347.0263.



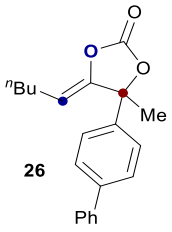
25

(*Z*)-4-methyl-5-pentylidene-4-(4-(trifluoromethyl)phenyl)-1,3-dioxolan-2-one (25): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 4.81 (t, *J* = 7.6 Hz, 1H), 2.28-2.12 (m, 2H), 1.93 (s, 3H), 1.44-1.26 (m, 4H), 0.90 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 149.3, 144.1, 131.3 (q, *J* = 32.0 Hz), 126.0 (q, *J* = 4.0 H), 125.3, 123.9 (q, *J* = 271.0 Hz), 105.8, 86.3, 31.3, 27.8, 25.0, 22.3, 13.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.81 (s). IR (neat, cm^{-1}) 1822, 1715, 1620, 1413, 1325, 1223, 1167, 1123, 1082, 1047, 1000, 843, 766; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{17}F_3O_3Na$: 337.1022, found: 337.1030.



P25

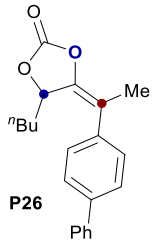
(*E*)-4-butyl-5-(1-(4-(trifluoromethyl)phenyl)ethylidene)-1,3-dioxolan-2-one (P25): white solid; 29.5 mg, 94% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.1 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 5.51-5.31 (m, 1H), 2.10 (d, *J* = 1.7 Hz, 3H), 1.45-1.35 (m, 1H), 1.32-1.03 (m, 5H), 0.74 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 143.2, 141.9, 130.2 (q, *J* = 32.0 Hz), 128.2, 126.1 (q, *J* = 4.0 Hz), 124.0 (q, *J* = 271.0 Hz), 112.3, 79.7, 32.3, 25.6, 21.9, 17.9, 13.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.70 (s); IR (neat, cm^{-1}) 1825, 1707, 1617, 1408, 1325, 1227, 1148, 1126, 1074, 1016, 847, 766; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{17}F_3O_3Na$: 337.1022, found: 337.1029.



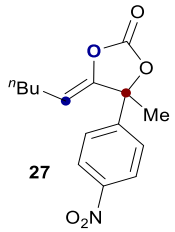
26

(*Z*)-4-([1,1'-biphenyl]-4-yl)-4-methyl-5-pentylidene-1,3-dioxolan-2-one (26): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 15.7, 7.7 Hz, 4H), 7.54 (d, *J* = 7.3 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 6.8 Hz, 1H), 4.80 (t, *J* = 7.6 Hz, 1H), 2.32-2.17 (m, 2H), 1.97 (s, 3H), 1.48-1.29 (m, 4H), 0.93 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 150.0, 142.0, 140.1, 138.9, 129.0, 127.9, 127.6, 127.2, 125.4, 105.1, 86.9, 31.4, 27.7, 24.9, 22.3, 13.9; IR (neat, cm^{-1}) 1816, 1714, 1487, 1379, 1222, 1081,

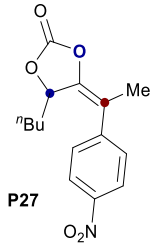
1046, 1001, 841, 765, 733, 697; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{21}H_{22}O_3Na$: 345.1461, found: 345.1471.



(*E*)-4-(1-([1,1'-biphenyl]-4-yl)ethylidene)-5-butyl-1,3-dioxolan-2-one (P26): white solid; 21.6 mg, 67% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 7.64-7.55 (m, 4H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.3 Hz, 1H), 7.26 (d, *J* = 7.8 Hz, 2H), 5.57-5.38 (m, 1H), 2.12 (d, *J* = 1.7 Hz, 3H), 1.52-1.42 (m, 1H), 1.37-1.02 (m, 5H), 0.75 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 142.3, 140.8, 140.3, 136.9, 129.0, 128.1, 127.8, 127.7, 127.1, 113.2, 80.0, 32.2, 25.6, 21.9, 18.0, 13.7; IR (neat, cm^{-1}) 1818, 1705, 1600, 1487, 1347, 1225, 1147, 1074, 1021, 1007, 843, 766, 734, 698; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{21}H_{22}O_3Na$: 345.1461, found: 345.1473.

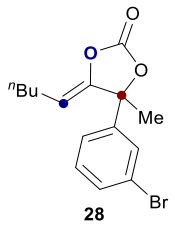


(*Z*)-4-methyl-4-(4-nitrophenyl)-5-pentylidene-1,3-dioxolan-2-one (27): ^1H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 4.84 (t, *J* = 7.6 Hz, 1H), 2.26-2.14 (m, 2H), 1.95 (s, 3H), 1.44-1.27 (m, 4H), 0.89 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 148.9, 148.2, 146.9, 125.9, 124.2, 106.3, 86.0, 31.2, 27.9, 25.0, 22.3, 13.9; IR (neat, cm^{-1}) 1823, 1715, 1607, 1523, 1348, 1224, 1096, 1079, 1050, 1002, 857, 763, 700; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}NO_5Na$: 314.0999, found: 314.1005.



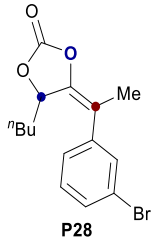
(*E*)-4-butyl-5-(1-(4-nitrophenyl)ethylidene)-1,3-dioxolan-2-one (P27): yellow solid; 19.2 mg, 66% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.6 Hz, 2H), 7.40 (d, *J* = 8.6 Hz, 2H), 5.55-5.35 (m, 1H), 2.12 (d, *J* = 1.6 Hz, 3H), 1.45-1.36 (m, 1H), 1.34-1.03 (m, 5H), 0.75 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 147.3, 145.1, 143.9, 128.7, 124.4, 111.7, 79.7, 32.4, 25.6, 21.9, 17.7, 13.7; IR (neat, cm^{-1}) 1817, 1703,

1597, 1518, 1344, 1226, 1148, 1075, 1052, 1014, 858, 765, 701; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}NO_5Na$: 314.0999, found: 314.1009.



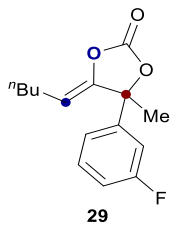
28

(*Z*)-4-(3-bromophenyl)-4-methyl-5-pentylidene-1,3-dioxolan-2-one (28): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (t, *J* = 1.8 Hz, 1H), 7.55-7.45 (m, 1H), 7.43-7.34 (m, 1H), 7.29 (d, *J* = 7.9 Hz, 1H), 4.77 (t, *J* = 7.6 Hz, 1H), 2.26-2.12 (m, 2H), 1.90 (s, 3H), 1.45-1.26 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 149.4, 142.4, 132.2, 130.6, 128.1, 123.6, 123.1, 105.7, 86.2, 31.3, 27.8, 25.0, 22.3, 13.9; IR (neat, cm^{-1}) 1818, 1714, 1594, 1568, 1475, 1467, 1418, 1379, 1221, 1115, 1095, 1068, 1046, 999, 880, 786, 765, 696, 643; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}BrO_3Na$: 347.0253, found: 347.0266.



P28

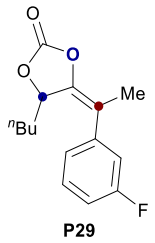
(*E*)-4-(1-(3-bromophenyl)ethylidene)-5-butyl-1,3-dioxolan-2-one (P28): white solid; 23.7 mg, 73% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 7.9 Hz, 1H), 7.34 (s, 1H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 5.39 (d, *J* = 1.2 Hz, 1H), 2.06 (d, *J* = 1.0 Hz, 3H), 1.47-1.38 (m, 1H), 1.33-1.07 (m, 5H), 0.76 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 143.0, 140.1, 131.1, 130.8, 130.7, 126.4, 123.1, 112.2, 79.7, 32.2, 25.5, 21.9, 17.9, 13.7; IR (neat, cm^{-1}) 1820, 1709, 1592, 1560, 1475, 1346, 1225, 1147, 1078, 788, 765, 699, 681; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}BrO_3Na$: 347.0253, found: 347.0266.



29

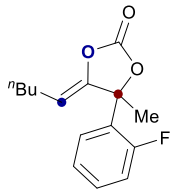
(*Z*)-4-(3-fluorophenyl)-4-methyl-5-pentylidene-1,3-dioxolan-2-one (29): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.33 (m, 1H), 7.29-7.20 (m, 1H), 7.20-7.12 (m, 1H), 7.11-7.00 (m, 1H), 4.77 (t, *J* = 7.6 Hz, 1H), 2.26-2.14 (m, 2H), 1.90 (s, 3H), 1.44-1.24 (m, 4H), 0.90 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, *J* = 246.0 Hz), 151.5, 149.5, 142.7 (d, *J* = 7.0 Hz), 130.7 (d, *J* = 8.0 Hz), 120.5 (d, *J* = 3.0 Hz), 116.1 (d,

J = 20.0 Hz), 112.3 (d, *J* = 23.0 Hz), 105.5, 86.3 (d, *J* = 2.0 Hz), 31.4, 27.8, 25.0, 22.3, 13.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.29 (s). IR (neat, cm^{-1}) 1818, 1714, 1614, 1591, 1488, 1440, 1269, 1253, 1223, 1201, 1101, 1047, 1001, 926, 874, 827, 787, 766, 701; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}FO_3Na$: 287.1054, found: 287.1053.



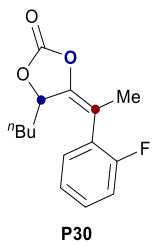
P29

(*E*)-4-butyl-5-(1-(3-fluorophenyl)ethylidene)-1,3-dioxolan-2-one (P29): white solid; 18.5 mg, 70% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.30 (m, 1H), 7.04-6.95 (m, 2H), 6.90 (d, *J* = 9.5 Hz, 1H), 5.48-5.35 (m, 1H), 2.07 (d, *J* = 1.6 Hz, 3H), 1.47-1.38 (m, 1H), 1.32-1.08 (m, 5H), 0.75 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1 (d, *J* = 246.0 Hz), 152.5, 142.8, 140.2 (d, *J* = 8.0 Hz), 130.8 (d, *J* = 8.0 Hz), 123.4 (d, *J* = 3.0 Hz), 115.0 (d, *J* = 19.0 Hz), 114.8 (d, *J* = 19.0 Hz), 112.4 (d, *J* = 2.0 Hz), 79.8, 32.2, 25.6, 21.9, 17.9, 13.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.80 (s); IR (neat, cm^{-1}) 1822, 1708, 1611, 1584, 1487, 1433, 1348, 1264, 1239, 1180, 1146, 1080, 896, 790, 766, 699; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}FO_3Na$: 287.1054, found: 287.1060.



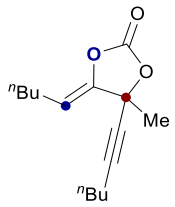
30

(*Z*)-4-(2-fluorophenyl)-4-methyl-5-pentylidene-1,3-dioxolan-2-one (30): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.43 (m, 1H), 7.42-7.33 (m, 1H), 7.22-7.06 (m, 2H), 4.69 (t, *J* = 7.6 Hz, 1H), 2.20-2.12 (m, 2H), 1.98 (s, 3H), 1.39-1.22 (m, 4H), 0.87 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7 (d, *J* = 249.0 Hz), 151.8, 149.7, 131.5 (d, *J* = 9.0 Hz), 127.2 (d, *J* = 10.0 Hz), 126.7 (d, *J* = 3.0 Hz), 124.2 (d, *J* = 3.0 Hz), 117.0 (d, *J* = 22.0 Hz), 104.3 (d, *J* = 8.0 Hz), 84.4, 31.3, 26.3 (d, *J* = 2.0 Hz), 24.9, 22.2, 13.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.16 (s); IR (neat, cm^{-1}) 1821, 1715, 1616, 1586, 1491, 1458, 1380, 1235, 1219, 1130, 1090, 1068, 1047, 1000, 759; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}FO_3Na$: 287.1054, found: 287.1050.



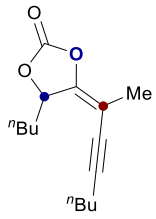
P30

(*E*)-4-butyl-5-(1-(2-fluorophenyl)ethylidene)-1,3-dioxolan-2-one (P30): white solid; 23.5 mg, 89% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.27 (m, 1H), 7.21-7.05 (m, 3H), 5.25 (s, 1H), 2.06 (d, *J* = 1.7 Hz, 3H), 1.44-1.34 (m, 1H), 1.30-1.02 (m, 5H), 0.75 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7 (d, *J* = 245.0 Hz), 158.4, 152.6, 130.12 (d, *J* = 8.0 Hz), 130.07 (d, *J* = 2.0 Hz), 125.2 (d, *J* = 16.0 Hz), 124.8 (d, *J* = 4.0 Hz), 116.2 (d, *J* = 21.0 Hz), 107.4, 79.9 (d, *J* = 4.0 Hz), 32.1, 25.4, 21.9, 17.4 (d, *J* = 1.0 Hz), 13.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.73 (s); IR (neat, cm^{-1}) 1824, 1714, 1492, 1448, 1346, 1263, 1232, 1204, 1147, 1109, 1079, 1051, 762; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{17}FO_3Na$: 287.1054, found: 287.1065.



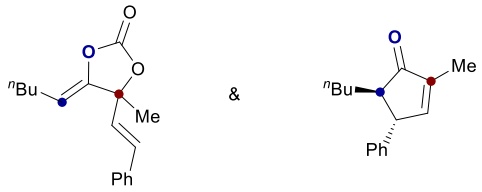
31

(*Z*)-4-(hex-1-yn-1-yl)-4-methyl-5-pentylidene-1,3-dioxolan-2-one (31): ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.81 (t, *J* = 7.6 Hz, 1H), 2.23 (t, *J* = 7.0 Hz, 2H), 2.19-2.05 (m, 2H), 1.76 (s, 3H), 1.52-1.44 (m, 2H), 1.42-1.27 (m, 6H), 0.90 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 148.5, 103.8, 89.3, 78.7, 77.1, 31.2, 30.2, 29.5, 24.8, 22.2, 22.0, 18.4, 13.9, 13.6; IR (neat, cm^{-1}) 1828, 1719, 1466, 1377, 1209, 1078, 1046, 997, 764; HRMS (ESI): *m/z*: $[M-CO_2+H]^+$ calcd for $C_{14}H_{23}O$: 207.1743, found: 207.1748.



P31

(*E*)-4-butyl-5-(oct-3-yn-2-ylidene)-1,3-dioxolan-2-one (P31): colorless oil; 24.0 mg, 96% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.34-5.26 (m, 1H), 2.32 (t, *J* = 6.9 Hz, 2H), 2.16-2.07 (m, 1H), 1.91-1.80 (m, 4H), 1.53-1.34 (m, 8H), 0.95-0.89 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 149.9, 96.0, 95.7, 81.1, 76.3, 32.4, 30.8, 26.1, 22.3, 22.1, 19.2, 16.1, 13.9, 13.7; IR (neat, cm^{-1}) 1826, 1690, 1466, 1337, 1224, 1125, 1080, 1050, 763; HRMS (ESI): *m/z*: $[M-CO_2+Na]^+$ calcd for $C_{14}H_{122}ONa$: 229.1563, found: 229.1565.

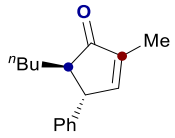


32 : **P32**

1.1 : 1

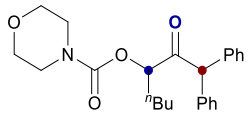
*Note: Cyclic carbonate **32** are not quite stable. A mixture of cyclic carbonate **32** and **P32** (ratio = 1.1:1) was synthesized according to the published method.*[2] *The yield reported in the main text (Fig. 2b) is the isolated yield without taking account of compound **P32** in the starting mixture.*

(*Z*)-4-methyl-5-pentylidene-4-((E)-styryl)-1,3-dioxolan-2-one (32): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.32 (m, 5H), 6.72 (d, *J* = 16.0 Hz, 1H), 6.21 (d, *J* = 16.0 Hz, 1H), 4.68 (t, *J* = 7.6 Hz, 1H), 2.24-2.16 (m, 2H), 1.76 (s, 3H), 1.37-1.27 (m, 4H), 0.92 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 148.9, 135.3, 131.4, 128.91, 128.86, 127.6, 127.1, 104.3, 85.8, 31.5, 26.4, 24.9, 22.3, 14.0; IR (neat, cm^{-1}) 1819, 1450, 1222, 1089, 1046, 968, 795, 693; HRMS (ESI): *m/z*: $[M\text{-}CO_2+H]^+$ calcd for $C_{16}H_{21}O$: 229.1587, found: 229.1594.



P32

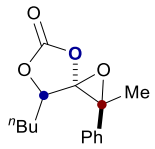
***trans*-5-butyl-2-methyl-4-phenylcyclopent-2-en-1-one (P32):** colorless oil; 21.6 mg, 95% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.29 (m, 2H), 7.28-7.22 (m, 1H), 7.19 (s, 1H), 7.14 (d, *J* = 7.2 Hz, 2H), 3.70-3.61 (m, 1H), 2.36-2.24 (m, 1H), 1.90-1.79 (m, 4H), 1.60-1.51 (m, 1H), 1.39-1.23 (m, 4H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.0, 159.2, 142.6, 141.0, 129.0, 127.5, 127.1, 55.6, 51.7, 31.0, 29.4, 22.9, 14.0, 10.4; IR (neat, cm^{-1}) 1700, 1639, 1601, 1494, 1454, 1331, 1075, 1030, 890, 805, 759; HRMS (ESI): *m/z*: $[M\text{-}CO_2+H]^+$ calcd for $C_{16}H_{21}O$: 229.1587, found: 229.1595.



33

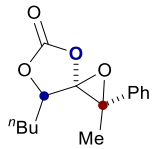
2-oxo-1,1-diphenylheptan-3-yl morpholine-4-carboxylate (33): colourless oil; 34.8 mg, 88% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (t, *J* = 7.3 Hz, 4H), 7.28-7.20 (m, 6H), 5.33 (s, 1H), 5.28-5.21 (m, 1H), 3.72-3.52 (m, 4H), 3.45-3.33 (m, 4H), 1.76-1.63 (m, 2H), 1.32-1.17 (m, 4H), 0.82 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.2, 154.5, 138.2, 137.6, 129.2, 129.1, 128.8, 128.7, 127.5, 127.4, 79.6, 66.7, 66.5, 60.1, 44.4, 44.0, 30.8, 27.4, 22.3, 13.9; IR (neat, cm^{-1}) 1699, 1494, 1426, 1276, 1238,

1115, 1091, 1077, 983, 856, 745, 700; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{24}H_{29}NO_4Na$: 418.1989, found: 418.1975.



trans-**34**

(*trans*)-7-butyl-2-methyl-2-phenyl-1,4,6-trioxaspiro[2.4]heptan-5-one (*trans*-34): colourless oil; 20.7 mg, 79% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.31 (m, 5H), 4.68-4.61 (m, 1H), 1.92 (s, 3H), 1.26-1.14 (m, 2H), 1.12-0.97 (m, 3H), 0.88-0.80 (m, 1H), 0.71 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 136.7, 129.1, 129.0, 125.4, 93.7, 80.2, 65.5, 29.4, 25.4, 21.9, 19.2, 13.6; IR (neat, cm^{-1}) 1827, 1468, 1447, 1342, 1279, 1225, 1051, 765, 749, 701; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{18}O_4Na$: 285.1097 found: 285.1117.



cis-**34**

(*cis*)-7-butyl-2-methyl-2-phenyl-1,4,6-trioxaspiro[2.4]heptan-5-one (*cis*-34): colourless oil; 20.0 mg, 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.33 (m, 5H), 4.93-4.76 (m, 1H), 2.01-1.85 (m, 2H), 1.75 (s, 3H), 1.54-1.38 (m, 4H), 0.97 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 135.9, 128.8, 128.6, 126.1, 93.8, 80.4, 65.5, 30.6, 26.0, 22.4, 22.0, 14.0; IR (neat, cm^{-1}) 1813, 1447, 1343, 1228, 1069, 1048, 899, 843, 765, 695, 644; HRMS (ESI): *m/z*: $[M+Na]^+$ calcd for $C_{15}H_{18}O_4Na$: 285.1097, found: 285.1122.

8. X-ray crystallographic information of product P13

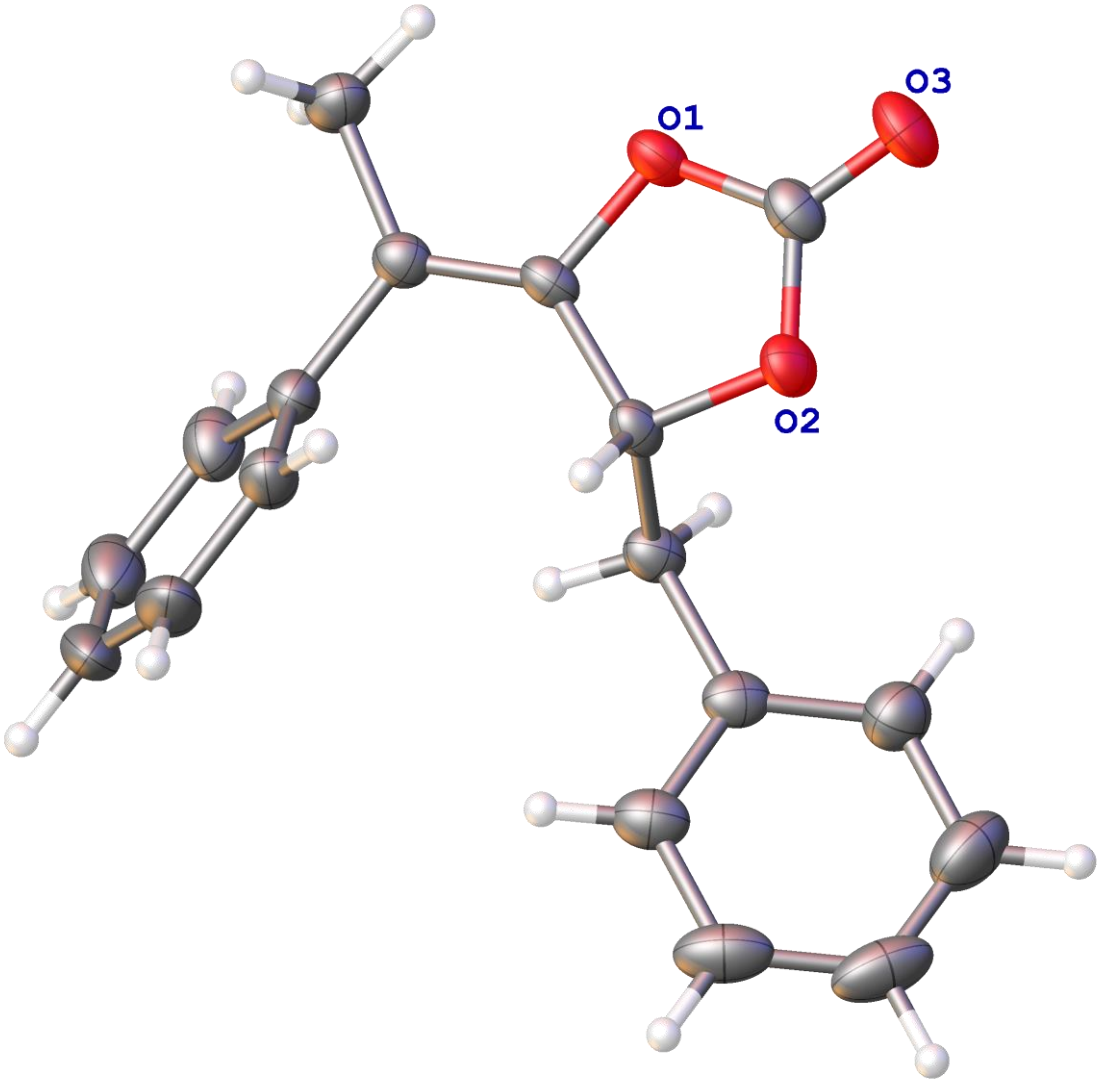


Fig. S1 X-ray crystallography of **P13** (CCDC: 2419557).

Table S3 Crystal data and structure refinement for P13.

Identification code	**P13**
Empirical formula	$C_{18}H_{16}O_3$
Formula weight	280.31
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.9241(2)

b/Å	9.1060(2)
c/Å	10.2978(2)
α/°	70.545(2)
β/°	74.245(2)
γ/°	74.481(2)
Volume/Å^3	744.80(3)
Z	2
ρ_{calc}g/cm^3	1.250
μ/mm^{-1}	0.682
F(000)	296.0
Crystal size/mm^3	0.16 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.298 to 142.834
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 9, -12 ≤ l ≤ 12
Reflections collected	6720
Independent reflections	2797 [R_{int} = 0.0181, R_{sigma} = 0.0176]
Data/restraints/parameters	2797/0/192
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0406, wR_2 = 0.1103
Final R indexes [all data]	R_1 = 0.0416, wR_2 = 0.1111
Largest diff. peak/hole / e Å^{-3}	0.24/-0.22

Crystal structure determination of [P13]

Crystal Data for $C_{18}H_{16}O_3$ (*M* =280.31 g/mol): triclinic, space group P-1 (no. 2), *a* = 8.9241(2) Å, *b* = 9.1060(2) Å, *c* = 10.2978(2) Å, *α* = 70.545(2) °, *β* = 74.245(2) °, *γ* = 74.481(2) °, *V* = 744.80(3) Å^3, *Z* = 2, *T* = 150.00(10) K, μ(Cu Kα) = 0.682 mm^{-1}, *Dcalc* = 1.250 g/cm^3, 6720 reflections measured (9.298° ≤ 2Θ ≤ 142.834°), 2797 unique (R_{int} = 0.0181, R_{sigma} = 0.0176) which were used in all calculations. The final R_1 was 0.0406 (I > 2σ(I)) and wR_2 was 0.1111 (all data).

Table S4 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for P13. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	802.5(10)	6419.7(10)	5011.8(9)	29.4(2)
O2	3220.4(10)	5534.1(10)	3907.9(9)	30.0(2)
O3	1633.0(13)	7609.1(12)	2724.6(10)	40.9(3)
C1	1614.6(15)	3589.4(15)	8447.9(13)	27.9(3)
C2	3066.8(15)	3692.5(18)	8641.2(14)	35.2(3)
C3	3833.2(18)	2478(2)	9617.8(16)	49.5(4)
C4	3152(2)	1180(2)	10414.8(16)	55.1(5)
C5	1706(2)	1078.2(18)	10236.9(16)	50.2(4)
C6	940.6(19)	2275.9(17)	9263.0(15)	39.0(3)
C7	780.4(14)	4869.7(14)	7394.1(13)	26.0(3)
C8	-847.5(15)	5730.5(17)	7913.7(15)	35.6(3)
C9	1501.1(13)	5204.6(13)	6056.4(12)	24.0(3)
C10	3095.0(14)	4481.9(14)	5335.6(12)	24.7(3)
C11	3272.8(14)	2778.6(14)	5310.4(13)	27.8(3)
C12	4929.9(15)	2124.5(14)	4624.0(14)	28.9(3)
C13	6092.0(16)	1390.2(16)	5424.9(16)	36.0(3)
C14	7625.2(17)	787.5(18)	4815(2)	47.3(4)
C15	8010.9(18)	913.8(19)	3401(2)	52.8(5)
C16	6869(2)	1640(2)	2586.9(19)	52.9(4)
C17	5332.7(18)	2246.6(18)	3195.7(16)	40.3(4)
C18	1871.4(16)	6611.4(15)	3779.8(13)	29.9(3)

Table S5 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for P13. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	26.6(4)	27.9(5)	28.9(5)	0.0(4)	-10.6(4)	-2.8(3)
O2	31.5(5)	27.3(5)	24.4(5)	1.3(4)	-3.2(3)	-7.9(4)
O3	51.4(6)	34.1(5)	31.9(5)	6.5(4)	-16.7(4)	-10.8(4)
C1	28.4(6)	28.1(6)	22.6(6)	-6.8(5)	-2.8(5)	-0.7(5)
C2	27.6(6)	43.2(8)	28.0(7)	-7.3(6)	-5.4(5)	0.4(5)
C3	33.8(7)	65.3(11)	35.6(8)	-12.8(7)	-11.5(6)	15.6(7)
C4	66.8(11)	44.4(9)	28.4(8)	-3.8(7)	-11.0(7)	24.4(8)
C5	73.7(12)	30.5(8)	31.6(8)	-2.4(6)	-3.0(7)	-1.7(7)
C6	50.5(8)	33.2(7)	29.8(7)	-5.3(6)	-3.7(6)	-11.3(6)
C7	23.1(6)	25.8(6)	28.2(6)	-5.9(5)	-6.0(5)	-4.7(5)
C8	27.5(7)	41.4(8)	34.6(7)	-13.0(6)	-6.2(5)	1.7(5)
C9	22.8(6)	20.7(6)	27.1(6)	-1.1(5)	-9.7(5)	-4.2(4)
C10	22.6(6)	25.6(6)	21.9(6)	0.8(5)	-4.8(4)	-7.4(4)
C11	24.0(6)	25.3(6)	30.3(6)	-2.3(5)	-4.8(5)	-6.2(5)
C12	25.7(6)	22.2(6)	36.1(7)	-5.4(5)	-3.8(5)	-6.6(5)
C13	30.6(7)	30.0(7)	47.8(8)	-10.1(6)	-11.5(6)	-4.3(5)
C14	28.4(7)	35.0(8)	80.6(12)	-19.6(8)	-15.4(7)	-0.7(6)
C15	29.1(7)	41.4(8)	82.7(13)	-28.0(9)	9.0(8)	-5.7(6)
C16	49.3(9)	50.5(10)	50.9(10)	-21.4(8)	11.8(7)	-9.8(7)
C17	37.8(8)	40.1(8)	37.9(8)	-9.8(6)	-2.4(6)	-5.9(6)
C18	34.1(7)	25.6(6)	29.1(7)	-0.5(5)	-10.0(5)	-9.8(5)

Table S6 Bond Lengths for P13.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C9	1.4044(14)	C7	C8	1.5031(17)
O1	C18	1.3543(16)	C7	C9	1.3222(18)
O2	C10	1.4567(14)	C9	C10	1.5028(16)
O2	C18	1.3406(16)	C10	C11	1.5246(17)
O3	C18	1.1900(16)	C11	C12	1.5109(17)
C1	C2	1.3948(19)	C12	C13	1.3888(19)
C1	C6	1.3925(19)	C12	C17	1.389(2)
C1	C7	1.4908(17)	C13	C14	1.389(2)
C2	C3	1.389(2)	C14	C15	1.374(3)
C3	C4	1.381(3)	C15	C16	1.383(3)
C4	C5	1.382(3)	C16	C17	1.391(2)
C5	C6	1.381(2)			

Table S7 Bond Angles for P13.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C18	O1	C9	109.10(9)	O2	C10	C9	102.12(9)
C18	O2	C10	110.19(9)	O2	C10	C11	109.71(10)
C2	C1	C7	120.79(11)	C9	C10	C11	115.73(10)
C6	C1	C2	119.11(12)	C12	C11	C10	112.11(10)
C6	C1	C7	120.10(12)	C13	C12	C11	119.87(12)
C3	C2	C1	119.88(14)	C13	C12	C17	118.60(13)
C4	C3	C2	120.33(16)	C17	C12	C11	121.53(12)
C3	C4	C5	120.05(14)	C12	C13	C14	120.85(15)
C6	C5	C4	120.00(15)	C15	C14	C13	120.09(15)
C5	C6	C1	120.62(15)	C14	C15	C16	119.88(14)
C1	C7	C8	117.93(11)	C15	C16	C17	120.14(16)
C9	C7	C1	118.99(11)	C12	C17	C16	120.45(15)
C9	C7	C8	123.07(11)	O2	C18	O1	111.23(10)
O1	C9	C10	106.89(9)	O3	C18	O1	123.99(12)
C7	C9	O1	122.08(11)	O3	C18	O2	124.78(13)
C7	C9	C10	131.03(11)				

Table S8 Torsion Angles for P13.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C9	C10	O2	6.58(11)	C8	C7	C9	C10	-179.31(12)
O1	C9	C10	C11	-112.53(11)	C9	O1	C18	O2	3.75(13)
O2	C10	C11	C12	67.68(13)	C9	O1	C18	O3	-176.35(12)
C1	C2	C3	C4	-1.0(2)	C9	C10	C11	C12	-177.47(10)
C1	C7	C9	O1	-178.48(10)	C10	O2	C18	O1	0.79(14)
C1	C7	C9	C10	1.2(2)	C10	O2	C18	O3	-179.11(12)
C2	C1	C6	C5	-0.9(2)	C10	C11	C12	C13	87.73(14)
C2	C1	C7	C8	-119.61(13)	C10	C11	C12	C17	-91.86(15)
C2	C1	C7	C9	59.91(17)	C11	C12	C13	C14	-179.68(12)
C2	C3	C4	C5	0.5(2)	C11	C12	C17	C16	179.74(13)
C3	C4	C5	C6	-0.1(2)	C12	C13	C14	C15	0.1(2)
C4	C5	C6	C1	0.3(2)	C13	C12	C17	C16	0.1(2)
C6	C1	C2	C3	1.2(2)	C13	C14	C15	C16	-0.1(2)
C6	C1	C7	C8	59.86(16)	C14	C15	C16	C17	0.2(2)
C6	C1	C7	C9	-120.62(14)	C15	C16	C17	C12	-0.2(2)
C7	C1	C2	C3	-179.28(12)	C17	C12	C13	C14	-0.1(2)
C7	C1	C6	C5	179.63(12)	C18	O1	C9	C7	173.21(11)
C7	C9	C10	O2	-173.14(12)	C18	O1	C9	C10	-6.54(12)
C7	C9	C10	C11	67.76(17)	C18	O2	C10	C9	-4.56(12)
C8	C7	C9	O1	1.01(19)	C18	O2	C10	C11	118.71(11)

Table S9 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for P13.

Atom	*x*	*y*	*z*	U(eq)
H2	3530.98	4591.49	8105.96	42
H3	4830.67	2540.45	9737.76	59
H4	3677.66	356.87	11086.08	66
H5	1239.56	184.11	10784.6	60
H6	-55.49	2203.01	9148.06	47
H8A	-1587.71	4995.19	8275.87	53
H8B	-1206.25	6612.71	7137.45	53
H8C	-809.86	6145	8666.52	53
H10	3944.75	4548.31	5766.04	30
H11A	3019.57	2099.52	6285.81	33
H11B	2503.17	2743.56	4791.89	33
H13	5834.91	1298.97	6402.71	43
H14	8408.12	287.21	5375.11	57
H15	9060.09	502.68	2983.87	63
H16	7134.11	1725.92	1610.01	63
H17	4553.98	2747.42	2630.84	48

9. Additional DFT computational data

All calculations were carried out using Gaussian 16 software.[3] All the structures were optimized using B3LYP[4] functional with Grimme's D3 dispersion correction[5], and Becke Johnson damping scheme[6] in the gas phase. A 6-31g(d) basis set was used for all the atoms.[7] Frequency calculations were performed on the optimized geometries to make sure that they were the equilibrium geometries. Transition states were characterized by a single imaginary frequency, and the absence of imaginary frequency characterized all the intermediates.

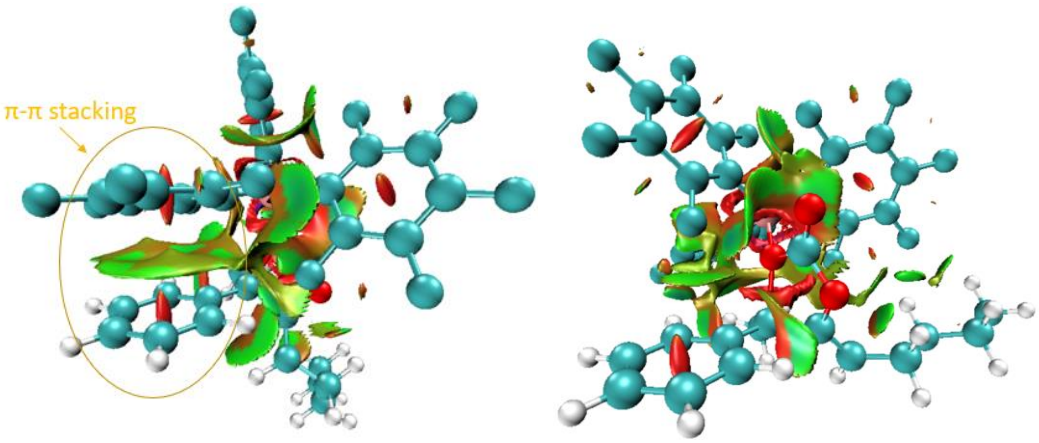
The single point energy calculation, NCI plot[8], and AIM[9] analysis on the optimized geometries were performed using the 6-311++g(d,p) basis set[7] and M06-2x functional[10] with Grimme's D3 dispersion correction. The solvation effects were considered in these single-point calculations using the SMD solvation model for the solvent Z-1,2-DichloroEthene (dielectric constant, ε=9.2). The actual solvent for the reaction medium was Trifluoro toluene (ε=9.18) since it was not in the gaussian solvent library, Z-1,2-DichloroEthene with a similar dielectric constant was taken for the single point energy calculation.[11] The 3D images of the transition state structures were generated using CYLView software.[12]

Non-Covalent Interactions (NCI) analysis was done using Multiwfn[13] software and the interactions were visualized using VMD[14] Software. AIM analysis for the transition states was also carried out using Multiwfn software.

All the reported energies are in Gibbs free energies (kcal mol^{-1}).

NCI analysis

A careful analysis of the ring opening transition states **TS1** and **TS1'** using the Non-Covalent Interaction (NCI) plot suggests that the *π-π stacking* which is present in **TS1** makes it more stable than **TS1'** (Fig. S2).



TS1 **TS1'**

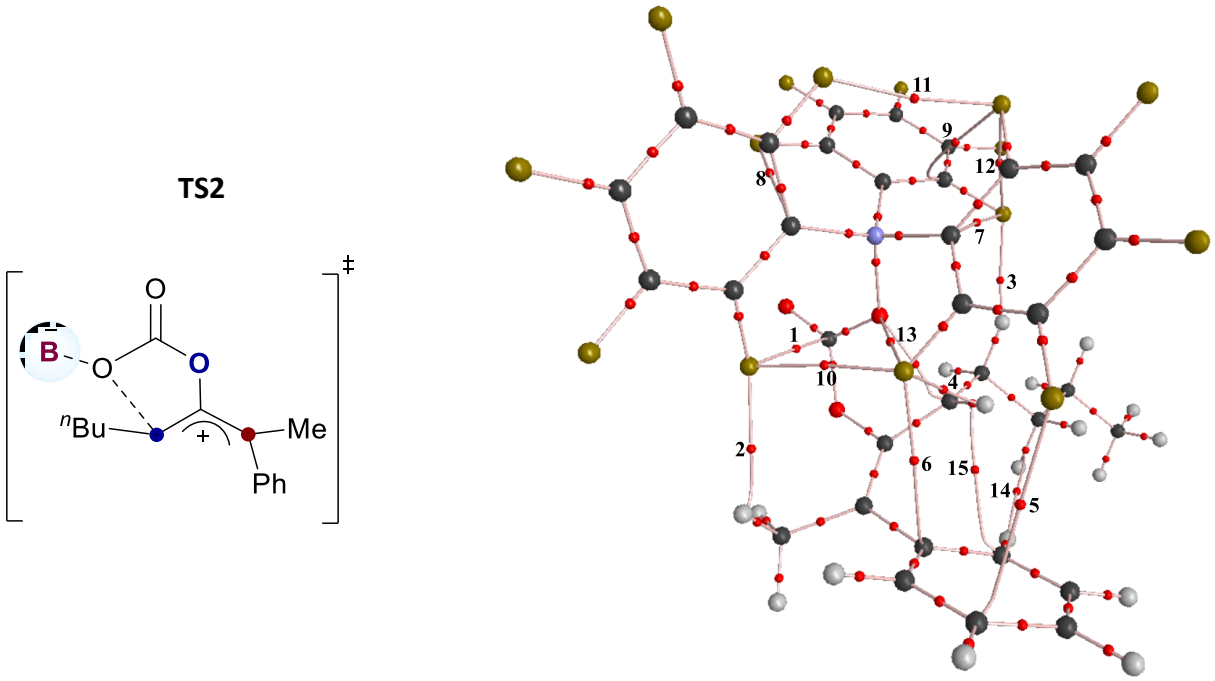
Fig. S2 NCI plot for the $B(C_6F_5)_3$ assisted ring opening transition states **TS1** and **TS1'**. Green colour represents attractive interactions and red color represents strong repulsive interactions.

AIM Analysis

The transition states **TS2** and **TS2'** involved in the final cyclization step were analyzed using Atoms In Molecules (AIM) analysis. The details are provided in Table S10 and

Table S11. The higher number of non-covalent interactions for the transition state **TS2** can be accounted for its extra stability.

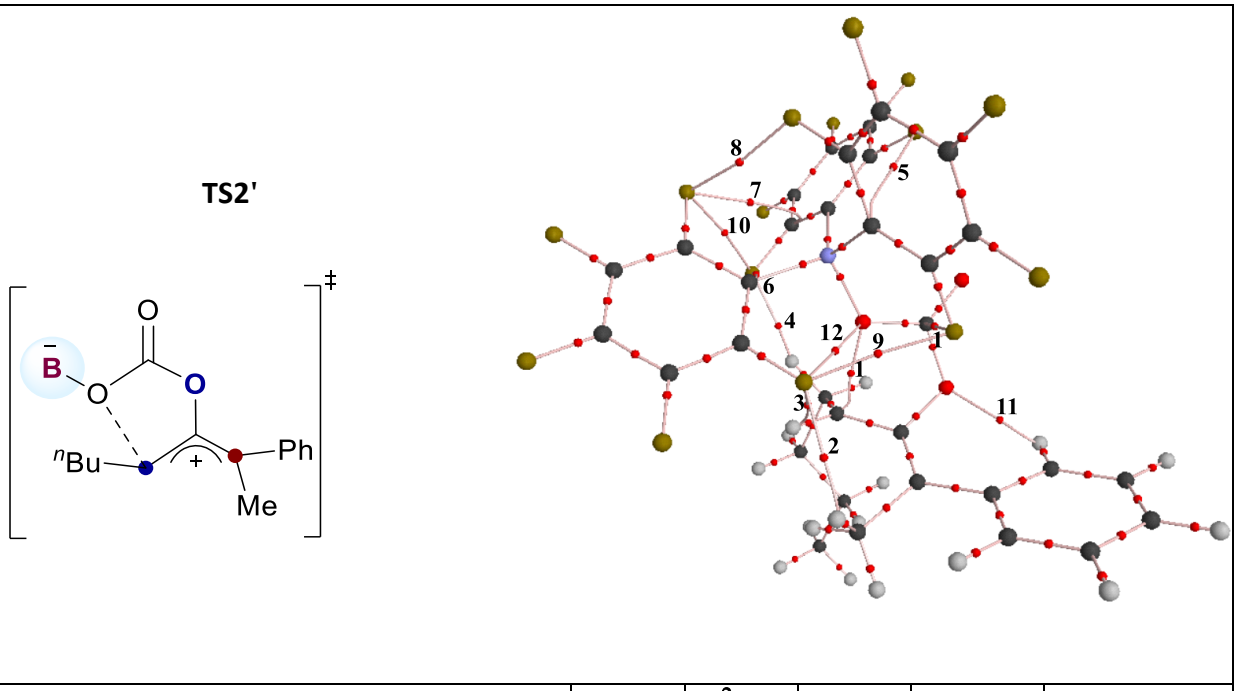
Table S10 Bond critical points along the bond pathways and estimated strengths of the important noncovalent interactions in the transition state **TS2**.



TS2 -Types of Interactions	**ρ**	**∇^2 ρ**	**G**	**V= 1/4∇^2 ρ-2G**	**E=1/2(V) (kcal mol^{-1})**
1. C-F(Lewis acid) – C (carbonate carbon)	0.016	-0.018	0.016	-0.037	-11.570
2. C-F (Lewis acid) – H-C (Methyl)	0.009	-0.010	0.008	-0.019	-6.092
3. C-F(Lewis acid) – H-C (n-butyl)	0.016	-0.016	0.014	-0.032	-9.997
4. C-F(Lewis acid) – H-C (carbonate)	0.011	-0.012	0.010	-0.024	-7.503
5. C-F (Lewis acid) – π (Phenyl)	0.005	-0.004	0.004	-0.008	-2.595
6. C-F (Lewis acid) – π (Phenyl)	0.008	-0.007	0.006	-0.015	-4.562
7. C-F (Lewis acid) – π (Lewis acid)	0.010	-0.011	0.009	-0.021	-6.685
8. C-F (Lewis acid) – π (Lewis acid)	0.013	-0.013	0.012	-0.027	-8.439
9. C-F (Lewis acid) – π (Lewis acid)	0.012	-0.012	0.011	-0.025	-7.716
10. C-F (Lewis acid) – F-C (Lewis acid)	0.009	-0.011	0.010	-0.023	-7.084

11. C-F (Lewis acid) – F-C (Lewis acid)	0.006	-0.007	0.006	-0.014	-4.438
12. C-F (Lewis acid) – F-C (Lewis acid)	0.011	-0.014	0.013	-0.028	-8.923
13. O (Carbonate) – F-C (Lewis acid)	0.012	-0.013	0.012	-0.027	-8.448
14. C-H (n-butyl) – H-C (Phenyl)	0.006	-0.005	0.004	-0.010	-3.065
15. C-H (Carbonate) – π (Phenyl)	0.013	-0.012	0.010	-0.023	-7.077

Table S11 Bond critical points along the bond pathways and estimated strengths of the important noncovalent interactions in the transition state **TS2'**.



TS2' -Types of Interactions	**ρ**	**∇^2 ρ**	**G**	**V= 1/4∇^2 ρ-2G**	**E=1/2(V) (kcal mol^{-1})**
1. C-F (Lewis acid) – C (carbonate carbon)	0.016	-0.018	0.017	-0.038	-11.824
2. C-F (Lewis acid) – H-C (Methyl)	0.009	-0.009	0.008	-0.018	-5.757
3. C-F (Lewis acid) – H-C (n-butyl)	0.015	-0.015	0.013	-0.030	-9.274
4. C-F (Lewis acid) – H-C (n-butyl)	0.011	-0.011	0.010	-0.023	-7.139
5. C-F (Lewis acid) – π (Lewis acid)	0.013	-0.013	0.012	-0.027	-8.346
6. C-F (Lewis acid) – π (Lewis acid)	0.011	-0.011	0.009	-0.022	-6.803
7. C-F (Lewis acid) – π (Lewis acid)	0.012	-0.012	0.011	-0.024	-7.672
8. C-F (Lewis acid) – F-C (Lewis acid)	0.006	-0.007	0.006	-0.014	-4.503

9. C-F (Lewis acid) – F-C (Lewis acid)	0.009	-0.010	0.009	-0.022	-6.756
10. C-F (Lewis acid) – F-C (Lewis acid)	0.011	-0.013	0.012	-0.027	-8.459
11. C-H (Methyl) – O (Carbonate)	0.018	-0.019	0.016	-0.037	-11.753
12. O (Carbonate) – F-C (Lewis acid)	0.012	-0.013	0.012	-0.027	-8.506

Other Possible Pathway: For the major product formation, a possible pathway which involves the change in the coordination site of the $B(C_6F_5)_3$ after the ring opening step was analyzed in detail (Fig. S3). Even though the cyclization transition state **TS4** in this pathway is highly favorable than the respective transition state in pathway a (**TS2**), the energy barrier for the intramolecular transfer of Lewis acid tansition state before the cyclization step was found to be 39.9 kcal mol^{-1}, which makes it unfavorable.

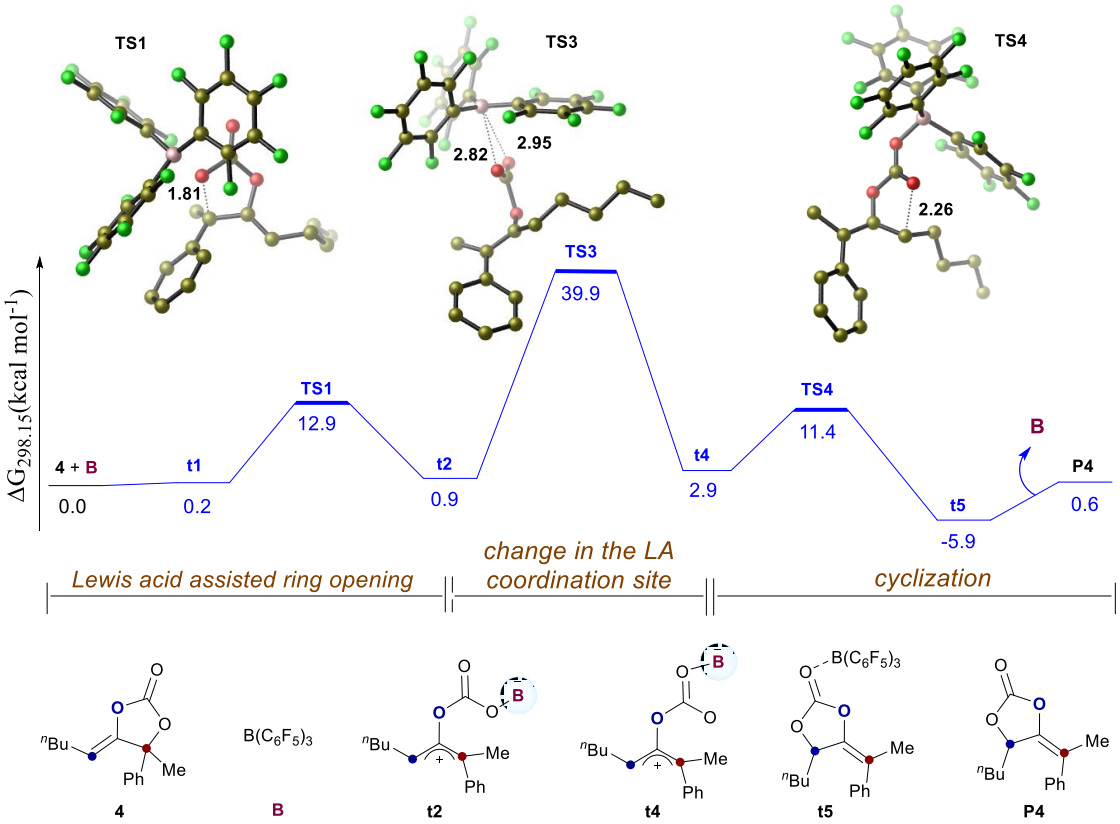


Fig. S3 Computed Gibbs free energy profile diagram for the $B(C_6F_5)_3$ catalyzed cyclic carbonate editing involving a change in the coordination site of $B(C_6F_5)_3$ at the M06-2X-D3/6-311++G(d,p)+SMD(Z-1,2-DichloroEthene)// B3LYP-D3(BJ)/6-31G(d) level of theory.

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11. NMR spectra

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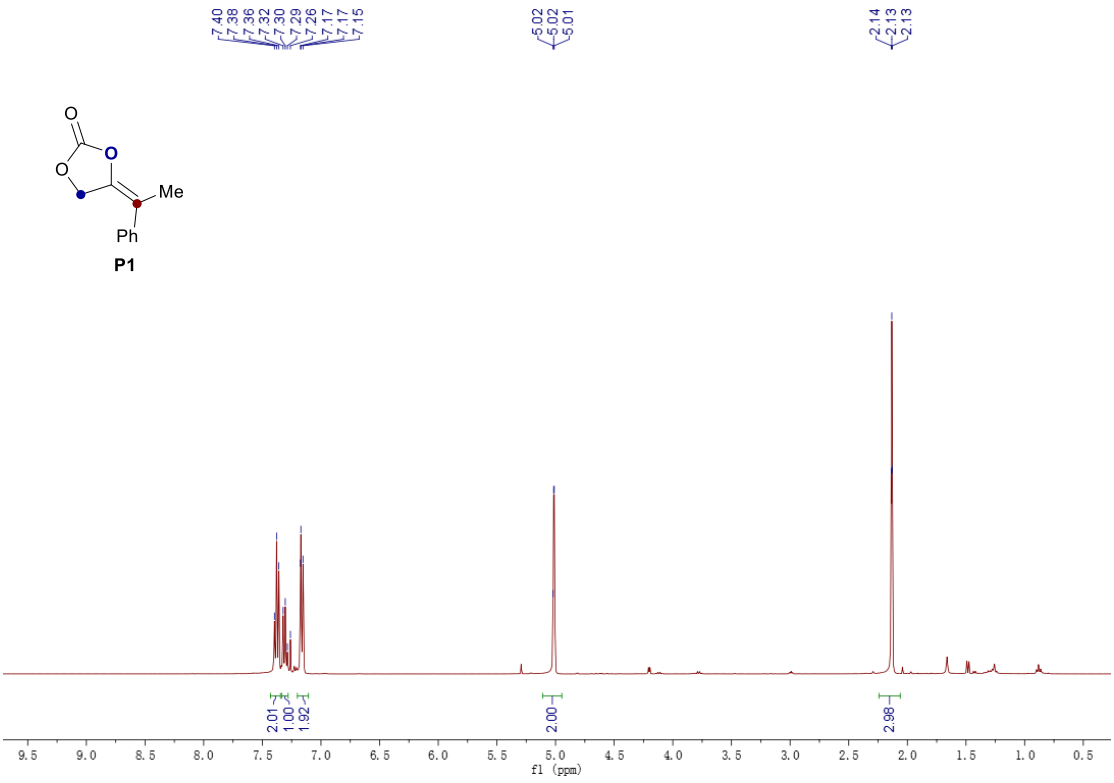

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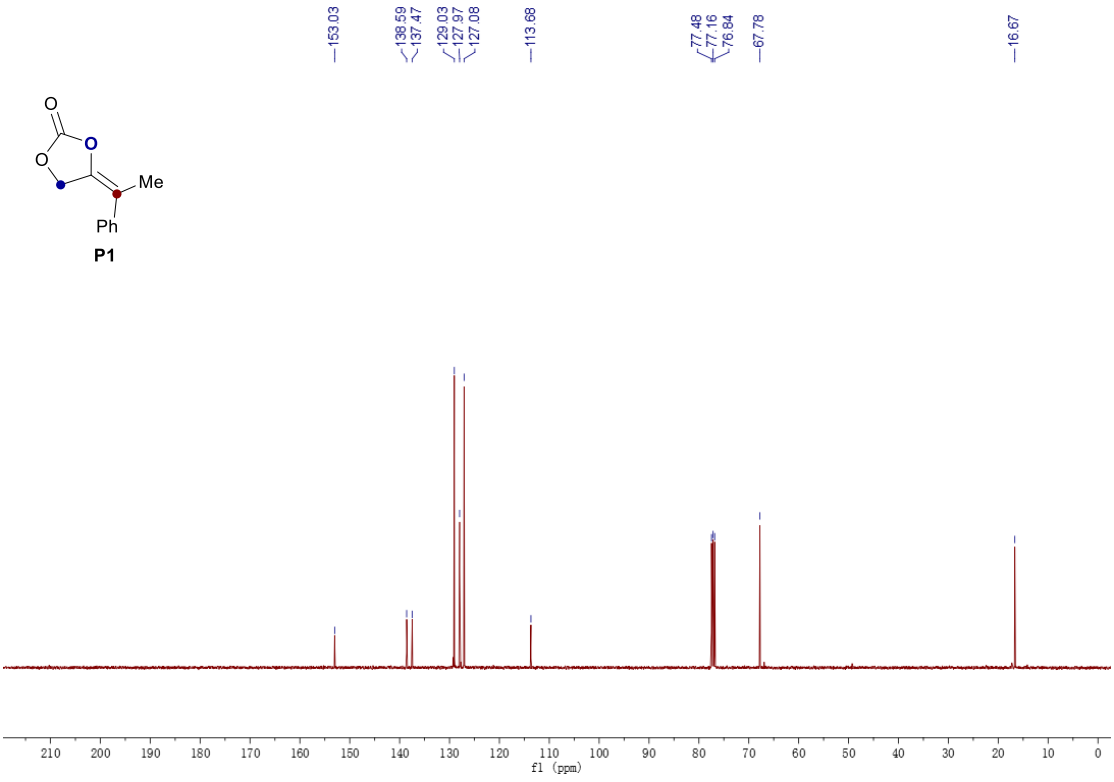

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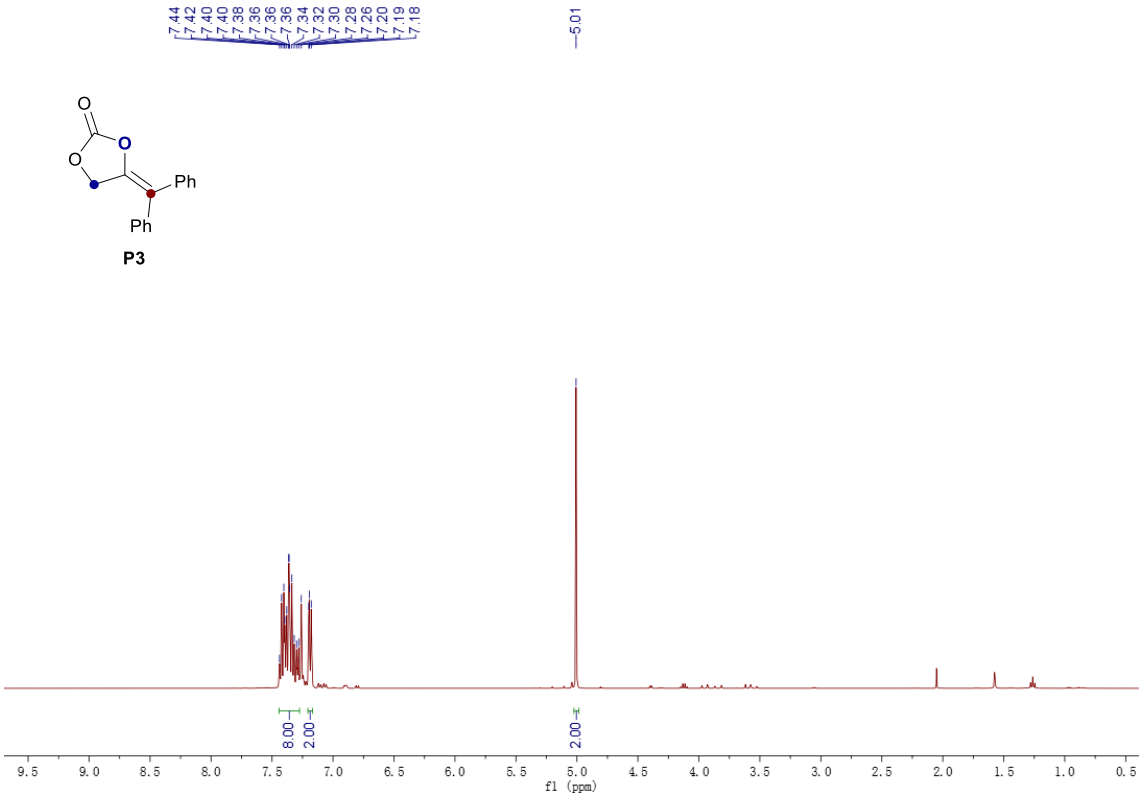

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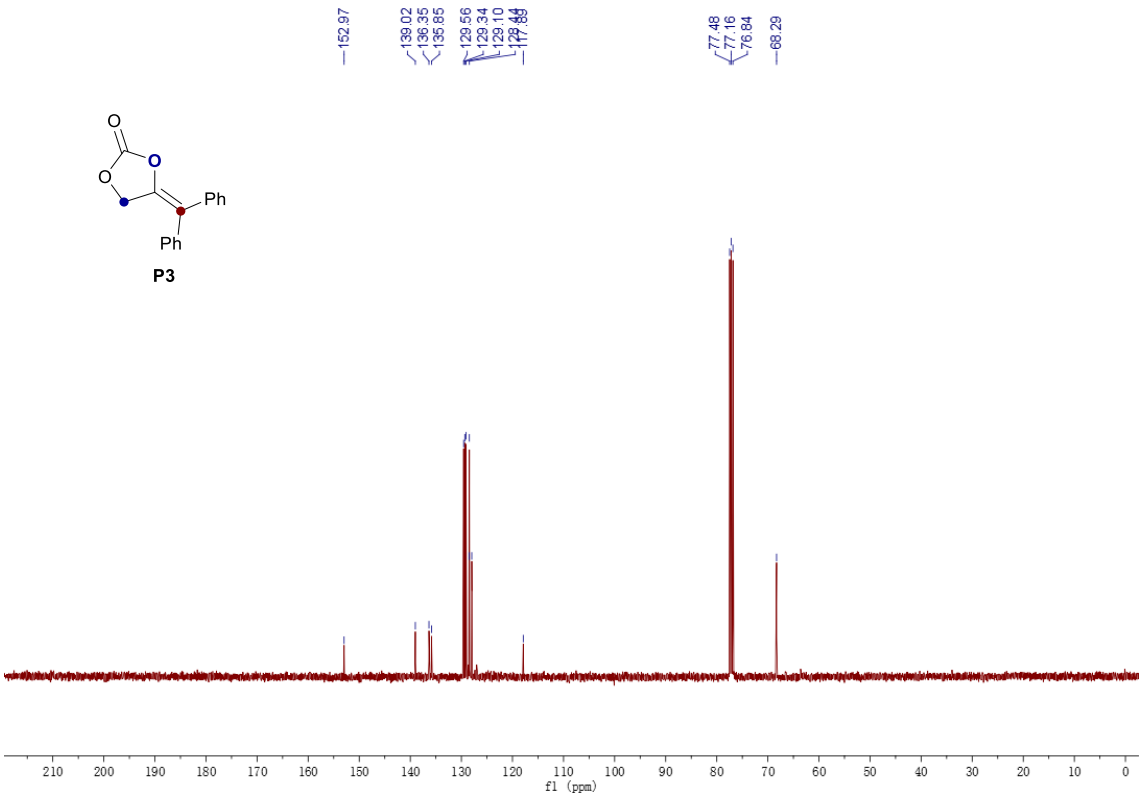

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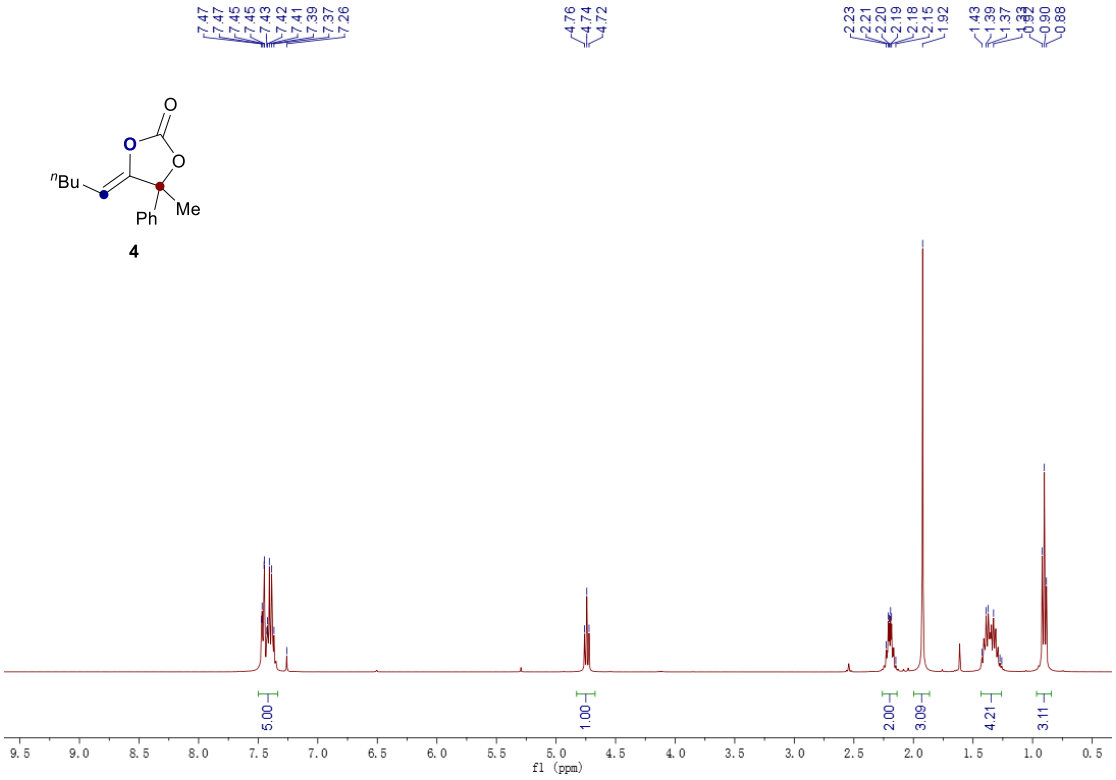

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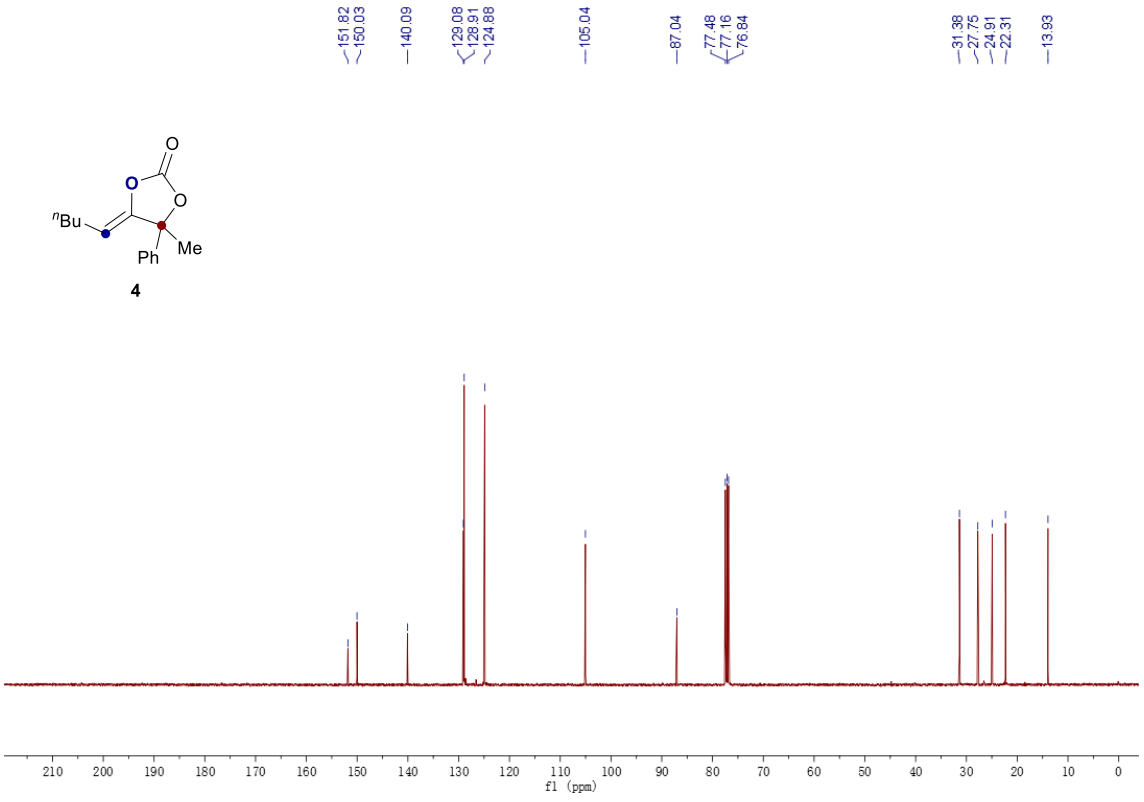

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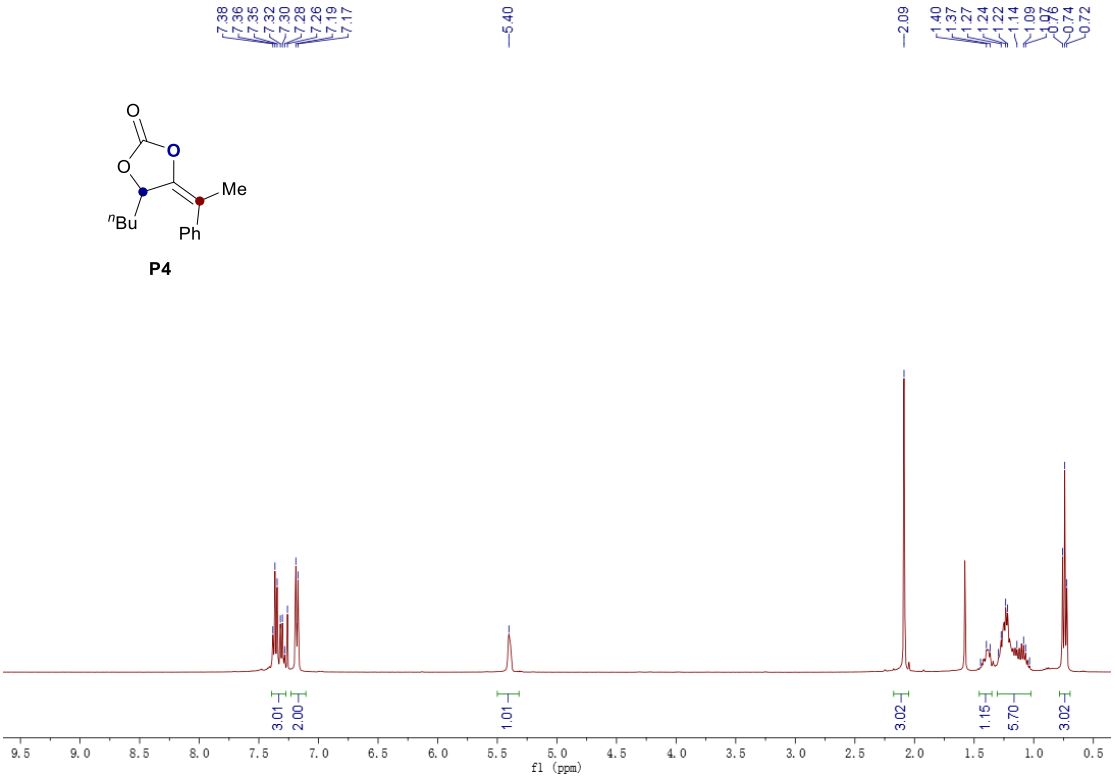

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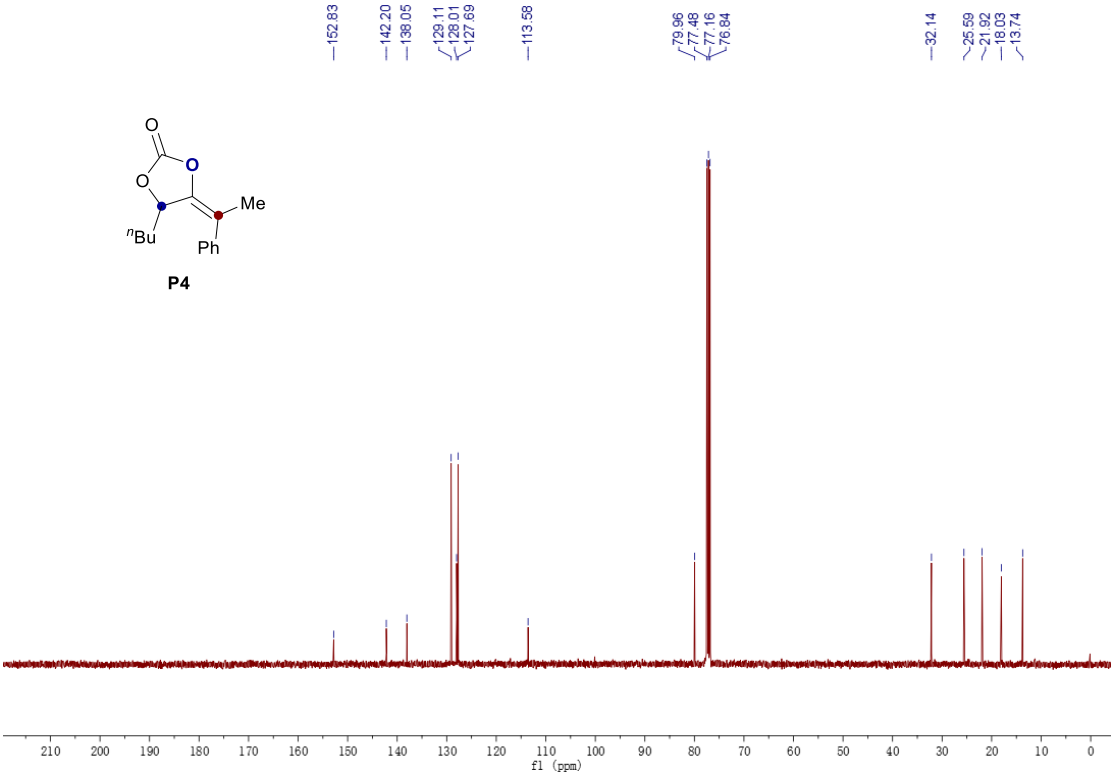

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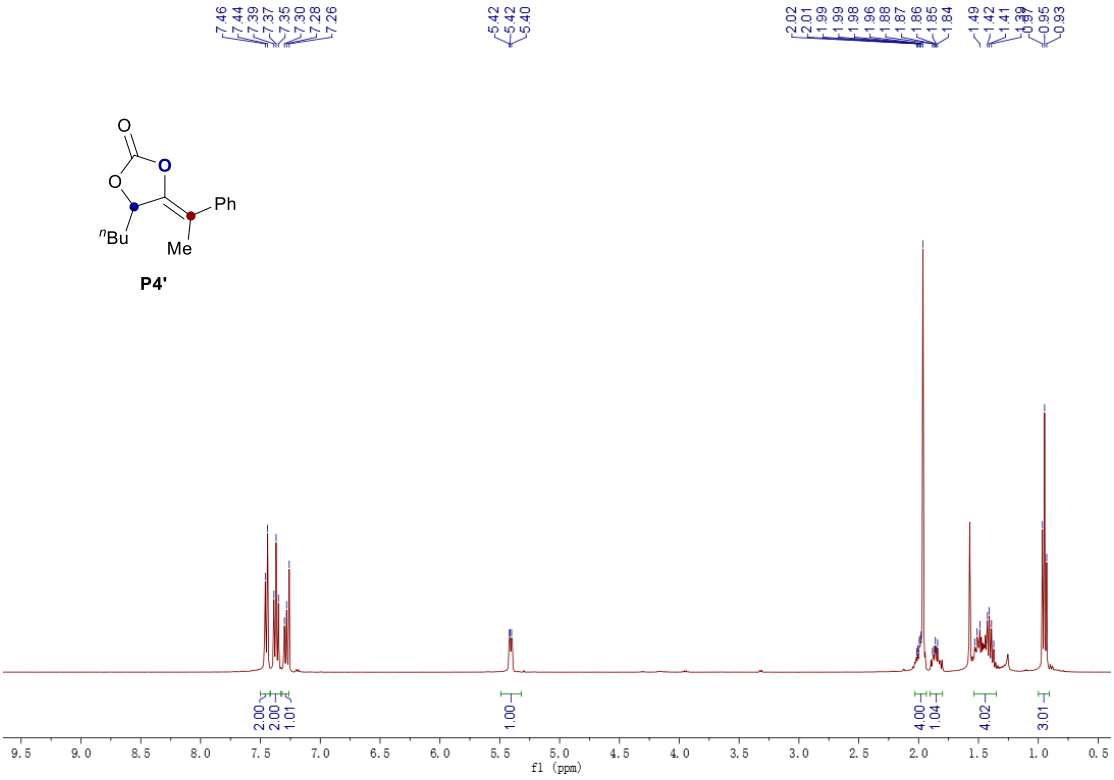

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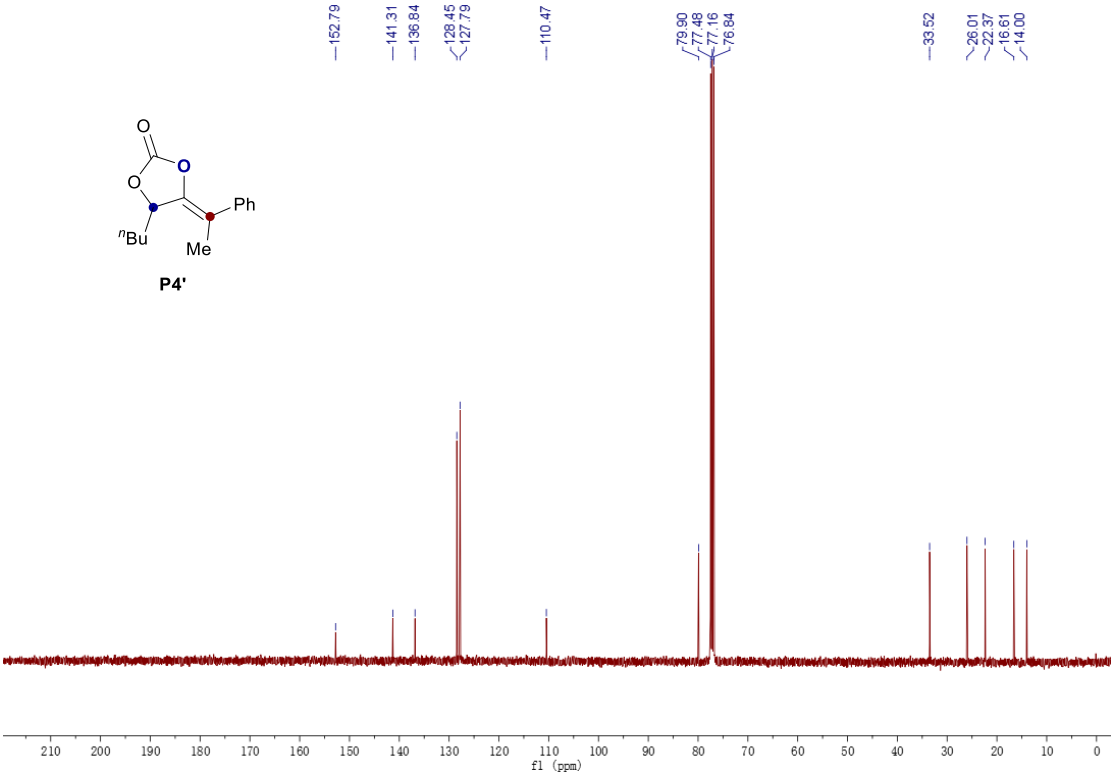

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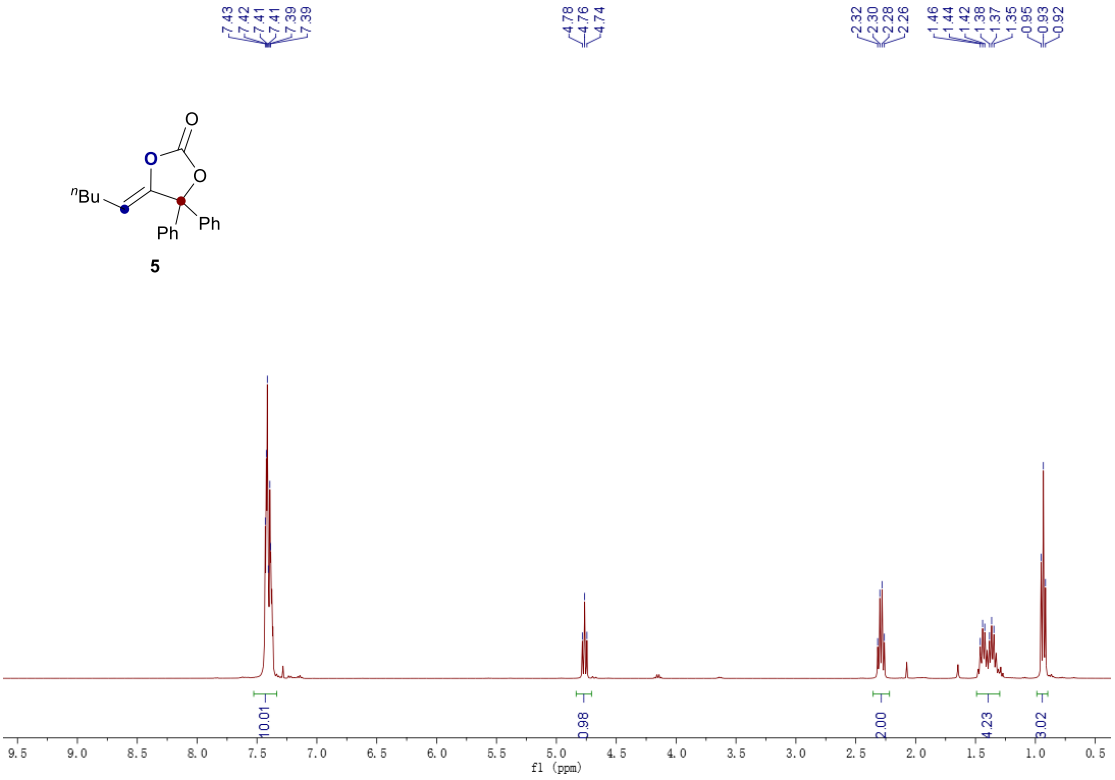

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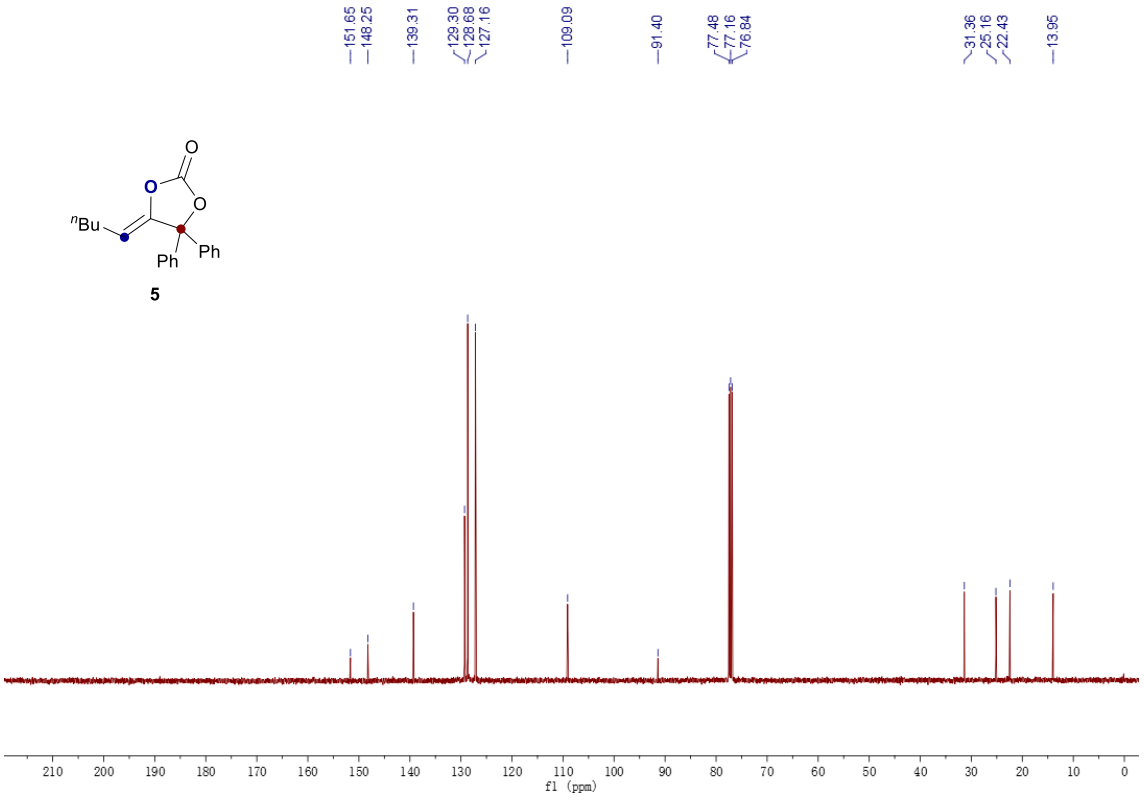

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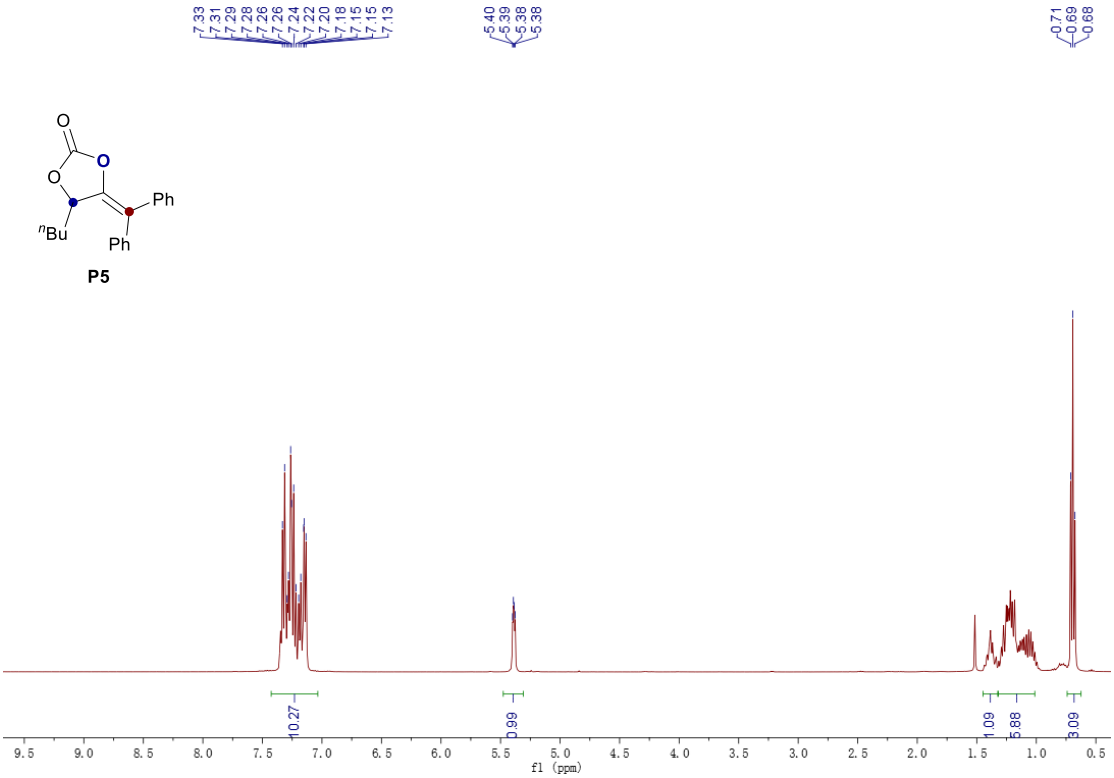

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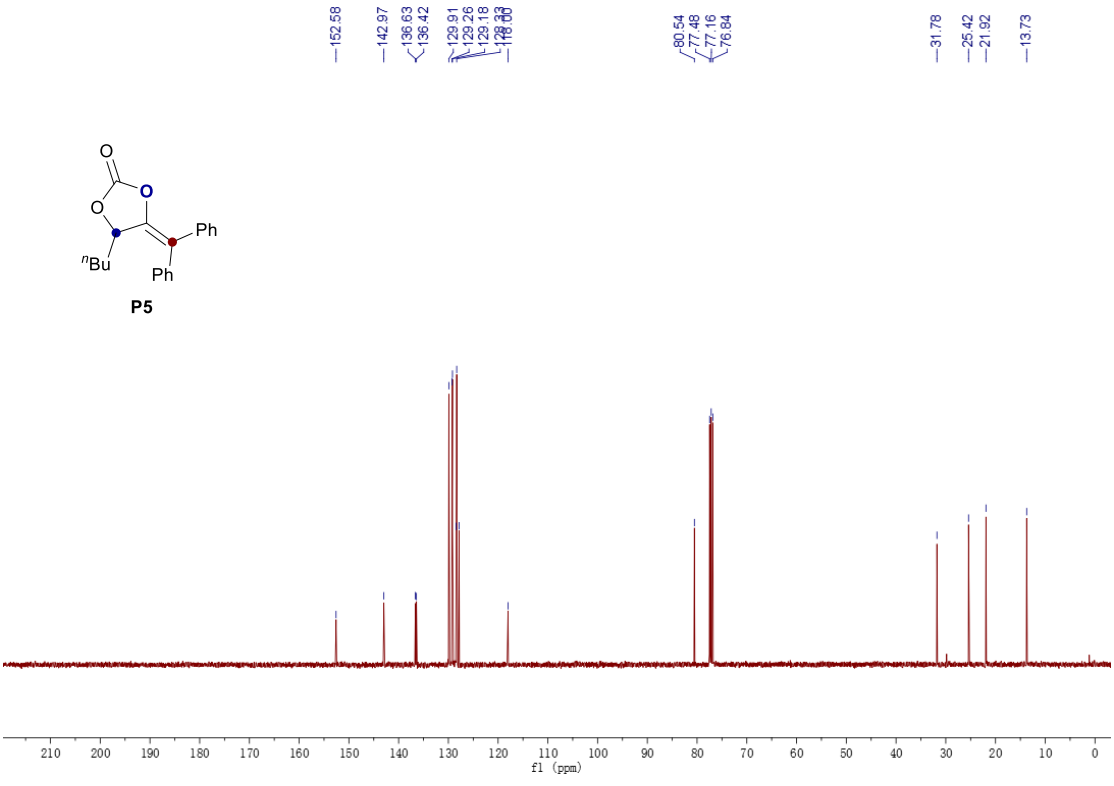

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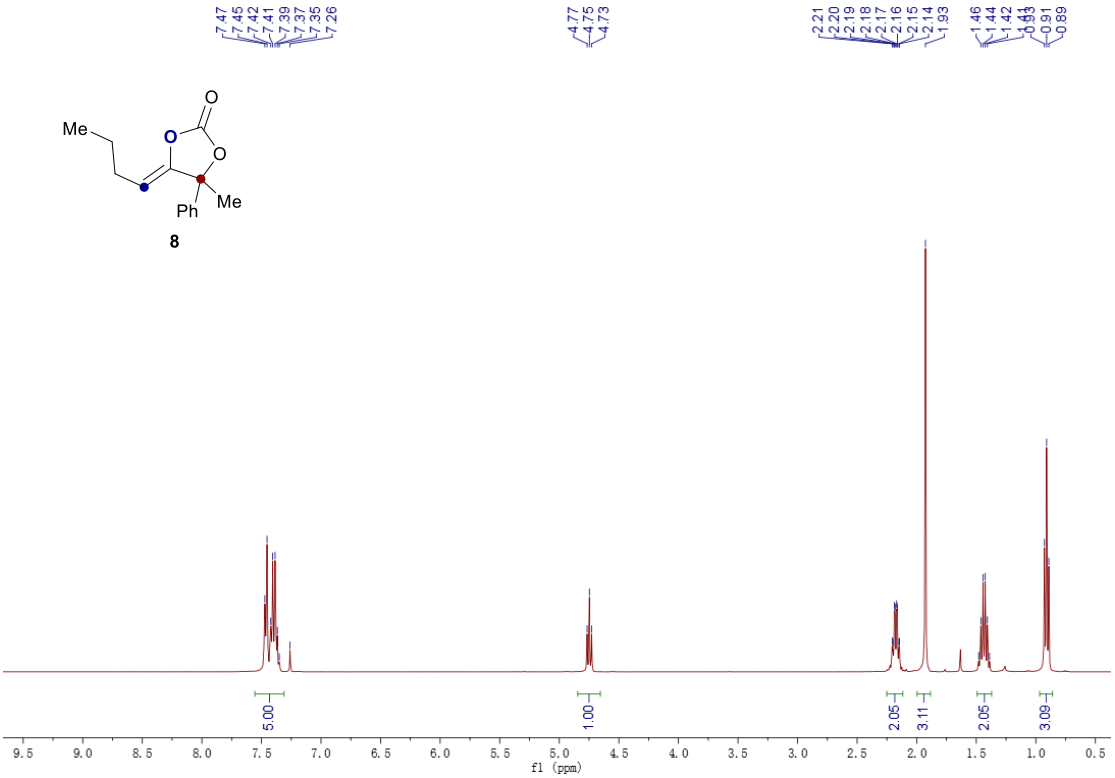

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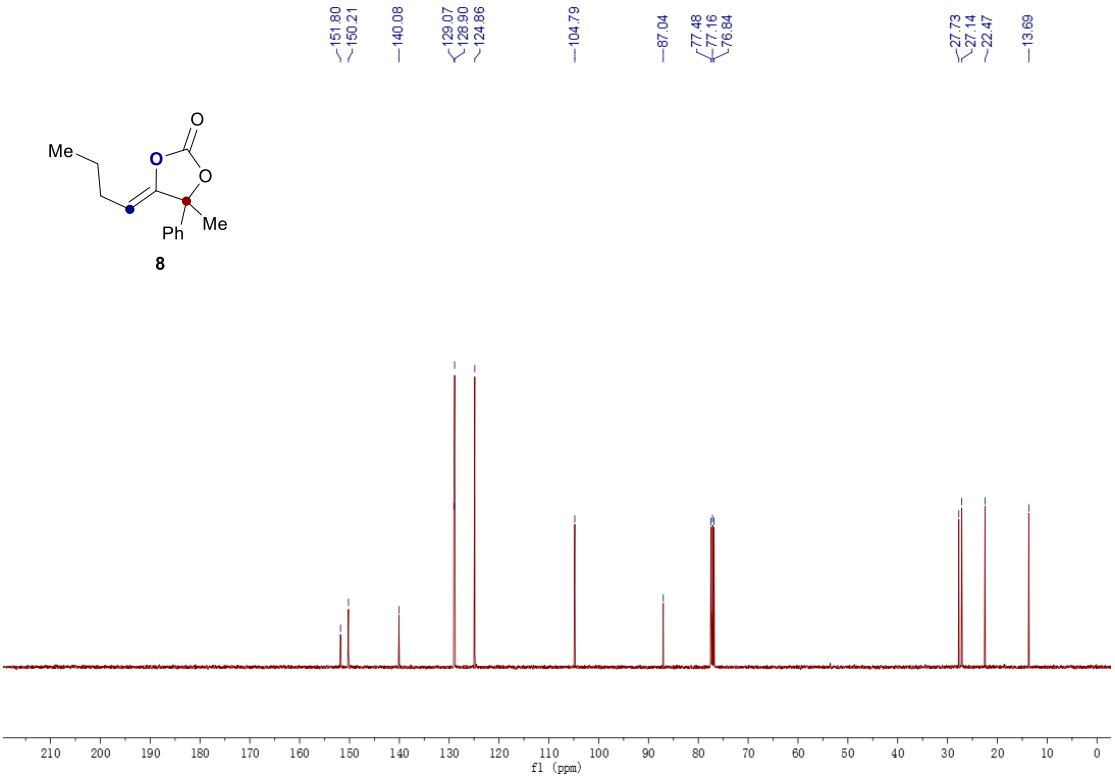

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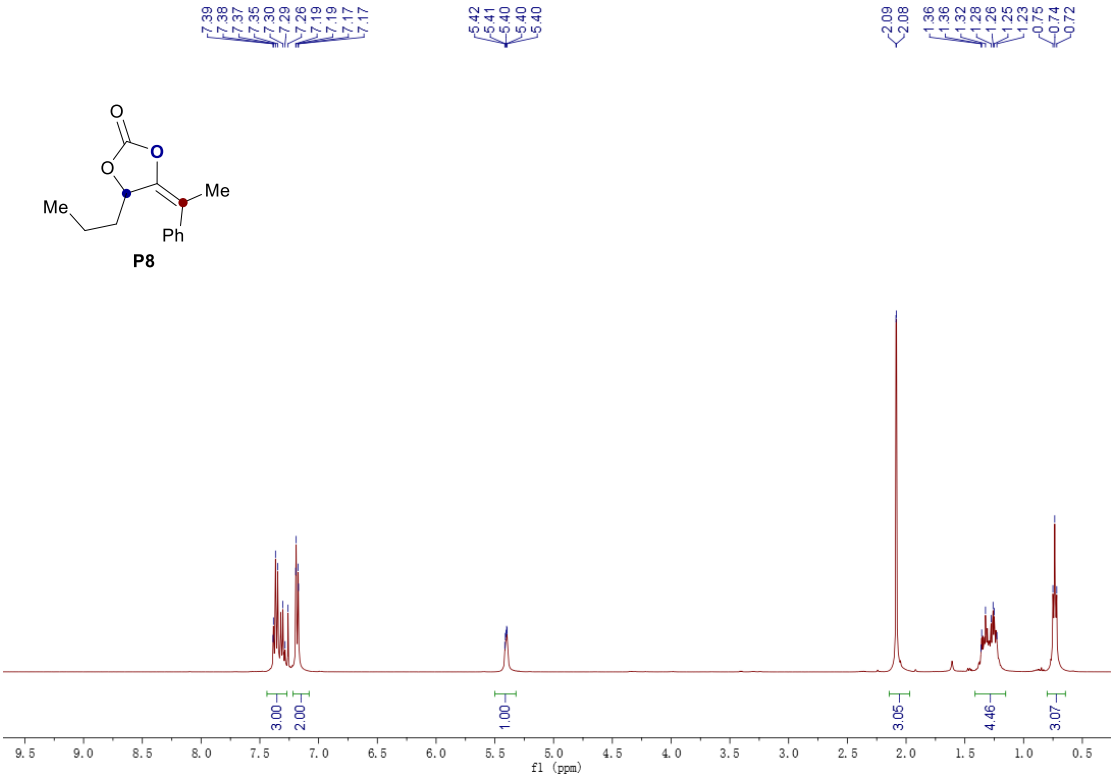

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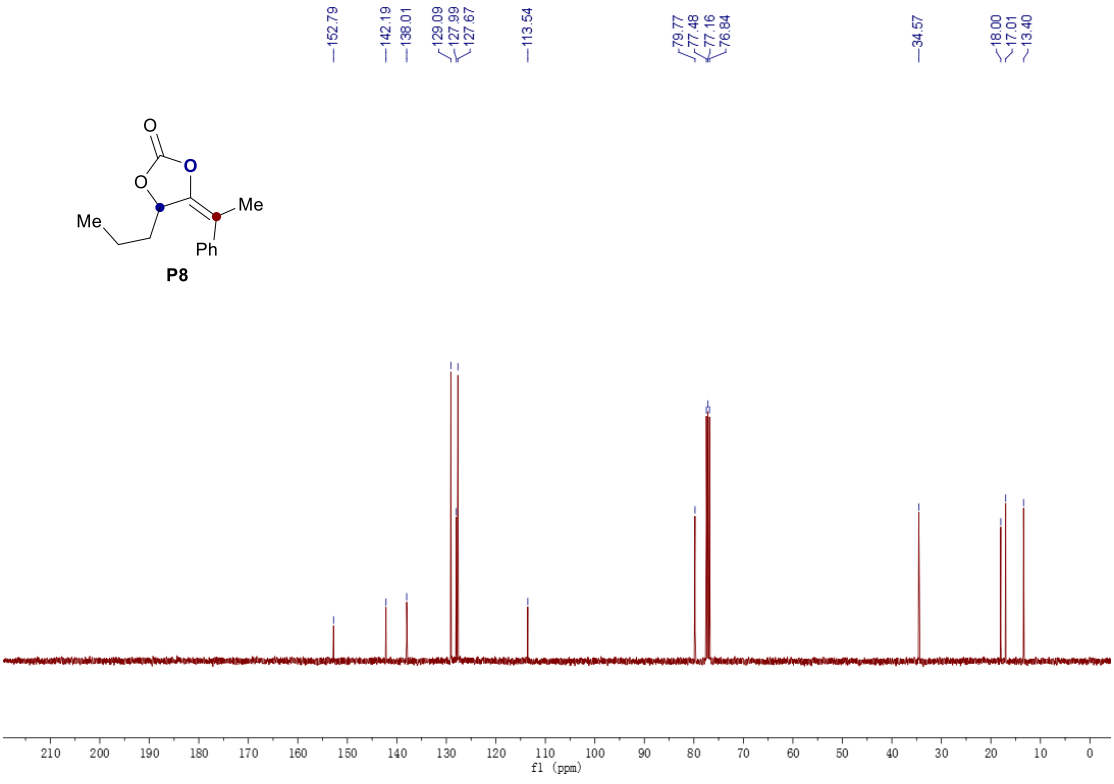

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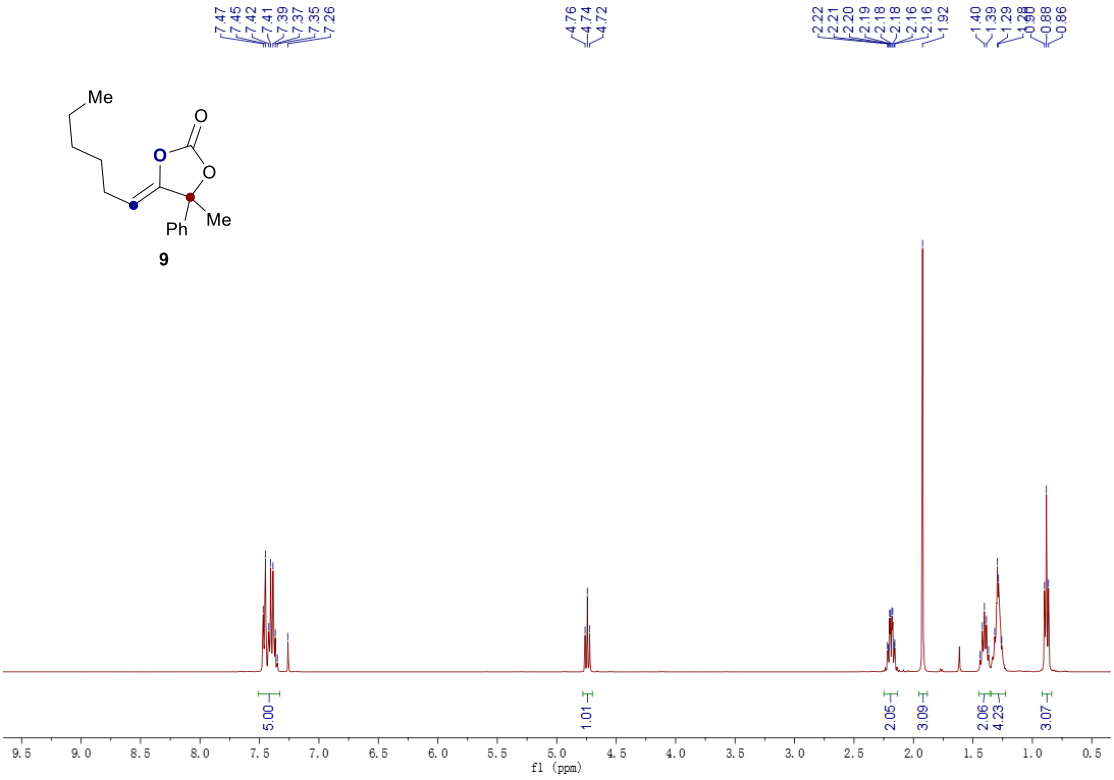

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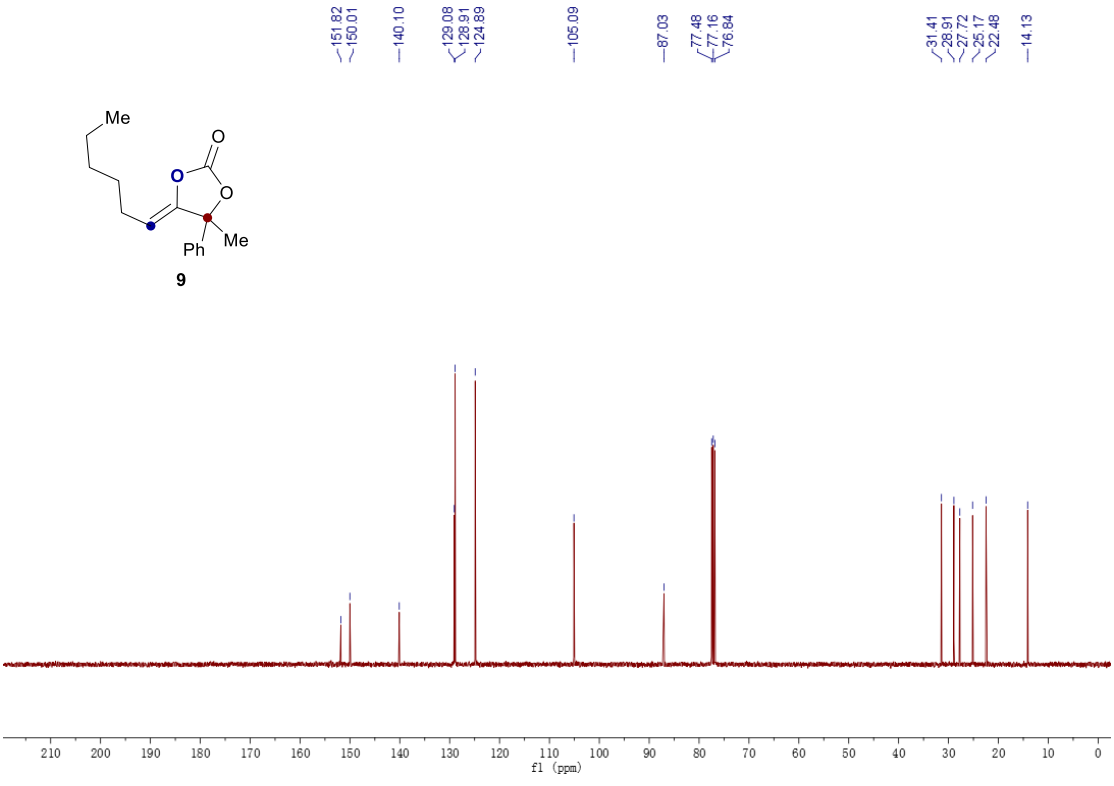

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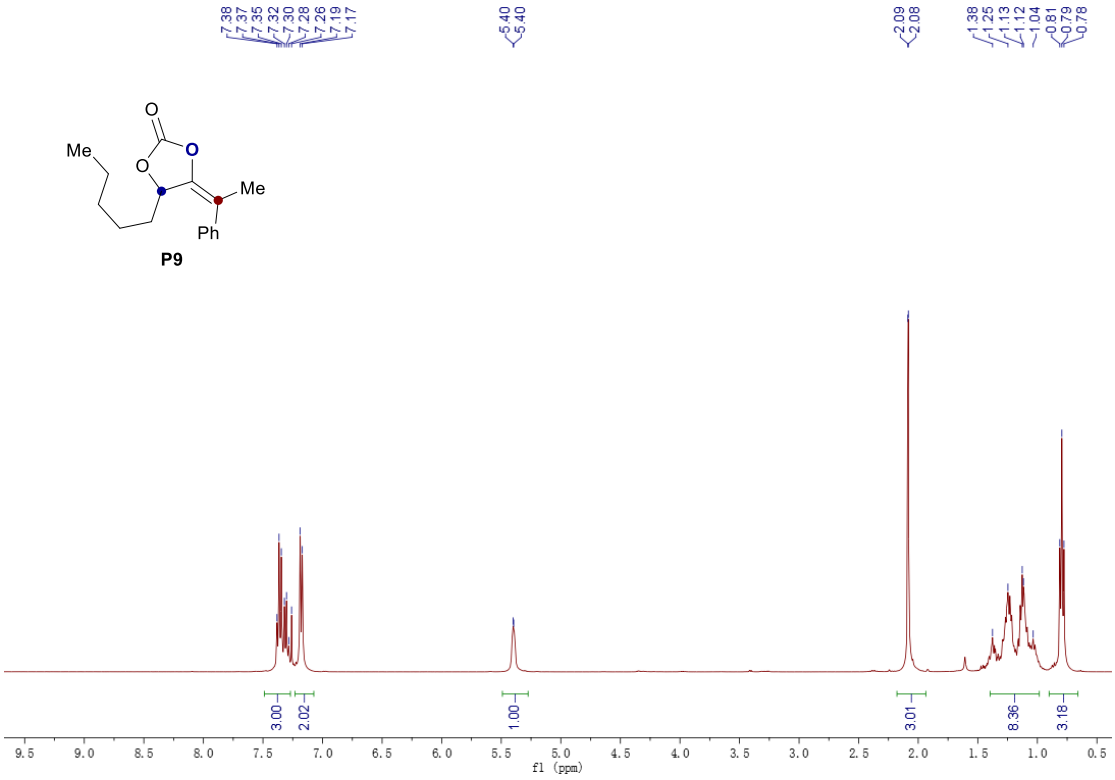

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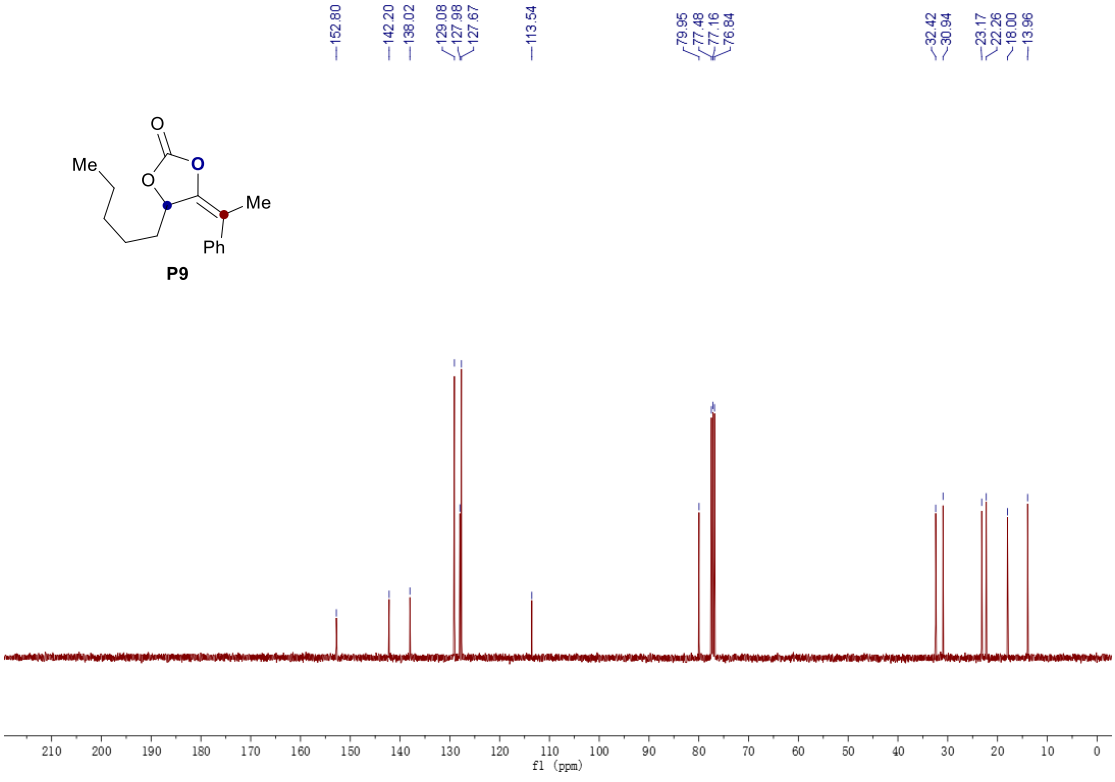

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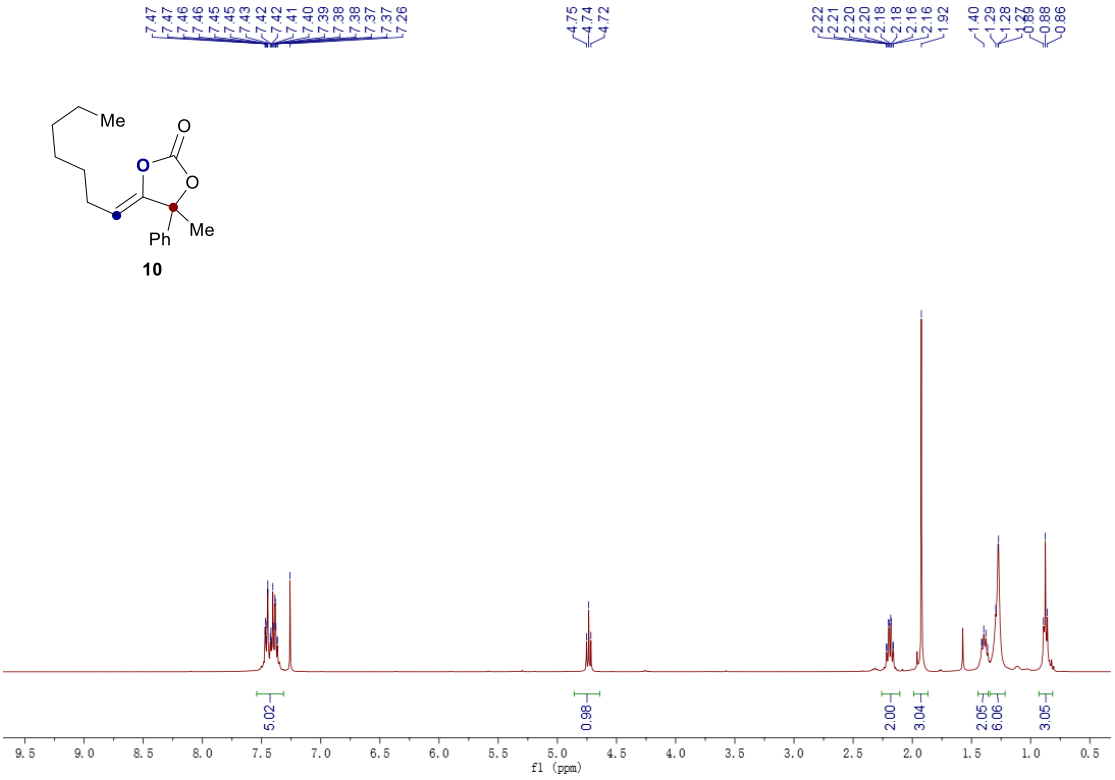

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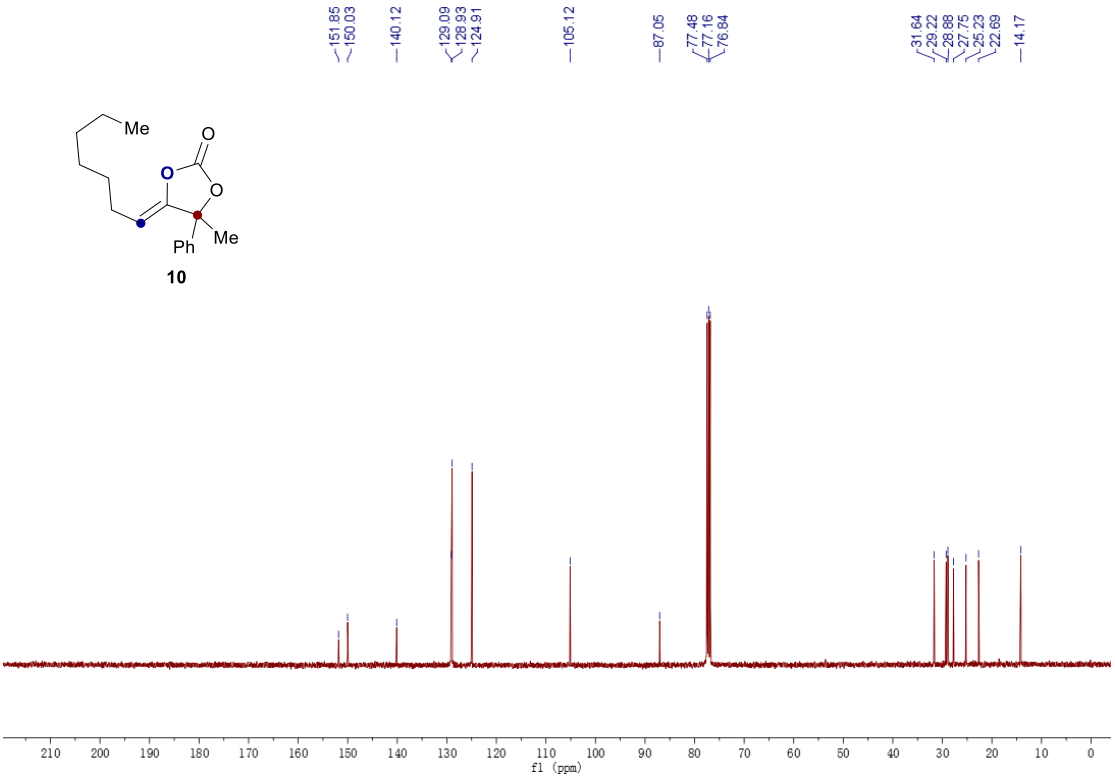

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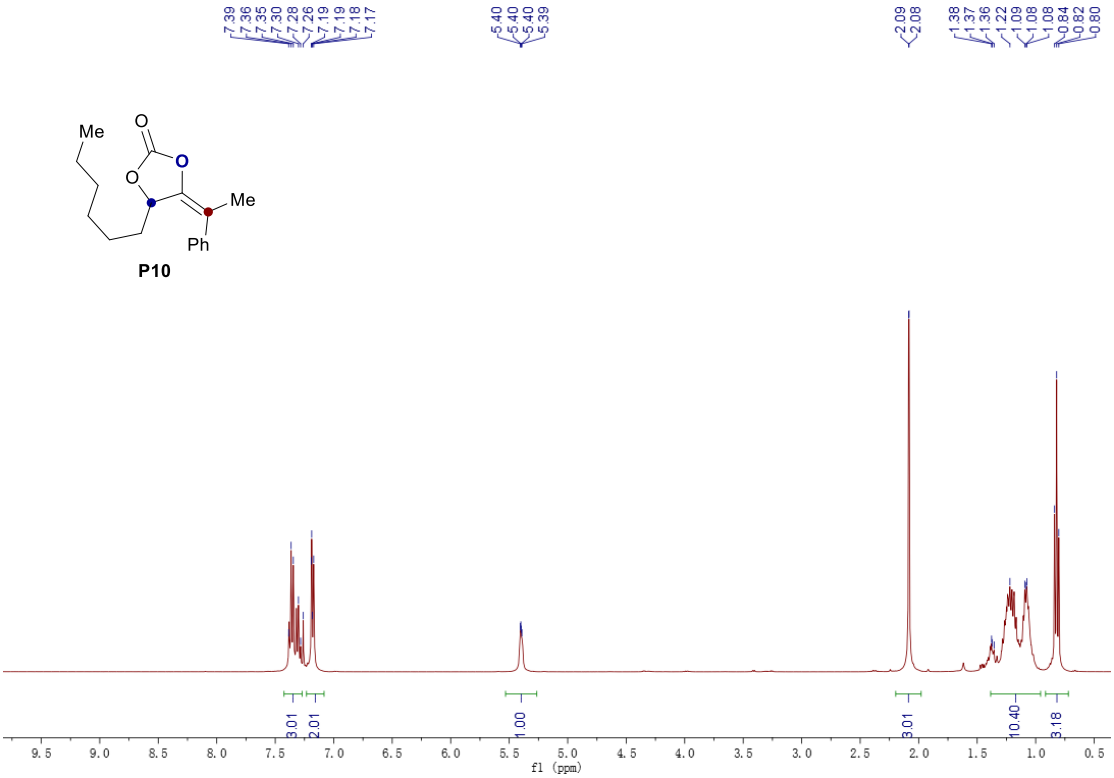

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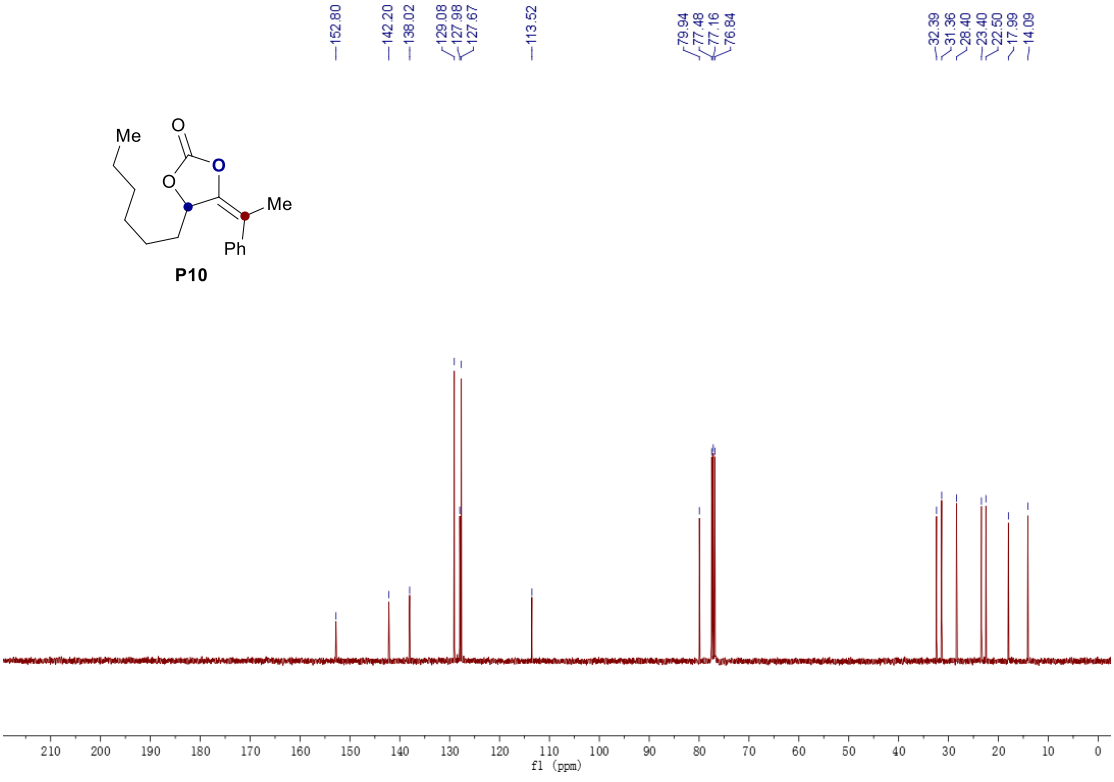

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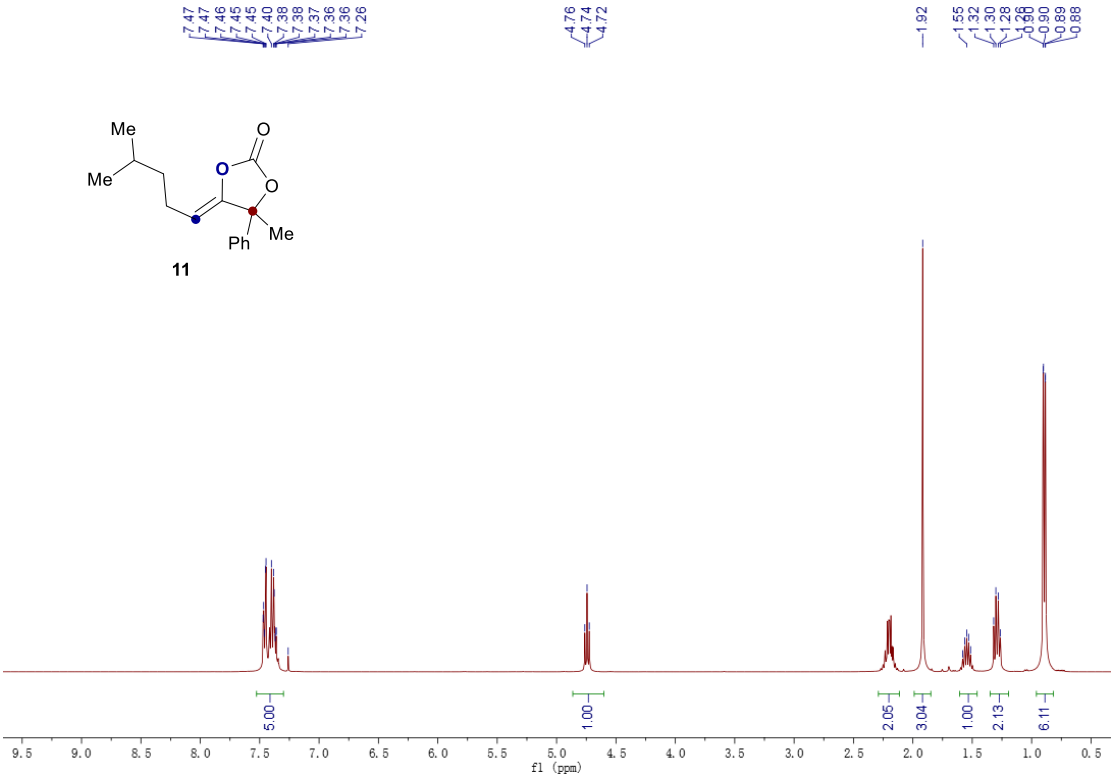

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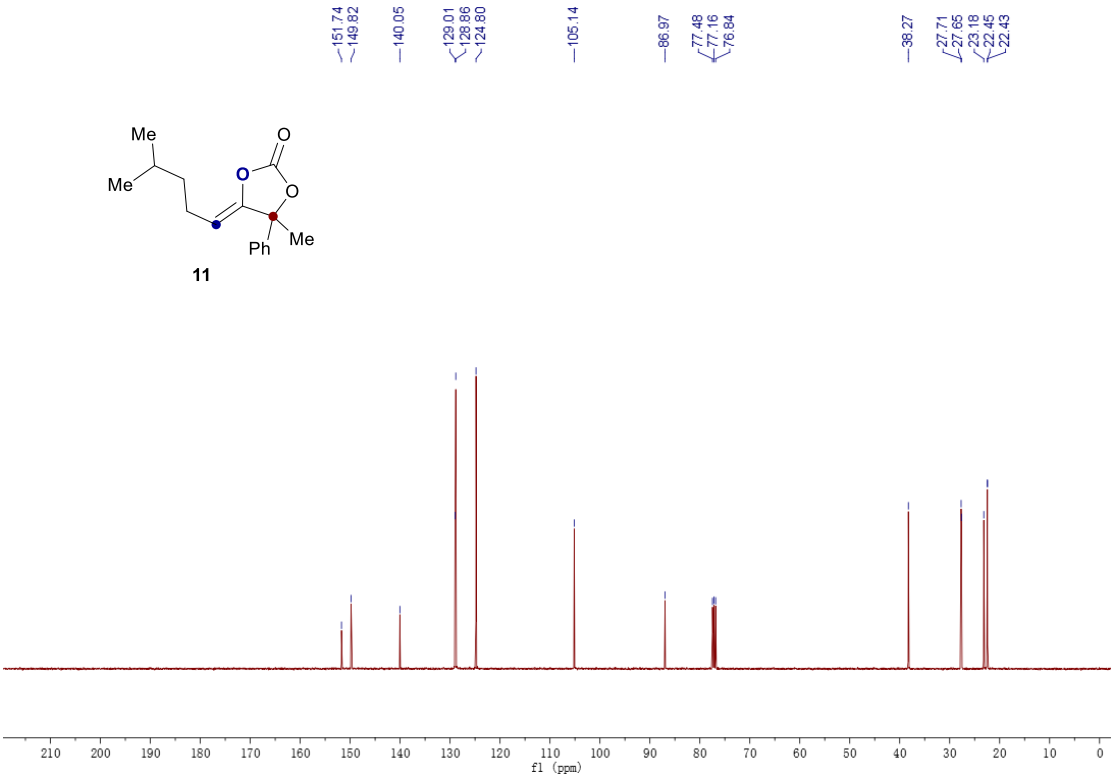

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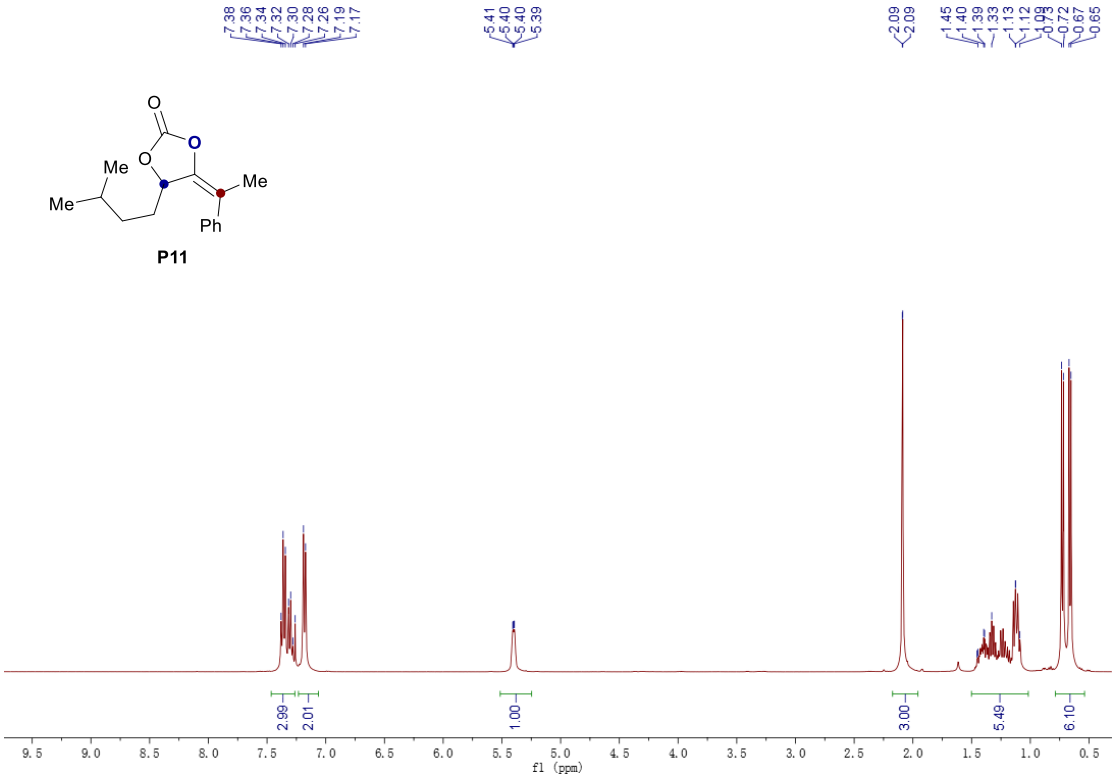

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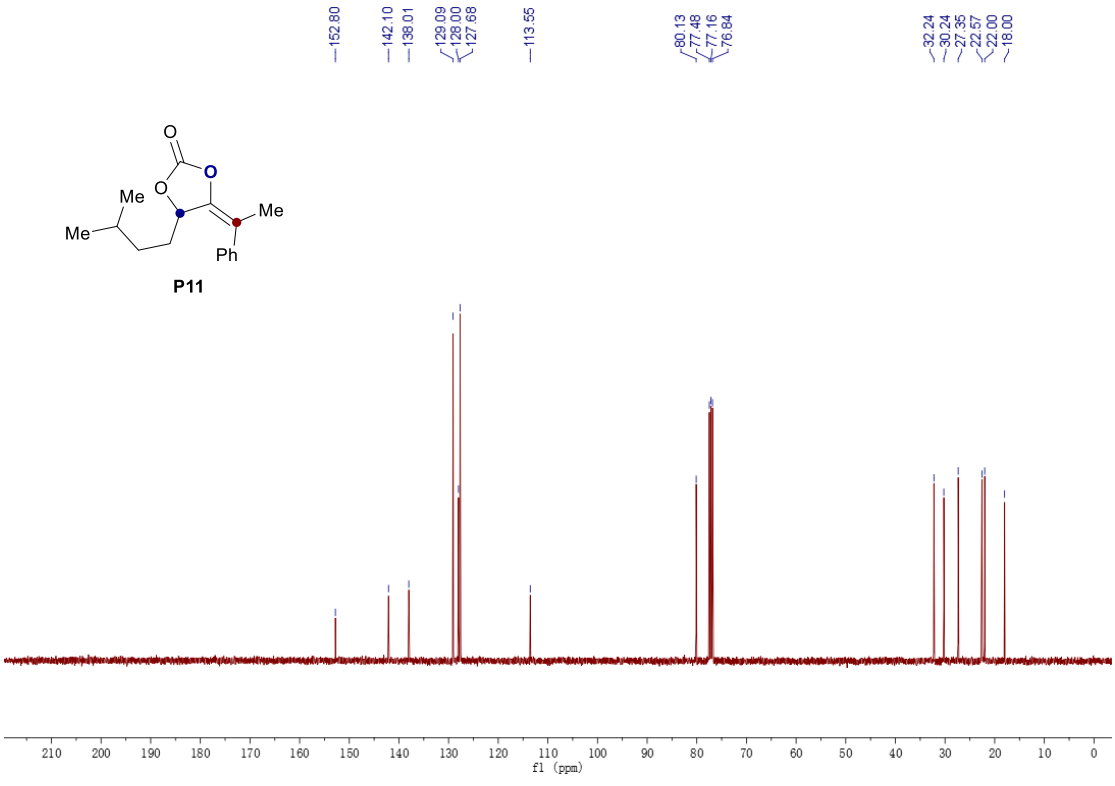

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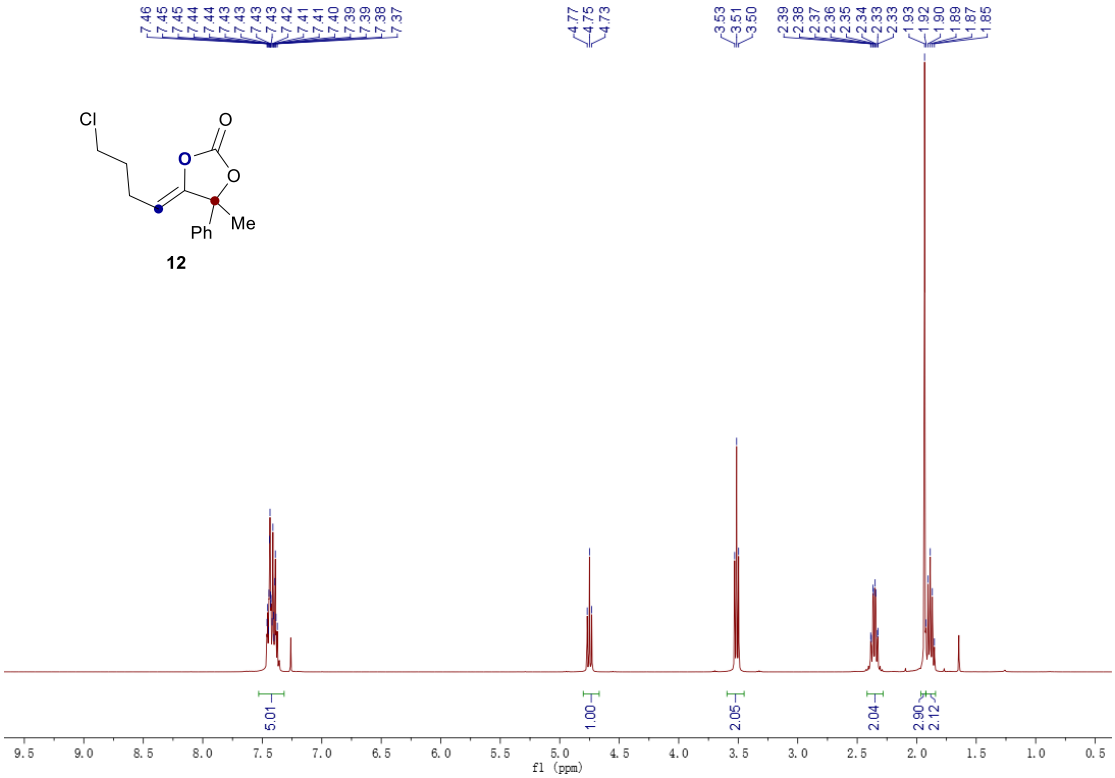

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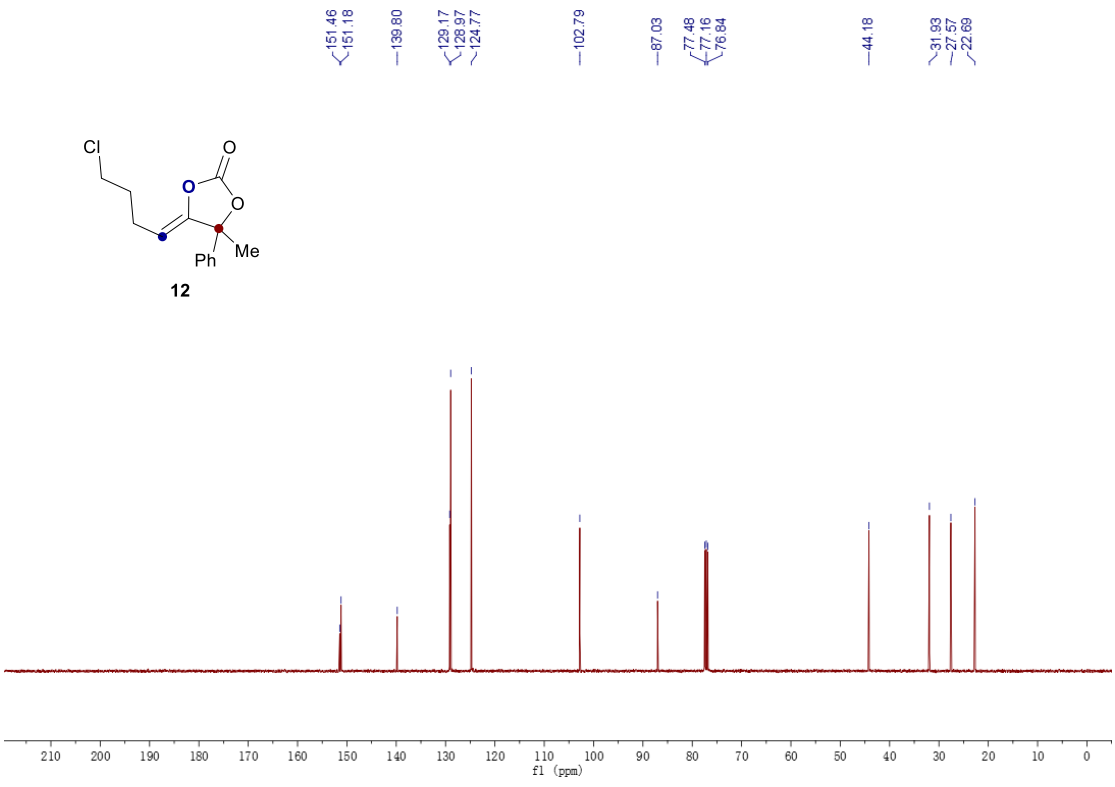

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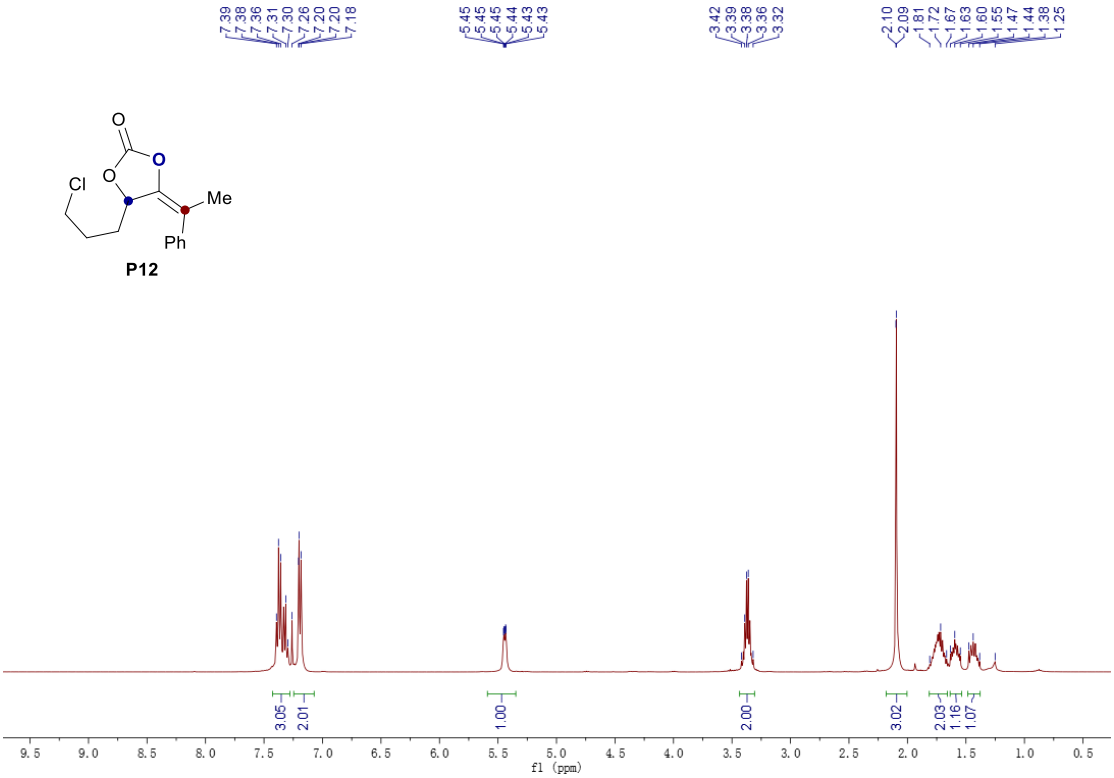

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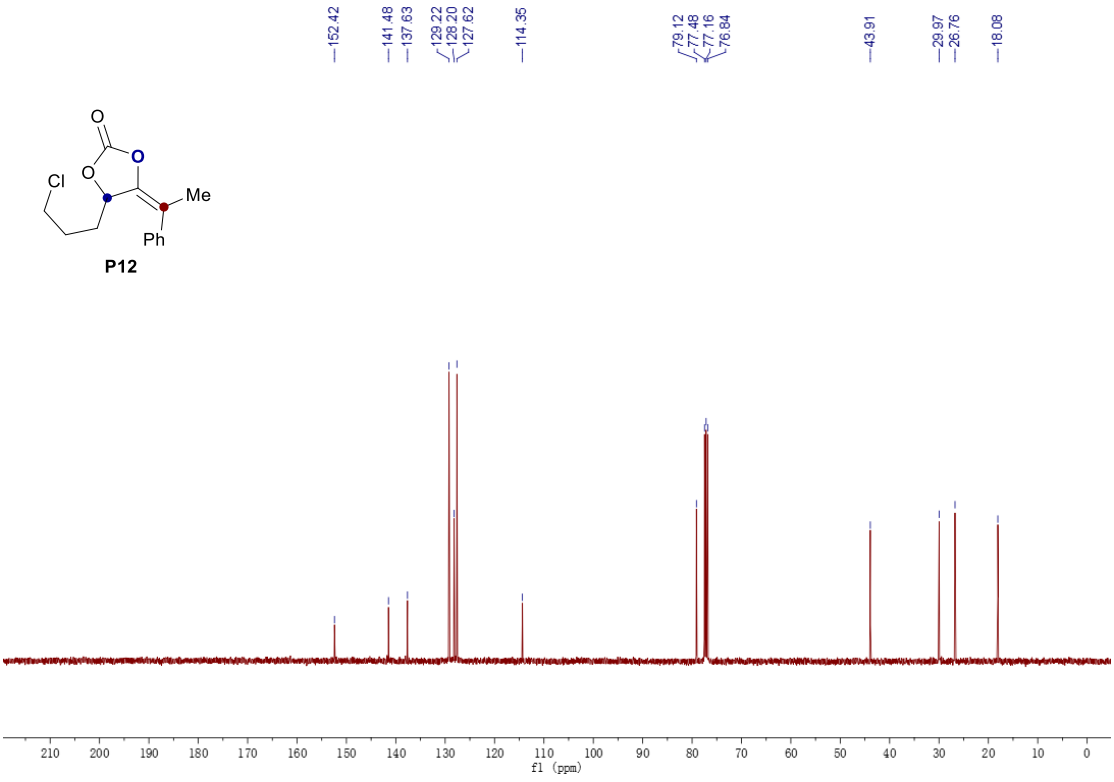

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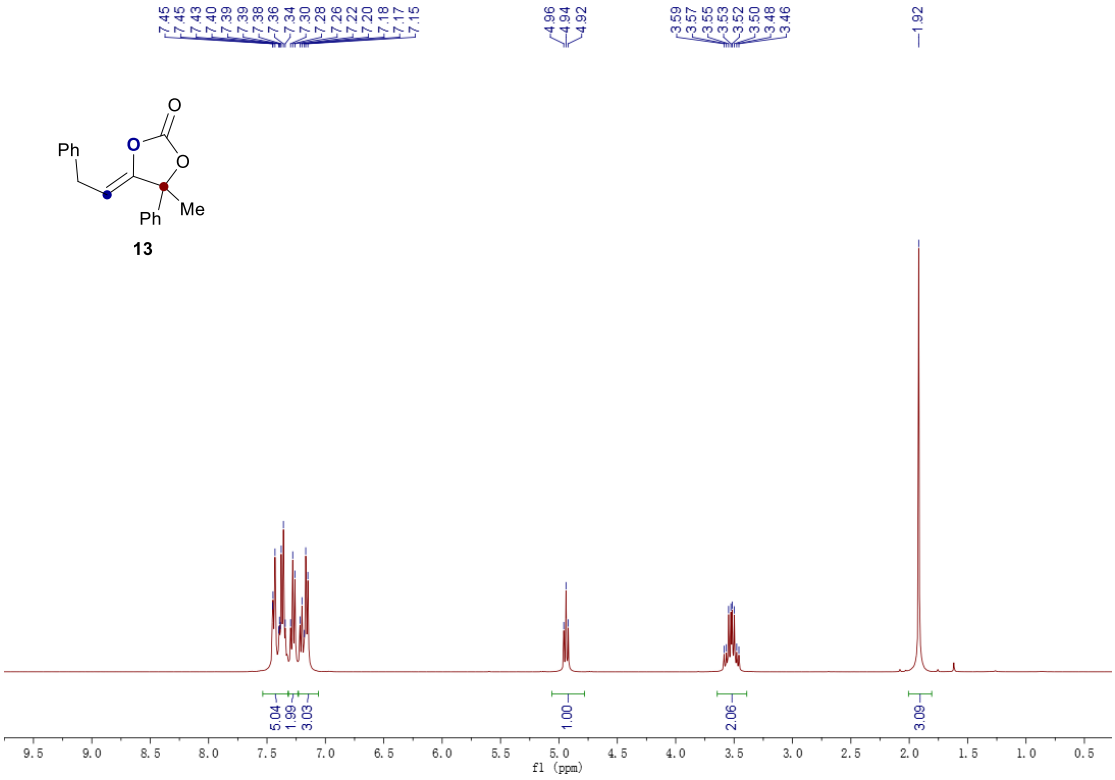

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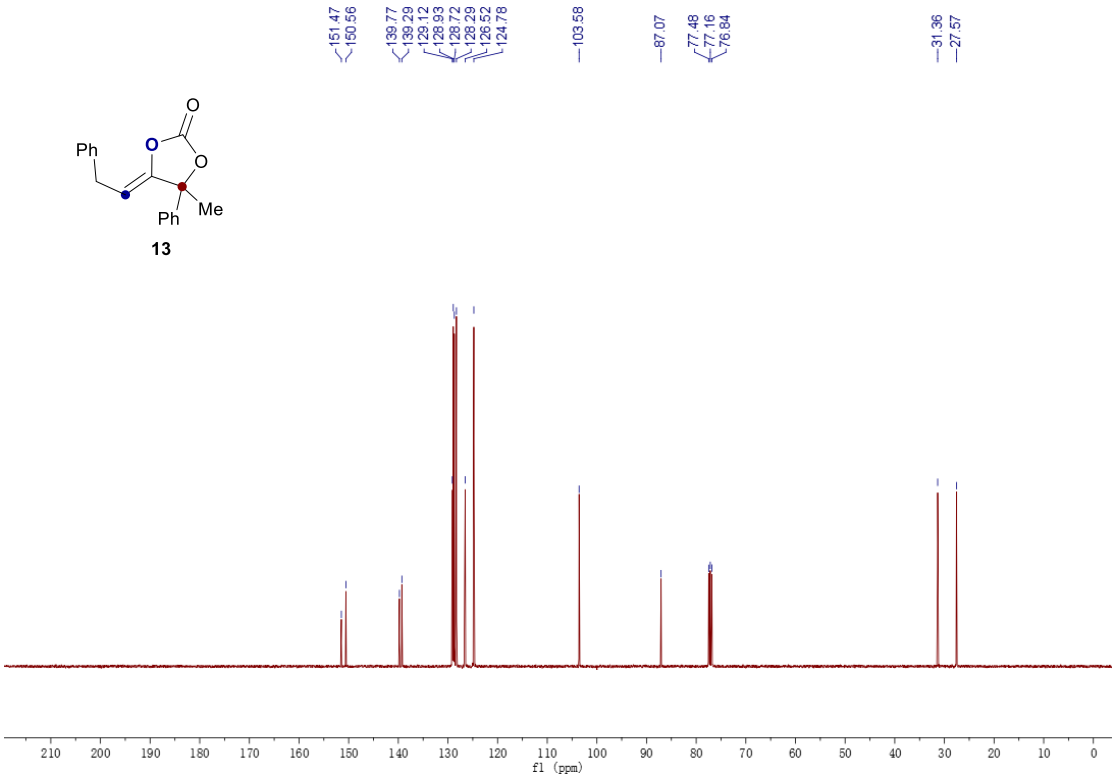

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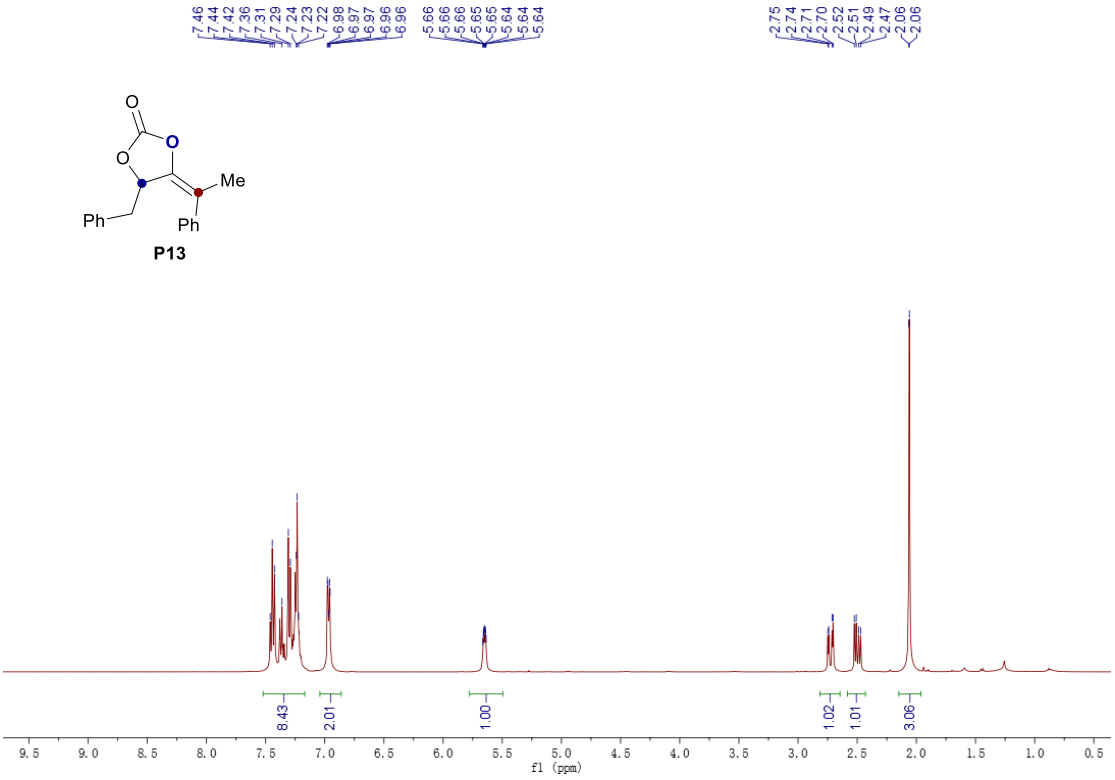

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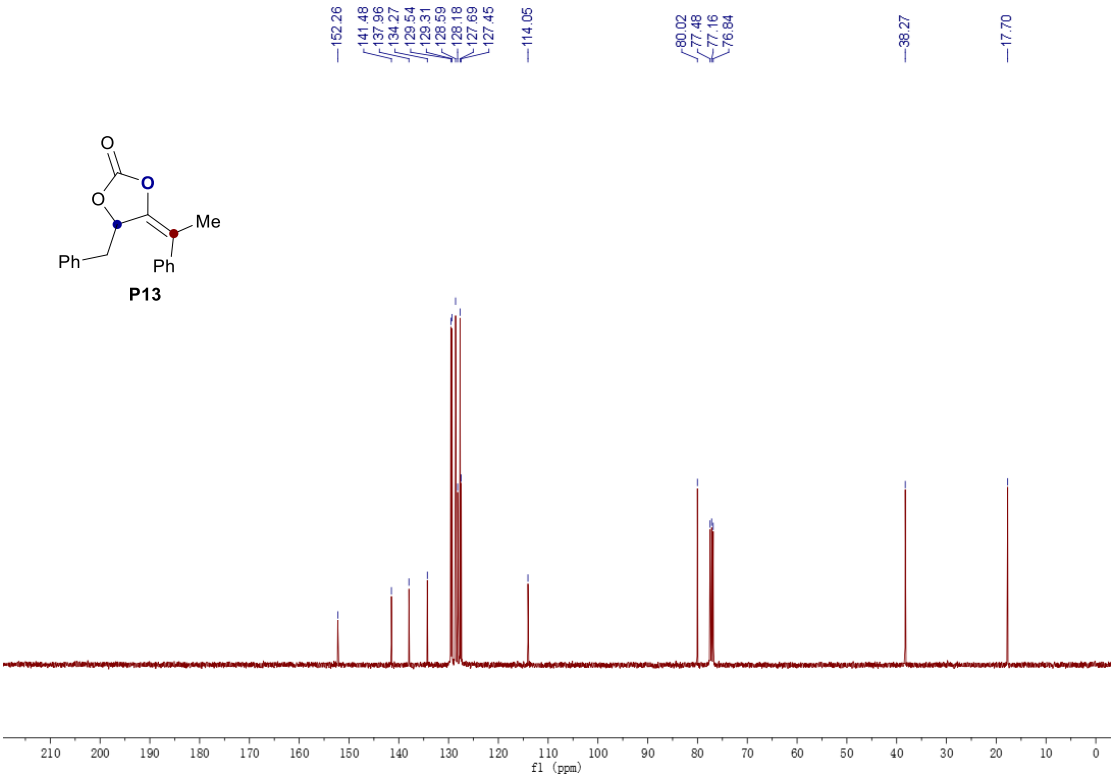

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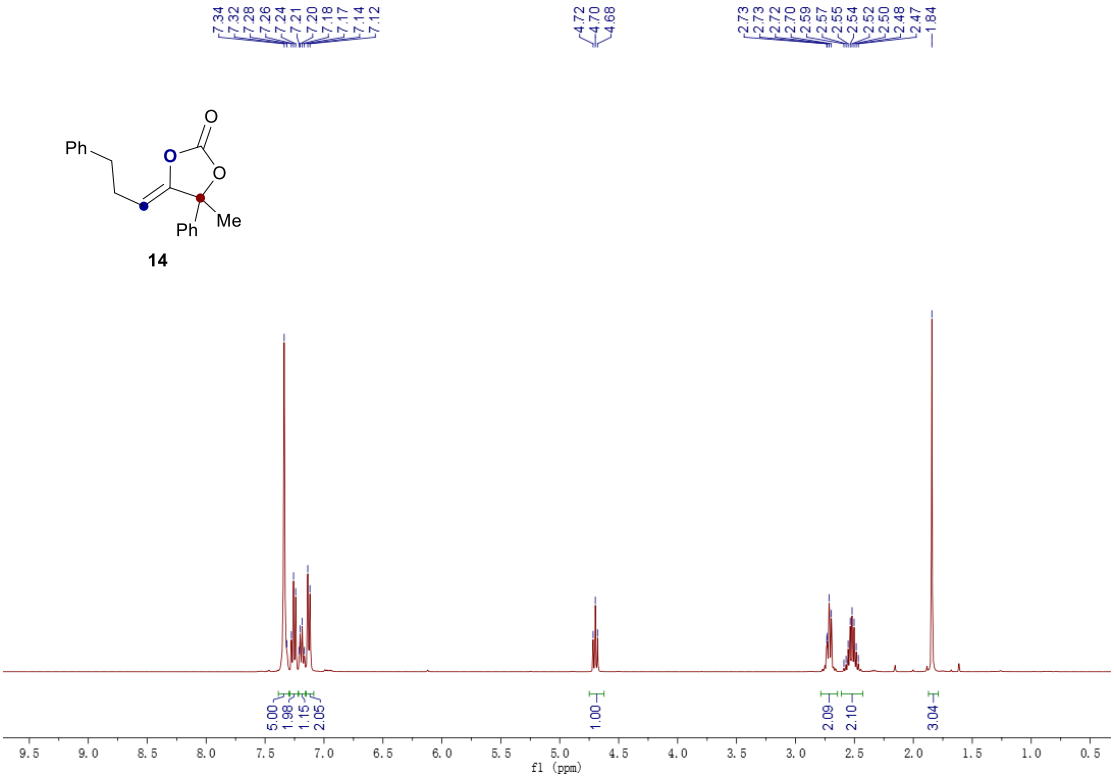

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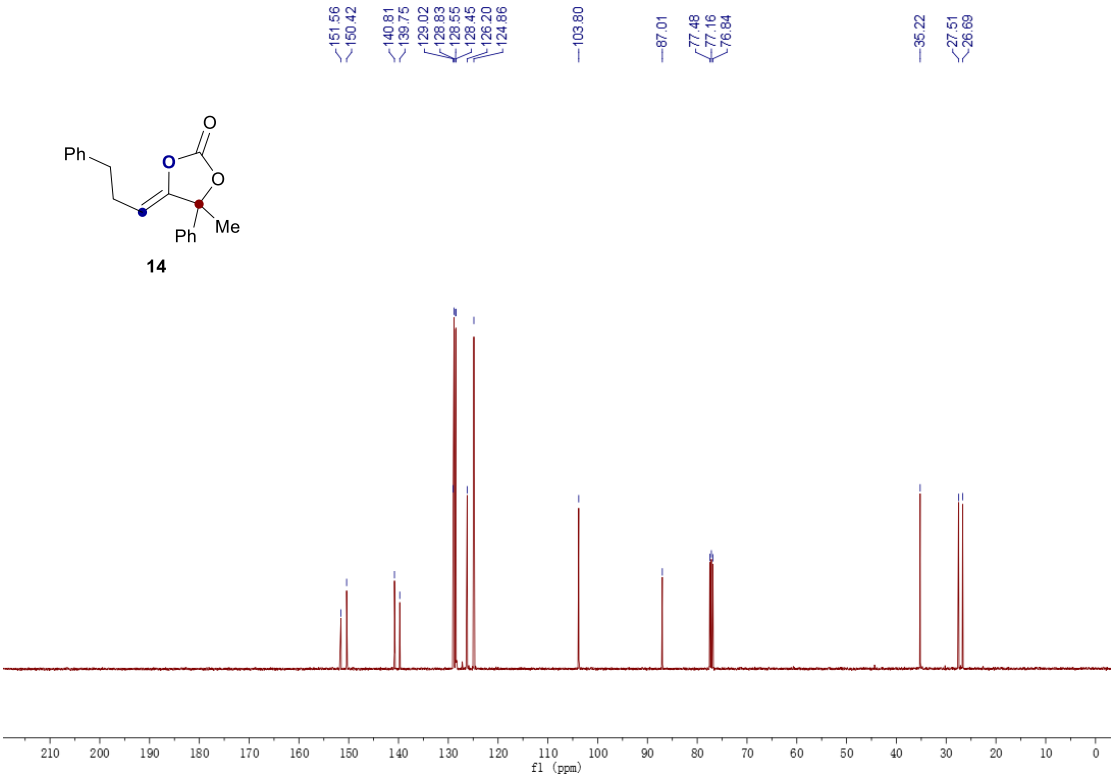

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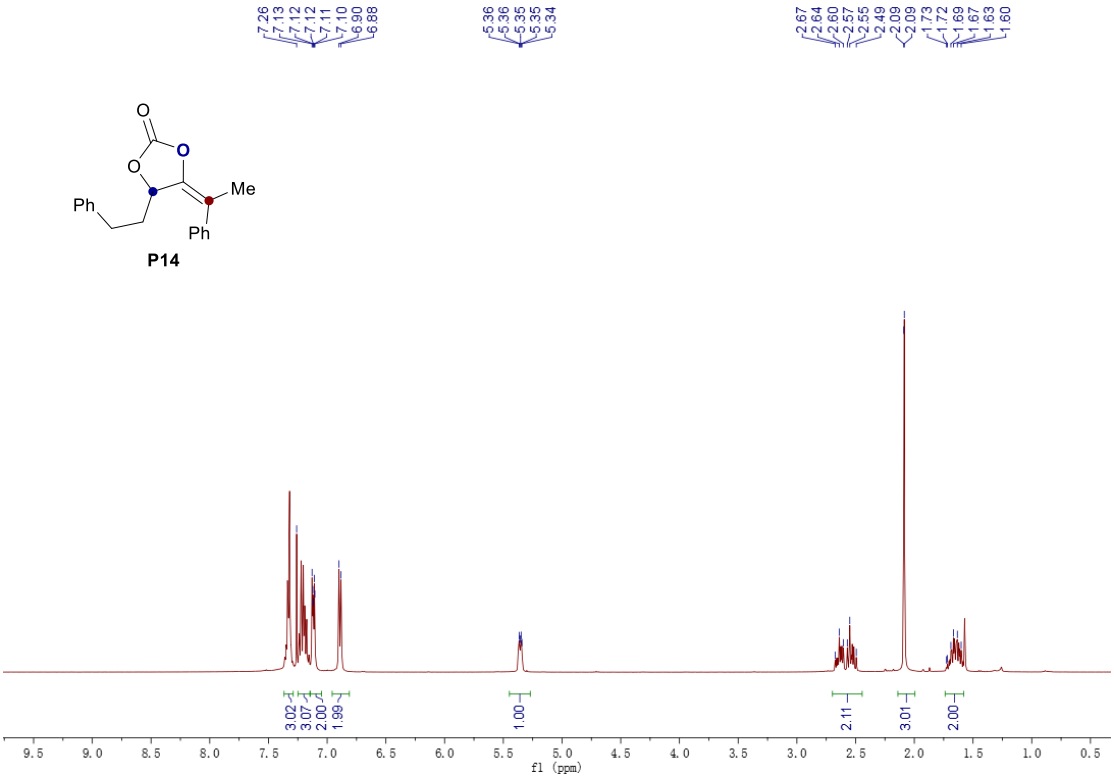

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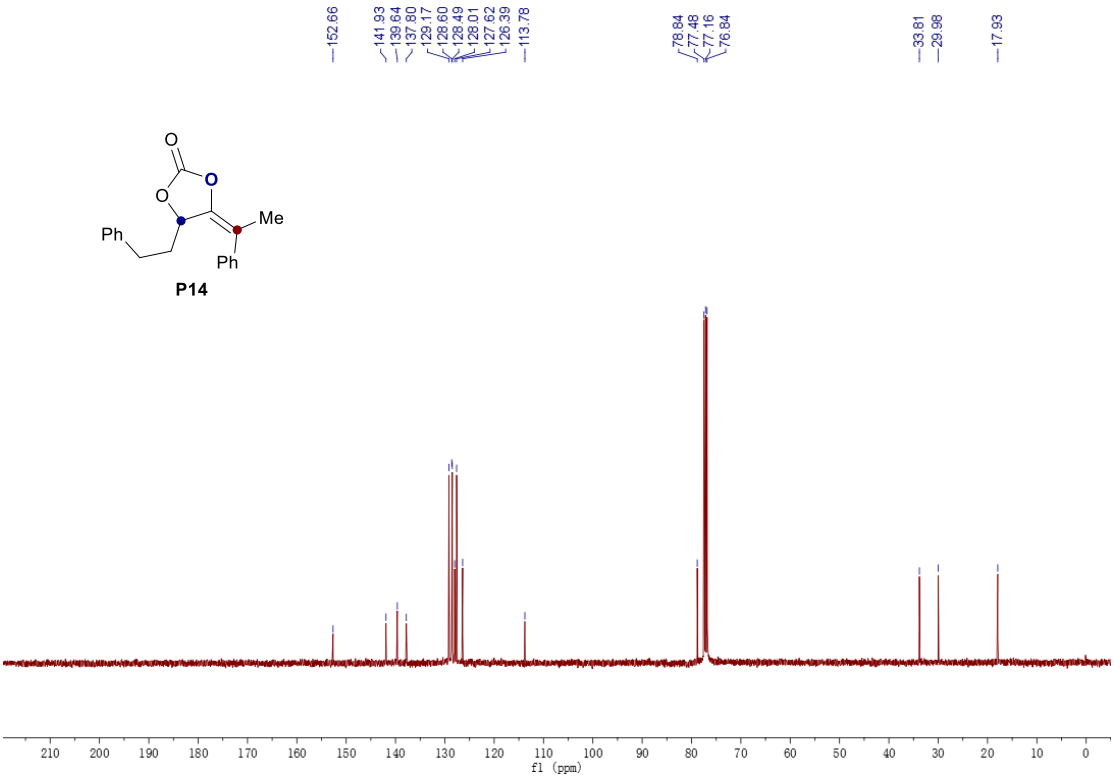

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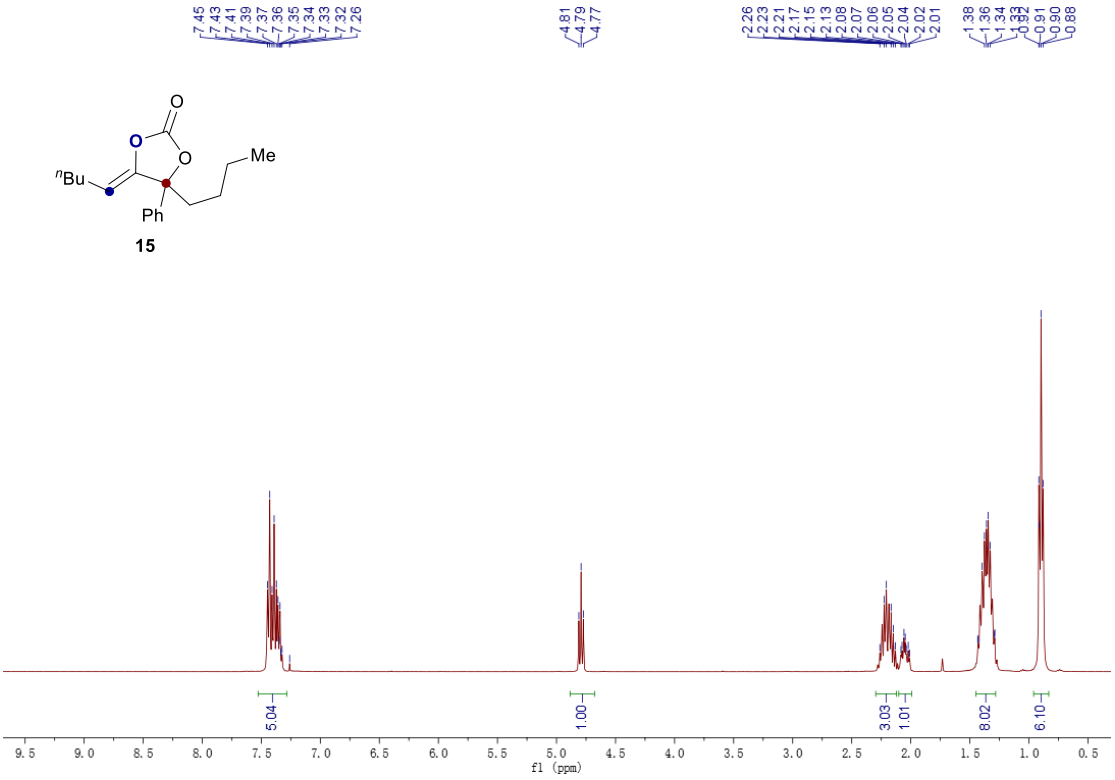
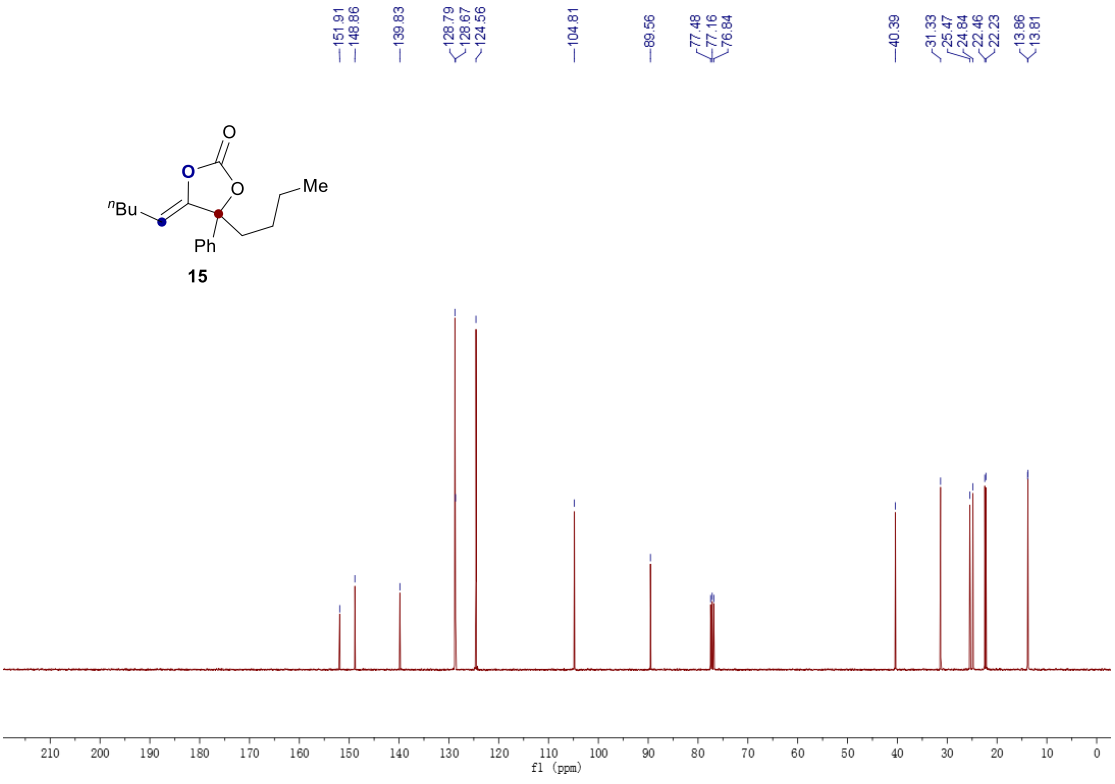
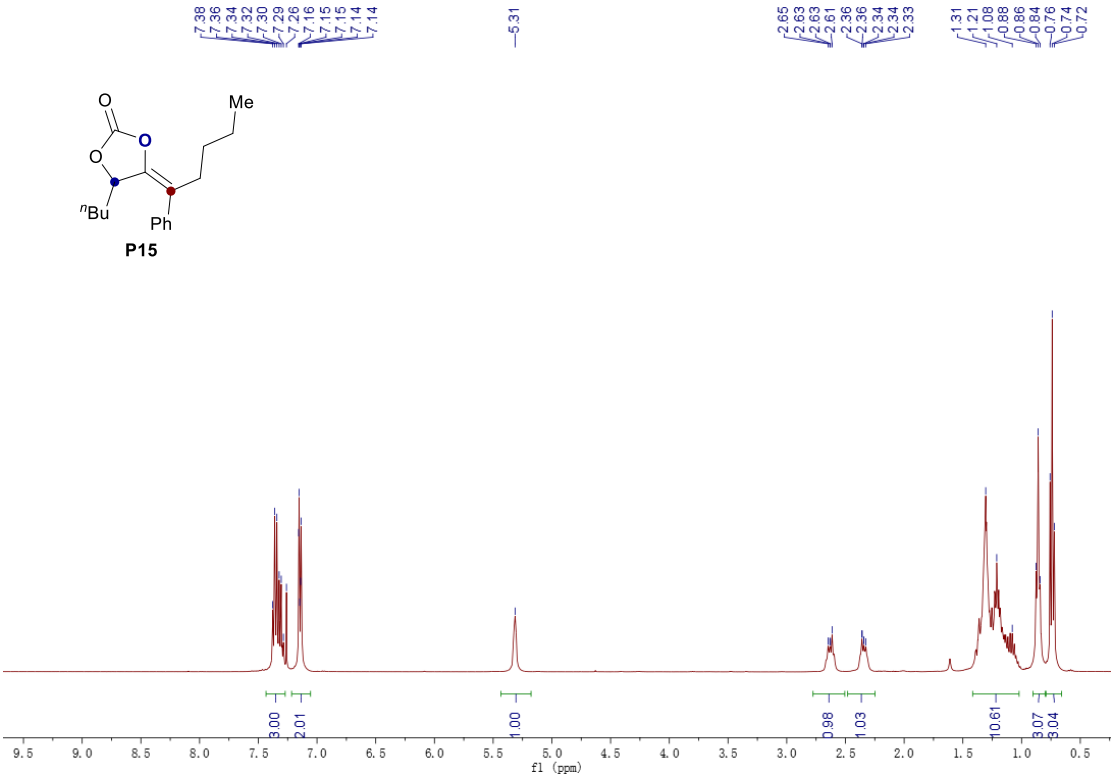


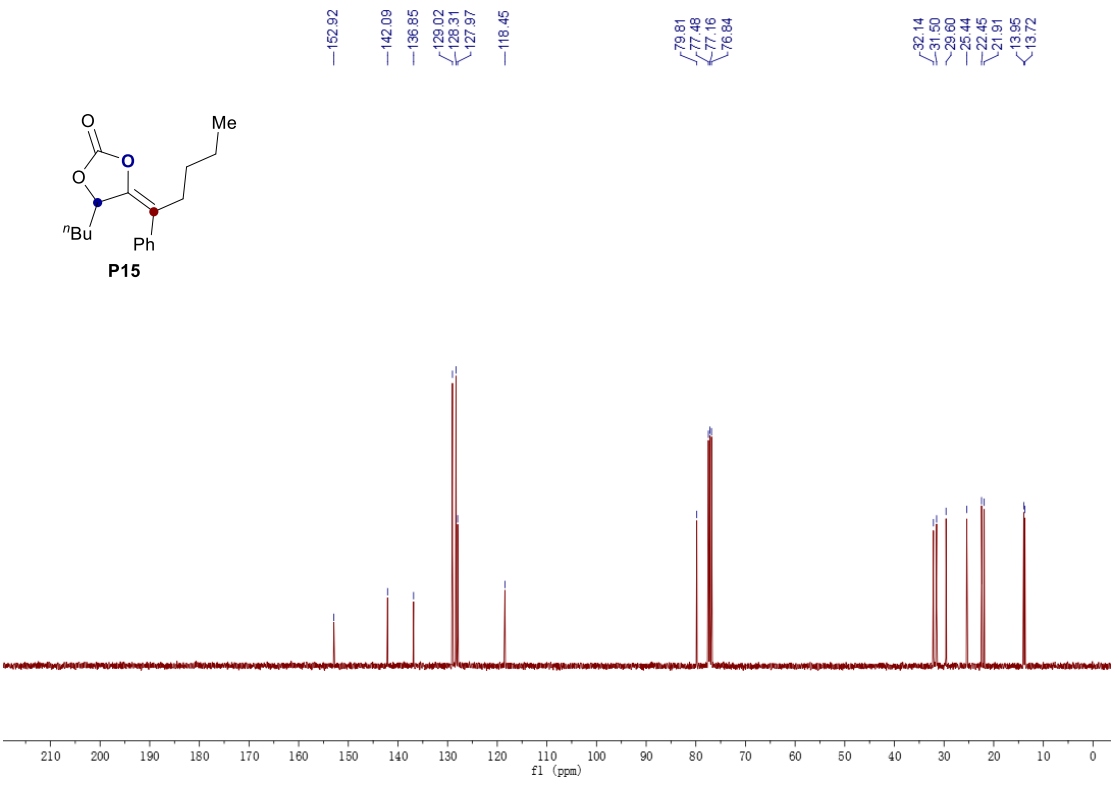
^{13}C NMR (100 MHz, $CDCl_3$)



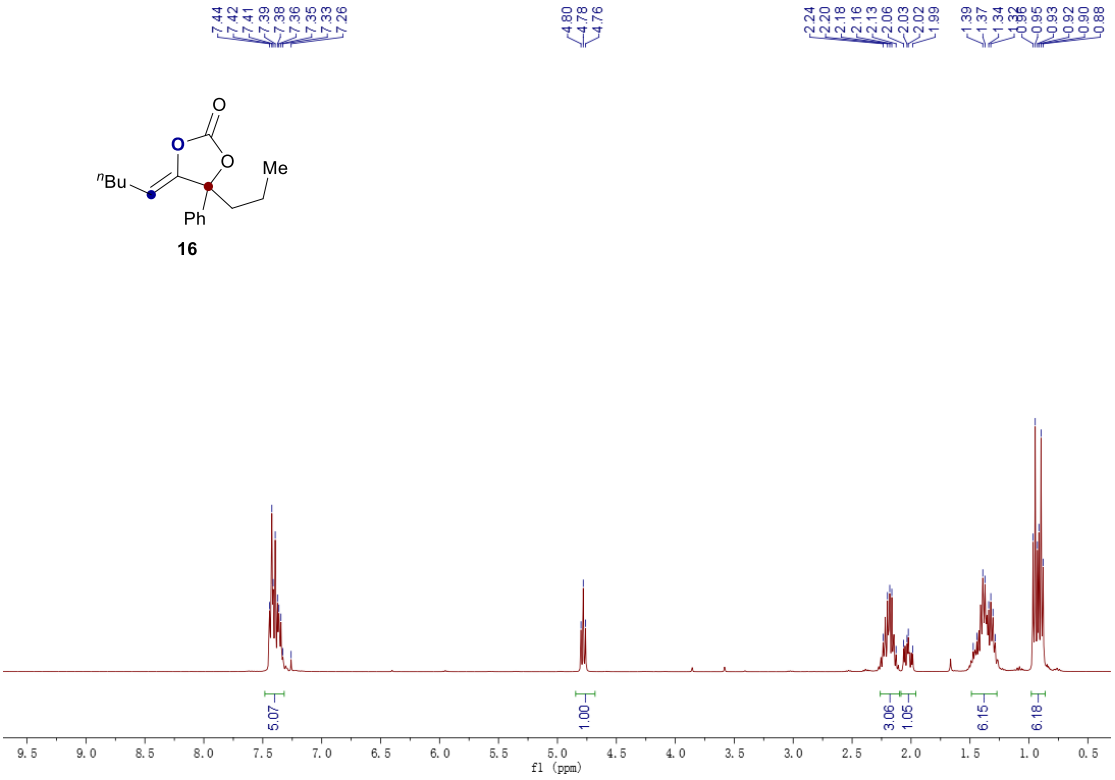
^{1}H NMR (400 MHz, $CDCl_3$)



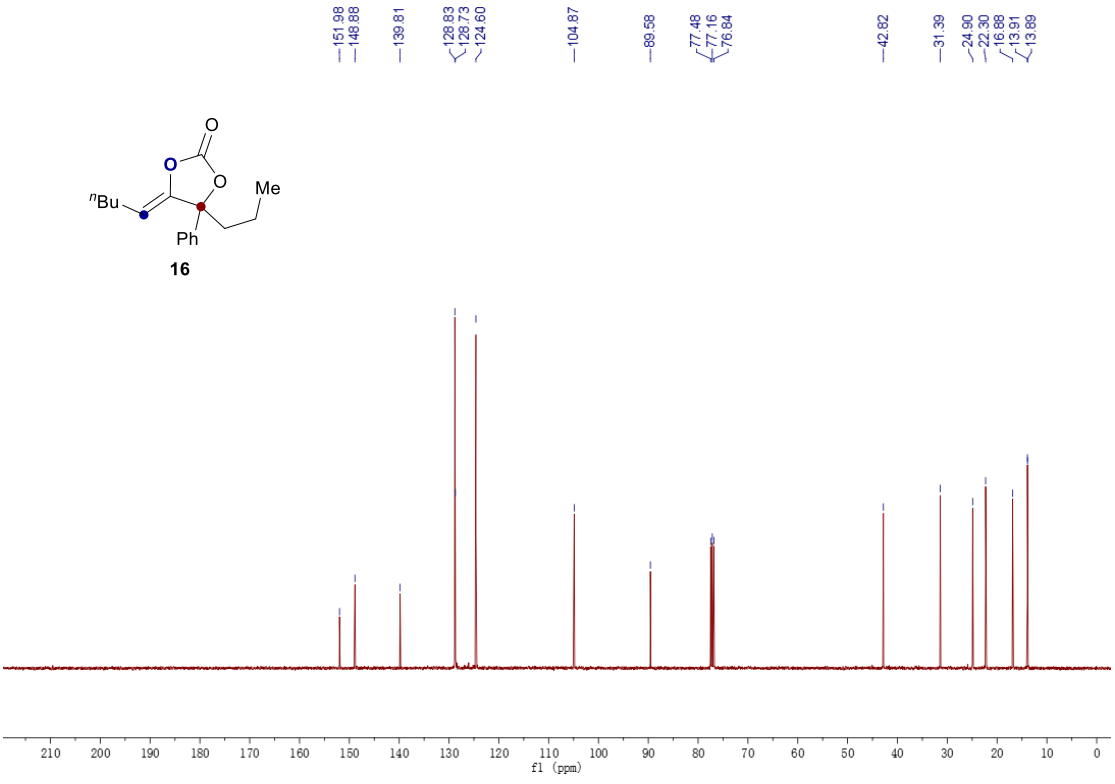
^{13}C NMR (100 MHz, $CDCl_3$)



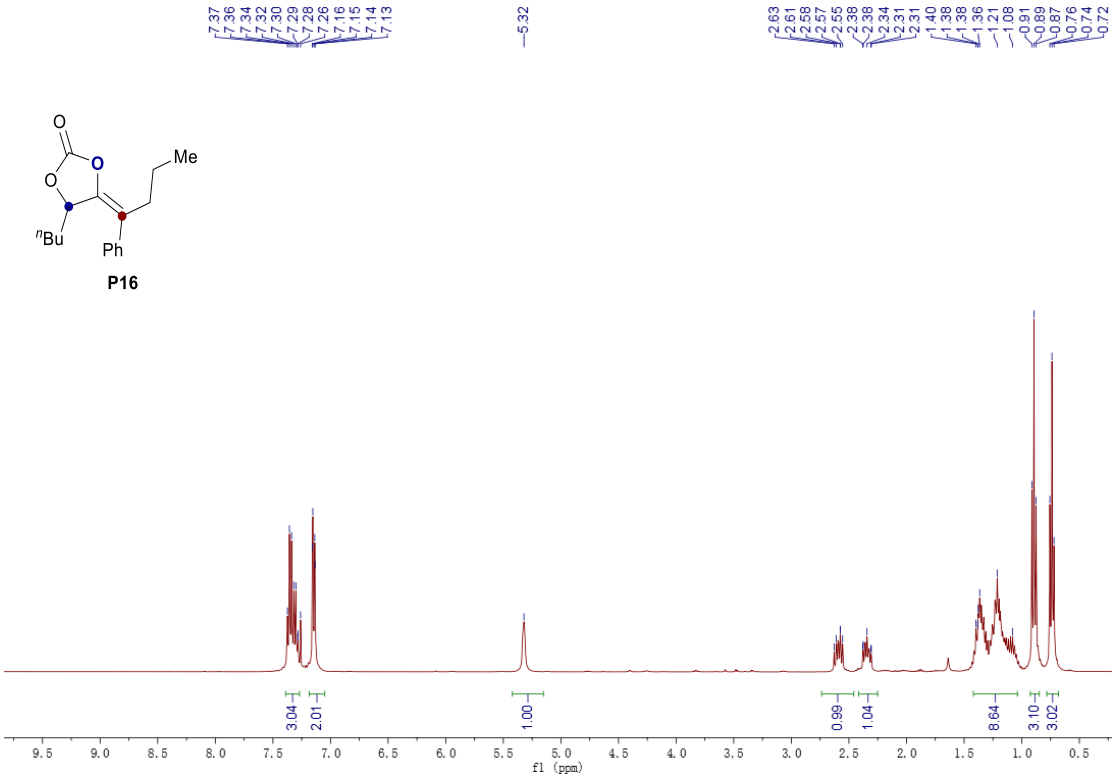
^{1}H NMR (400 MHz, $CDCl_3$)



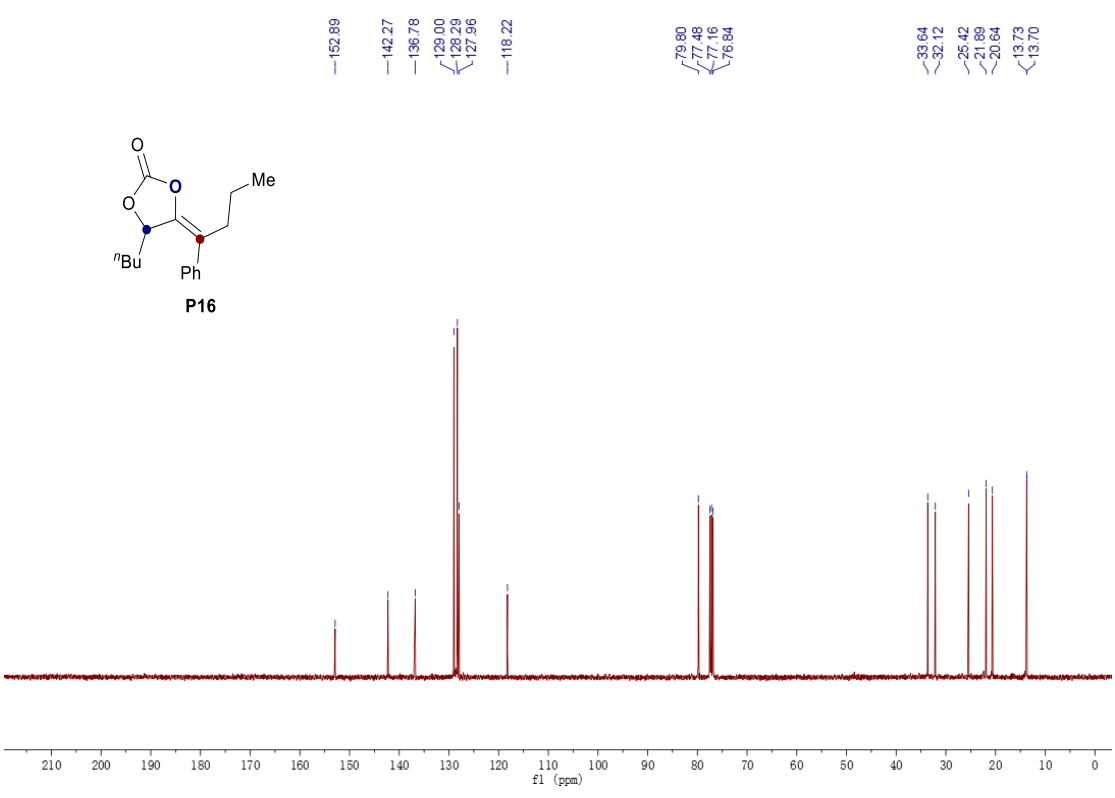
^{13}C NMR (100 MHz, $CDCl_3$)



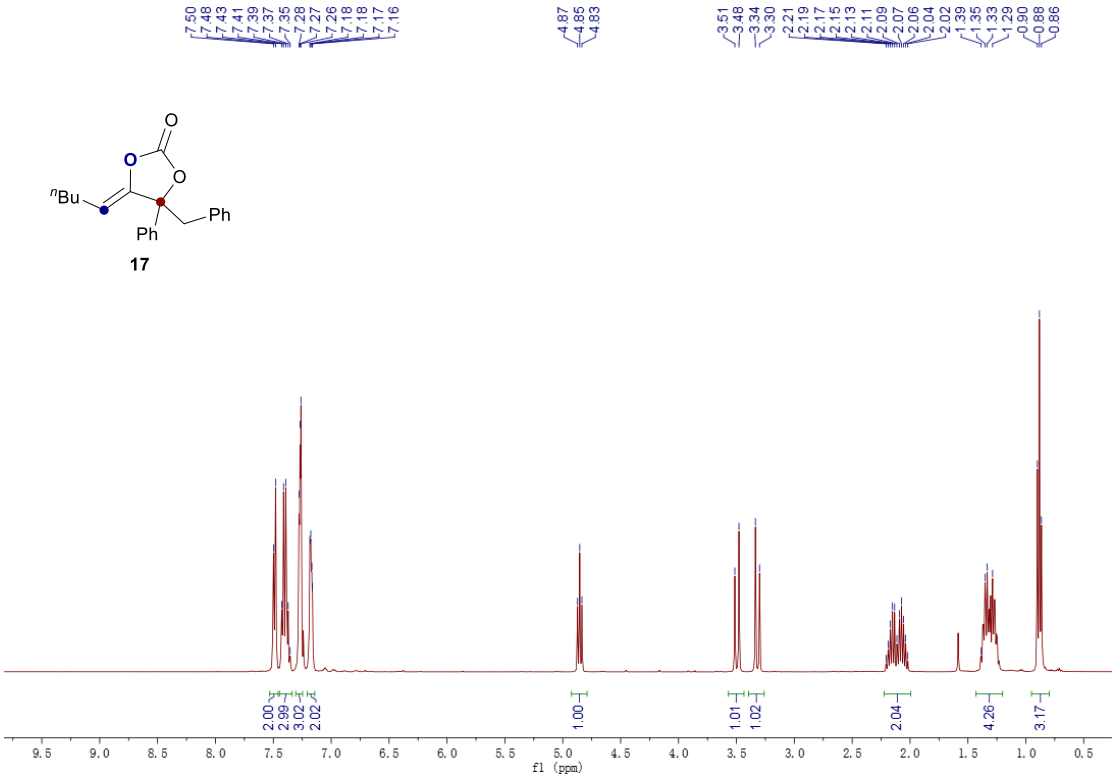
^{1}H NMR (400 MHz, $CDCl_3$)



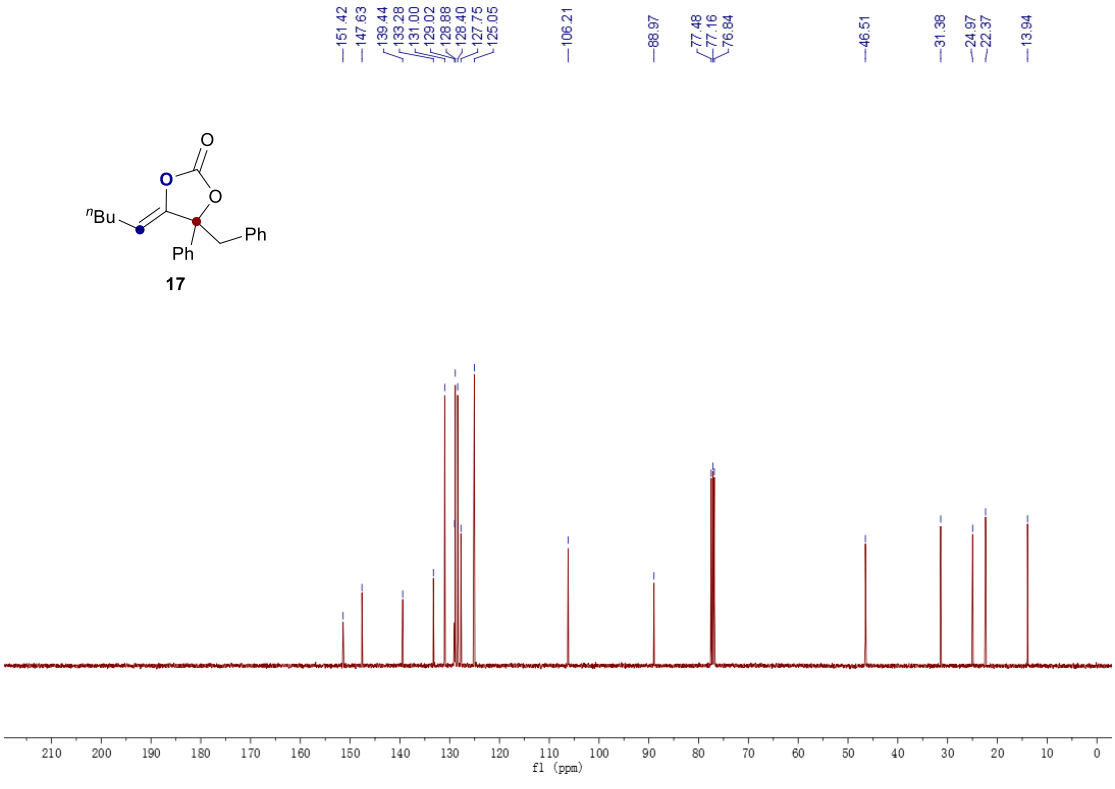
^{13}C NMR (100 MHz, $CDCl_3$)



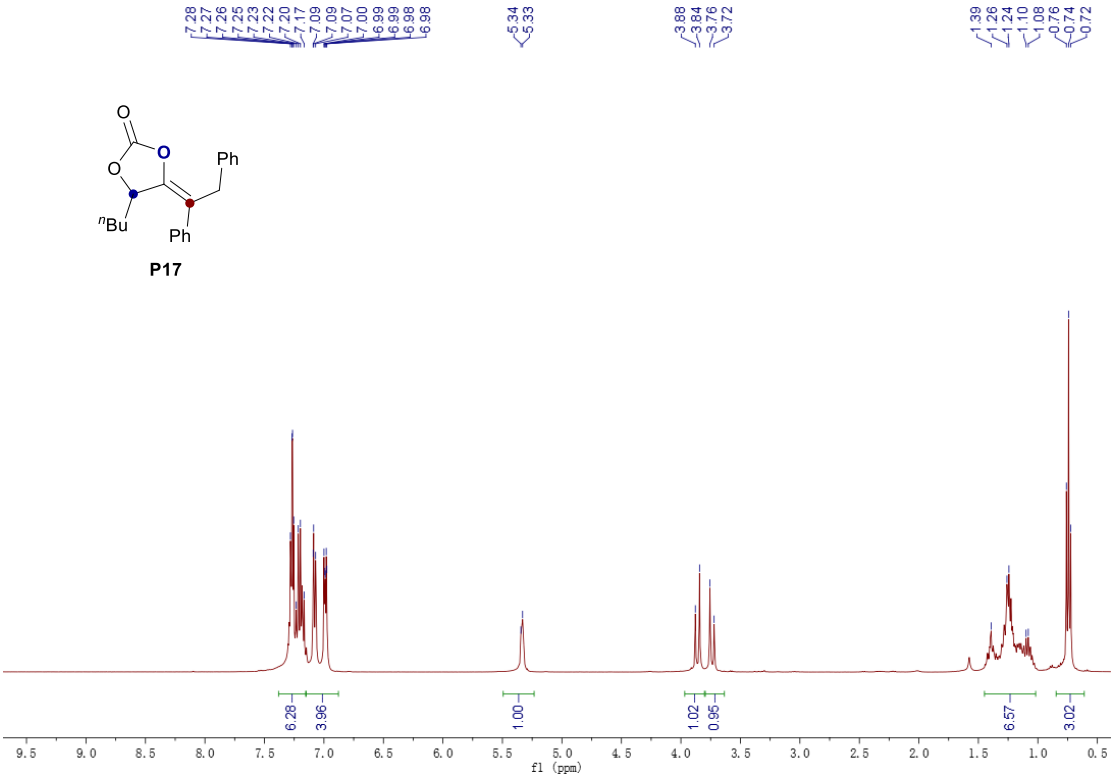
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)

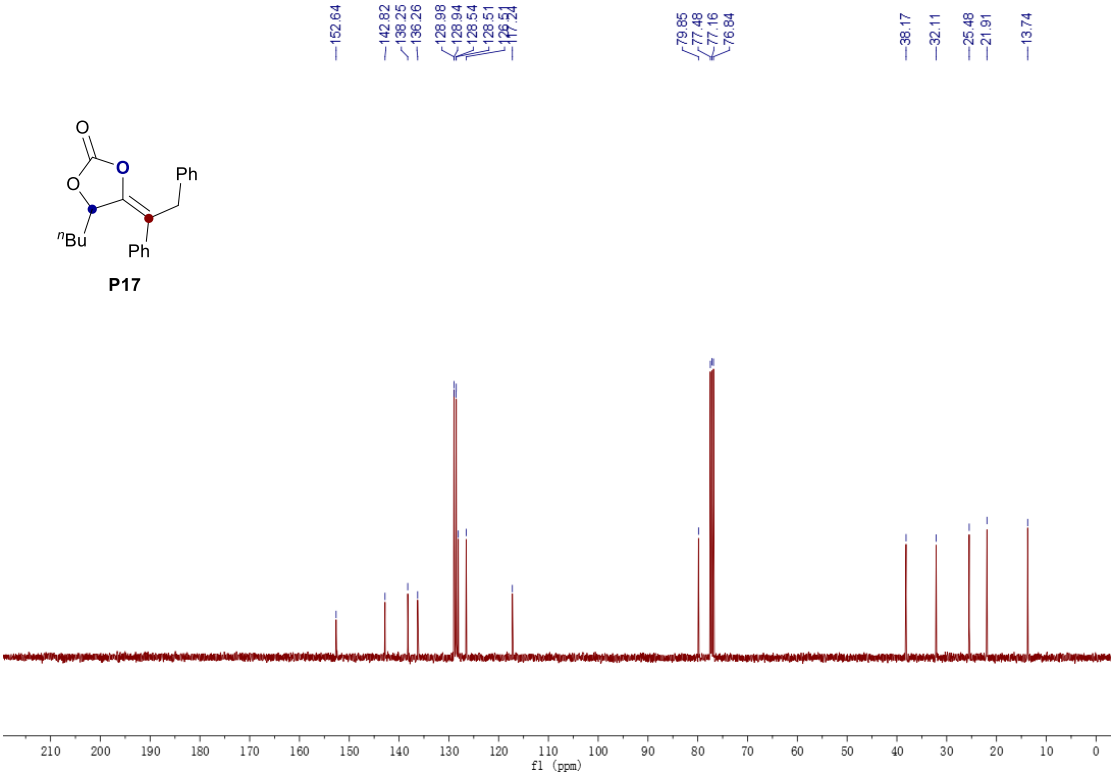


^{1}H NMR (400 MHz, $CDCl_3$)



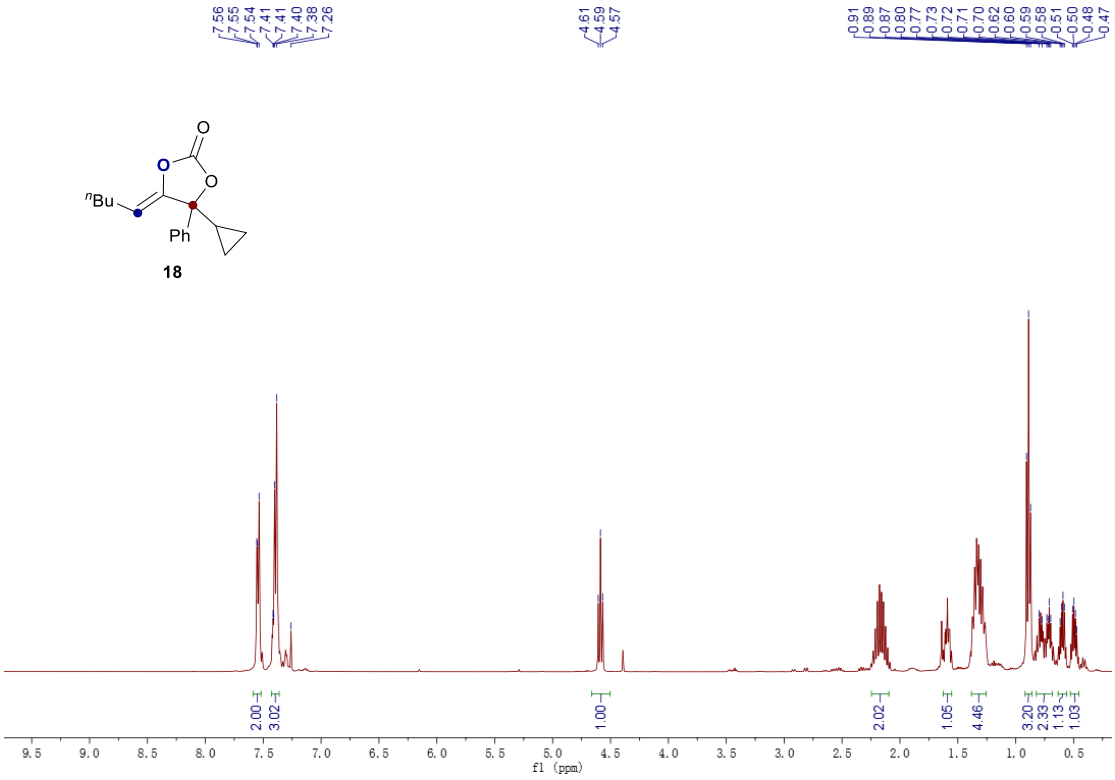
P17

^{13}C NMR (100 MHz, $CDCl_3$)

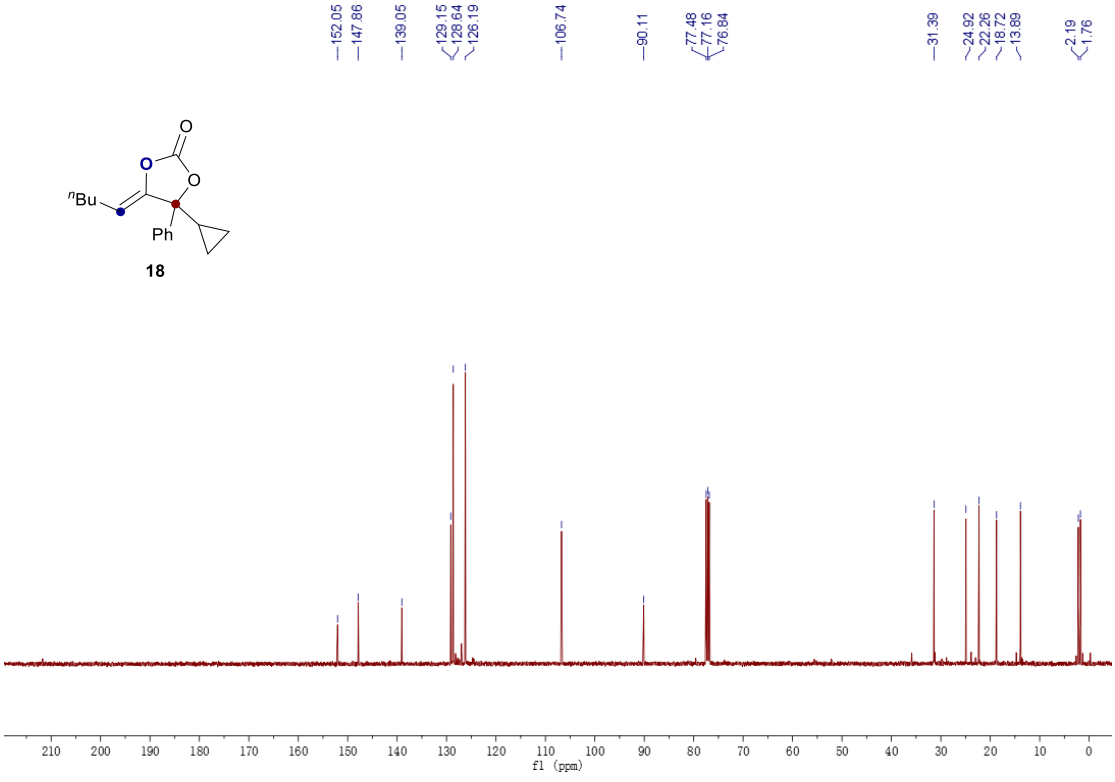


P17

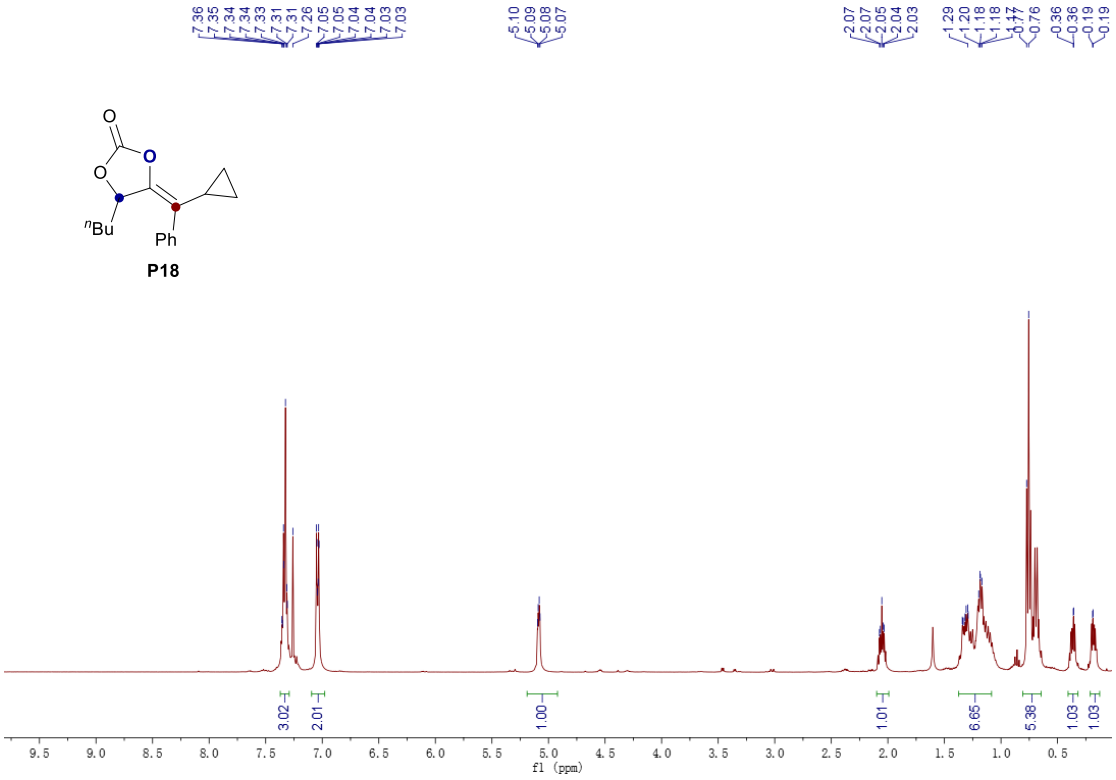
^{1}H NMR (400 MHz, $CDCl_3$)



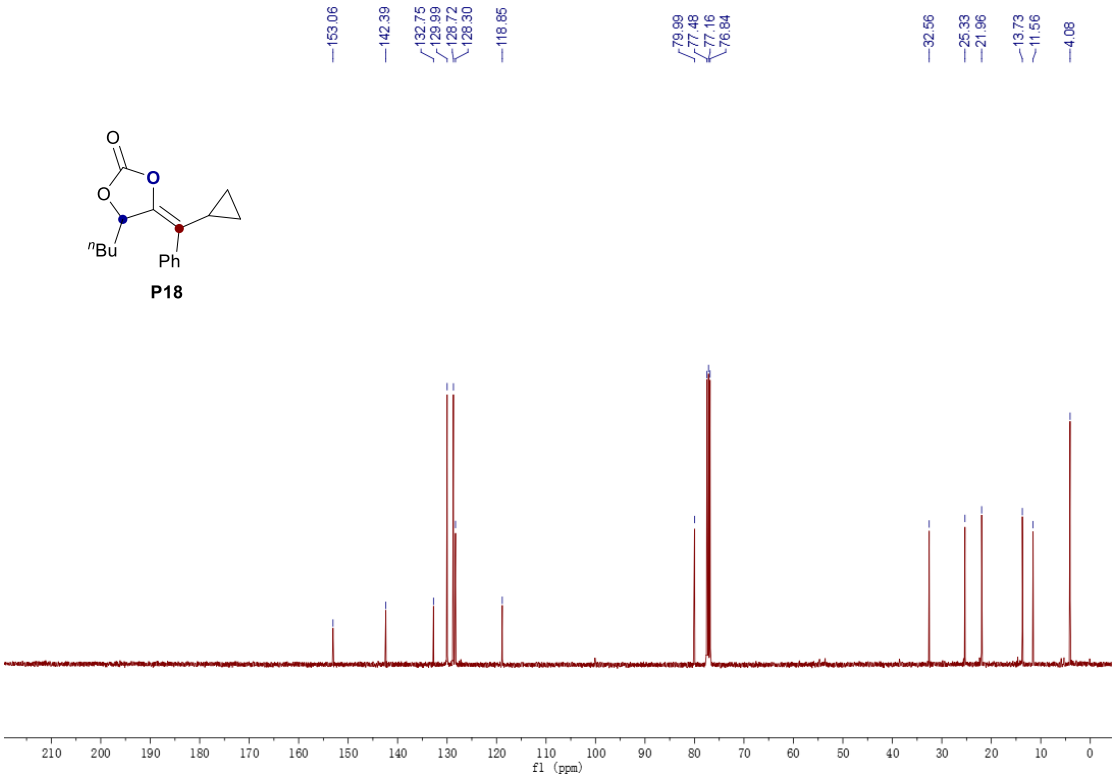
^{13}C NMR (100 MHz, $CDCl_3$)



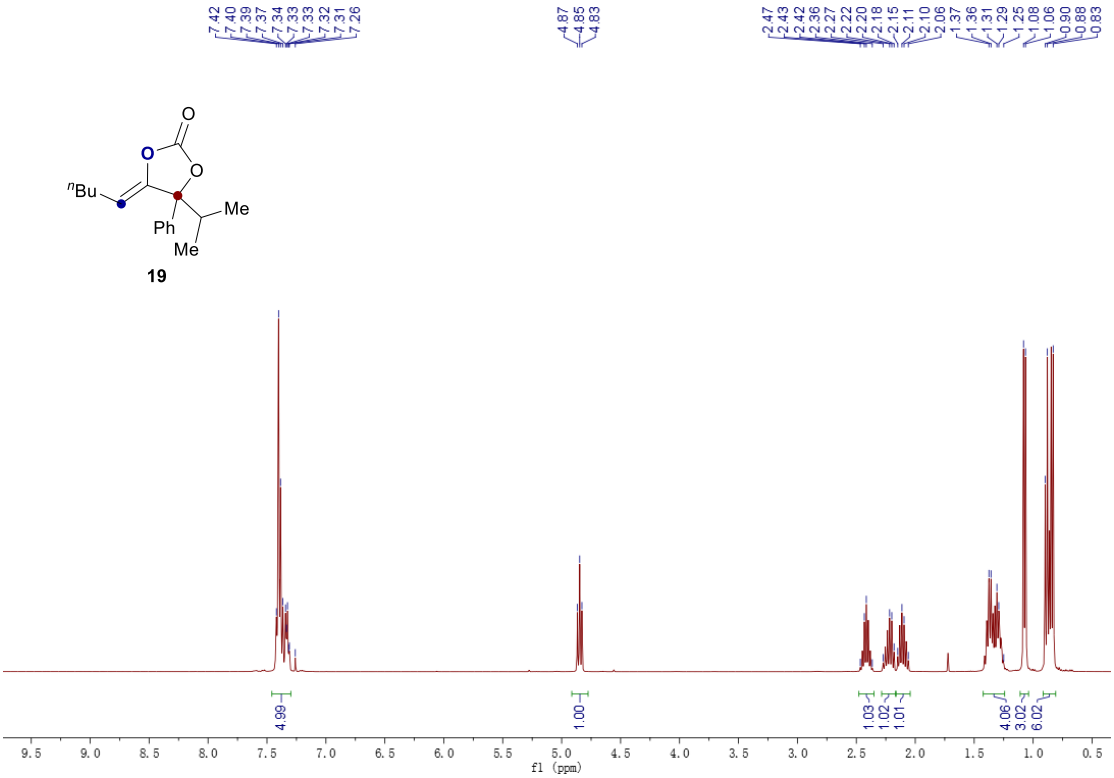
^{1}H NMR (400 MHz, $CDCl_3$)



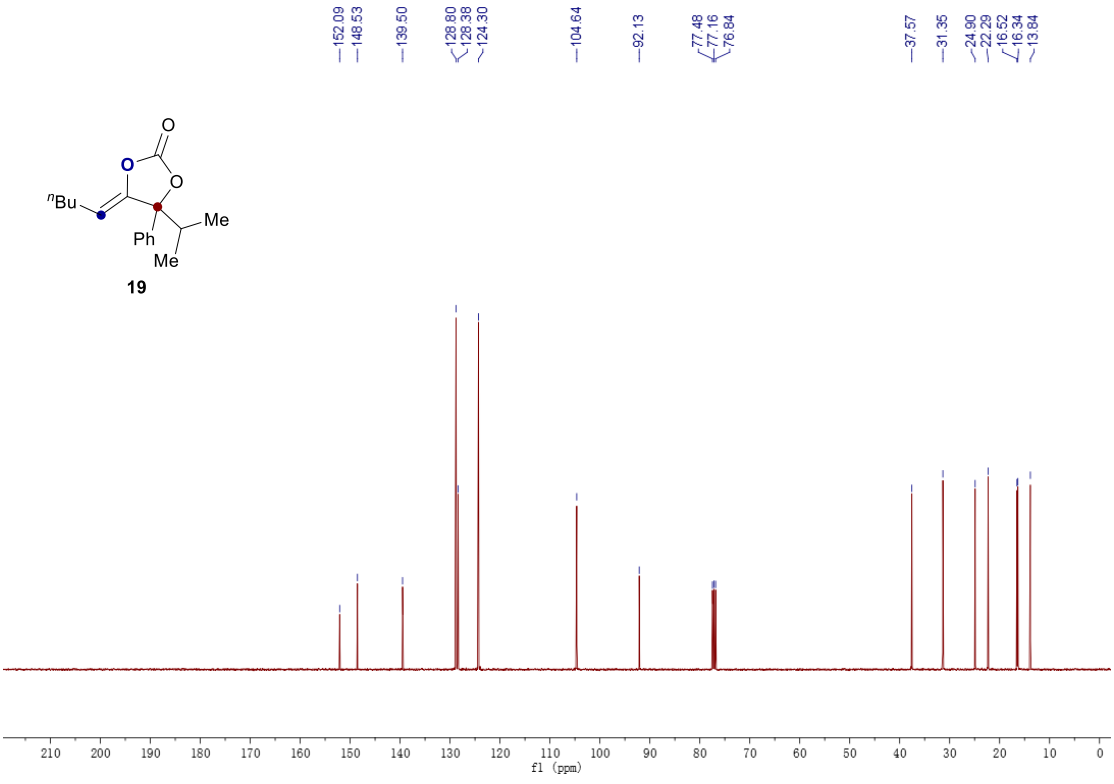
^{13}C NMR (100 MHz, $CDCl_3$)



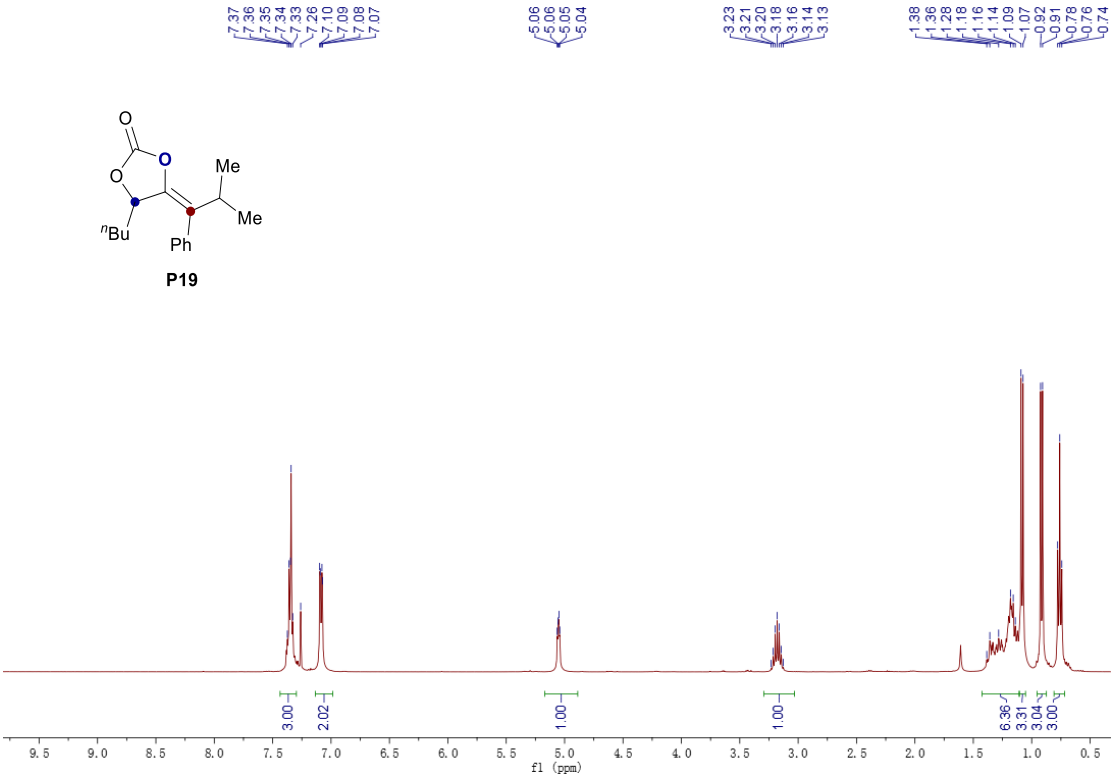
^{1}H NMR (400 MHz, $CDCl_3$)



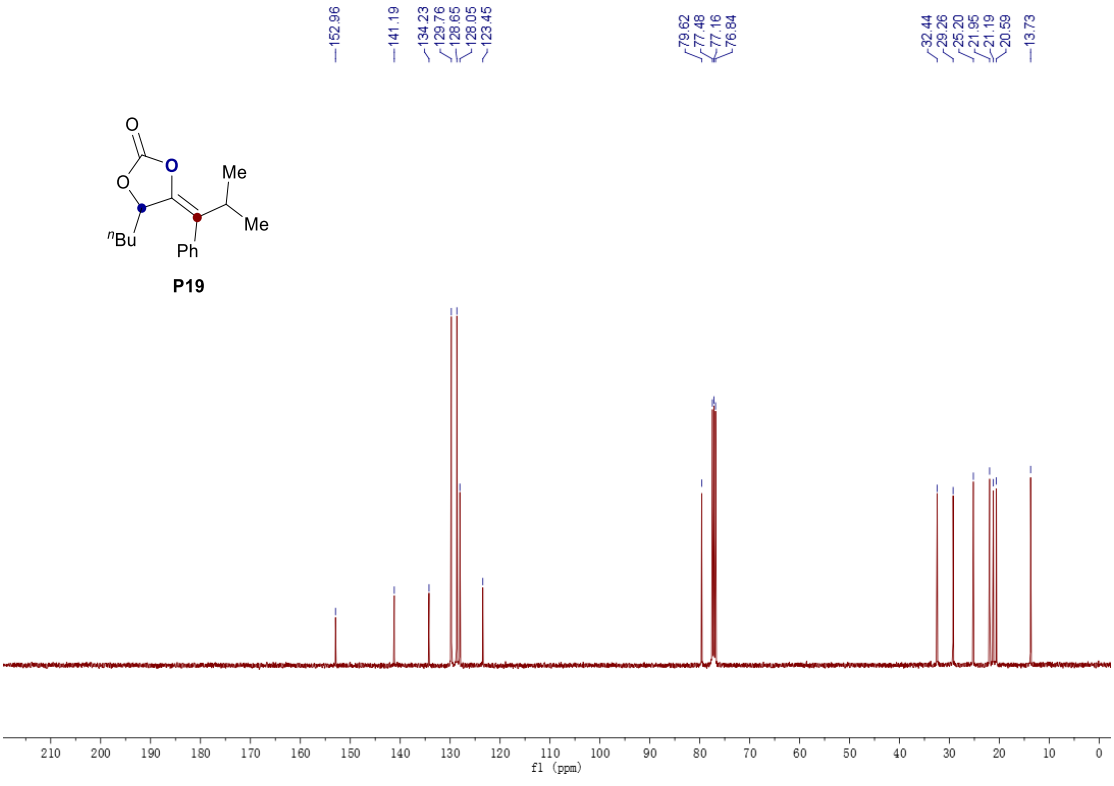
^{13}C NMR (100 MHz, $CDCl_3$)



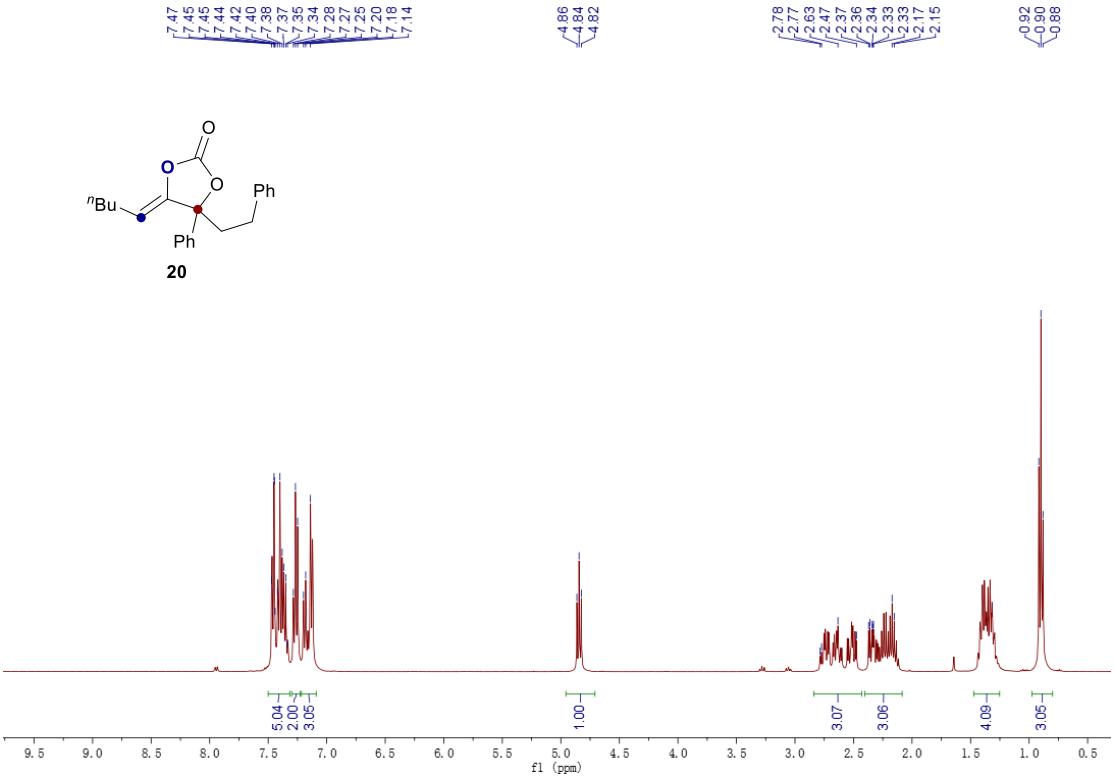
^{1}H NMR (400 MHz, $CDCl_3$)



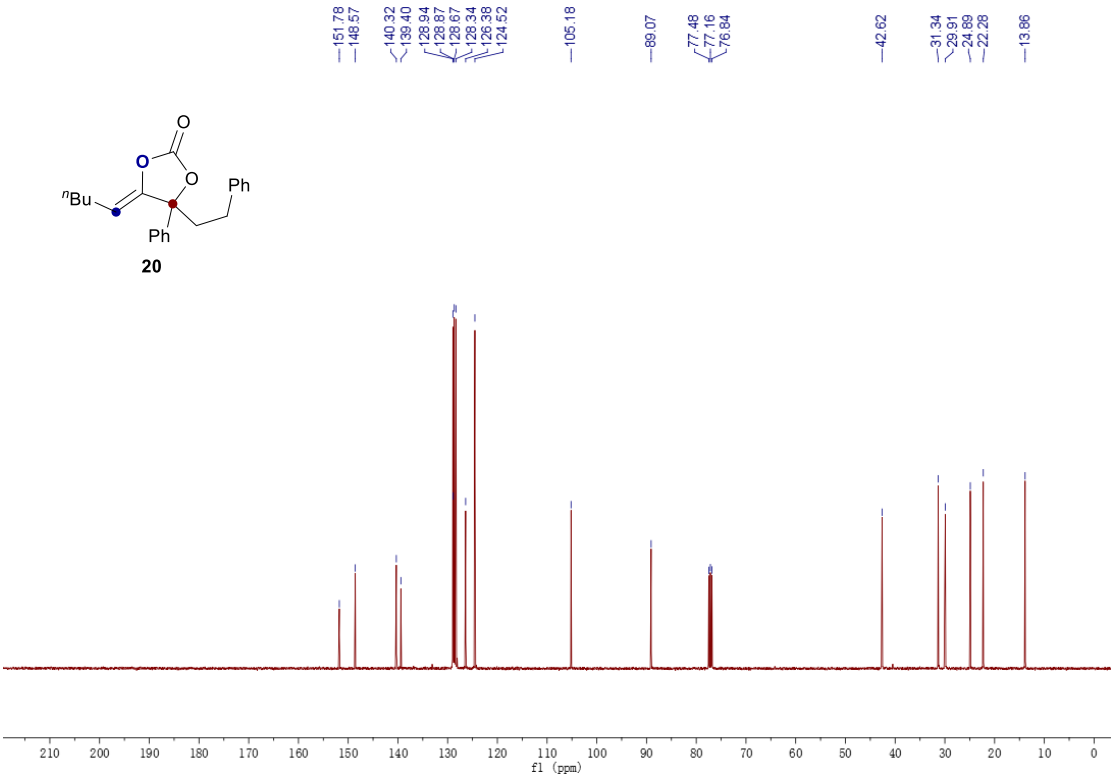
^{13}C NMR (100 MHz, $CDCl_3$)



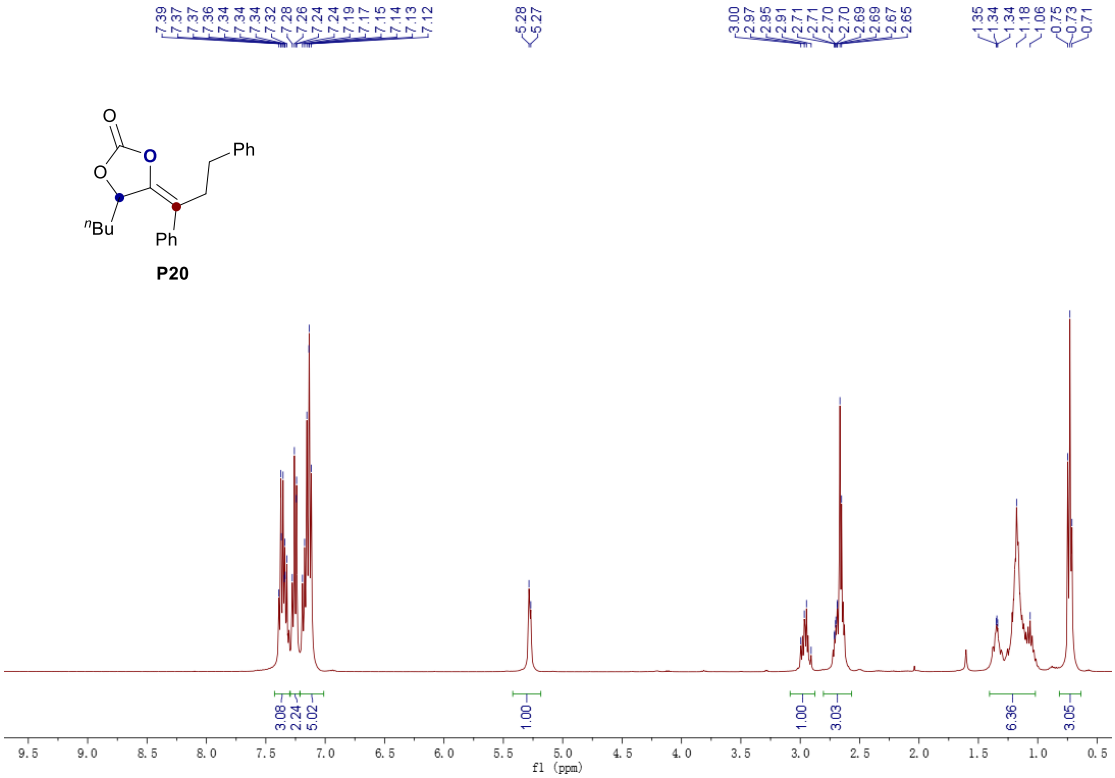
^{1}H NMR (400 MHz, $CDCl_3$)



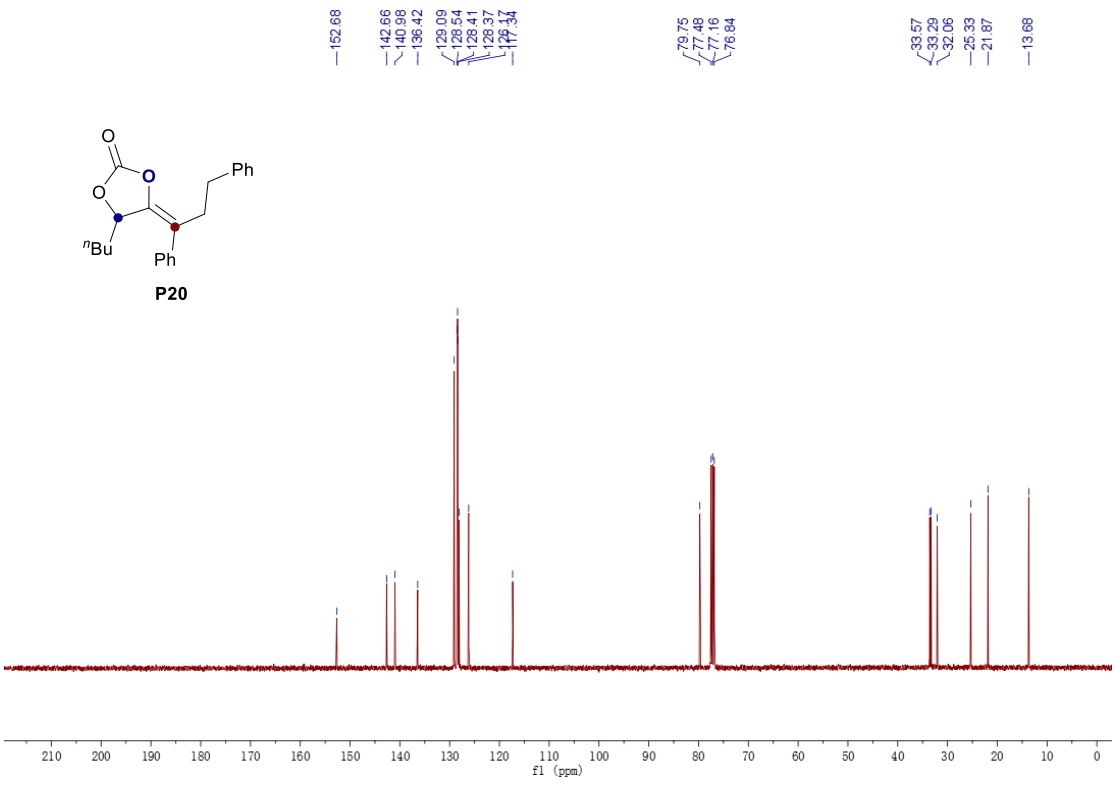
^{13}C NMR (100 MHz, $CDCl_3$)



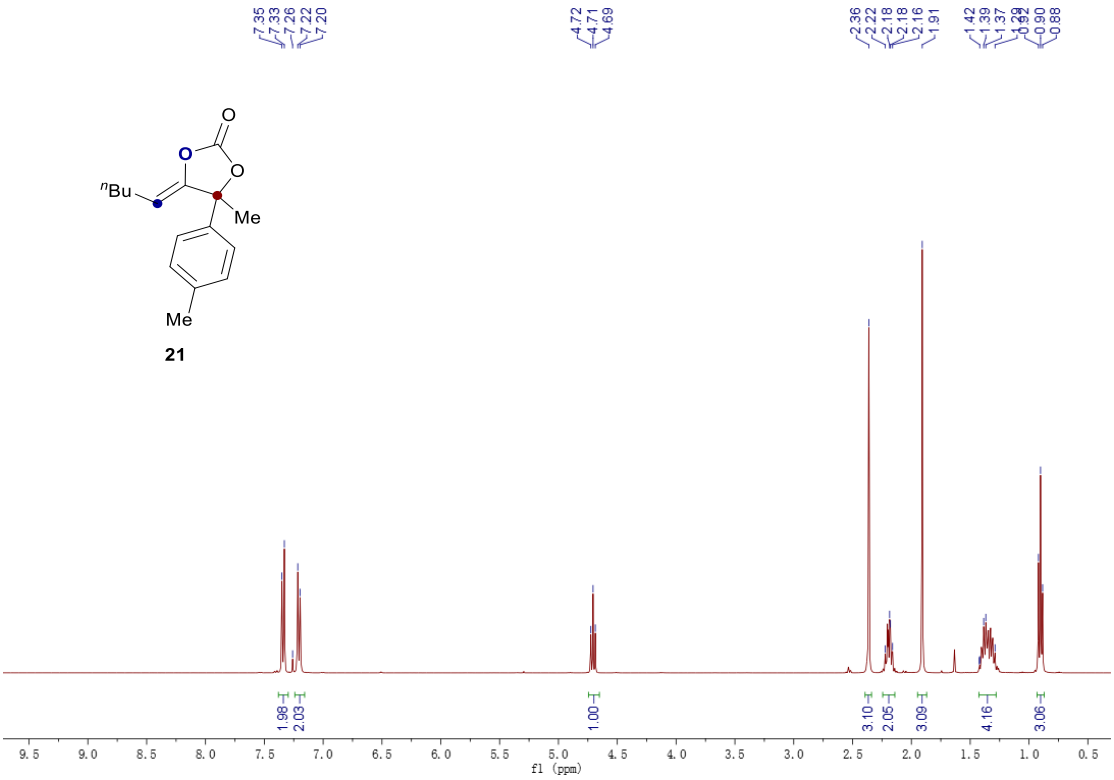
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)

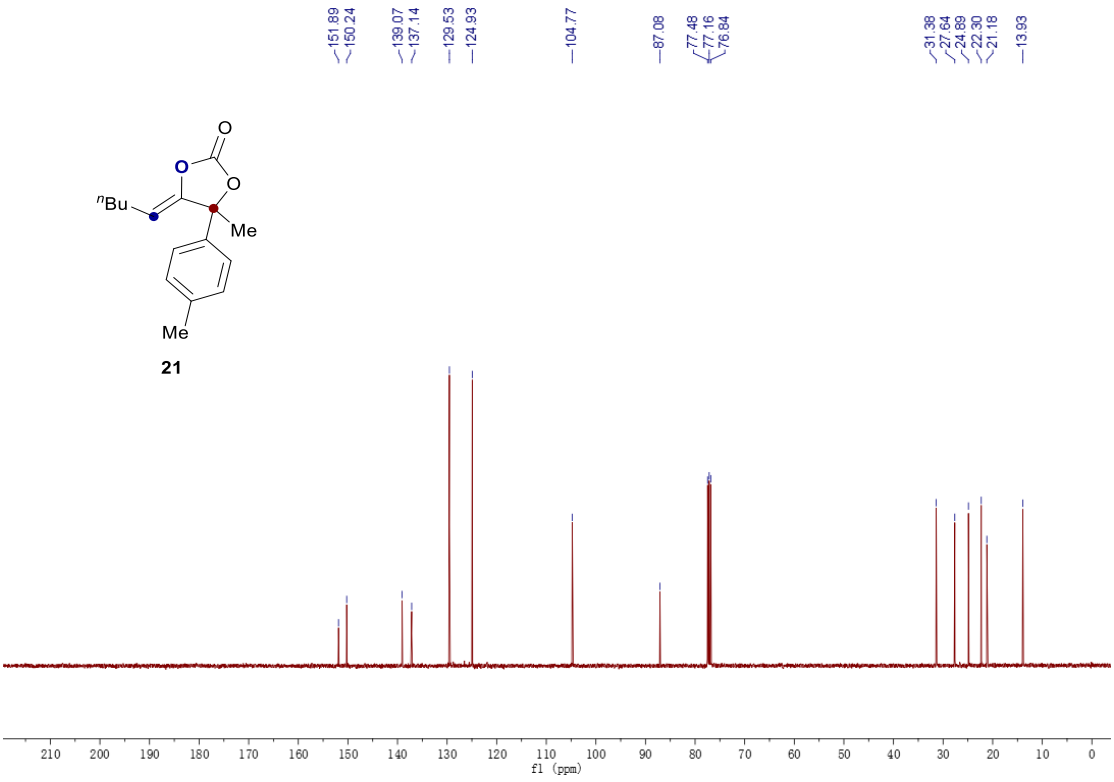


^{1}H NMR (400 MHz, $CDCl_3$)



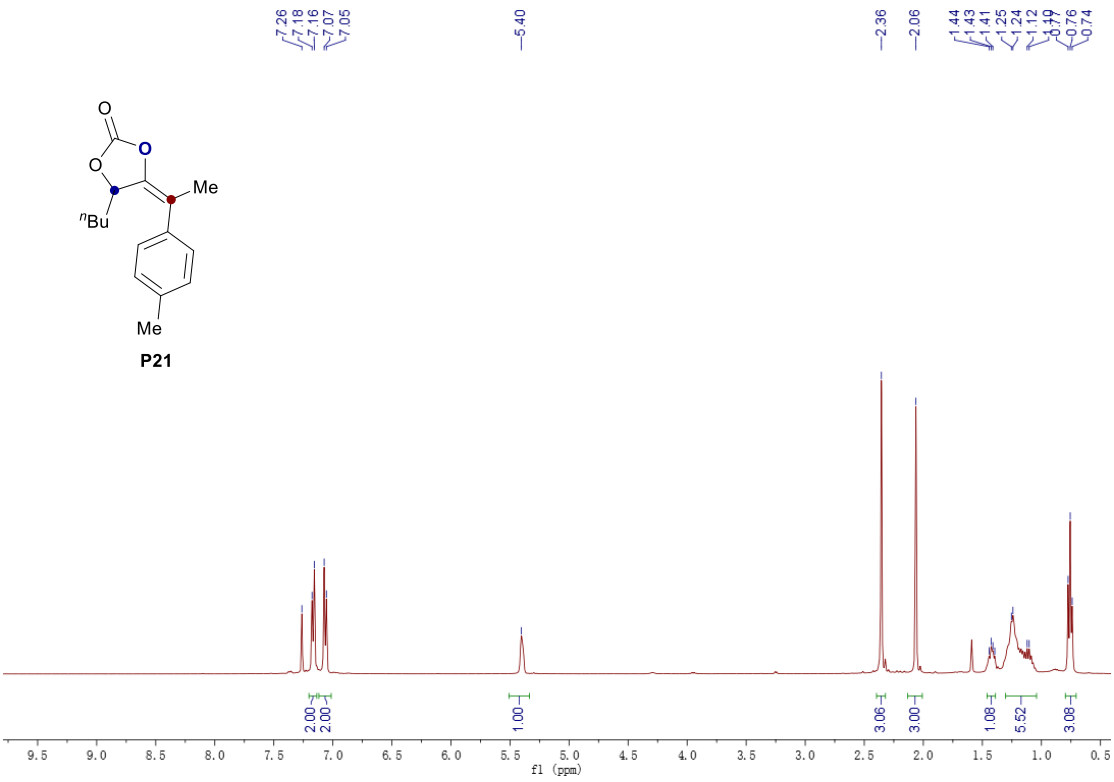
21

^{13}C NMR (100 MHz, $CDCl_3$)

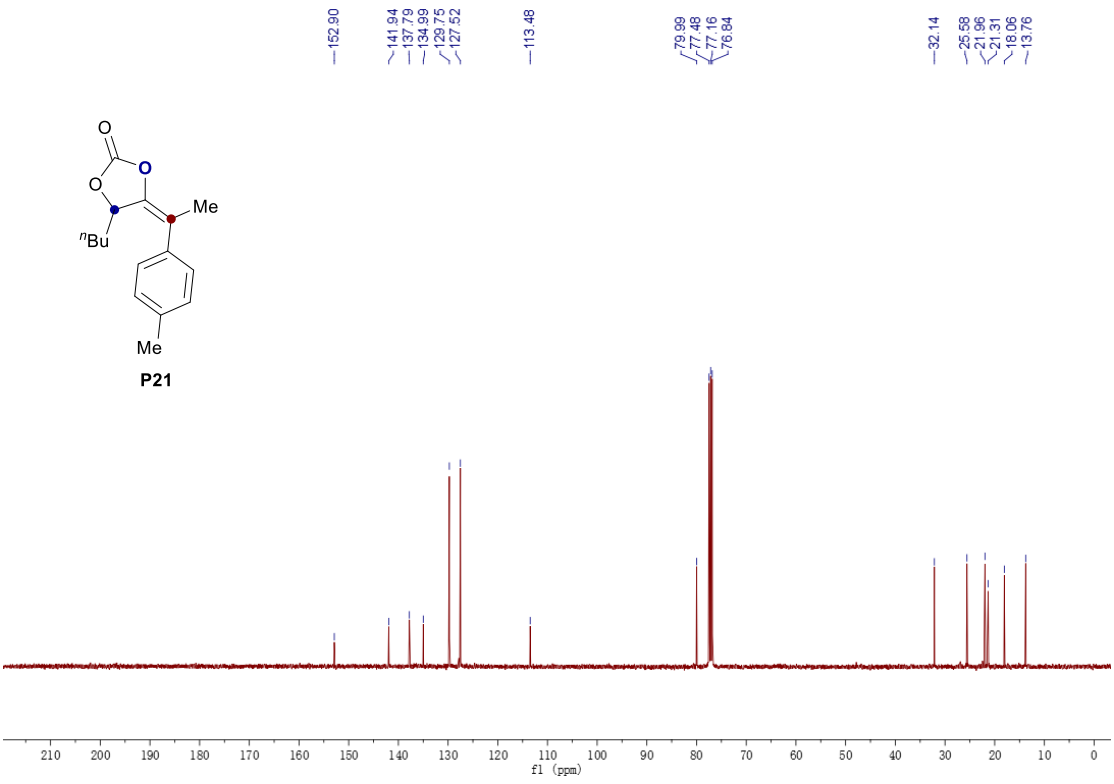


21

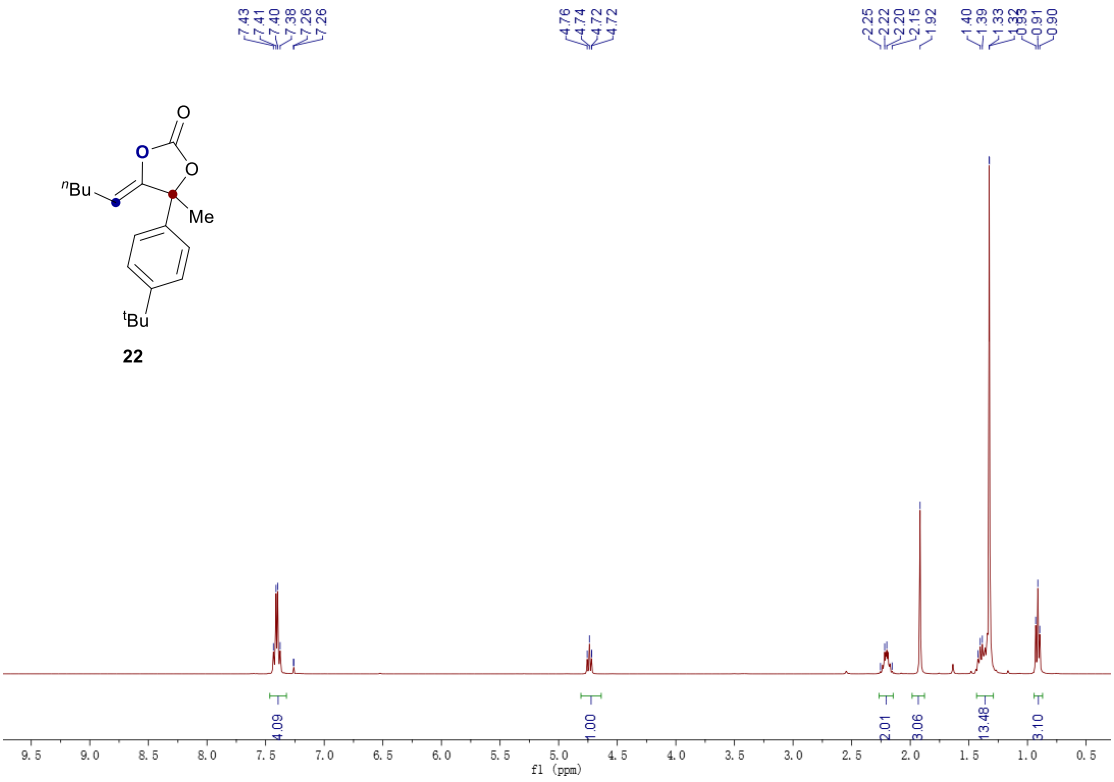
^{1}H NMR (400 MHz, $CDCl_3$)



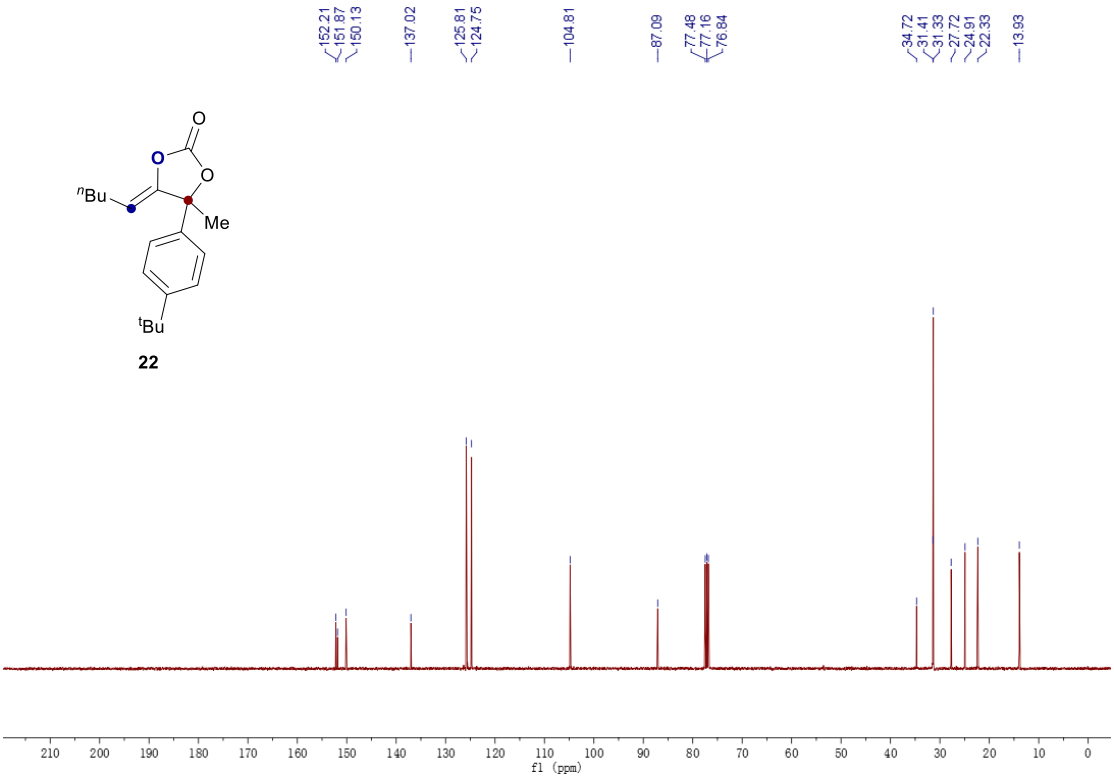
^{13}C NMR (100 MHz, $CDCl_3$)



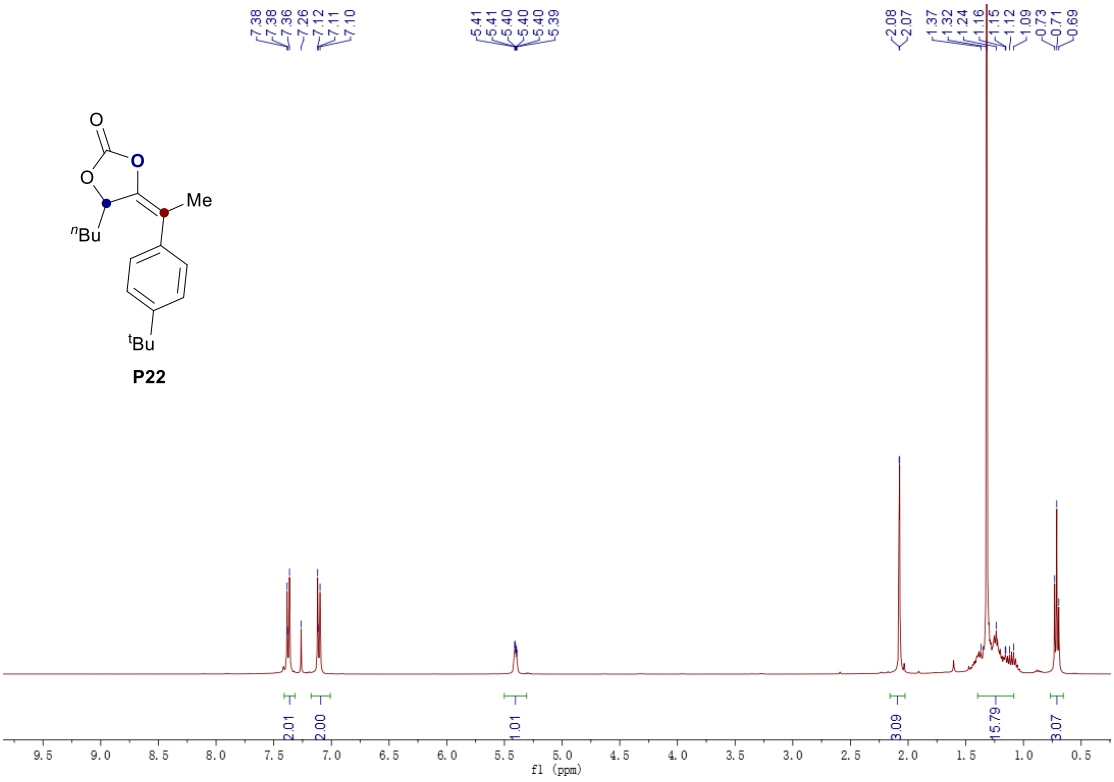
^{1}H NMR (400 MHz, $CDCl_3$)



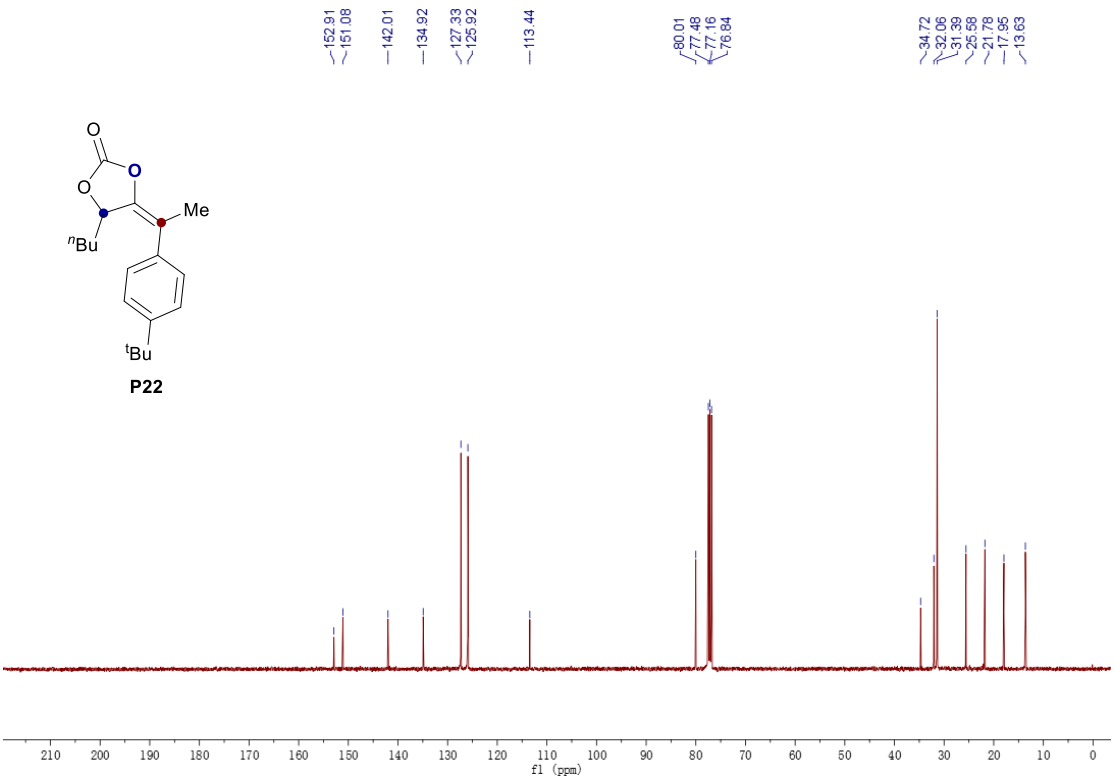
^{13}C NMR (100 MHz, $CDCl_3$)



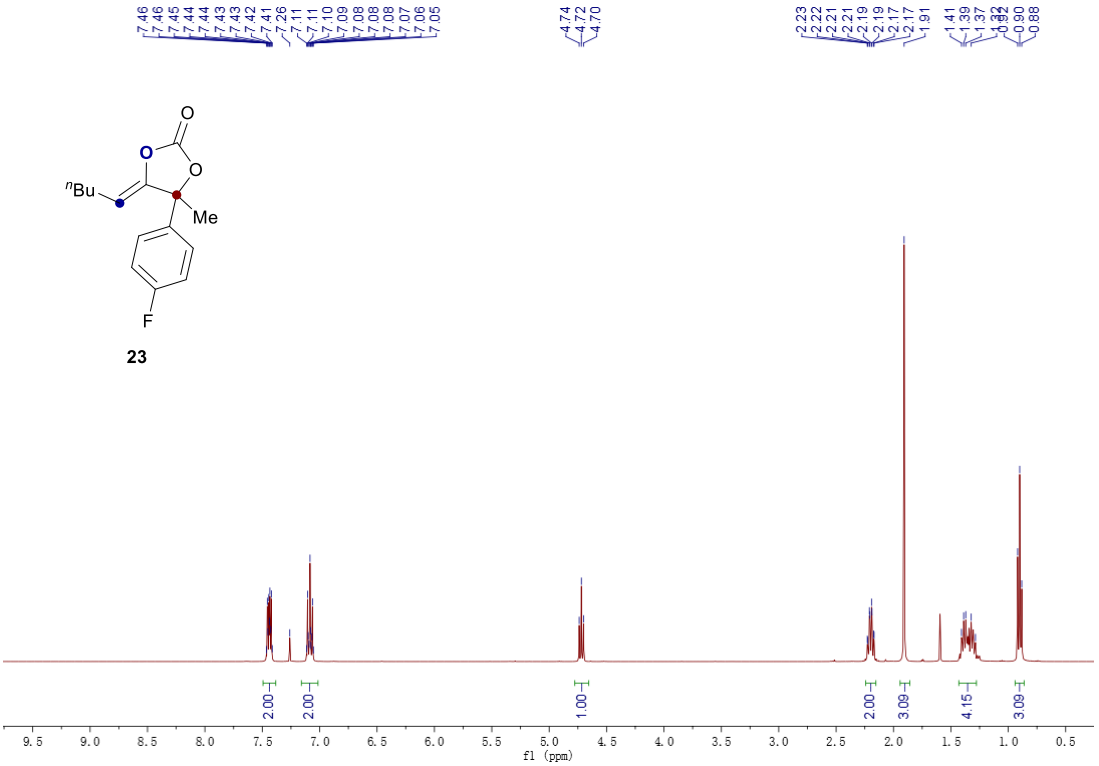
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)

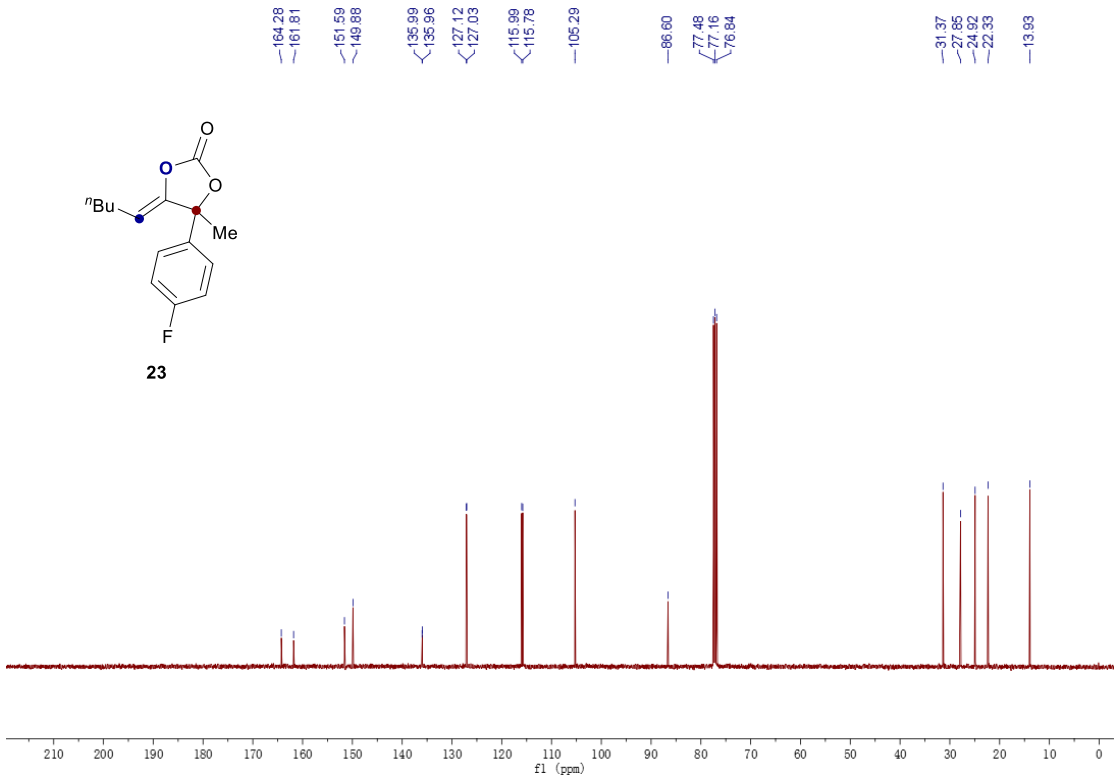


^{1}H NMR (400 MHz, $CDCl_3$)



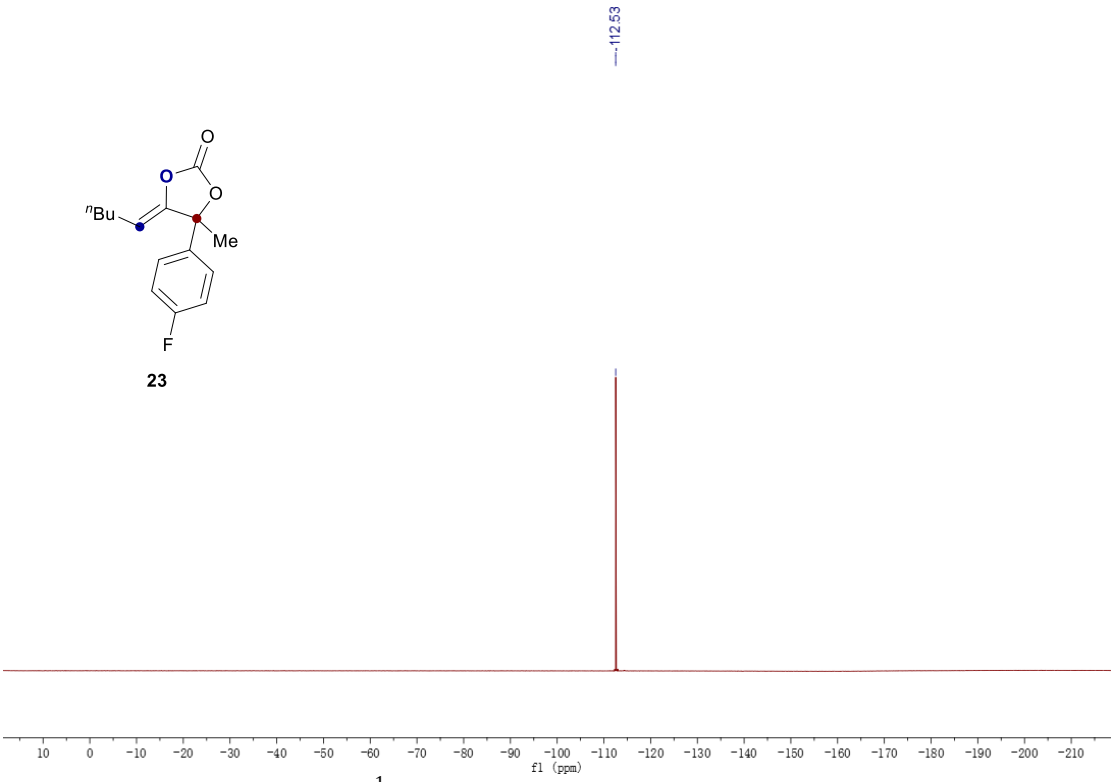
23

^{13}C NMR (100 MHz, $CDCl_3$)

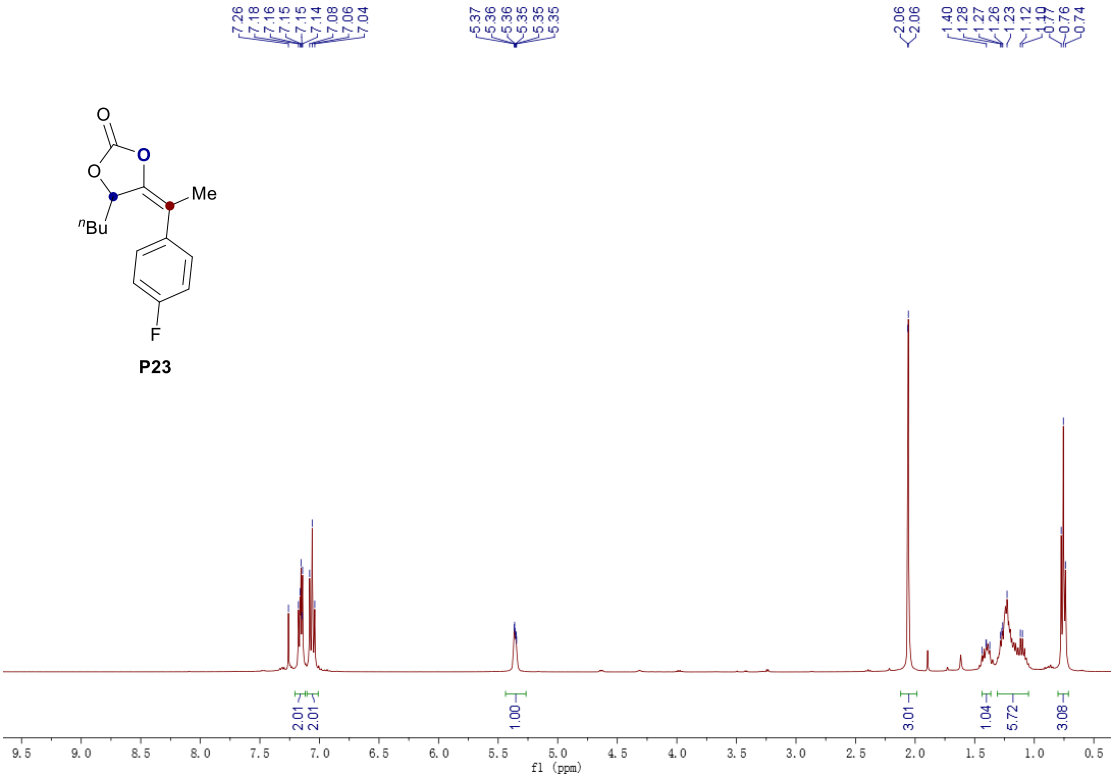


23

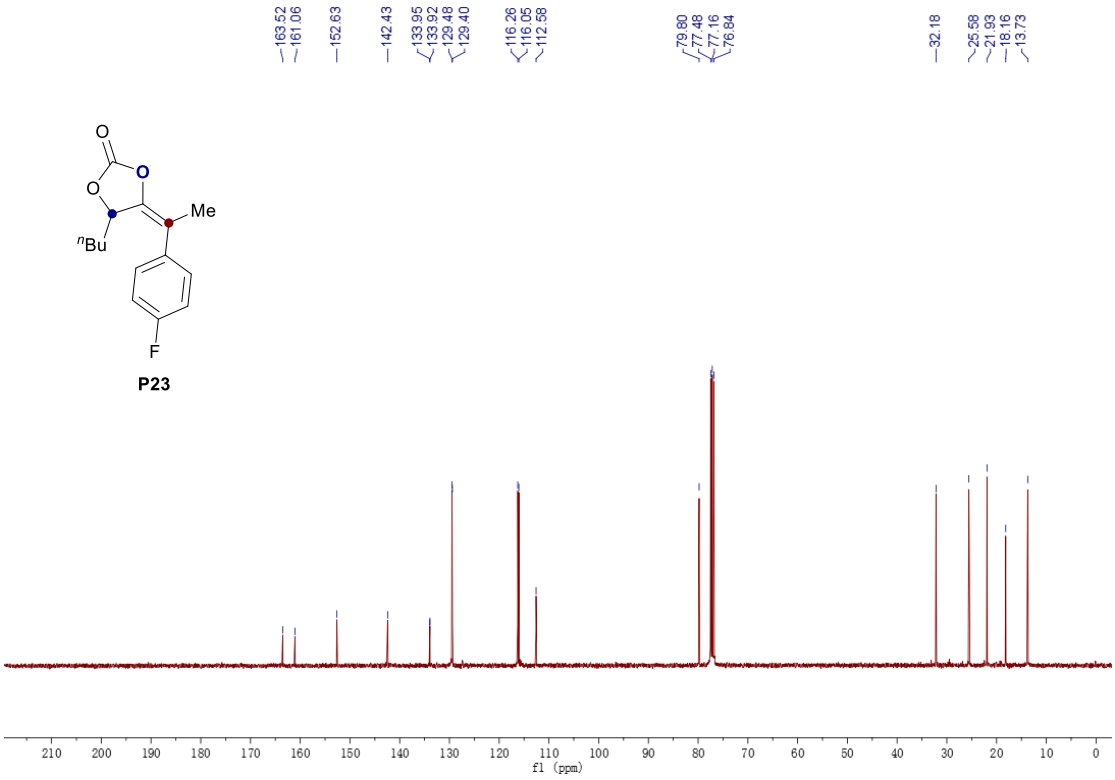
^{19}F NMR (376 MHz, $CDCl_3$)



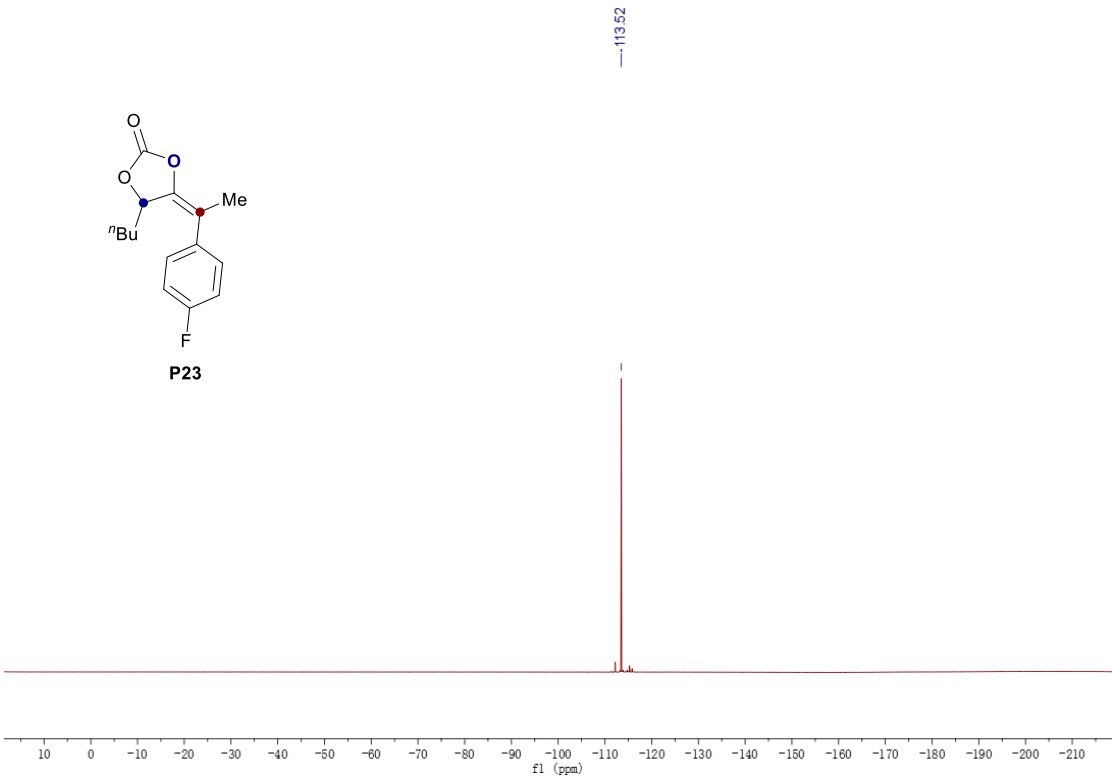
^{1}H NMR (400 MHz, $CDCl_3$)



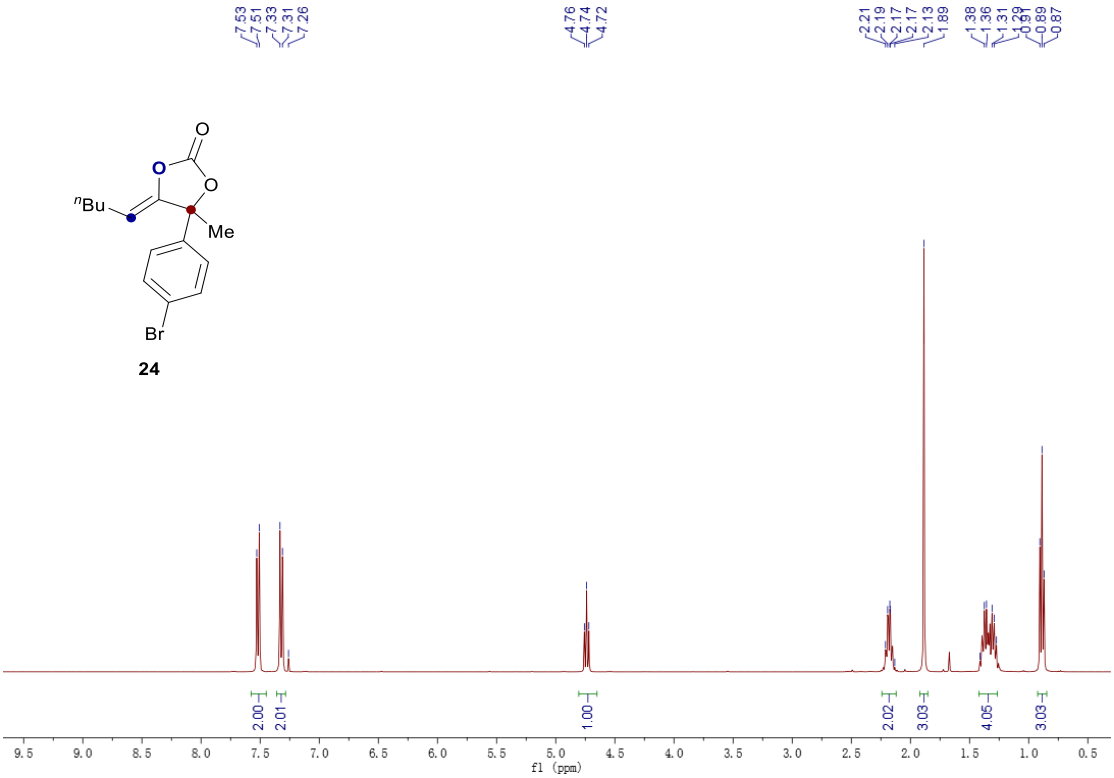
^{13}C NMR (100 MHz, $CDCl_3$)



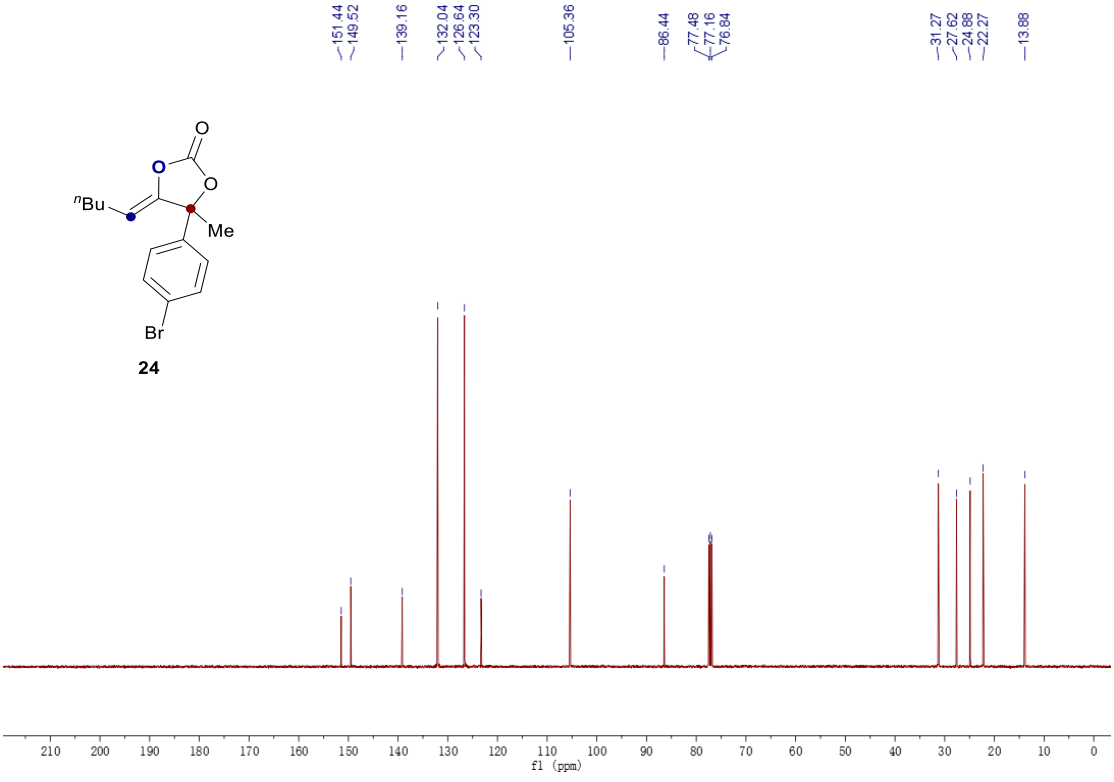
^{19}F NMR (376 MHz, $CDCl_3$)



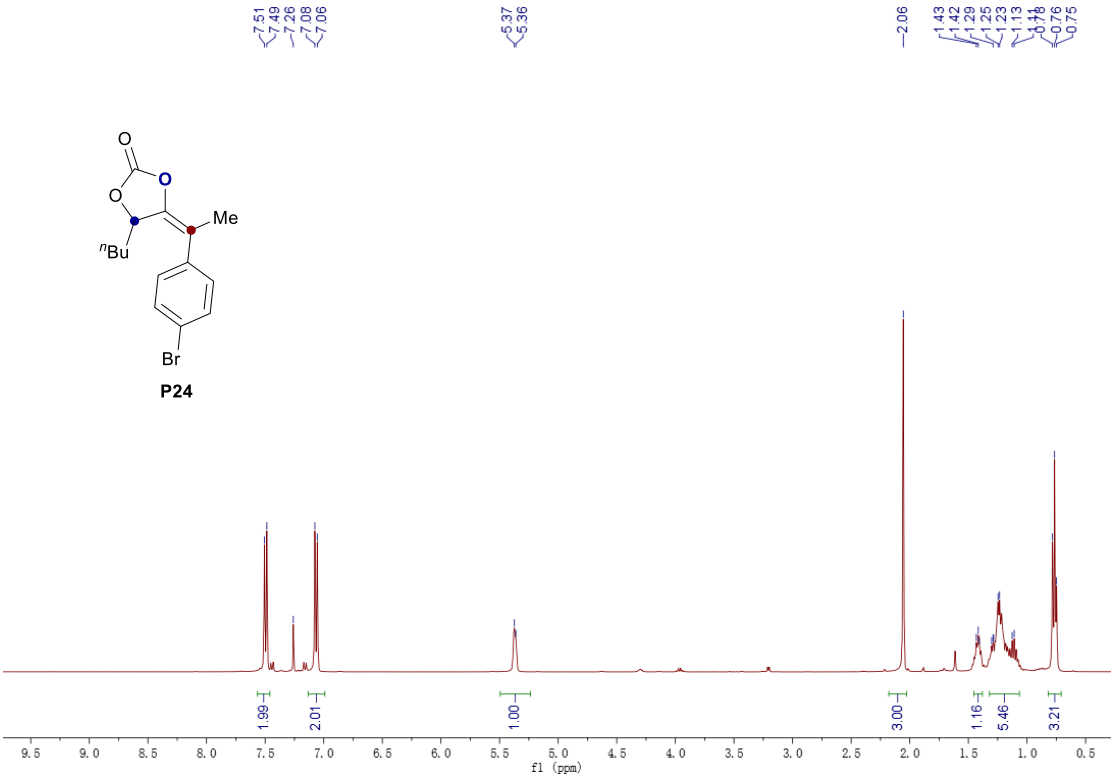
^{1}H NMR (400 MHz, $CDCl_3$)



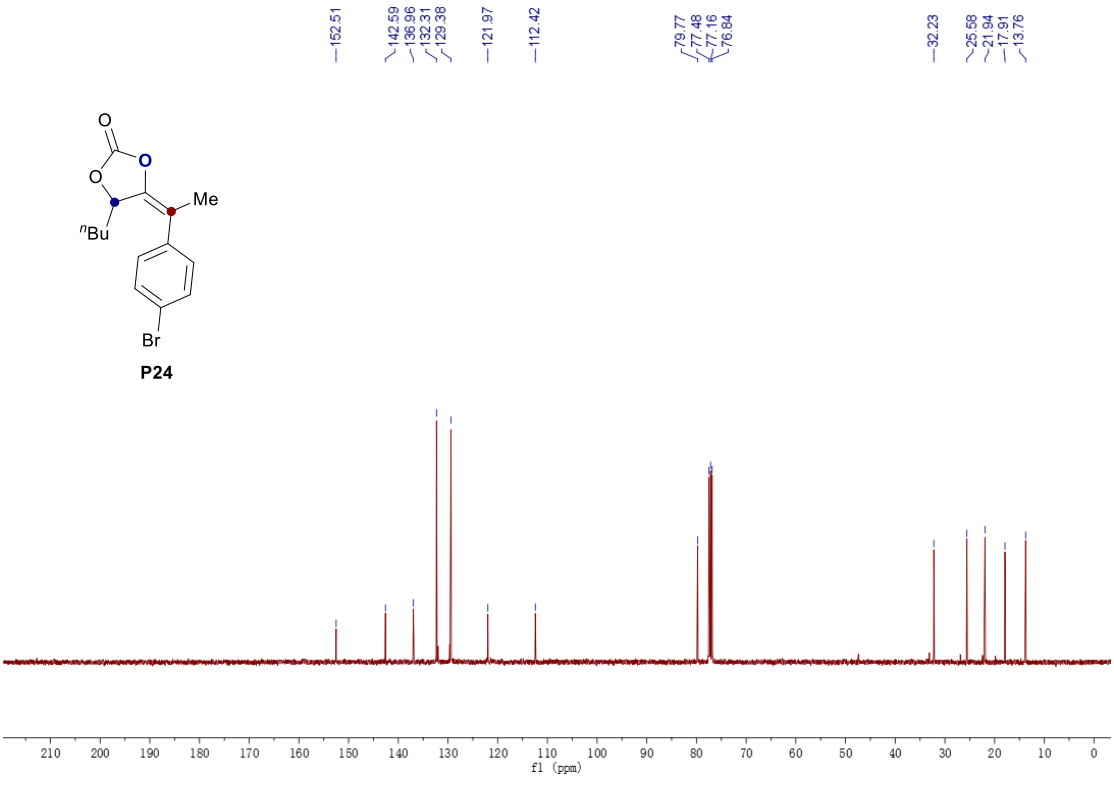
^{13}C NMR (100 MHz, $CDCl_3$)



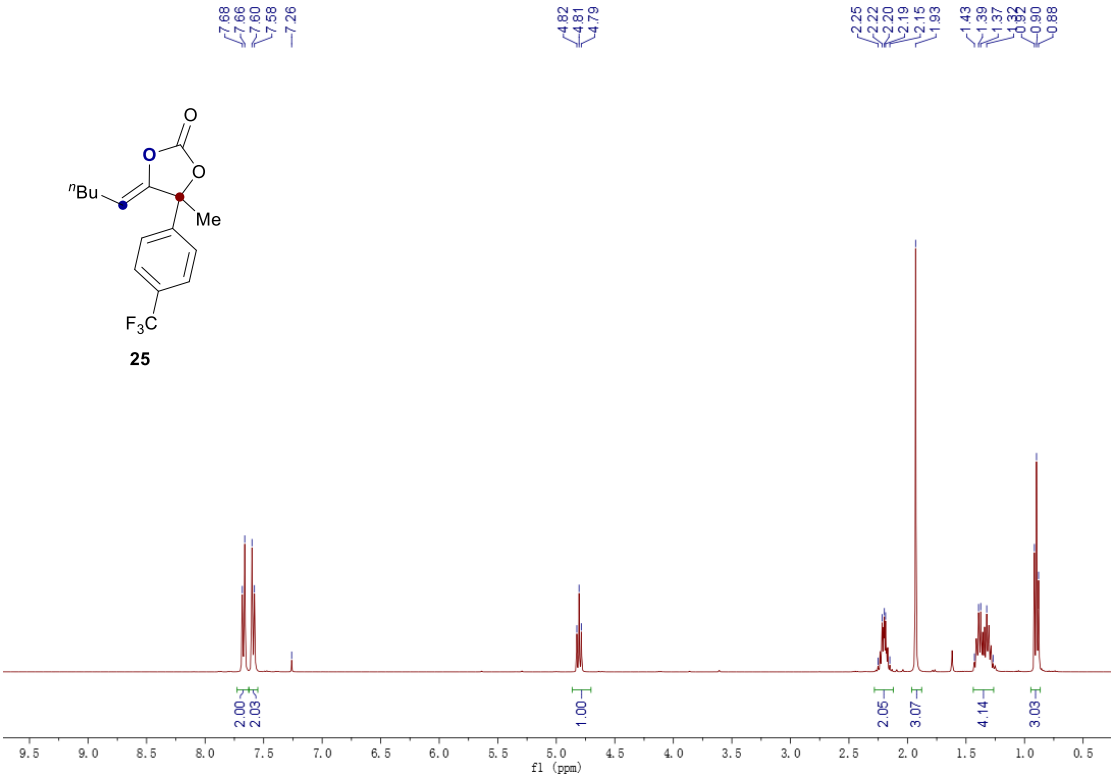
^{1}H NMR (400 MHz, $CDCl_3$)



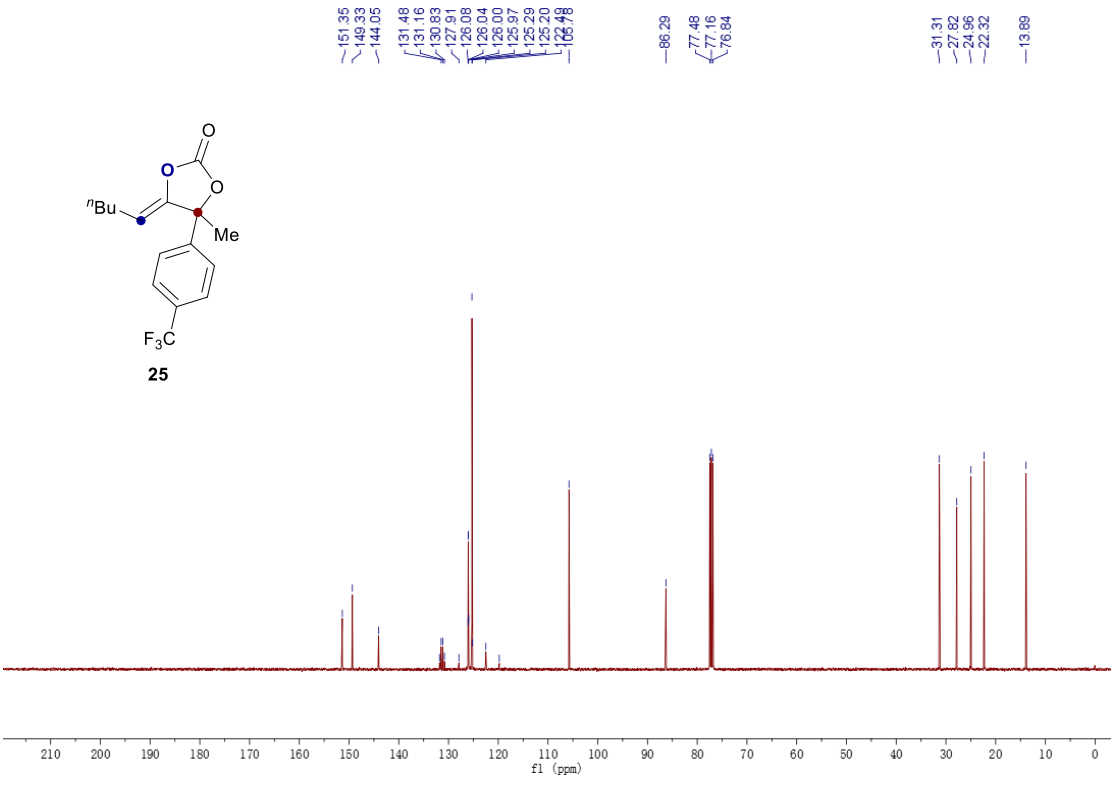
^{13}C NMR (100 MHz, $CDCl_3$)



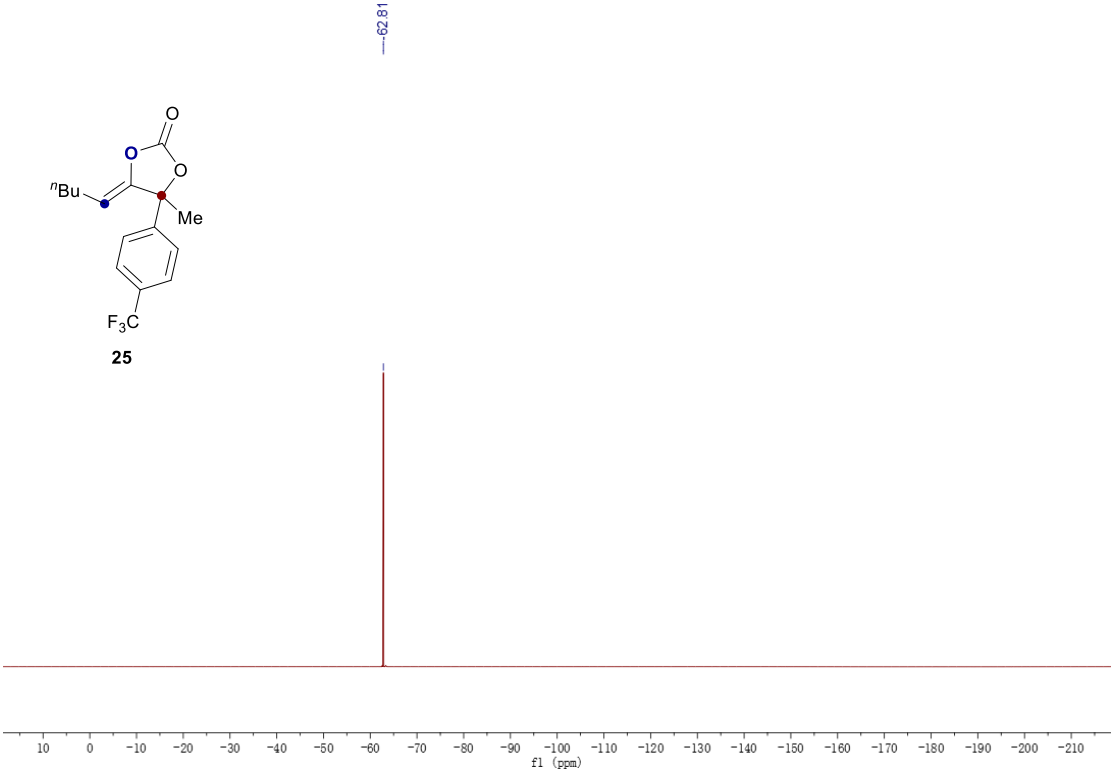
^{1}H NMR (400 MHz, $CDCl_3$)



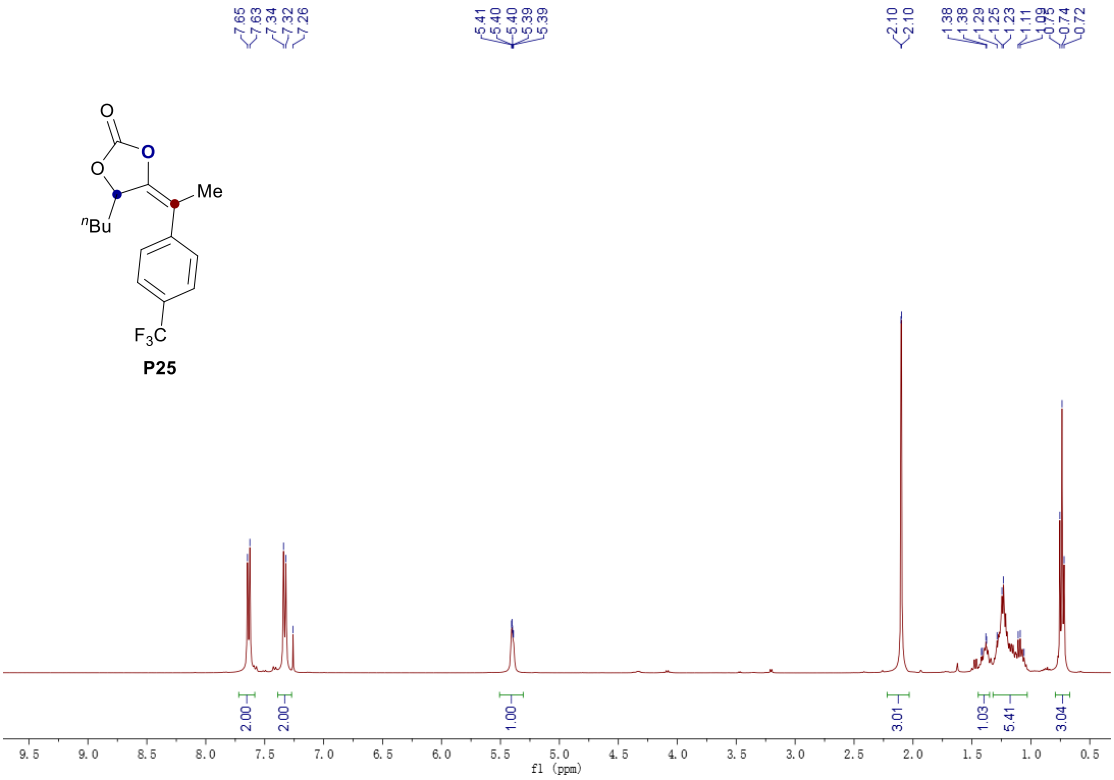
^{13}C NMR (100 MHz, $CDCl_3$)



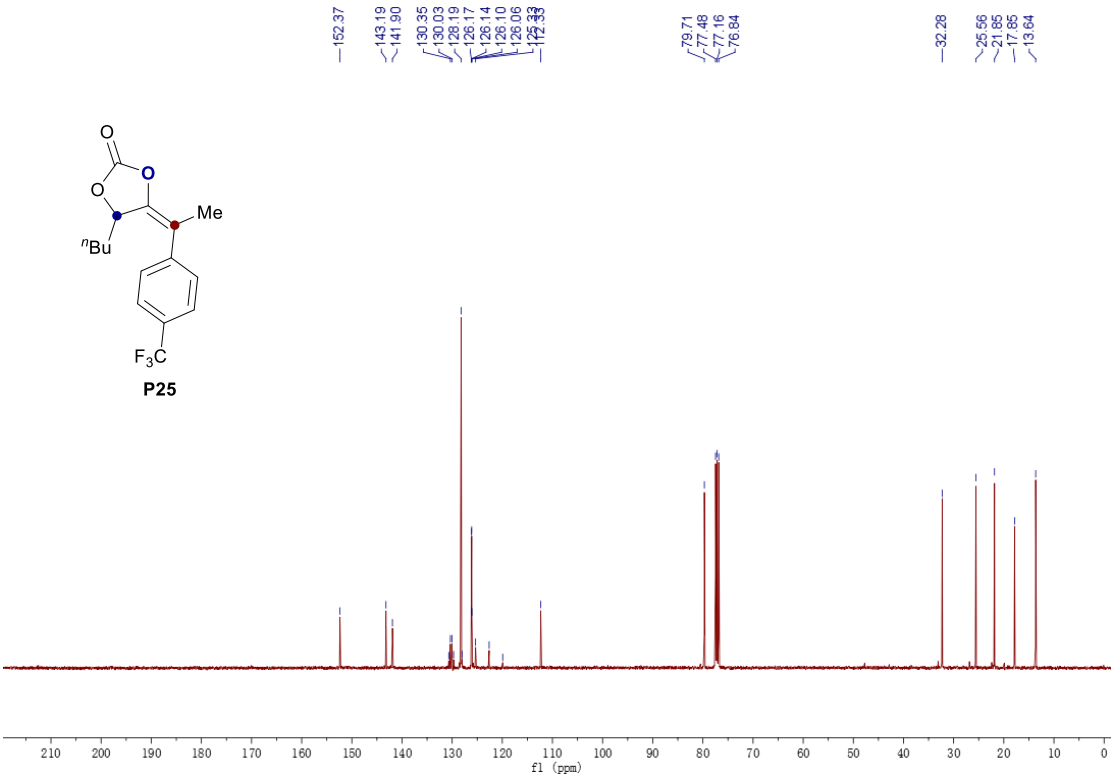
^{19}F NMR (376 MHz, $CDCl_3$)



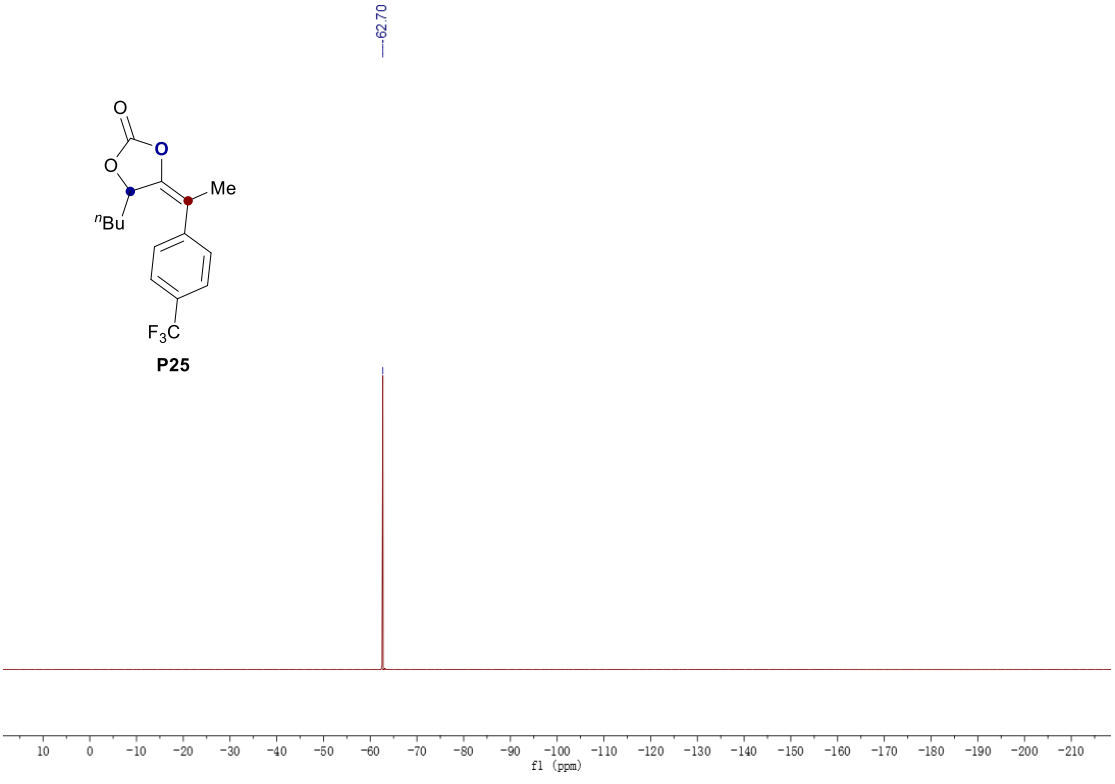
^{1}H NMR (400 MHz, $CDCl_3$)



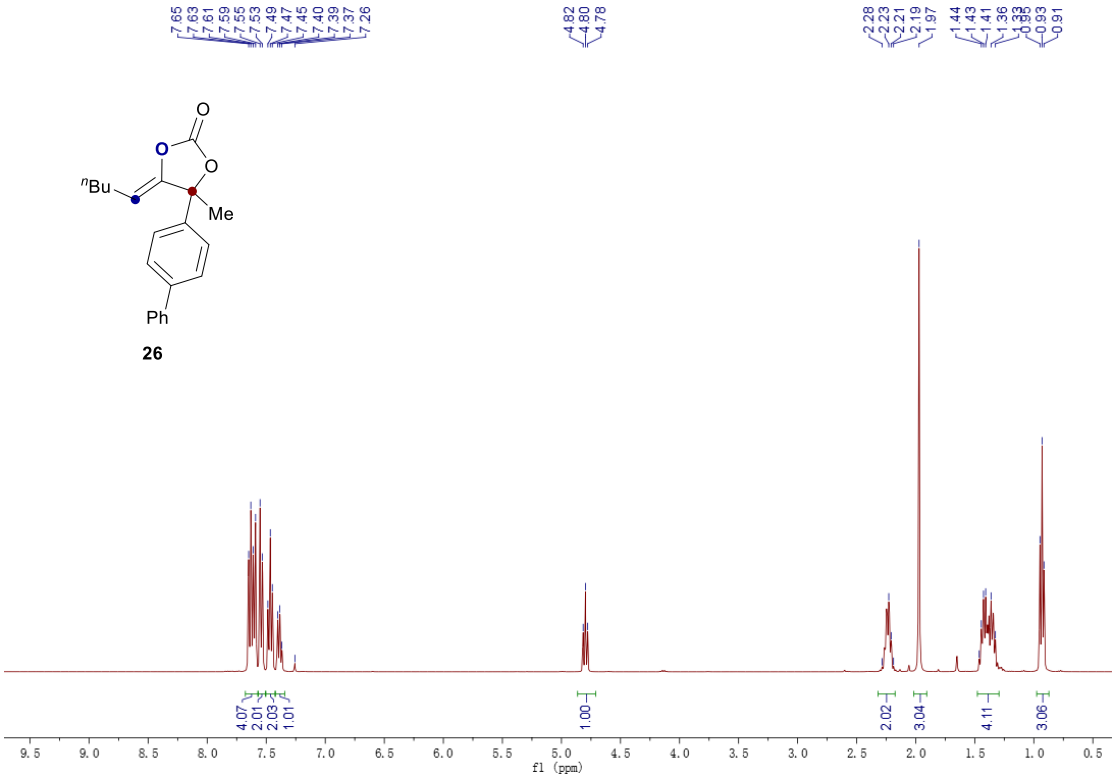
^{13}C NMR (100 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)

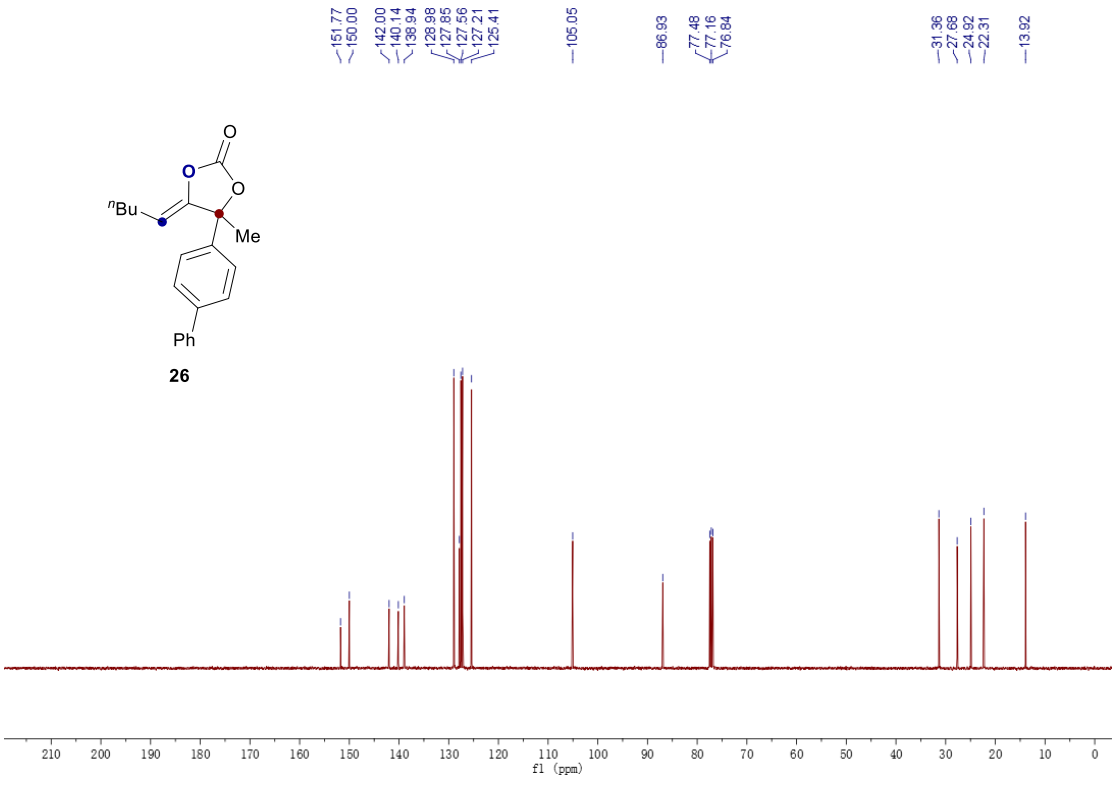


^{1}H NMR (400 MHz, $CDCl_3$)



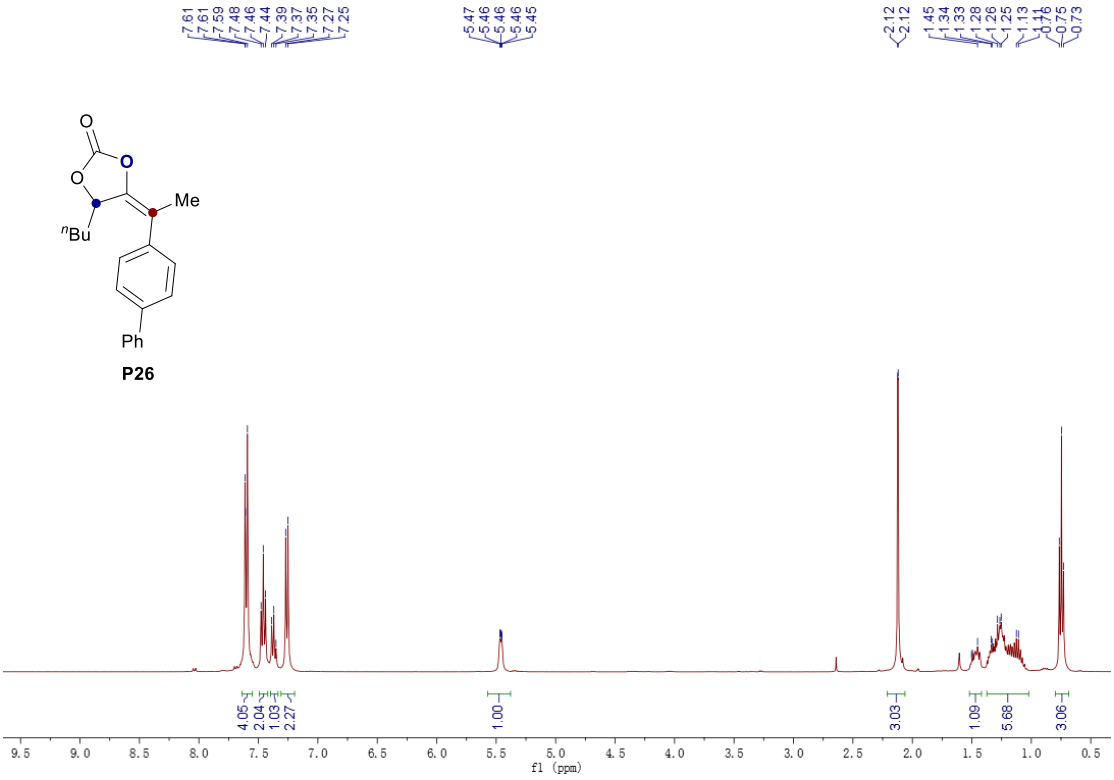
26

^{13}C NMR (100 MHz, $CDCl_3$)

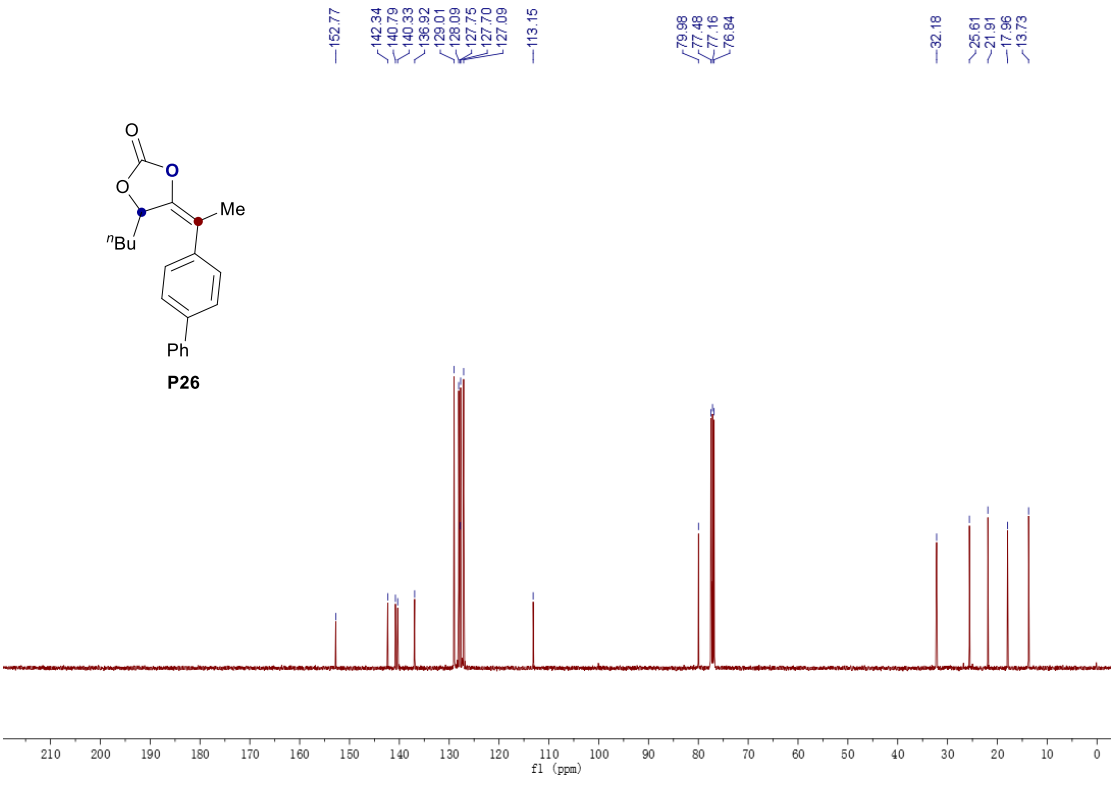


26

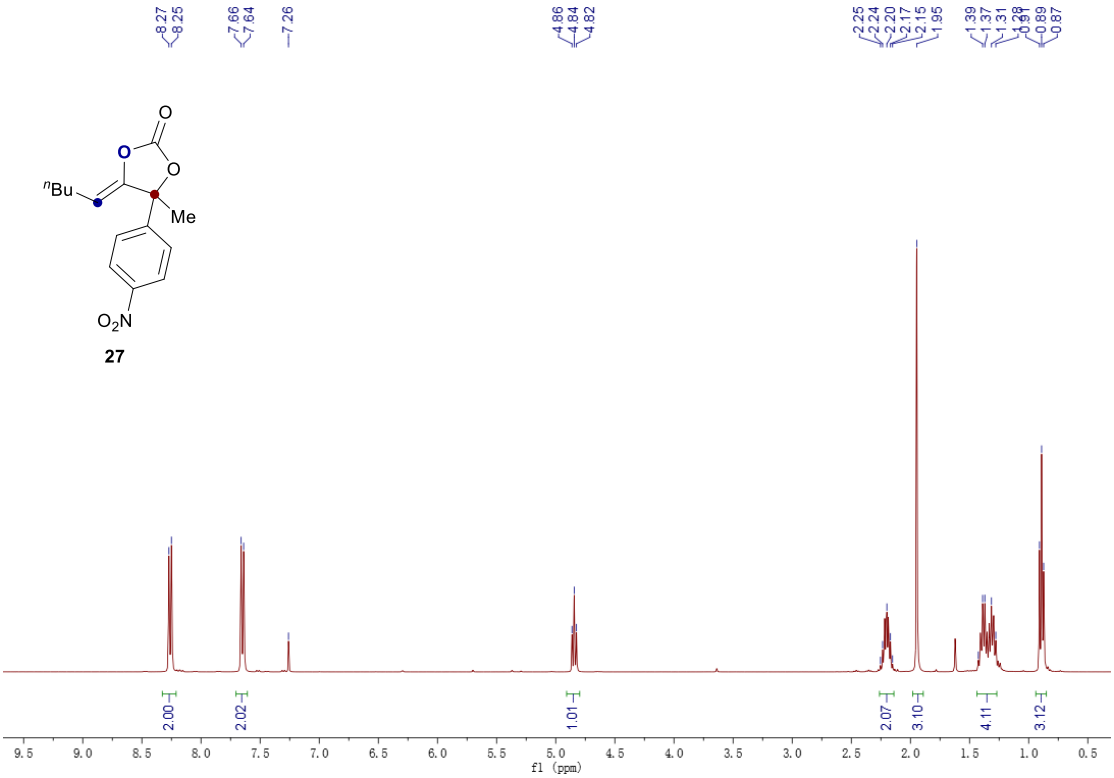
^{1}H NMR (400 MHz, $CDCl_3$)



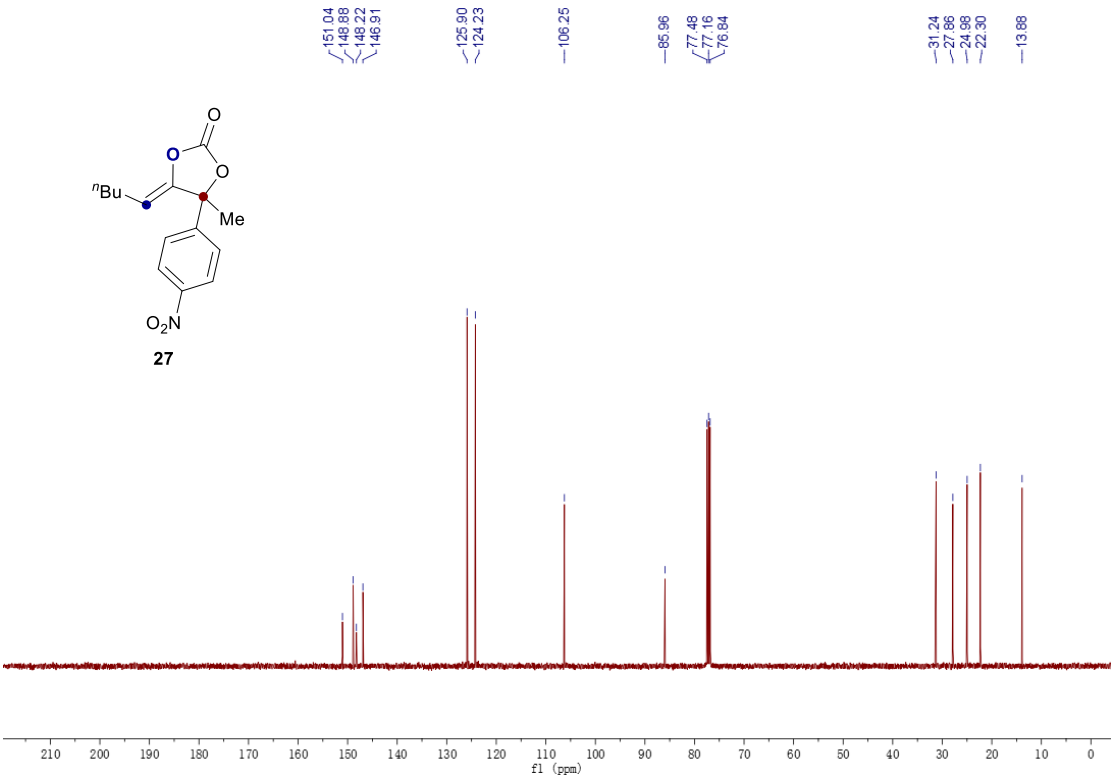
^{13}C NMR (100 MHz, $CDCl_3$)



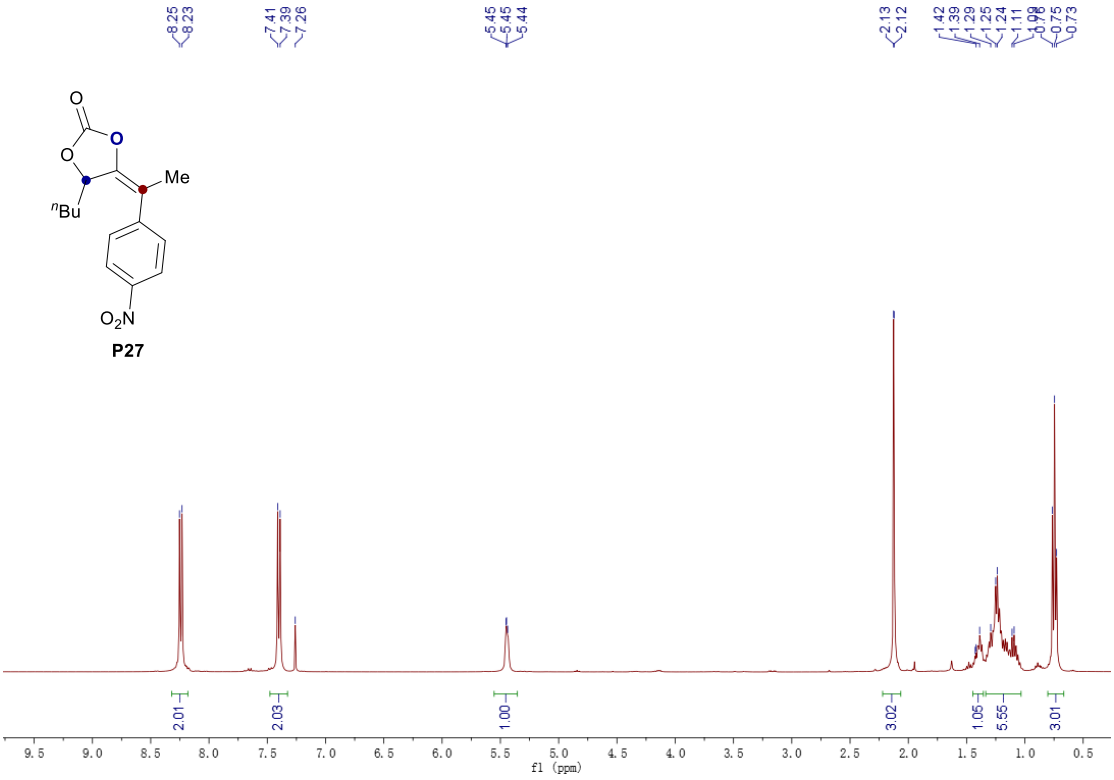
^{1}H NMR (400 MHz, $CDCl_3$)



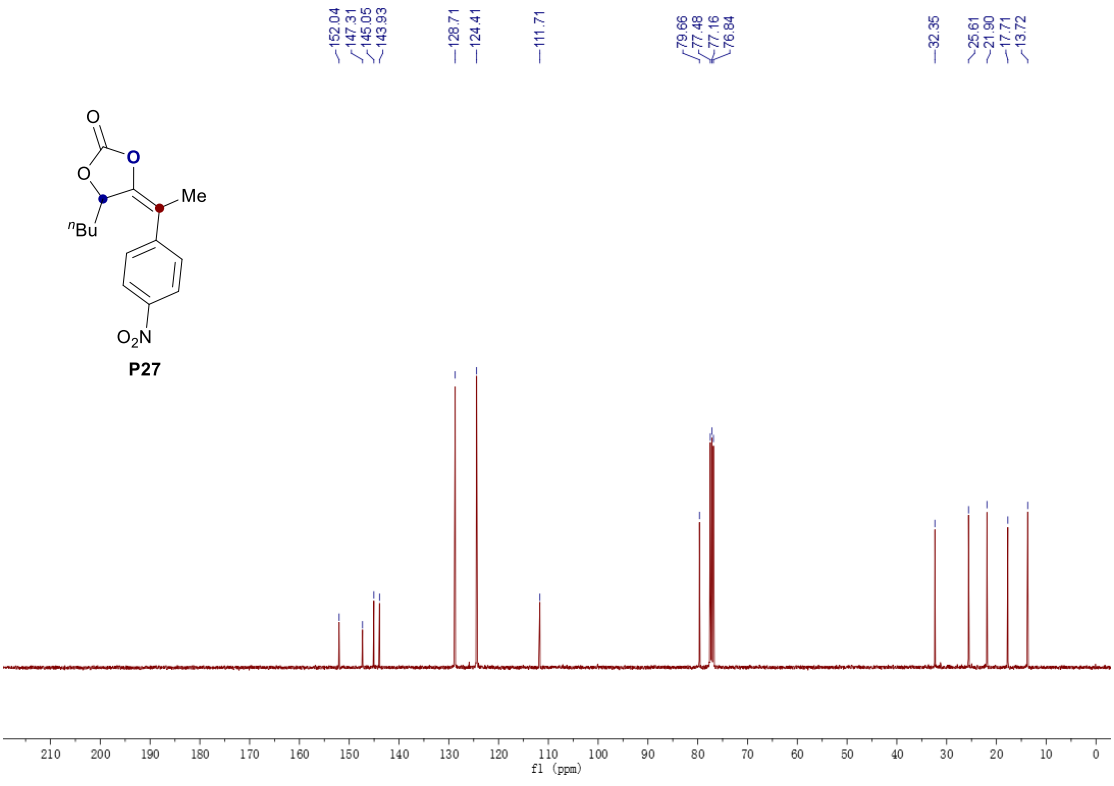
^{13}C NMR (100 MHz, $CDCl_3$)



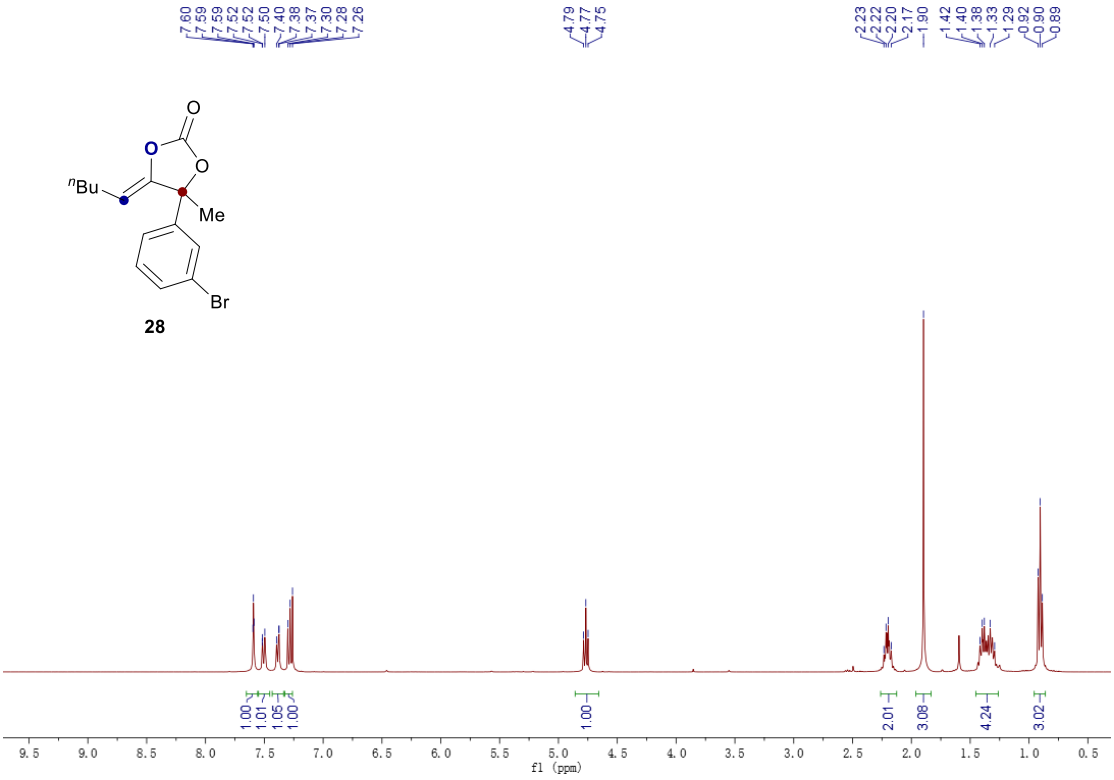
^{1}H NMR (400 MHz, $CDCl_3$)



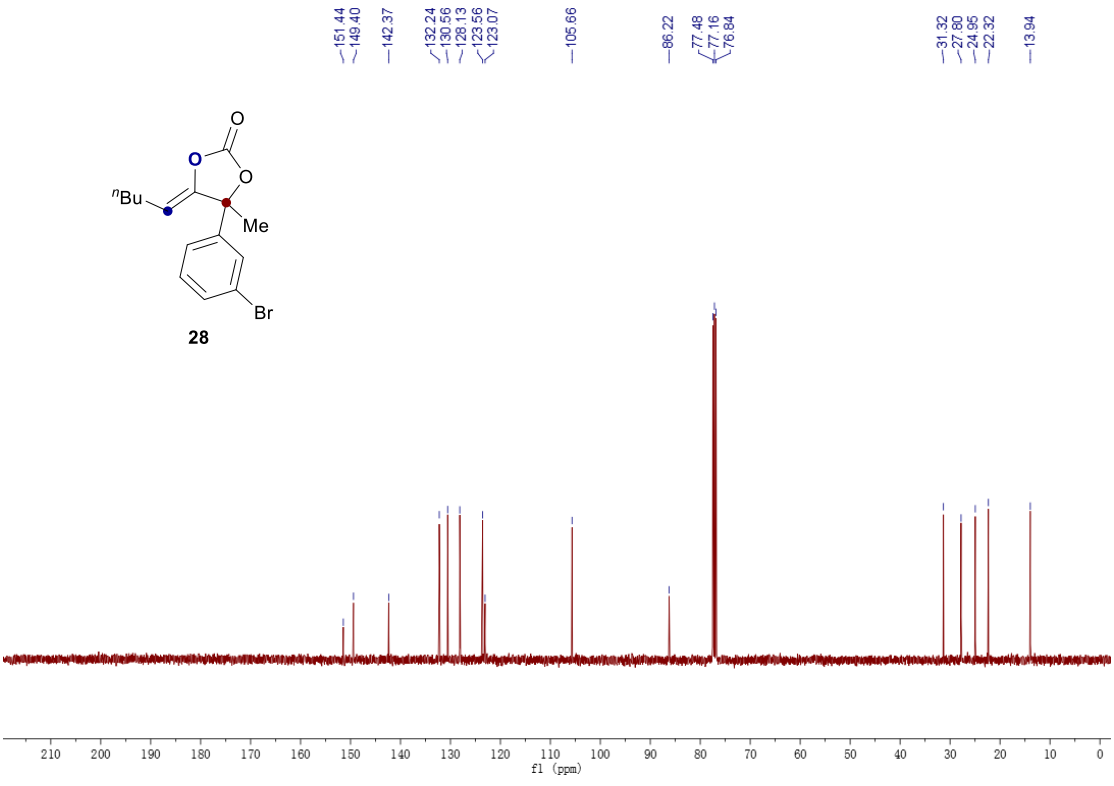
^{13}C NMR (100 MHz, $CDCl_3$)



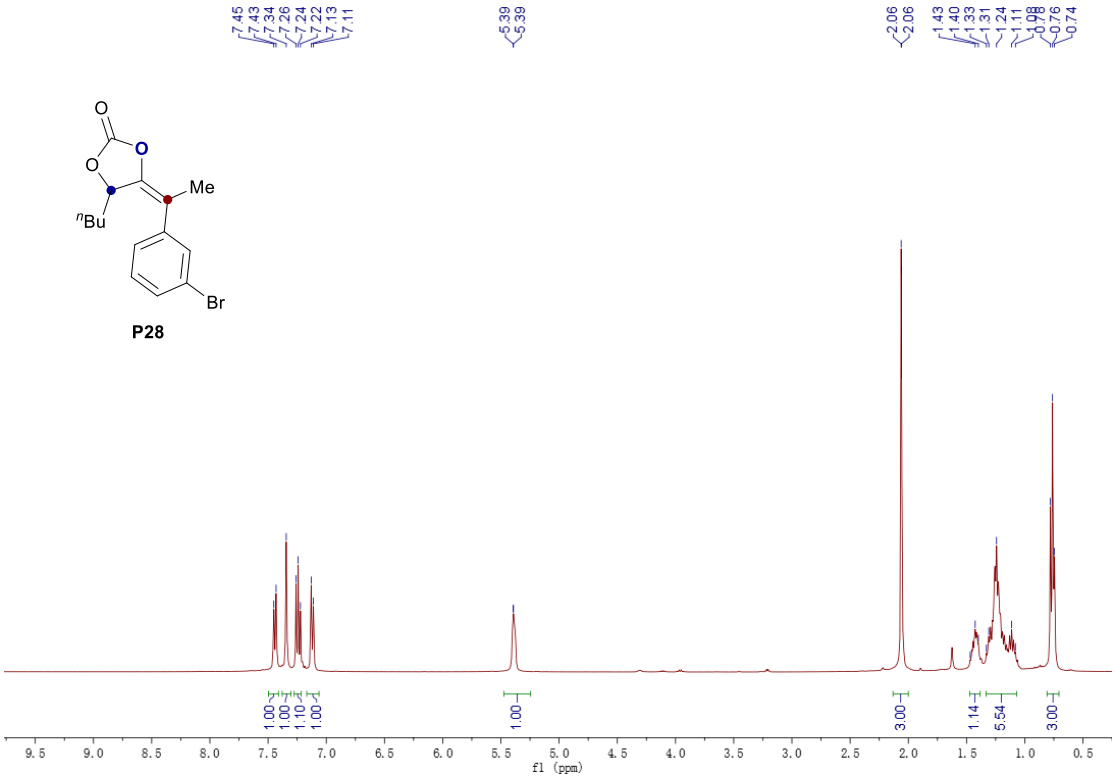
^{1}H NMR (400 MHz, $CDCl_3$)



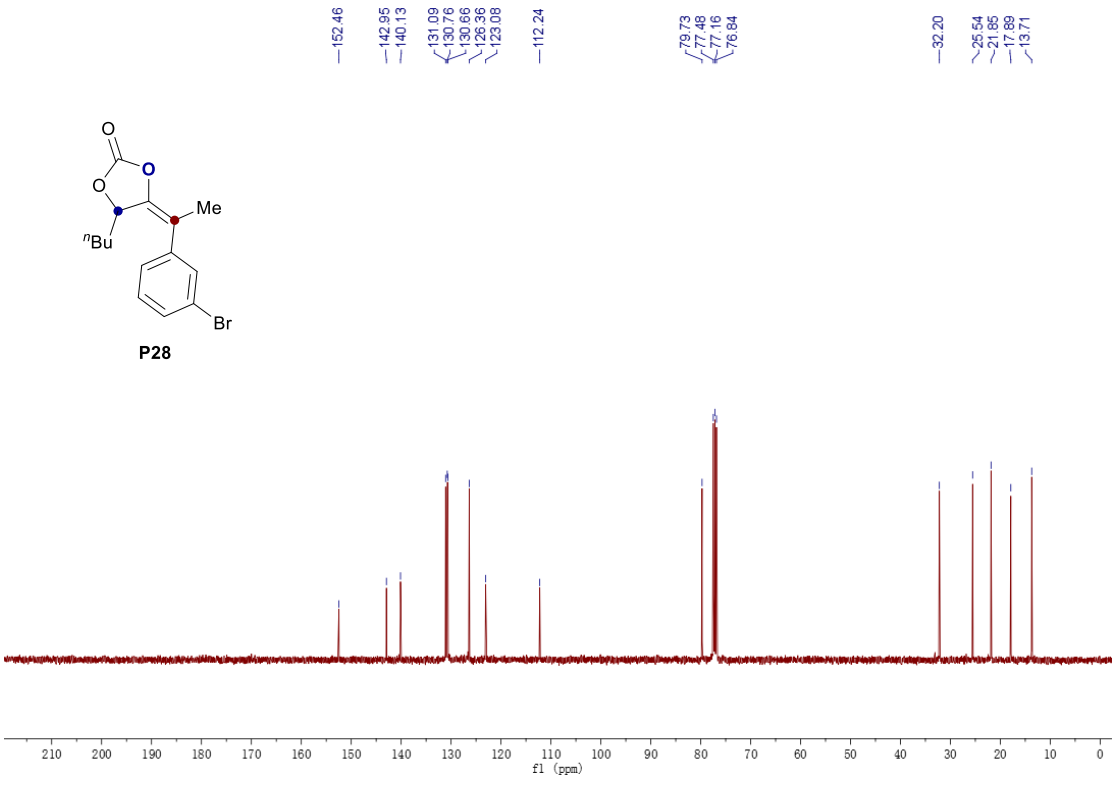
^{13}C NMR (100 MHz, $CDCl_3$)



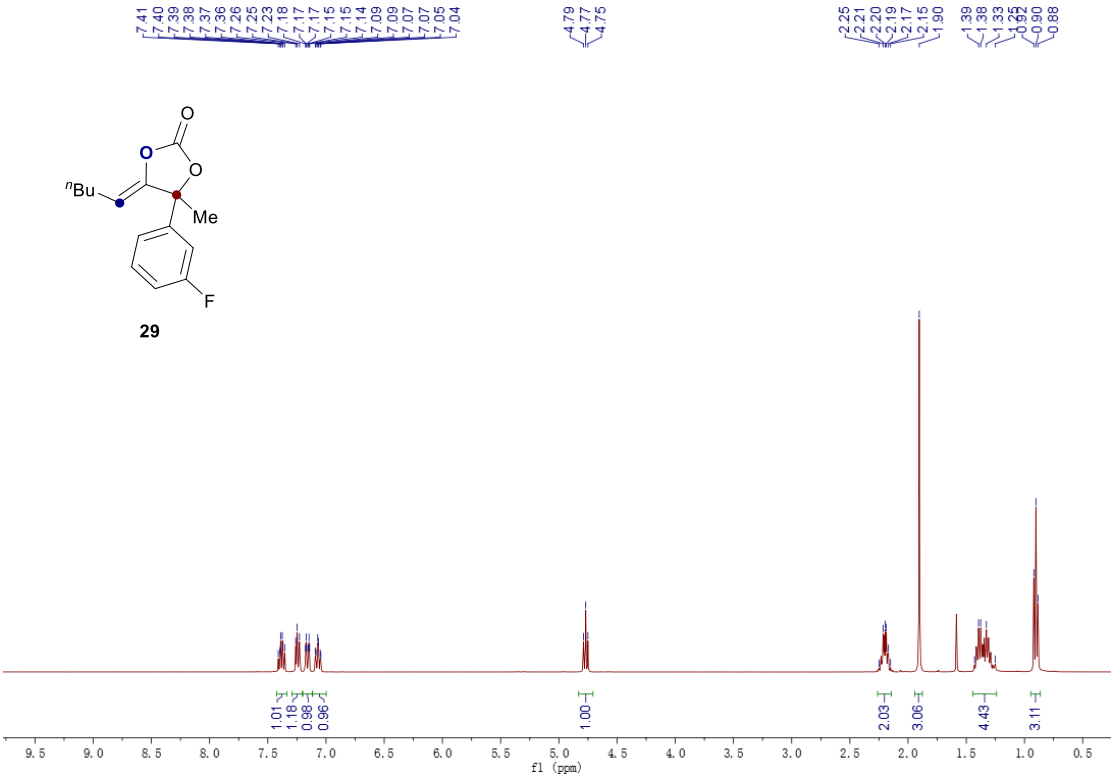
^{1}H NMR (400 MHz, $CDCl_3$)



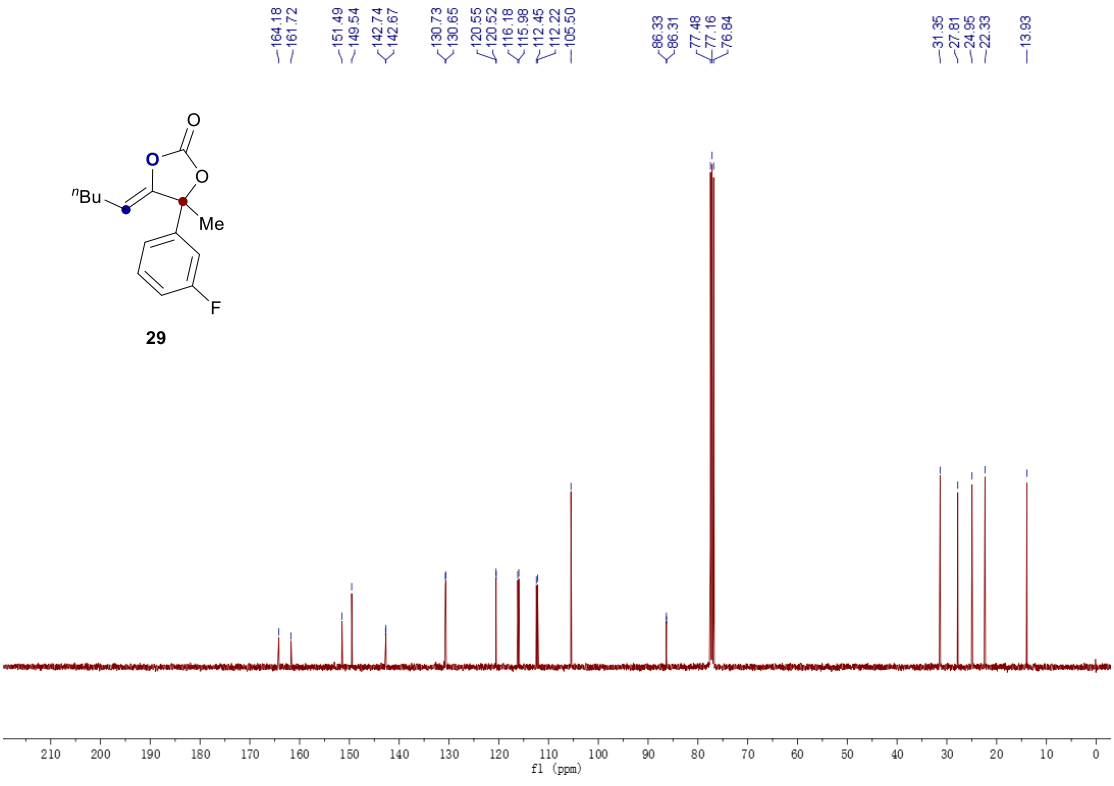
^{13}C NMR (100 MHz, $CDCl_3$)



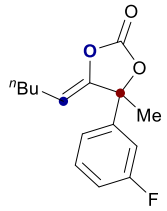
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)

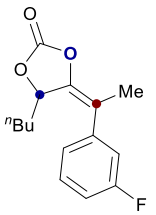


^{19}F NMR (376 MHz, $CDCl_3$)



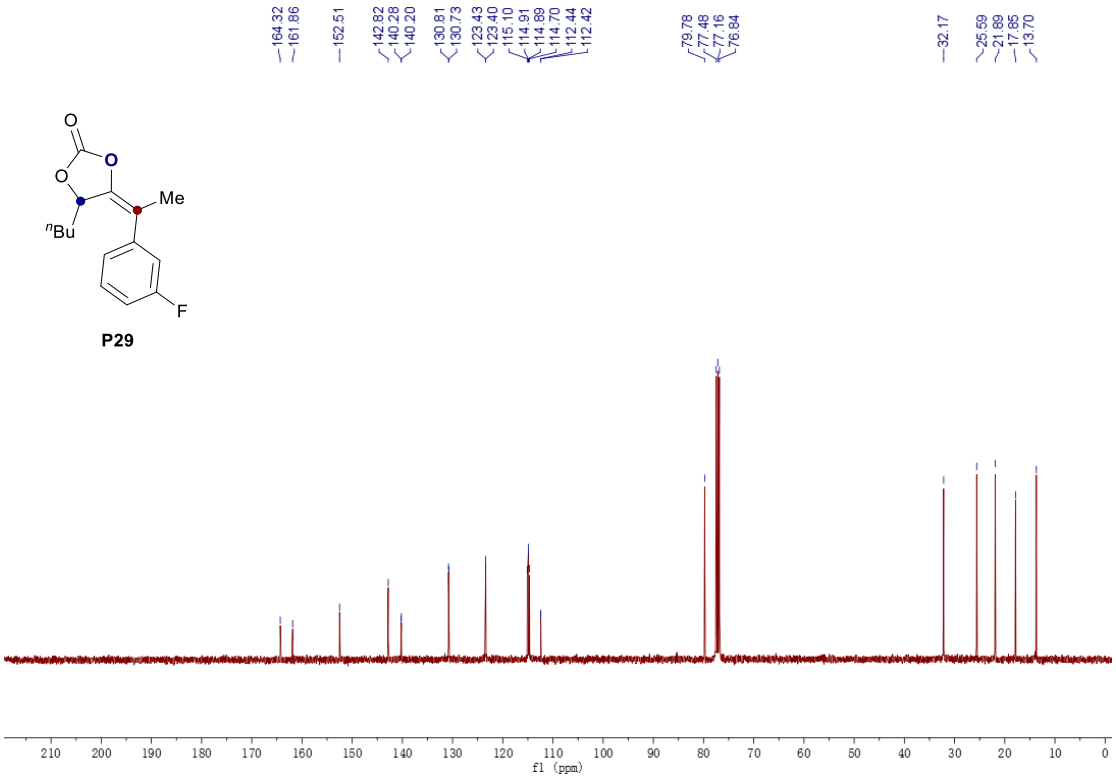
29

^1H NMR (400 MHz, $CDCl_3$)

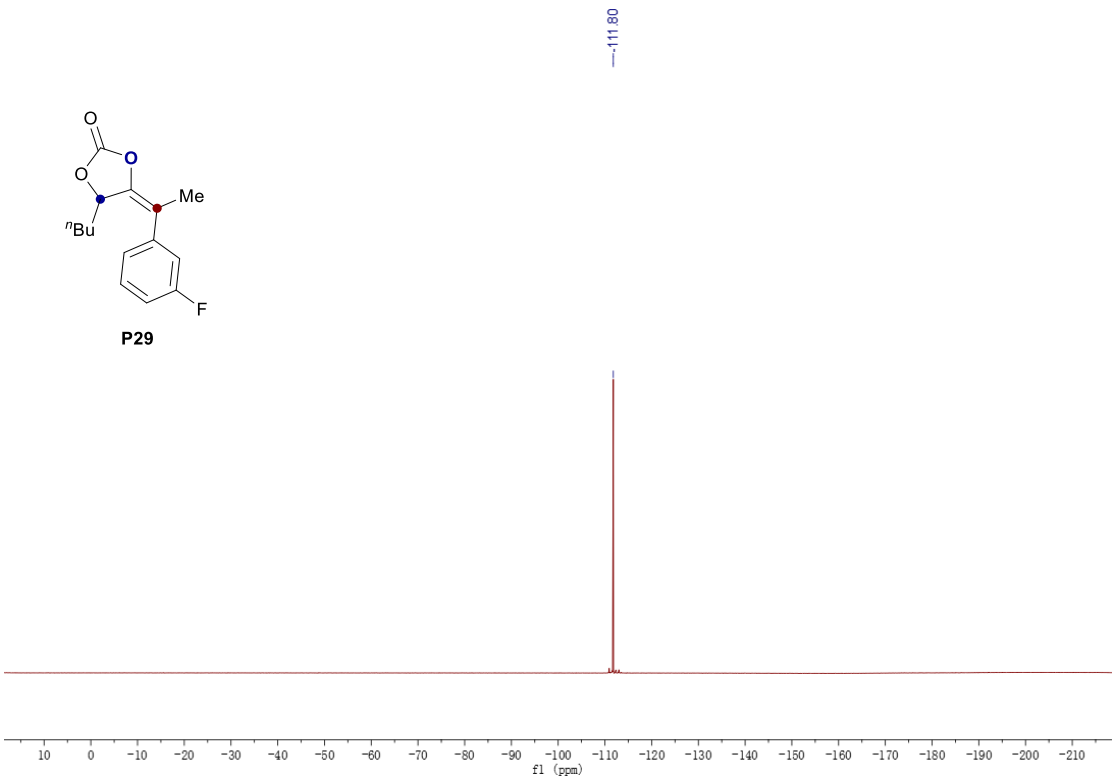


P29

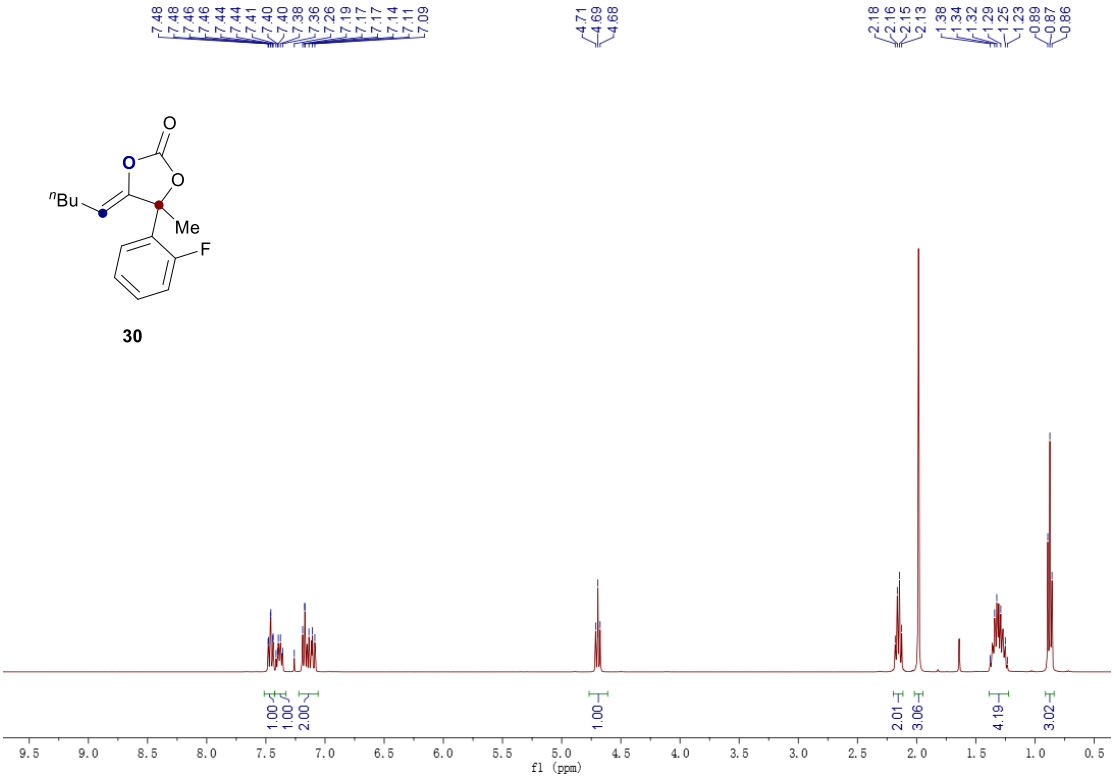
^{13}C NMR (100 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)

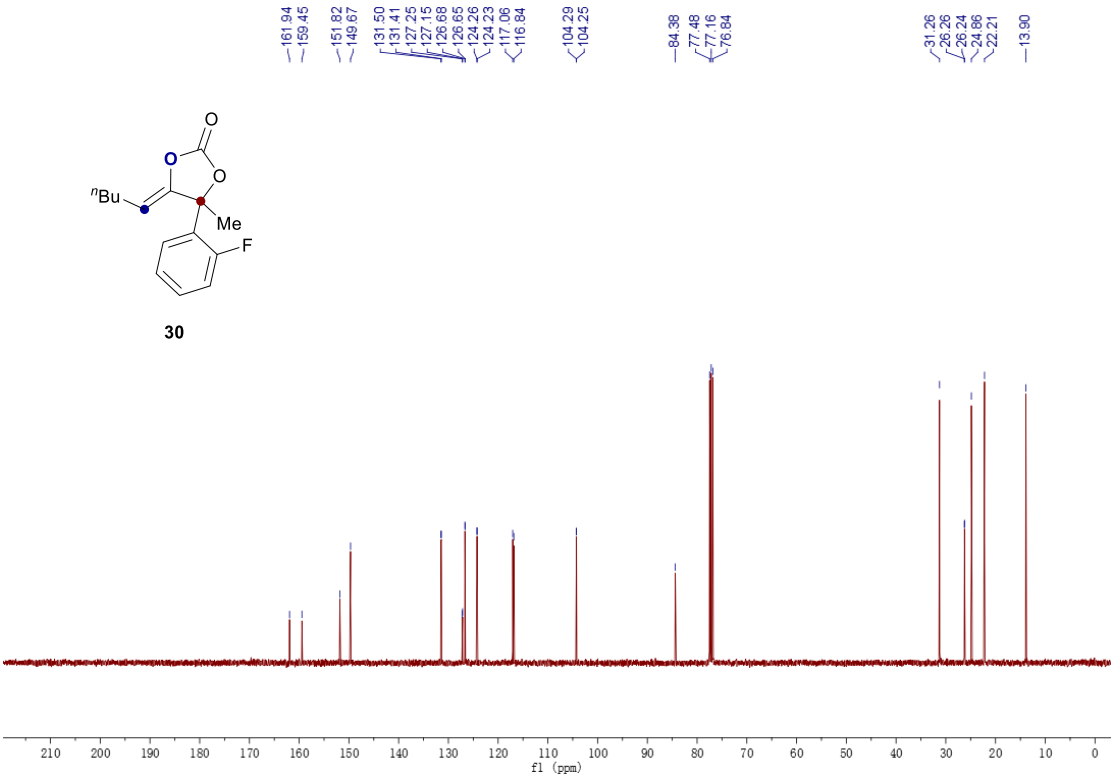


^{1}H NMR (400 MHz, $CDCl_3$)



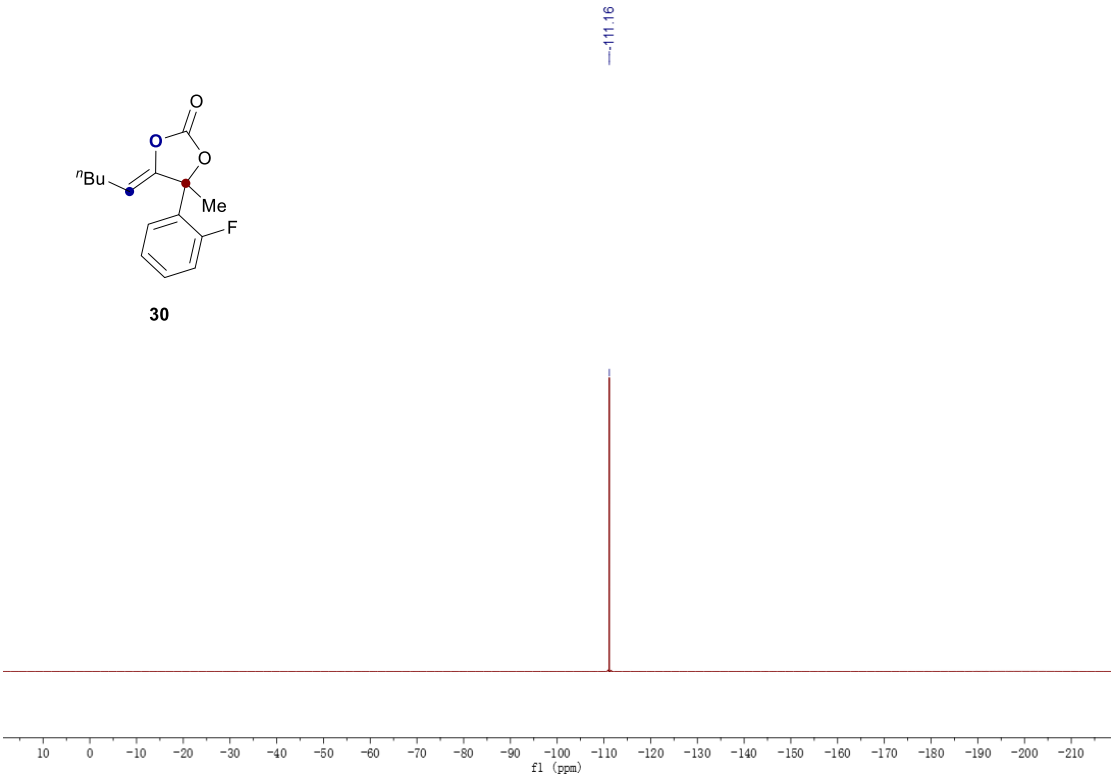
30

^{13}C NMR (100 MHz, $CDCl_3$)

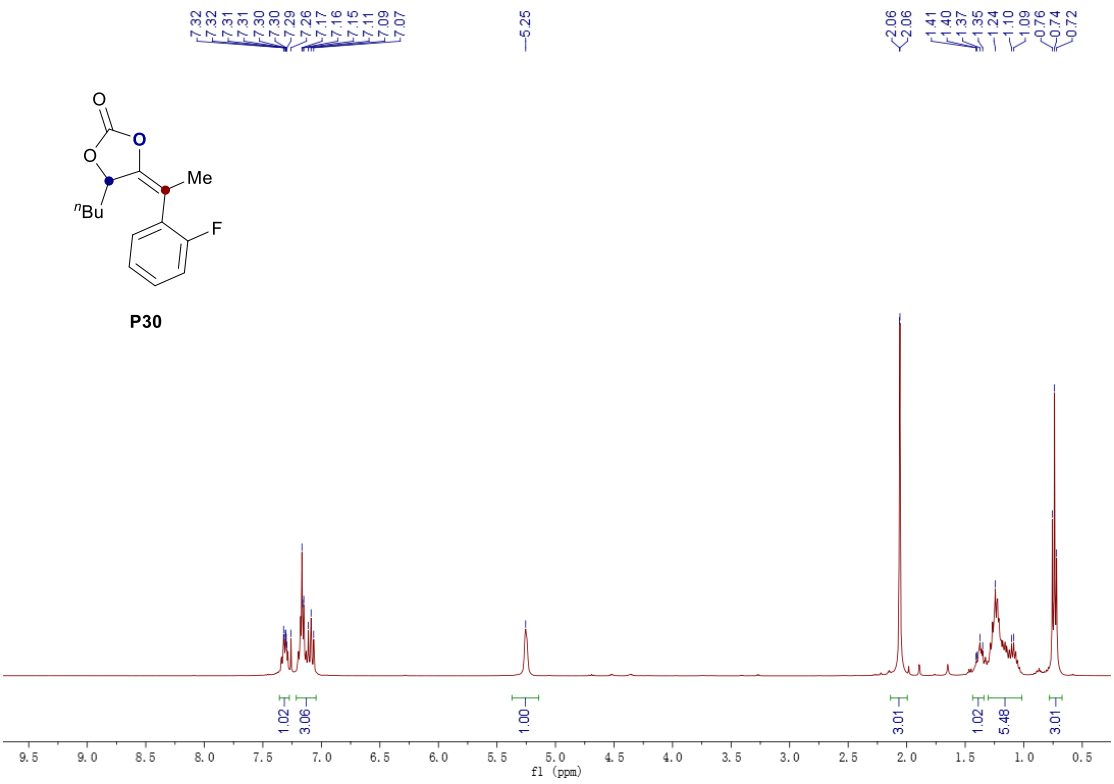


30

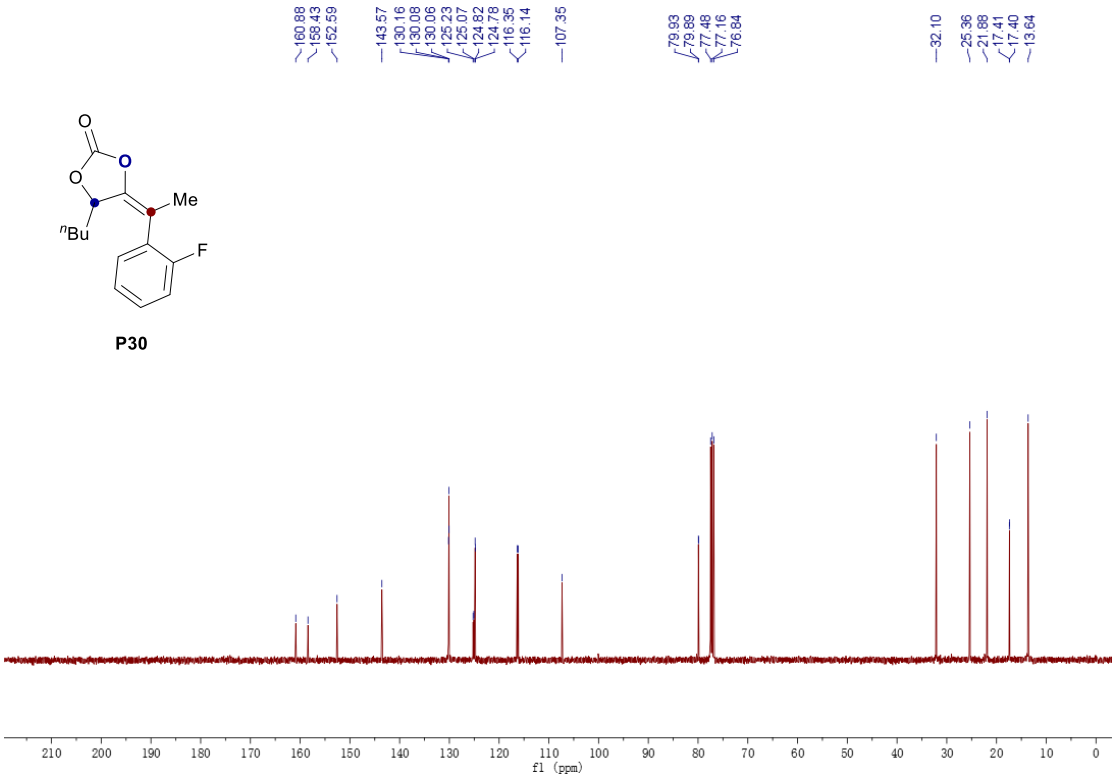
^{19}F NMR (376 MHz, $CDCl_3$)



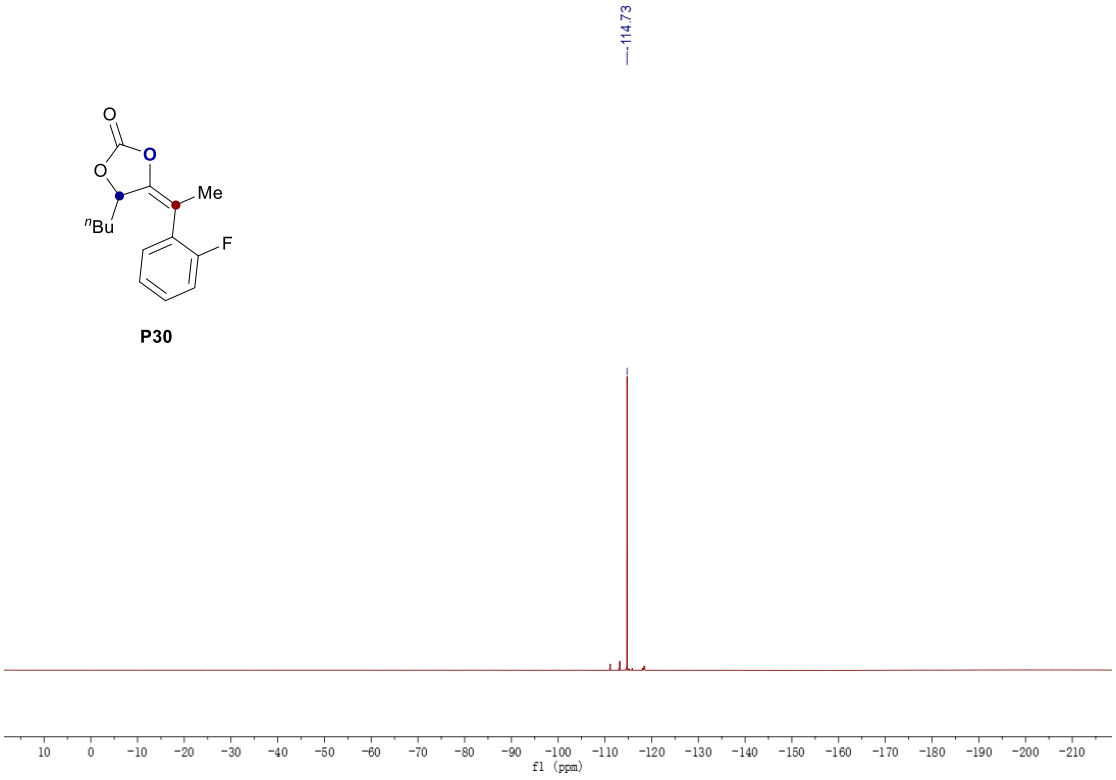
^{1}H NMR (400 MHz, $CDCl_3$)



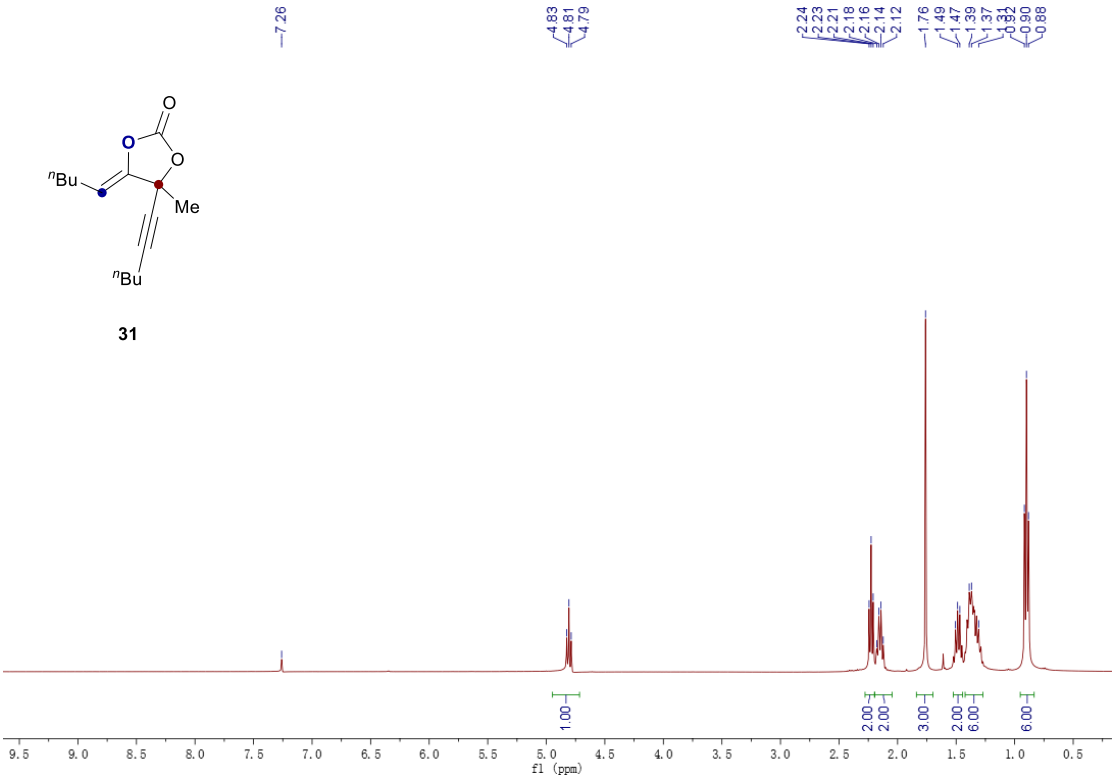
^{13}C NMR (100 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)

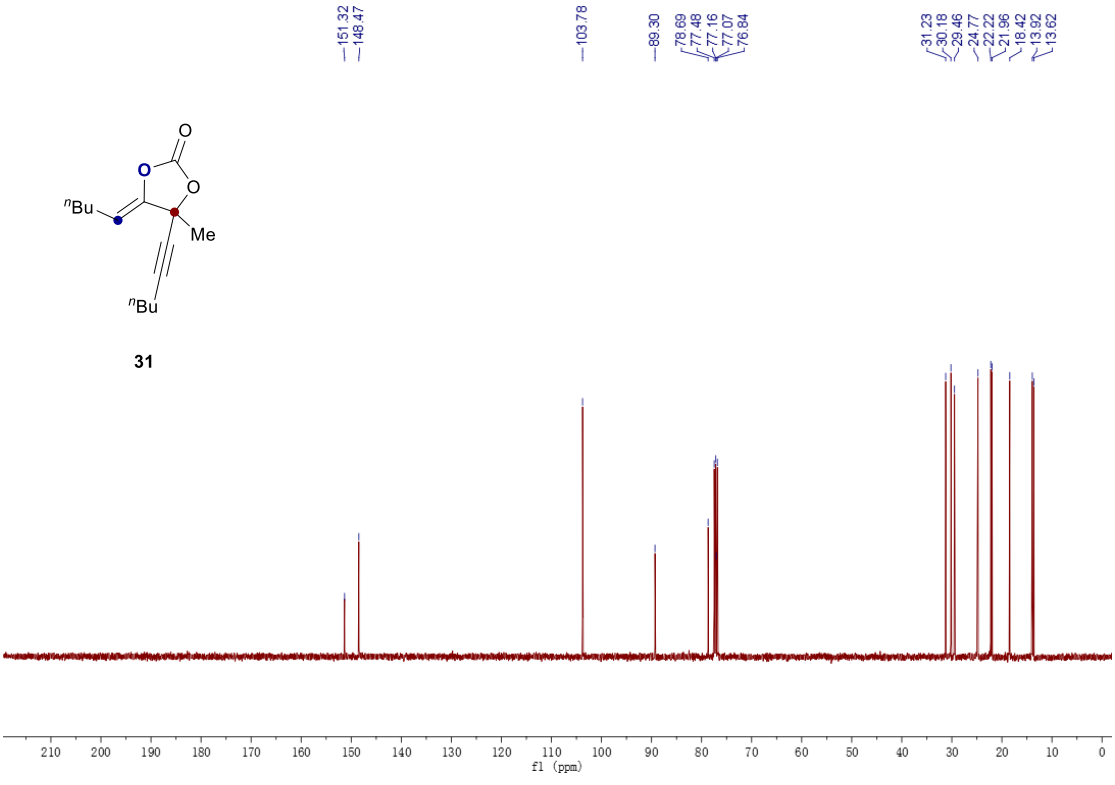


^{1}H NMR (400 MHz, $CDCl_3$)



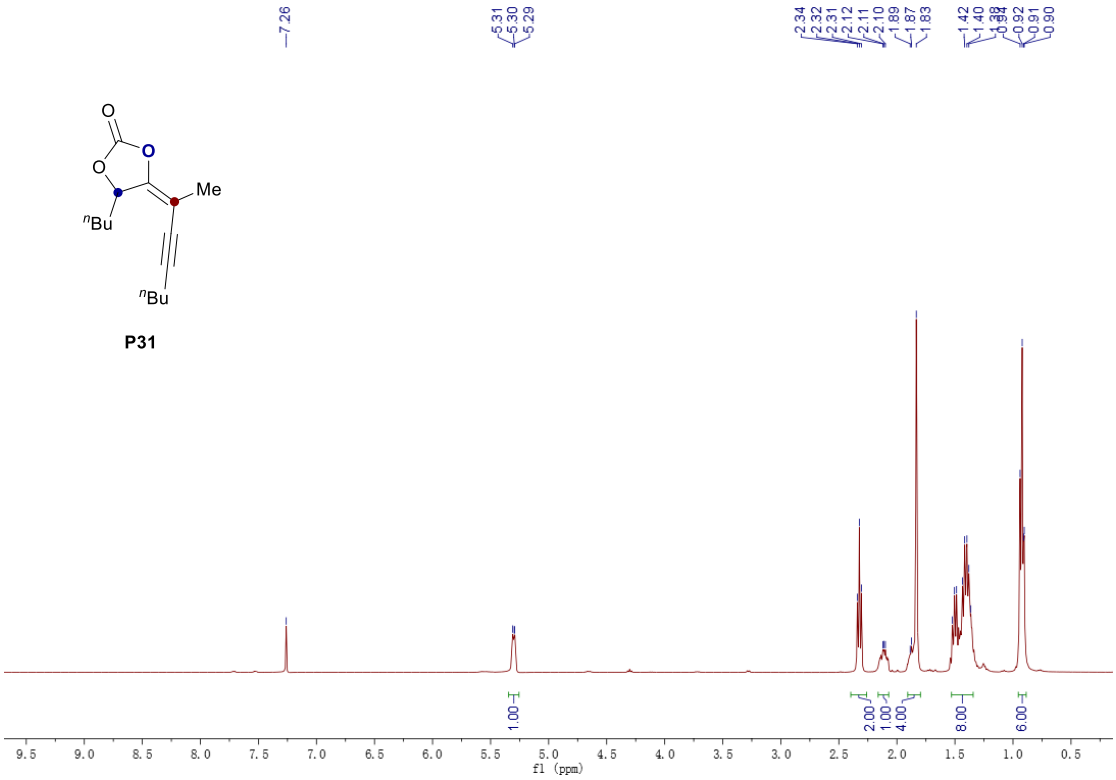
31

^{13}C NMR (100 MHz, $CDCl_3$)

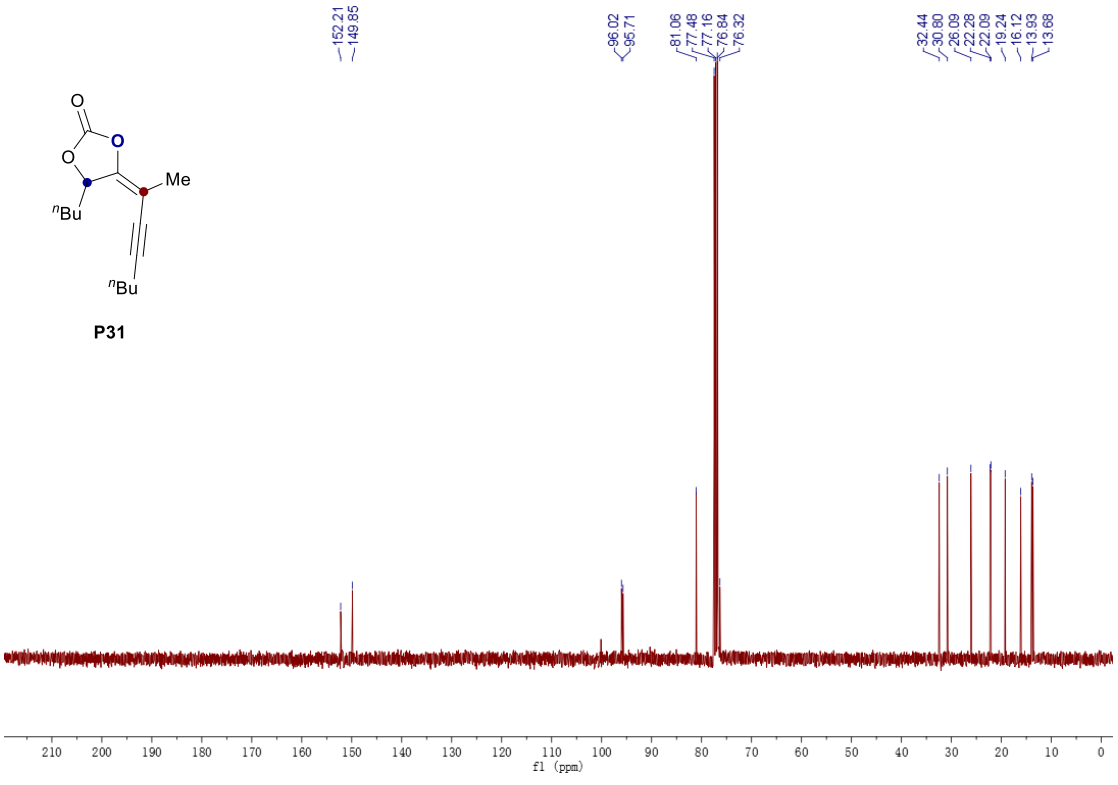


31

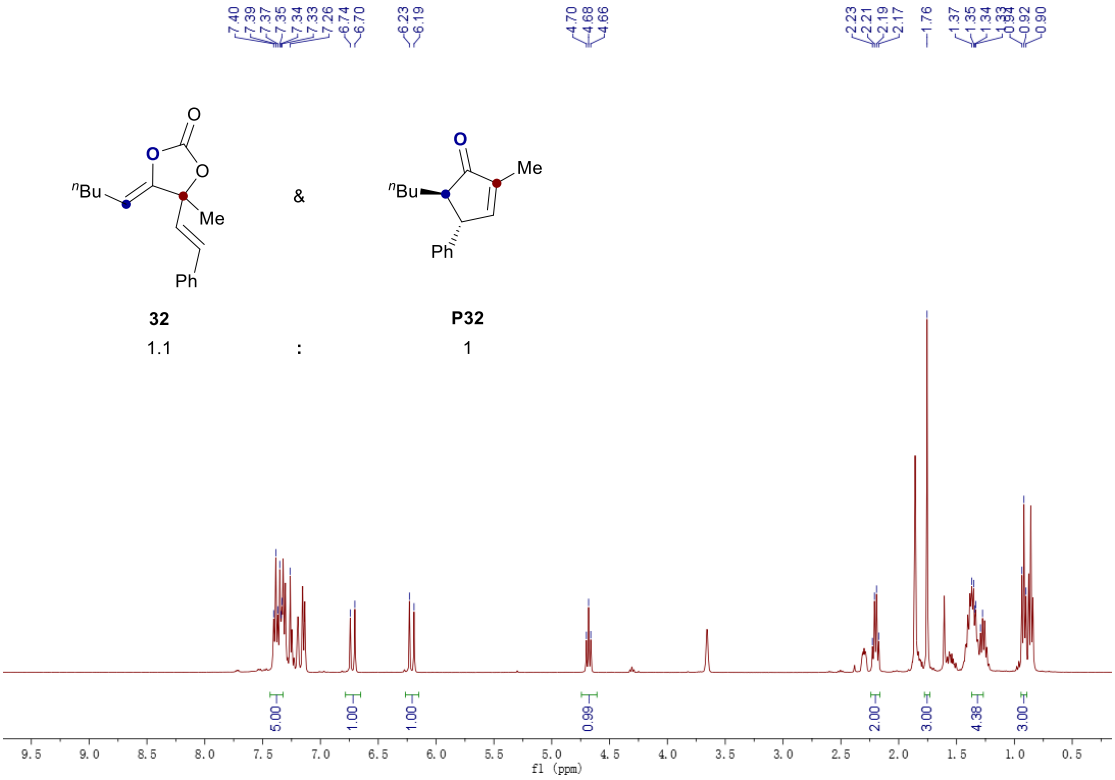
^{1}H NMR (400 MHz, $CDCl_3$)



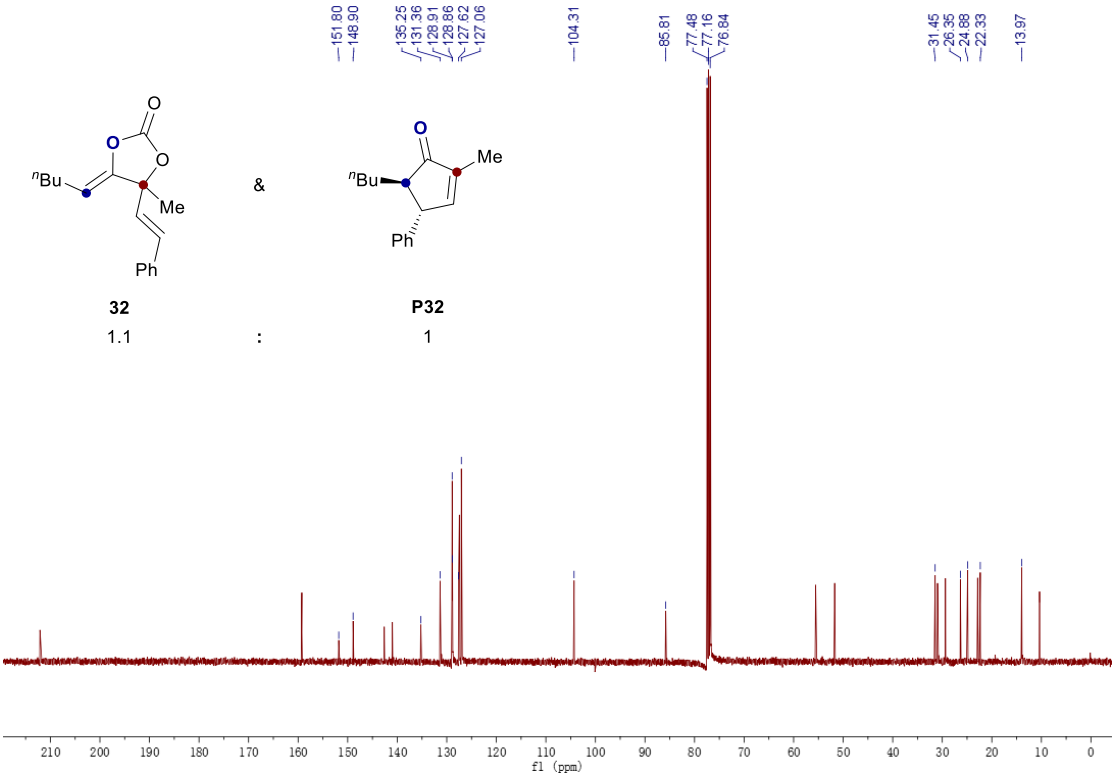
^{13}C NMR (100 MHz, $CDCl_3$)



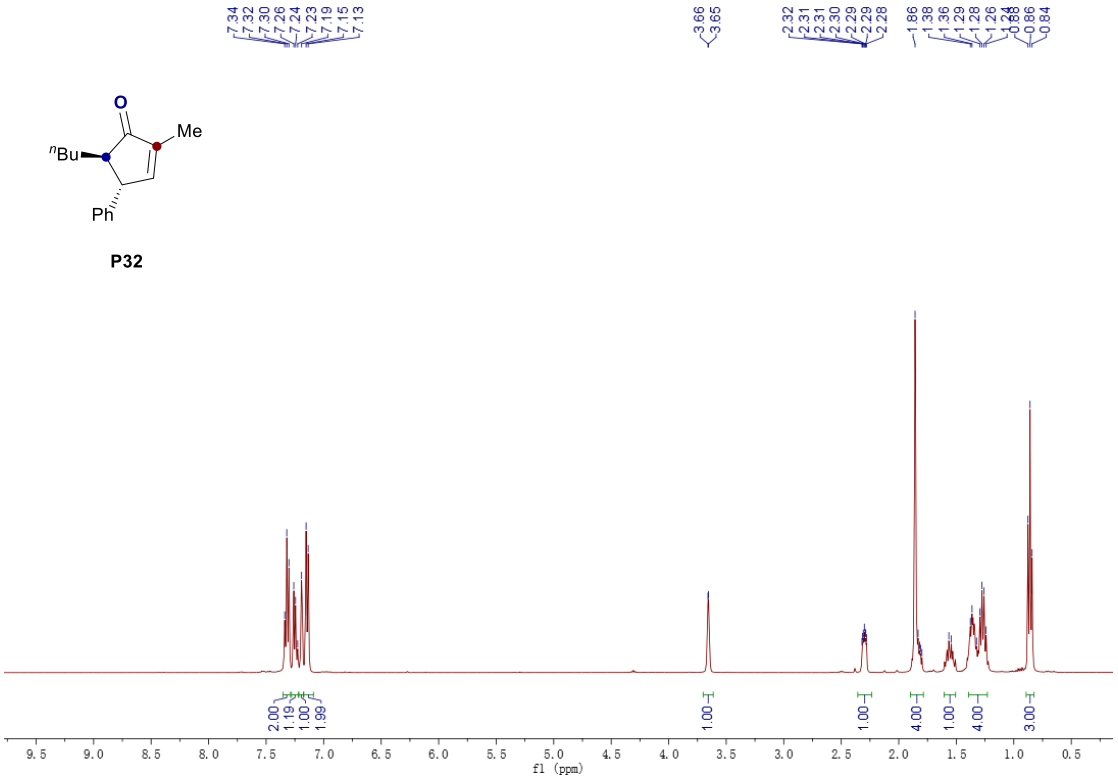
^{1}H NMR (400 MHz, $CDCl_3$)



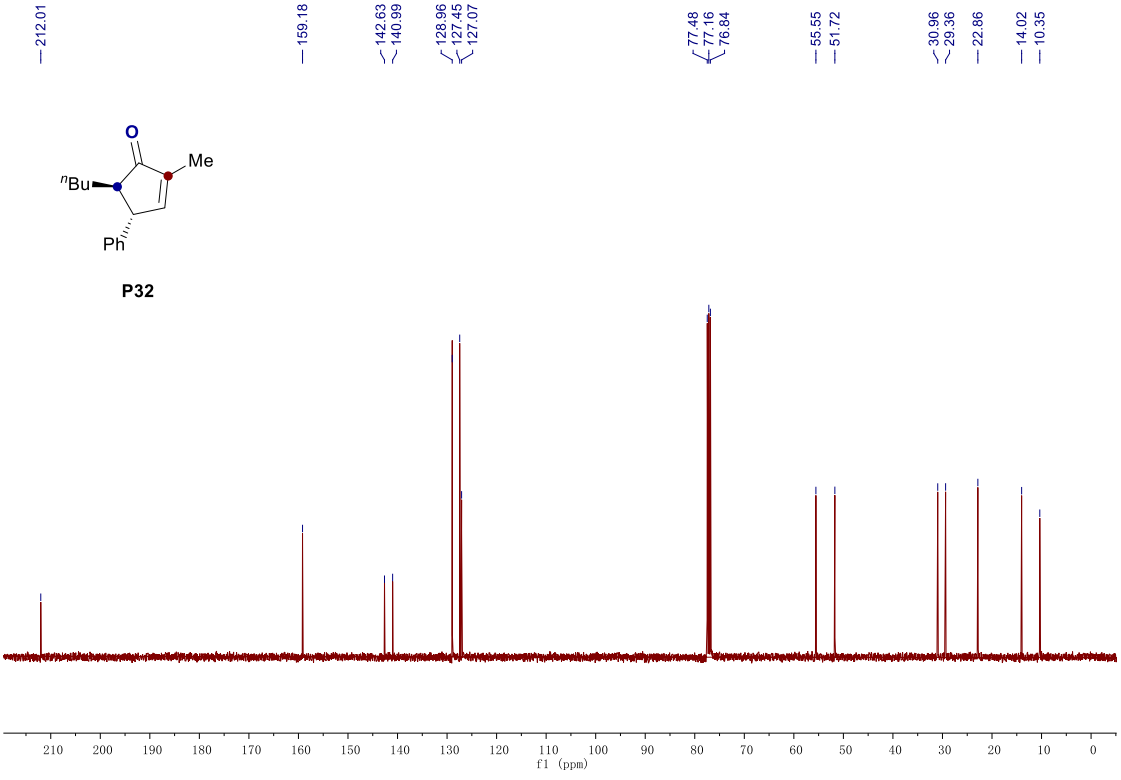
^{13}C NMR (100 MHz, $CDCl_3$)



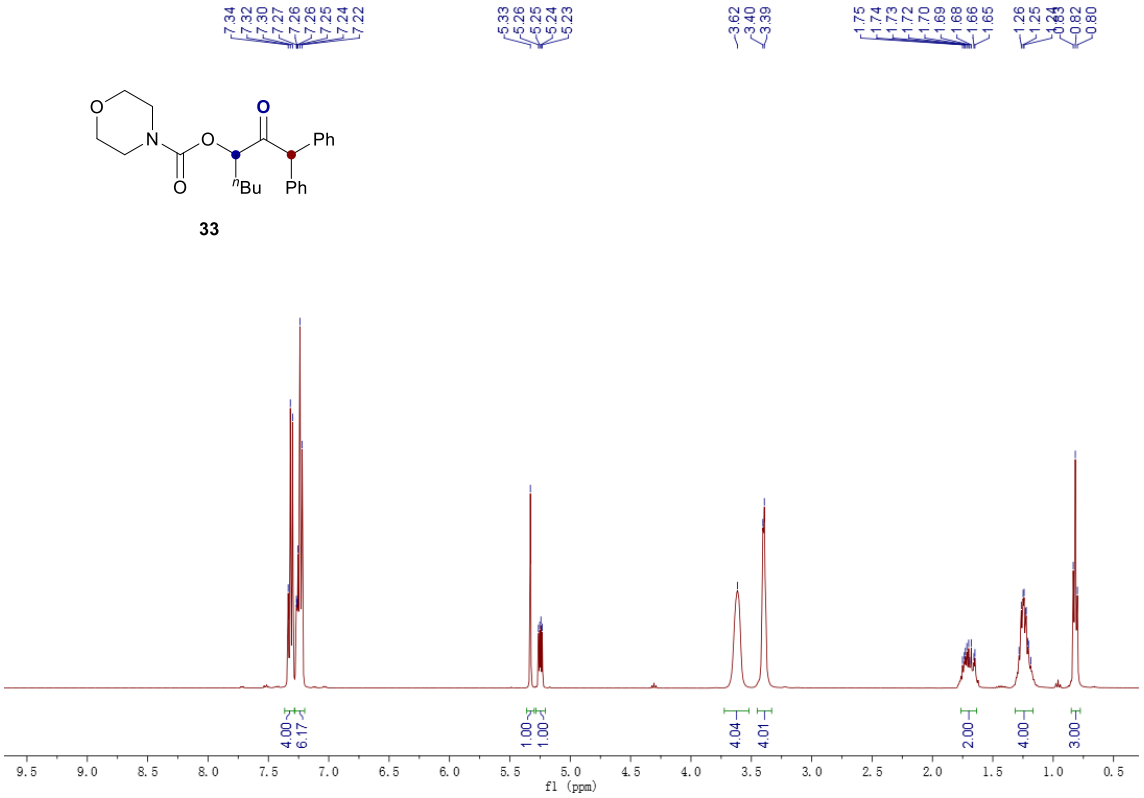
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)

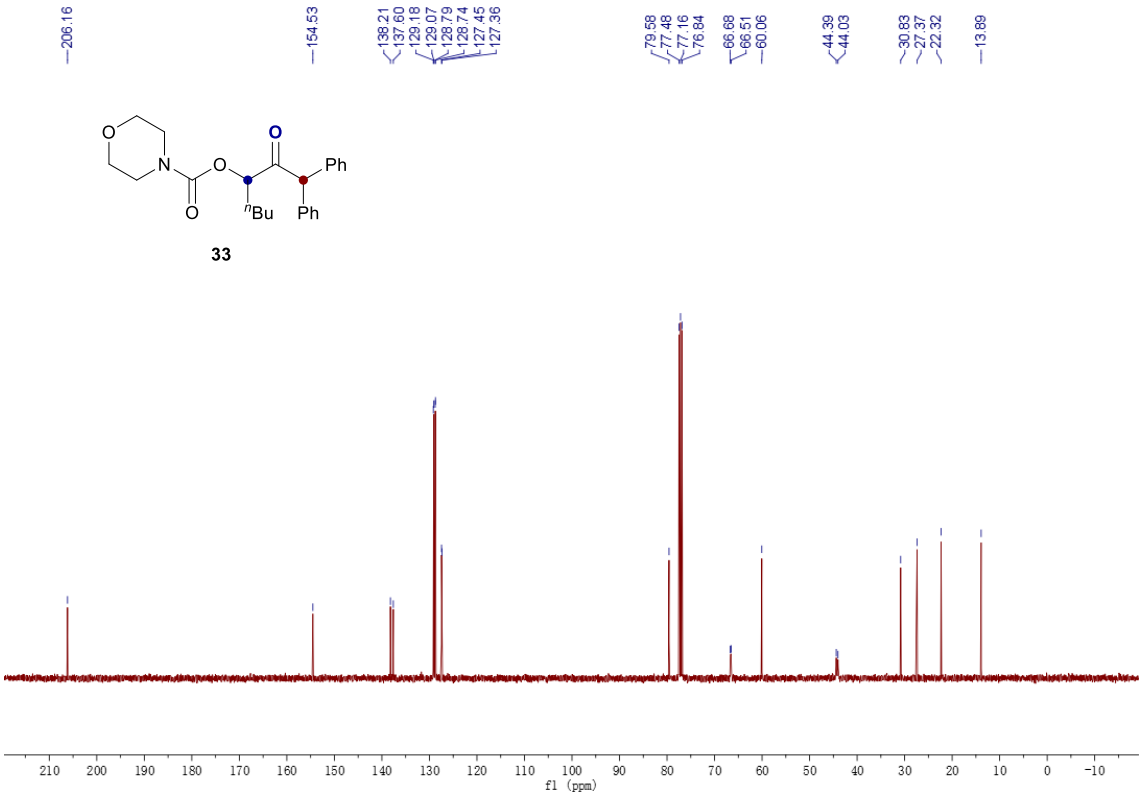


^{1}H NMR (400 MHz, $CDCl_3$)



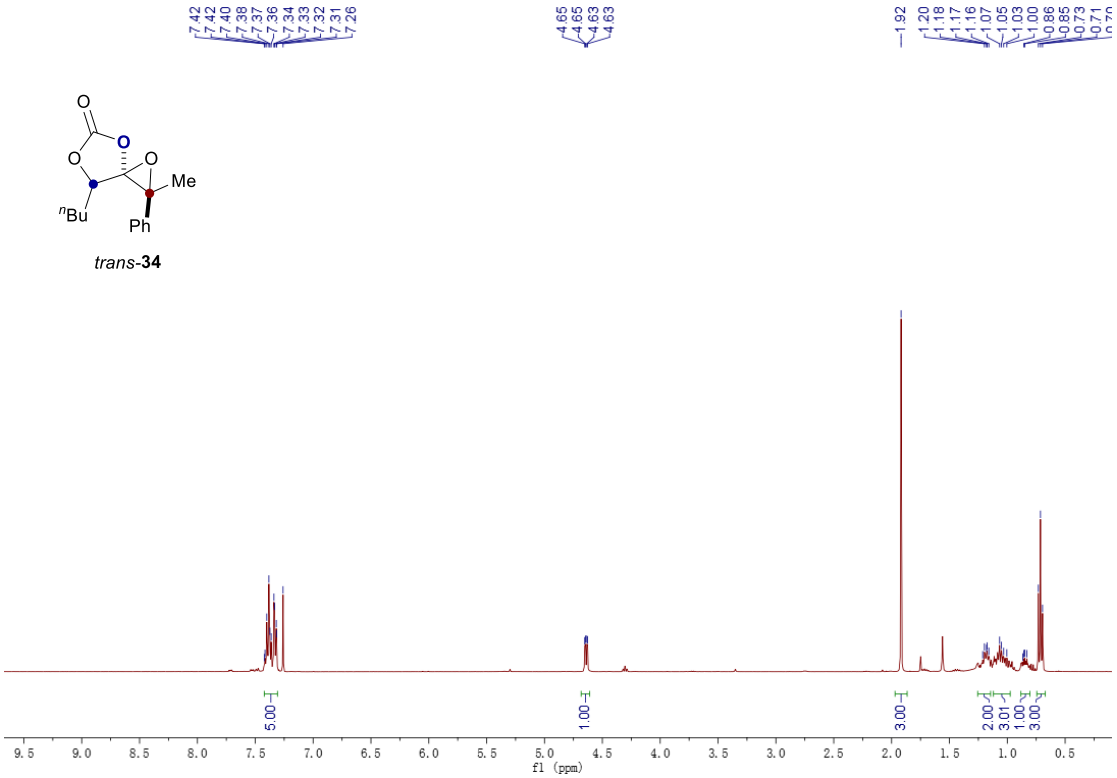
33

^{13}C NMR (100 MHz, $CDCl_3$)

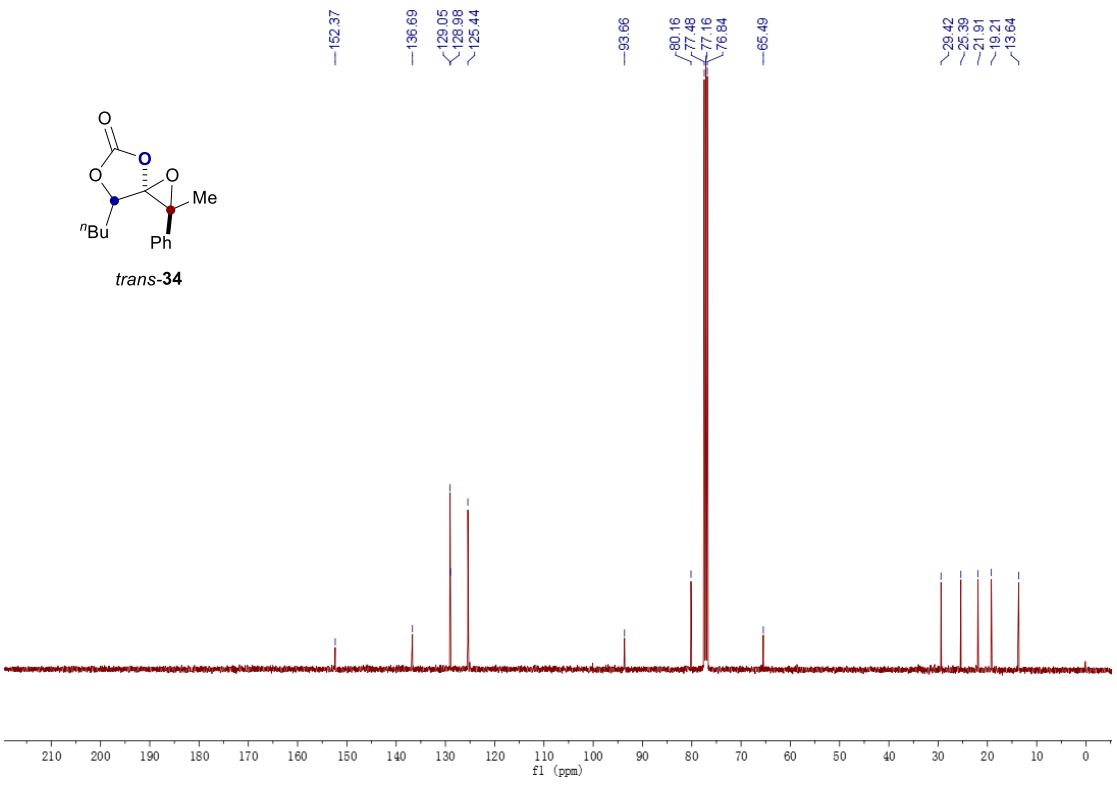


33

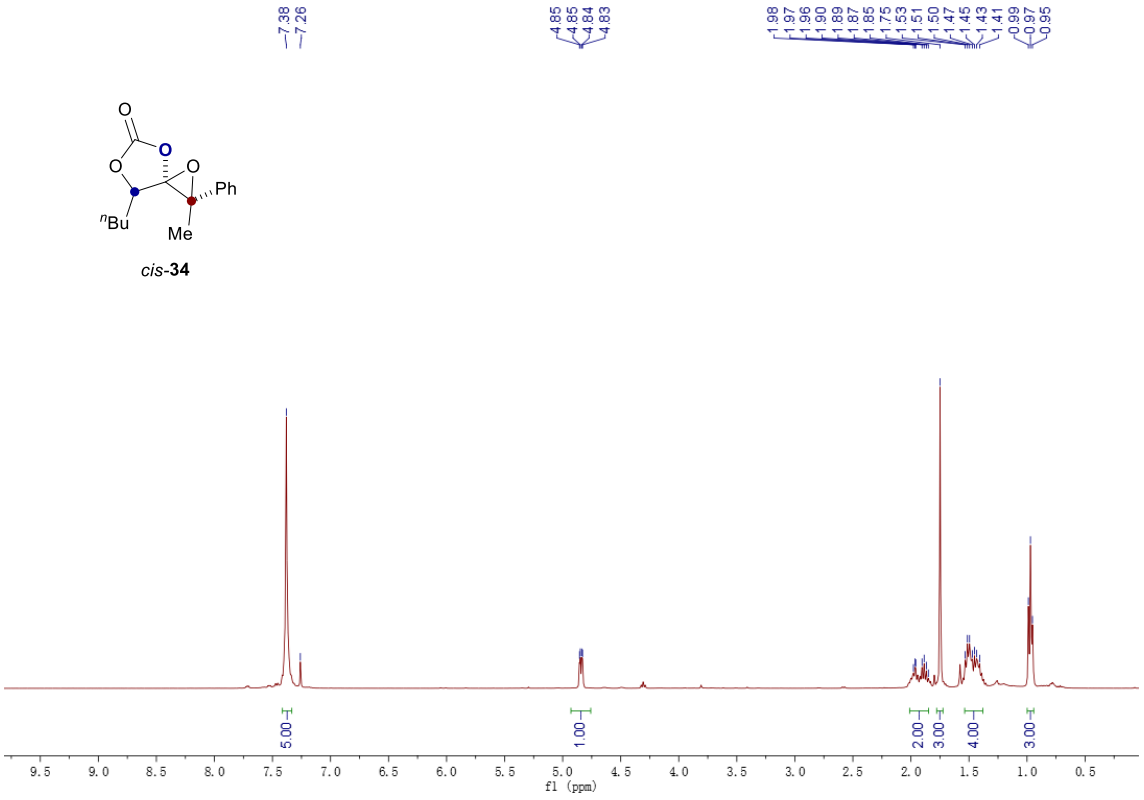
^{1}H NMR (400 MHz, $CDCl_3$)



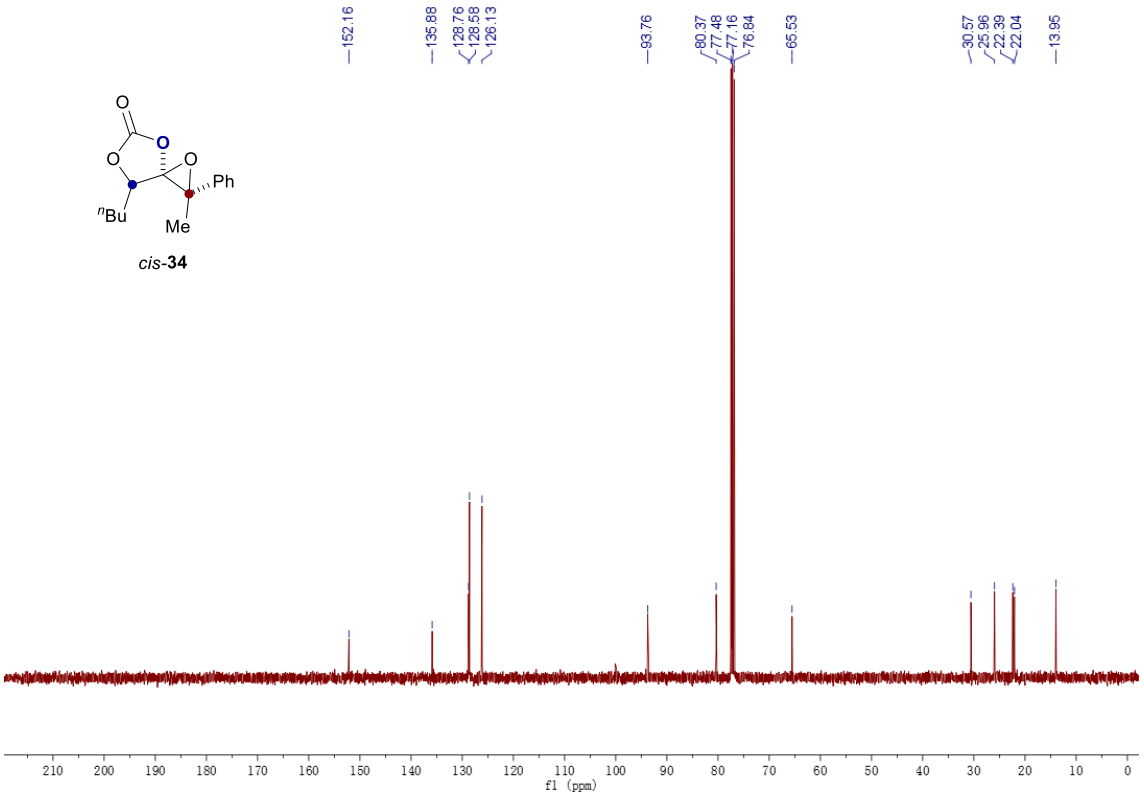
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



12. Cartesian Coordinates of the Optimized Geometries

Cyclic carbonate 4

SCF Energy = -808.020205

Thermal correction to Gibbs Free Energy = 0.254553

Charge = 0, Multiplicity = 1

C	-1.17271600	-1.06519300	0.43982600
C	-0.14923000	-2.47231400	-1.08816100
O	0.85055100	-2.02211400	-0.26447800
O	-1.32666900	-1.90451100	-0.74186800
O	0.01458800	-3.24719300	-1.98239000
C	0.33599700	-1.10520300	0.63982100
C	1.09617000	-0.40736900	1.47519800
C	3.57036300	2.34833500	-1.05703200
C	2.89292600	1.09191700	-0.50515300
H	3.31288500	2.51162600	-2.10953000
H	3.26355300	3.23995000	-0.49624900
H	4.66260400	2.27409800	-0.98806100
C	3.22925600	0.83711500	0.96807400
H	1.80502200	1.18163200	-0.61788200
H	3.19080200	0.21657200	-1.09870900
C	2.59594400	-0.45402200	1.52735600
H	4.31908800	0.77428400	1.09122500
H	2.89915400	1.69593800	1.57035800
H	2.95835900	-1.31572100	0.95671800
H	2.92447200	-0.59437900	2.56583500
H	0.58460000	0.31467300	2.10824500
C	-1.92138500	-1.74842200	1.58379700

H	-1.73135700	-1.23493500	2.52975700
H	-2.99710700	-1.75933700	1.38702000
H	-1.56689800	-2.77799600	1.68216200
C	-1.64554300	0.34274000	0.11133400
C	-1.34675400	0.88895700	-1.14422500
C	-2.30697600	1.13374400	1.05426100
C	-1.70223600	2.20016500	-1.44790500
H	-0.84492600	0.28086300	-1.88946500
C	-2.65990900	2.45118500	0.75089000
H	-2.55302500	0.73312700	2.03148100
C	-2.35887600	2.98816400	-0.49894100
H	-1.46813300	2.60695900	-2.42734700
H	-3.17414400	3.05277500	1.49484500
H	-2.63488500	4.01161900	-0.73535000

$B(C_6F_5)_3$

SCF Energy = -2208.224713

Thermal correction to Gibbs Free Energy = 0.094370

Charge = 0, Multiplicity = 1

B	0.00000000	0.00000000	-0.00034800
C	0.00000000	0.00000000	1.56185100
C	0.00002600	1.35300500	-0.78117700
C	-0.00002600	-1.35300500	-0.78117700
C	0.74921900	0.92026000	2.30874900
C	-0.74921900	-0.92026000	2.30874900
C	0.77108100	0.92848000	3.69816100
C	-0.77108100	-0.92848000	3.69816100

C	0.00000000	0.00000000	4.39602500
F	1.51774100	1.83117500	1.68133100
F	-1.51774100	-1.83117500	1.68133100
F	1.51740300	1.81386700	4.36975200
F	-1.51740300	-1.81386700	4.36975200
F	0.00000000	0.00000000	5.72947500
C	0.74705200	1.53912800	-1.95316200
C	-0.74694700	2.46087200	-0.35585200
C	0.76880300	2.73837000	-2.65482000
C	-0.76875900	3.66841700	-1.04316400
C	0.00000000	3.80782600	-2.19780900
F	1.51352300	0.53967900	-2.43018300
F	-1.51334400	2.37383600	0.74823500
F	1.51293400	2.87662800	-3.75893800
F	-1.51293200	4.69355200	-0.61044400
F	-0.00002600	4.96273200	-2.86430300
C	0.74694700	-2.46087200	-0.35585200
C	-0.74705200	-1.53912800	-1.95316200
C	0.76875900	-3.66841700	-1.04316400
C	-0.76880300	-2.73837000	-2.65482000
C	0.00000000	-3.80782600	-2.19780900
F	1.51334400	-2.37383600	0.74823500
F	-1.51352300	-0.53967900	-2.43018300
F	1.51293200	-4.69355200	-0.61044400
F	-1.51293400	-2.87662800	-3.75893800
F	0.00002600	-4.96273200	-2.86430300

t1

SCF Energy = -3016.269197

Thermal correction to Gibbs Free Energy = 0.373510

Charge = 0, Multiplicity = 1

C	2.12550900	0.89493700	0.09240900
C	1.99252300	-0.87782800	-1.39191400
O	3.28966400	-0.45352900	-1.42910000
O	1.26475200	-0.07499500	-0.58048300
O	1.57256000	-1.81721800	-2.00126400
C	3.42856900	0.70050900	-0.66633400
C	4.54332300	1.42061900	-0.64502300
C	7.69227300	-1.26322800	1.16593000
C	6.56940700	-0.75343300	0.25963000
H	7.41832600	-2.20748400	1.64934400
H	8.61383100	-1.43457400	0.59642500
H	7.92260900	-0.53760800	1.95586700
C	6.91899900	0.56838800	-0.43108900
H	6.33582100	-1.50751000	-0.50427900
H	5.65146900	-0.62325400	0.84739700
C	5.81092900	1.07954100	-1.37489100
H	7.13436300	1.33336300	0.32894500
H	7.84219700	0.44378000	-1.01297300
H	6.17201200	1.97300900	-1.90077400
H	5.60392300	0.31980100	-2.13634700
H	4.53399300	2.30857300	-0.01665700
B	-1.68272000	-0.57271500	0.14433900
C	-1.64516700	-1.45384400	-1.14111000

C	-1.36405100	-1.23371500	1.53389000
C	-2.05411100	0.94861900	0.10229700
C	-1.93760600	-2.82683900	-1.10144700
C	-1.26092600	-0.96571900	-2.39824400
C	-1.85985400	-3.65349600	-2.21450500
C	-1.16193700	-1.76087200	-3.52948400
C	-1.46391600	-3.11569900	-3.43627100
F	-2.34477400	-3.40453700	0.04148500
F	-0.91583600	0.32420700	-2.55387100
F	-2.16547500	-4.95245500	-2.12564800
F	-0.76343700	-1.24381600	-4.69559000
F	-1.37794100	-3.89560300	-4.51197000
C	-0.29497300	-2.11726200	1.72262700
C	-2.12777600	-0.95587300	2.67321200
C	0.02900200	-2.65462800	2.96351200
C	-1.85375000	-1.49714100	3.92298300
C	-0.76051900	-2.34821400	4.06861500
F	0.49700200	-2.46353700	0.69628800
F	-3.18853400	-0.13401500	2.58589000
F	1.08568200	-3.46359700	3.10158300
F	-2.61863900	-1.20658900	4.98091600
F	-0.47095600	-2.86645100	5.26236700
C	-2.88830200	1.50013000	-0.88363400
C	-1.59023800	1.86490800	1.06089000
C	-3.20262800	2.85268300	-0.94744200
C	-1.90257600	3.21607000	1.04412600
C	-2.69720400	3.71707900	0.01882200

F	-3.45225200	0.71925500	-1.81642100
F	-0.78732200	1.46845200	2.06569100
F	-3.98792700	3.32760900	-1.92028600
F	-1.43904700	4.03889200	1.99029700
F	-2.97358100	5.01920500	-0.03440300
C	1.54157900	2.28326800	-0.10311700
C	0.91037000	2.59871700	-1.31362300
C	1.66401400	3.27100500	0.87785400
C	0.40399500	3.87695600	-1.53226800
H	0.79215700	1.83601400	-2.07224400
C	1.16710200	4.55652700	0.65180700
H	2.13510600	3.04558700	1.82806000
C	0.53316700	4.86310900	-0.55079500
H	-0.09593100	4.10197100	-2.46985400
H	1.25937100	5.31004400	1.42768300
H	0.13026500	5.85746900	-0.71822300
C	2.26240900	0.43923100	1.54730300
H	1.30717100	0.52854900	2.06580600
H	2.58635100	-0.60522100	1.56584300
H	3.01625900	1.03679200	2.06582100

TS1

SCF Energy = -3016.251839

Thermal correction to Gibbs Free Energy = 0.376335

Charge = 0, Multiplicity = 1

C	2.10218400	0.82055100	1.02287900
C	1.30159100	-1.54594700	0.95925600

O	2.66468300	-1.45952800	0.93873200
O	0.75164200	-0.33511900	0.66076000
O	0.71982800	-2.55722100	1.20773800
C	3.09828500	-0.18818900	0.59352000
C	4.29808100	0.01761200	0.04868800
C	7.20772400	-1.39350200	3.20210200
C	6.03251200	-1.35570800	2.22262000
H	6.87070100	-1.61371500	4.22080200
H	7.93488800	-2.16325600	2.91719600
H	7.73533600	-0.43203900	3.22423900
C	6.47040000	-1.04552000	0.78765500
H	5.50260600	-2.31745800	2.23775800
H	5.30376600	-0.60303600	2.55198700
C	5.30615200	-1.05711900	-0.22641000
H	6.97342000	-0.06850800	0.75864400
H	7.21383300	-1.78521300	0.46342900
H	5.70813400	-0.90737600	-1.23663800
H	4.81687800	-2.03606800	-0.21084500
H	4.57612600	1.04822200	-0.15105900
B	-0.82475200	-0.35041900	-0.02509500
C	-0.72489000	-1.60629000	-1.04122600
C	-1.90517500	-0.48915600	1.17037400
C	-0.99591700	1.11408000	-0.69672900
C	-1.53730900	-2.74315900	-0.99722700
C	0.27479200	-1.65391500	-2.01477800
C	-1.38740300	-3.82205500	-1.86847100
C	0.47041900	-2.70864300	-2.89437900

C	-0.37757900	-3.80922000	-2.82217600
F	-2.51790900	-2.87618400	-0.09084000
F	1.13947900	-0.61619300	-2.13541000
F	-2.20252800	-4.88003500	-1.77961400
F	1.45665900	-2.67378800	-3.80200100
F	-0.21857900	-4.84016700	-3.65678300
C	-1.68532600	-0.62677800	2.53673600
C	-3.24829800	-0.38514800	0.79881000
C	-2.71645000	-0.66861400	3.47486200
C	-4.30713500	-0.42486300	1.69557600
C	-4.03616100	-0.56761500	3.05401200
F	-0.43676200	-0.70572600	3.05002000
F	-3.55794400	-0.26486800	-0.51034300
F	-2.43870100	-0.79484200	4.78061800
F	-5.57404000	-0.33009700	1.27098000
F	-5.03532000	-0.60506600	3.94241000
C	-1.25320000	1.36598200	-2.04696000
C	-1.02647000	2.24666200	0.11904900
C	-1.46629800	2.64592400	-2.55724800
C	-1.23590100	3.53774600	-0.34499700
C	-1.44829400	3.74116000	-1.70326700
F	-1.31737400	0.37217700	-2.94866700
F	-0.79621800	2.12765100	1.44888200
F	-1.68155500	2.82769400	-3.86680100
F	-1.19236600	4.58411700	0.49280900
F	-1.61329200	4.97894600	-2.18110700
C	2.02248800	2.06698100	0.23848900

C	2.15709700	2.04318500	-1.16178100
C	1.85776700	3.30539400	0.88528800
C	2.11292700	3.22529300	-1.89202200
H	2.26643200	1.09759000	-1.67046500
C	1.84114800	4.48762700	0.15319300
H	1.73673100	3.35147900	1.95946900
C	1.95964900	4.44983700	-1.23721600
H	2.19196500	3.19040100	-2.97388900
H	1.71038900	5.43472100	0.66550700
H	1.92089800	5.37126100	-1.81039600
C	1.94844900	0.92362100	2.52535700
H	0.99529400	1.37338200	2.79495300
H	2.02647800	-0.05337200	3.00028400
H	2.76955000	1.54619300	2.89778900

t2

SCF Energy = -3016.269303

Thermal correction to Gibbs Free Energy = 0.374807

Charge = 0, Multiplicity = 1

C	2.10884300	1.51302600	1.82842600
C	0.64515600	-1.14905500	1.82126300
O	1.95592800	-0.83698500	2.27458500
O	0.22572700	-0.21459000	1.01717800
O	0.13641000	-2.16494700	2.20200000
C	2.57543400	0.18112200	1.59051200
C	3.64547600	-0.11766500	0.79589800
C	7.70448000	-1.60281300	2.07750200

C	6.18734900	-1.42752900	1.99277300
H	8.06821100	-1.44095900	3.09778000
H	8.00067000	-2.61374700	1.77346400
H	8.22228700	-0.89393000	1.42002700
C	5.64225600	-1.64808300	0.57755000
H	5.69152800	-2.12564400	2.68052400
H	5.91144200	-0.41902300	2.33475900
C	4.11400800	-1.49497600	0.49978500
H	6.11915800	-0.94322200	-0.11839100
H	5.90819200	-2.65340400	0.22988700
H	3.77172900	-1.72080000	-0.52425500
H	3.60778000	-2.20874900	1.15642700
H	4.20325100	0.70860300	0.36494300
B	-0.93169700	-0.41511500	0.02546200
C	-0.53704200	-1.80160500	-0.74417800
C	-2.37436200	-0.37722300	0.76811300
C	-0.86107700	0.94009900	-0.90115500
C	-1.25266200	-2.99819100	-0.71399800
C	0.71842800	-1.90209700	-1.34306900
C	-0.76741100	-4.19372000	-1.24820600
C	1.25455400	-3.06958300	-1.86452500
C	0.49813500	-4.23597700	-1.82099900
F	-2.46182300	-3.07456300	-0.13612000
F	1.53141800	-0.80806700	-1.42255900
F	-1.50361000	-5.31086700	-1.18962300
F	2.49823000	-3.07913100	-2.38290100
F	0.98505500	-5.37902200	-2.31747400

C	-2.60051900	-0.08872300	2.11055300
C	-3.52380900	-0.50049100	-0.01262400
C	-3.87700000	0.03365200	2.65841100
C	-4.81448800	-0.39141100	0.48808900
C	-4.99146400	-0.12204800	1.84325500
F	-1.57659100	0.10861300	2.97779500
F	-3.39235000	-0.74109900	-1.33507500
F	-4.03644600	0.31049700	3.96186400
F	-5.88213600	-0.53195600	-0.31072200
F	-6.22418900	-0.00637100	2.35339600
C	-0.83708600	0.97685300	-2.29505300
C	-0.86418500	2.19298200	-0.28430900
C	-0.76816100	2.16319800	-3.02695700
C	-0.80521200	3.39875200	-0.97237600
C	-0.74500300	3.38296300	-2.36019800
F	-0.86142000	-0.15578400	-3.01898100
F	-0.89578600	2.28986700	1.06664500
F	-0.70953600	2.13858400	-4.36631200
F	-0.74579900	4.56905700	-0.31395300
F	-0.63382400	4.53122600	-3.04328200
C	2.26984500	2.53354600	0.83169000
C	2.31224600	2.17728500	-0.54446100
C	2.30578300	3.90959700	1.17527500
C	2.43001000	3.15638700	-1.52236500
H	2.13913300	1.15033700	-0.82972400
C	2.42231800	4.87560400	0.19145200
H	2.28227900	4.20953500	2.21611400

C	2.48295500	4.50274400	-1.15914200
H	2.42775200	2.87147600	-2.56889000
H	2.45759800	5.92459000	0.46602100
H	2.54144500	5.26804700	-1.92694400
C	1.37992000	1.76677200	3.09959300
H	0.32949000	1.49108800	2.93279100
H	1.75546300	1.13569300	3.90812000
H	1.38953400	2.81864500	3.38651300

TS2

SCF Energy = -3016.243430

Thermal correction to Gibbs Free Energy = 0.375361

Charge = 0, Multiplicity = 1

C	3.03531800	-0.55343300	-2.32986100
C	-0.17697500	0.37708300	-2.40648900
O	1.03219400	0.52056900	-3.08587400
O	0.03127000	0.44723600	-1.08720100
O	-1.21098000	0.23918800	-2.98941200
C	2.10363300	0.43519700	-2.20635100
C	1.89910500	1.26276700	-1.06145600
C	3.52124500	6.00577400	-0.77287800
C	2.31356000	5.07718500	-0.91704000
H	3.20817000	7.05434400	-0.73577100
H	4.07847200	5.79051400	0.14666500
H	4.21181500	5.89249300	-1.61712000
C	2.71985600	3.59971300	-0.97119900
H	1.62256100	5.22750800	-0.07768700

H	1.75489200	5.33061000	-1.82740900
C	1.47815400	2.68465700	-1.12365000
H	3.40609100	3.43644400	-1.81237300
H	3.26602800	3.33388200	-0.05646100
H	0.78627200	2.88843200	-0.30397400
H	0.97256000	2.90250700	-2.06825300
H	2.33719600	0.92531800	-0.12907800
B	-0.99495600	-0.09731700	-0.00098300
C	-1.33981800	-1.66338000	-0.28162700
C	-0.14428500	-0.10031600	1.39539900
C	-2.23350200	0.94328100	-0.10696200
C	-0.68059500	-2.53669000	-1.13939600
C	-2.30254400	-2.26399600	0.53312100
C	-0.96386300	-3.89809100	-1.22252700
C	-2.62431300	-3.61451400	0.48534700
C	-1.94584600	-4.44327800	-0.40555100
F	0.31140900	-2.10442800	-1.96233900
F	-2.96603000	-1.50683700	1.43081300
F	-0.28438000	-4.68089800	-2.07550000
F	-3.56546900	-4.12717800	1.28860600
F	-2.23168200	-5.74881100	-0.46717300
C	1.10271600	-0.72931500	1.45014400
C	-0.61419400	0.35685600	2.62888100
C	1.88559800	-0.82182100	2.59544000
C	0.12816800	0.27186800	3.80709500
C	1.38992000	-0.31327200	3.79148100
F	1.62491100	-1.29912200	0.33450800

F	-1.83014300	0.91268700	2.74572500
F	3.09384500	-1.40686800	2.55688500
F	-0.36534800	0.74861000	4.95650200
F	2.11542600	-0.39184400	4.91218800
C	-2.08848400	2.26710800	0.30932800
C	-3.45035400	0.66156800	-0.73160100
C	-3.05947000	3.24763000	0.15492300
C	-4.45825300	1.60996500	-0.90166900
C	-4.26347100	2.91196000	-0.45637400
F	-0.93523900	2.66917700	0.90729700
F	-3.71427800	-0.55990100	-1.22239100
F	-2.84765900	4.50113800	0.58420100
F	-5.60823000	1.27934400	-1.50332400
F	-5.21832600	3.83420100	-0.61788800
C	4.10608700	-0.64345500	-1.33580500
C	4.75714300	0.50431500	-0.84462000
C	4.44280700	-1.89895800	-0.79216900
C	5.67700500	0.40714100	0.19929400
H	4.57739500	1.46181500	-1.32138000
C	5.34843200	-1.98800200	0.25631100
H	3.94328800	-2.79128000	-1.15346400
C	5.96345700	-0.83591500	0.76012900
H	6.17473300	1.30059900	0.56385000
H	5.56846100	-2.95603900	0.69524600
H	6.67181900	-0.91368500	1.57911700
C	2.92643800	-1.58010500	-3.41743600
H	3.91209900	-1.86987100	-3.79041000

H	2.43255400	-2.47370100	-3.01435400
H	2.30519200	-1.21983100	-4.23870700

t3

SCF Energy = -3016.260558

Thermal correction to Gibbs Free Energy = 0.371264

Charge = 0, Multiplicity = 1

C	2.96420000	-0.83511800	-2.69302200
C	0.06488300	1.11929000	-2.39569900
O	1.02560400	0.48418600	-3.12348900
O	0.43949200	1.17840600	-1.09777500
O	-0.95511000	1.56307200	-2.83828600
C	2.04090300	0.03586000	-2.27270700
C	1.81221500	0.73359700	-0.94981900
C	6.32777000	2.53175100	0.61191700
C	4.89213900	2.87562000	0.20673600
H	6.88356400	3.42405900	0.92002100
H	6.34035000	1.82163900	1.44756400
H	6.86928700	2.06682300	-0.22067400
C	4.10749300	1.63824100	-0.23825000
H	4.37323000	3.35723300	1.04718800
H	4.90351900	3.61236500	-0.60852900
C	2.67316300	1.96516700	-0.65834000
H	4.63549300	1.15592400	-1.06630100
H	4.09439600	0.90205100	0.57716400
H	2.15871100	2.51236500	0.14193100
H	2.67059600	2.61636500	-1.54217100

H	1.83382000	0.04753600	-0.10693200
B	-1.75010000	0.02070300	0.73092400
C	-2.34530300	-1.31344200	0.13172000
C	-0.68585600	-0.16009100	1.86698700
C	-2.23120800	1.39601200	0.22471500
C	-1.92858200	-1.91019000	-1.05155400
C	-3.35846300	-1.95681400	0.83408000
C	-2.49067800	-3.09086200	-1.52779500
C	-3.95320000	-3.13263100	0.39172700
C	-3.51166700	-3.70069300	-0.80198600
F	-0.92640100	-1.36231400	-1.76697800
F	-3.79371500	-1.40552400	1.98704000
F	-2.05708500	-3.64547600	-2.66448100
F	-4.93183100	-3.71721900	1.09090600
F	-4.06245800	-4.83308200	-1.24634100
C	0.33788200	-1.10663100	1.76079100
C	-0.73276500	0.55367100	3.06917200
C	1.28693100	-1.31375600	2.75375400
C	0.18456800	0.35897600	4.09628500
C	1.20454200	-0.57737400	3.93329400
F	0.47382500	-1.82936300	0.62943200
F	-1.70145800	1.45634200	3.27193700
F	2.26909200	-2.20977000	2.58729700
F	0.10049700	1.05666600	5.23206900
F	2.09881800	-0.76693300	4.90215300
C	-1.48801800	2.57659500	0.42268100
C	-3.35281200	1.52745700	-0.61655900

C	-1.80416700	3.77938300	-0.18663800
C	-3.70915800	2.72400100	-1.22401900
C	-2.92349000	3.85260000	-1.01399000
F	-0.38242500	2.57565400	1.18157600
F	-4.14877600	0.48041800	-0.86480200
F	-1.04755100	4.86501000	0.00536100
F	-4.78849200	2.80000300	-2.00646600
F	-3.24324900	5.00451900	-1.59521600
C	4.01778500	-1.32697400	-1.76477700
C	5.37265600	-1.22168900	-2.11660300
C	3.69072300	-1.89331700	-0.52378800
C	6.37187300	-1.62506100	-1.23267000
H	5.64547500	-0.79311000	-3.07664100
C	4.69015100	-2.29293300	0.36320000
H	2.64983800	-2.03069600	-0.25474600
C	6.03419900	-2.15262100	0.01552700
H	7.41544500	-1.52141000	-1.51625500
H	4.41256200	-2.71421600	1.32402300
H	6.81316800	-2.46091100	0.70677000
C	2.98242200	-1.33982800	-4.11477400
H	3.90511400	-1.03898000	-4.62640400
H	2.95504800	-2.43575600	-4.12564500
H	2.13506800	-0.95967700	-4.68757600

P4

SCF Energy = -808.021523

Thermal correction to Gibbs Free Energy = 0.256805

Charge = 0, Multiplicity = 1

C	-0.45025800	-1.46946000	-0.60595200
C	-3.50115700	0.06962900	0.21392500
O	-2.70076100	-0.69717400	-0.59701800
O	-2.73959100	0.73339900	1.11122600
O	-4.69129900	0.12140100	0.12741100
C	-1.38090100	-0.61639500	-0.16140200
C	-1.33469600	0.55650200	0.79574000
C	2.72304300	3.24146000	-0.76937900
C	1.22012100	3.25678600	-0.47853500
H	3.08496100	4.23104300	-1.06919000
H	3.29083700	2.92842000	0.11512600
H	2.95923700	2.53727300	-1.57627800
C	0.69959000	1.87877200	-0.05929500
H	1.00222100	3.98780100	0.31236900
H	0.67391400	3.59735700	-1.36920300
C	-0.80721900	1.86989700	0.20733200
H	0.93777100	1.15232900	-0.84221700
H	1.23945700	1.54258000	0.83641700
H	-1.06935700	2.66175300	0.92045400
H	-1.35784800	2.08149100	-0.71858100
H	-0.82232200	0.32414100	1.72992000
C	0.94196400	-1.42057000	-0.08629900
C	2.02877500	-1.32055200	-0.96896700
C	1.20494200	-1.48569900	1.28990300
C	3.33398900	-1.23959500	-0.48779400
H	1.84653200	-1.27757400	-2.03889800

C	2.51069900	-1.40588700	1.77370200
H	0.37850300	-1.61726500	1.98209200
C	3.57974900	-1.27326000	0.88656500
H	4.16056600	-1.14587000	-1.18643700
H	2.69256400	-1.45669800	2.84353400
H	4.59696500	-1.20864700	1.26155800
C	-0.77345900	-2.51403400	-1.64674400
H	-0.18815400	-2.35074000	-2.56038900
H	-0.51225300	-3.51261300	-1.27660100
H	-1.83147600	-2.50135900	-1.91343900

t1′

SCF Energy= -3016.261470

Thermal correction to Gibbs Free Energy = 0.373187

Charge = 0, Multiplicity = 1

C	1.34357600	2.13177800	1.15550600
C	1.22661300	2.08035800	-1.14486200
O	2.54019800	1.87075700	-0.82432600
O	0.47396900	2.07377900	-0.02091400
O	0.82329500	2.21493600	-2.26269800
C	2.65315700	1.67634700	0.55049100
C	3.72700700	1.12281800	1.10236600
C	6.28422900	-3.06060300	-0.13115300
C	6.15746400	-1.54662200	-0.31667800
H	6.50623600	-3.31462200	0.91260000
H	5.35079200	-3.56767100	-0.40407000
H	7.08463700	-3.47550300	-0.75379600

C	5.03893200	-0.93979000	0.53443600
H	7.11168700	-1.06062600	-0.06927800
H	5.96033800	-1.32132700	-1.37320200
C	4.90293700	0.58190400	0.34239300
H	4.08554700	-1.41203000	0.27355300
H	5.21923500	-1.16149000	1.59640500
H	5.82756300	1.07404500	0.67572400
H	4.78541900	0.80589300	-0.72182400
H	3.71233600	0.98591900	2.18116100
B	-1.34889000	-1.05508100	-0.46146900
C	-2.73490600	-0.33530600	-0.51824000
C	-0.30621900	-0.91747300	-1.61251600
C	-1.01549600	-1.92914000	0.79738300
C	-3.89101500	-0.92646700	0.01390500
C	-2.90545100	0.94856700	-1.05864300
C	-5.13157800	-0.30228000	0.01512000
C	-4.12774100	1.61154900	-1.05445700
C	-5.24682100	0.97965500	-0.51814700
F	-3.84123800	-2.16459200	0.53450900
F	-1.87014200	1.60447900	-1.58994800
F	-6.20783300	-0.91368900	0.52089800
F	-4.23971600	2.84273200	-1.56221300
F	-6.42635200	1.59821500	-0.51697100
C	-0.68464500	-0.68658100	-2.94486900
C	1.07935800	-1.00439400	-1.39513800
C	0.22886800	-0.54535200	-3.98191000
C	2.02008700	-0.85860800	-2.40291300

C	1.59037000	-0.62449800	-3.70672900
F	-1.98057900	-0.62149000	-3.28014500
F	1.56564500	-1.19229800	-0.15098400
F	-0.18566600	-0.33605100	-5.23319000
F	3.33078100	-0.92429700	-2.13874500
F	2.48009200	-0.48177400	-4.68385800
C	-1.38297200	-1.53789000	2.09114800
C	-0.33388900	-3.14892300	0.70465300
C	-1.07491500	-2.28106300	3.22379200
C	-0.02850100	-3.93208000	1.81128700
C	-0.39885900	-3.49068800	3.07973600
F	-2.02962500	-0.37505000	2.29094800
F	0.04395500	-3.62000600	-0.49454100
F	-1.42128000	-1.85122000	4.44143500
F	0.61561500	-5.09485900	1.67268200
F	-0.10420400	-4.22208800	4.15338200
C	1.35326900	3.57109000	1.66721000
C	0.21607500	4.37010200	1.50518300
C	2.45759500	4.07923000	2.35614300
C	0.18771900	5.66309500	2.02667300
H	-0.63589300	3.98206400	0.95756200
C	2.42531700	5.37113800	2.88159800
H	3.35001200	3.47177000	2.46689300
C	1.29066200	6.16658800	2.71832300
H	-0.69672100	6.27827300	1.88832700
H	3.29174800	5.75781000	3.41046500
H	1.26801700	7.17449700	3.12243000

C	0.79214500	1.16909600	2.20073600
H	0.82058900	0.14618500	1.82219100
H	1.39851800	1.23092000	3.10899800
H	-0.23461400	1.44006900	2.45642200

TS1′

SCF Energy= -3016.243472

Thermal correction to Gibbs Free Energy= 0.375394

Charge = 0, Multiplicity = 1

C	0.52609400	2.60369700	0.46773900
C	0.71482200	1.13881700	-1.57936500
O	1.75112100	2.02370500	-1.46435300
O	0.08291600	1.00223500	-0.38220400
O	0.45506300	0.57981700	-2.60086200
C	1.86167400	2.53149300	-0.17462900
C	3.04306700	2.87554700	0.33555600
C	7.32741000	0.21678300	0.32720500
C	6.51001400	1.30743900	-0.36974800
H	7.60538200	0.51931000	1.34420200
H	6.75018600	-0.71098000	0.39951500
H	8.25051900	-0.00002600	-0.22135400
C	5.21542500	1.63780800	0.37953400
H	7.11363500	2.21944600	-0.47839700
H	6.25936800	0.98120300	-1.38853500
C	4.35683400	2.68514900	-0.35775800
H	4.62747700	0.72482800	0.51577300
H	5.45405800	2.00406600	1.38816200

H	4.89961200	3.63936700	-0.39913600
H	4.18789700	2.36357800	-1.38987600
H	3.05671700	3.27789800	1.34473200
B	-0.45731100	-0.56507700	-0.05133500
C	-1.82304900	-0.80010300	-0.88224300
C	0.84360300	-1.42482700	-0.49720700
C	-0.83481800	-0.63047900	1.52827100
C	-2.40693900	-2.06375000	-0.78297800
C	-2.56360400	0.14178500	-1.59320500
C	-3.61618500	-2.40708400	-1.37271300
C	-3.78198700	-0.15938200	-2.20067700
C	-4.31136600	-1.43974300	-2.09353600
F	-1.76624300	-3.02558100	-0.08231700
F	-2.15511000	1.42152100	-1.71409700
F	-4.11737700	-3.64406200	-1.25187800
F	-4.45481800	0.78554800	-2.87463400
F	-5.48152300	-1.73825200	-2.67001900
C	0.89325000	-2.32746900	-1.56322500
C	2.06743000	-1.22054600	0.14568200
C	2.05403800	-3.00795300	-1.93301000
C	3.24272300	-1.87848700	-0.18609500
C	3.23880300	-2.78222200	-1.24347500
F	-0.18504300	-2.58416300	-2.31585500
F	2.15401400	-0.33416500	1.16999600
F	2.03819100	-3.86385600	-2.96151700
F	4.37821400	-1.64595300	0.49644900
F	4.35990500	-3.42168100	-1.58810000

C	-1.87651700	0.15613000	2.02346500
C	-0.31899600	-1.54313700	2.45430900
C	-2.33355000	0.12719500	3.33463000
C	-0.75530100	-1.62003900	3.77777200
C	-1.76503200	-0.77677800	4.22626700
F	-2.48283500	1.05272400	1.21028900
F	0.63679400	-2.42434300	2.11852000
F	-3.30475100	0.95934600	3.73840100
F	-0.21006900	-2.50692500	4.61848600
F	-2.18321600	-0.83206500	5.49331900
C	-0.44457900	3.56099200	-0.10460200
C	-1.71185500	3.75255500	0.47676800
C	-0.09688700	4.33250800	-1.23335000
C	-2.60267100	4.67480700	-0.05911000
H	-2.02360800	3.15964000	1.32269400
C	-0.99015200	5.25614600	-1.76233400
H	0.87591800	4.21605700	-1.69387100
C	-2.24767300	5.42709200	-1.18023900
H	-3.58021700	4.79985700	0.39544600
H	-0.70456700	5.84187700	-2.63023200
H	-2.94818800	6.14349300	-1.59882100
C	0.50936800	2.33984300	1.94152100
H	1.06274600	1.43430900	2.18035800
H	1.00713700	3.19557800	2.41669000
H	-0.49584400	2.28428300	2.34996800

t2′

SCF Energy= -3016.267234

Thermal correction to Gibbs Free Energy= 0.377920

Charge = 0, Multiplicity = 1

C	-1.51537400	3.06275800	-1.44932500
C	-0.17509700	0.30158600	-2.25301500
O	-0.19398700	1.59789400	-2.85748100
O	-0.19438000	0.42747000	-0.96699000
O	-0.14575800	-0.64641600	-2.98644100
C	-0.26671400	2.69477500	-2.03350200
C	0.88571700	3.39287600	-1.77309500
C	5.12323400	1.53509600	0.12116800
C	4.44136700	2.08964900	-1.13215100
H	5.15658800	2.27624300	0.92841400
H	4.58865600	0.65732100	0.49597900
H	6.15248700	1.23034400	-0.09712900
C	3.03912100	2.62979000	-0.82575600
H	5.04956900	2.88750000	-1.57964700
H	4.36254900	1.29067400	-1.87734000
C	2.24719200	2.94646000	-2.12716700
H	2.47686600	1.88693600	-0.25876600
H	3.10806500	3.53135700	-0.20276300
H	2.76920900	3.75115700	-2.66524200
H	2.21306000	2.06320600	-2.76655100
H	0.81052700	4.31322200	-1.20214800
B	0.06713400	-0.61533400	0.13597500
C	-1.36733700	-1.11834300	0.72512200
C	1.02426200	-1.80457200	-0.41975100

C	0.79421200	0.36636100	1.24470200
C	-1.49826600	-1.50505700	2.05938500
C	-2.54185900	-1.17446000	-0.01906400
C	-2.70522900	-1.88012400	2.64023600
C	-3.77310000	-1.54031100	0.52090300
C	-3.85957500	-1.88849200	1.86264200
F	-0.41130700	-1.54338500	2.85755100
F	-2.54418700	-0.86898200	-1.33442500
F	-2.76913300	-2.23176000	3.93252100
F	-4.88382800	-1.55149600	-0.24279500
F	-5.03762000	-2.23595300	2.39802600
C	0.82536700	-3.16769600	-0.20763000
C	2.16246500	-1.49856500	-1.16348900
C	1.68434300	-4.15122700	-0.70102400
C	3.04639600	-2.43491100	-1.67496600
C	2.80207700	-3.78508000	-1.44010700
F	-0.22606000	-3.62081100	0.50376800
F	2.46572700	-0.19734500	-1.41477700
F	1.43917400	-5.44800600	-0.46441100
F	4.12390100	-2.05285900	-2.37837500
F	3.63547700	-4.71667400	-1.91811900
C	0.14987000	1.55572000	1.58586800
C	2.05484800	0.21200800	1.81676800
C	0.71949800	2.56053300	2.35699900
C	2.65721300	1.18189600	2.62038500
C	1.99466500	2.37553700	2.88059200
F	-1.11132800	1.80103600	1.14163700

F	2.79568100	-0.88944700	1.59007300
F	0.05232500	3.71166900	2.58273500
F	3.88924100	0.98926600	3.11004200
F	2.57154000	3.33027300	3.61988400
C	-2.71357700	2.30672600	-1.69436000
C	-3.67972300	2.18654600	-0.65924600
C	-2.97055400	1.67796400	-2.94134200
C	-4.82270300	1.43210100	-0.85071300
H	-3.47731500	2.61507500	0.31481900
C	-4.15280200	0.98262200	-3.14055100
H	-2.25179200	1.76414200	-3.74378400
C	-5.06682100	0.83583900	-2.09432900
H	-5.52192200	1.28876900	-0.03426100
H	-4.34803700	0.52322300	-4.10368300
H	-5.96529500	0.24479700	-2.23845300
C	-1.58872000	4.24816400	-0.52357900
H	-1.06353900	4.05620600	0.41575300
H	-1.13219900	5.12448500	-0.99361500
H	-2.62293200	4.50369400	-0.29783500

TS2′

SCF Energy= -3016.236886

Thermal correction to Gibbs Free Energy= 0.373839

Charge = 0, Multiplicity = 1

C	3.54285600	-1.04113000	-0.06118500
C	0.74423100	-0.44941900	-1.83880100
O	1.98688700	-1.07154600	-1.91758000

O	0.19616200	-0.67615300	-0.63933800
O	0.28747100	0.15622200	-2.76199600
C	2.40345700	-1.50668900	-0.66286700
C	1.34872600	-2.22838000	-0.03101500
C	3.04743500	-6.37610000	-0.45596100
C	2.56193500	-4.96848500	-0.80894200
H	4.04941400	-6.56178800	-0.85664200
H	3.08887200	-6.51955000	0.63047000
H	2.37574400	-7.13938100	-0.86603400
C	1.15879400	-4.68493000	-0.26254500
H	3.27316900	-4.22711600	-0.42250900
H	2.55412300	-4.83904800	-1.89960800
C	0.56839700	-3.31082300	-0.68428800
H	0.46159900	-5.44875800	-0.62739000
H	1.15602600	-4.76785900	0.83313600
H	0.59475000	-3.21398200	-1.77277800
H	-0.46995900	-3.25106600	-0.35226500
H	1.30757300	-2.21792400	1.05284400
B	-0.96892600	0.23109500	-0.03593900
C	-0.50885000	1.79174700	-0.01558700
C	-2.24050700	-0.13926800	-0.96919400
C	-1.05553700	-0.20807200	1.53433100
C	-1.45739200	2.72862900	0.40077000
C	0.76768500	2.30647000	-0.22230200
C	-1.19000700	4.08167000	0.56401500
C	1.08458200	3.65537700	-0.07147500
C	0.09902000	4.55117600	0.32308600

F	-2.71342300	2.31435600	0.66876600
F	1.80352200	1.50811700	-0.58394400
F	-2.14820300	4.93152200	0.95665900
F	2.33501200	4.08814300	-0.29213100
F	0.38571500	5.84919100	0.47693800
C	-2.76202600	0.68658400	-1.96698900
C	-2.81225500	-1.41063000	-0.90961800
C	-3.79392100	0.29400200	-2.81864100
C	-3.83490200	-1.84901700	-1.74015700
C	-4.33505800	-0.98117800	-2.70611500
F	-2.27863600	1.92205800	-2.17150800
F	-2.36549300	-2.31217900	0.00507900
F	-4.25878000	1.13189800	-3.75448100
F	-4.33749700	-3.08728200	-1.62115800
F	-5.32078700	-1.37376100	-3.52010700
C	0.09879900	-0.21531900	2.31977800
C	-2.23560000	-0.44842100	2.24237100
C	0.12561800	-0.52219700	3.67500800
C	-2.26050600	-0.74521700	3.60538600
C	-1.07267100	-0.79042900	4.32817000
F	1.30067200	0.09185100	1.76382900
F	-3.43063200	-0.40438800	1.63384300
F	1.28860800	-0.54612500	4.34712700
F	-3.42117400	-0.98705000	4.22613600
F	-1.08221400	-1.08377400	5.63232000
C	4.47536300	-0.10754000	-0.69837300
C	4.55326600	0.07335500	-2.09673400

C	5.32974800	0.66488900	0.11899200
C	5.43783200	0.99612500	-2.64296300
H	3.92701200	-0.51214300	-2.75353900
C	6.19433100	1.60250000	-0.43215000
H	5.29525900	0.55726900	1.19649400
C	6.25462100	1.77065900	-1.81702800
H	5.48445800	1.11443100	-3.72108000
H	6.82209600	2.20220200	0.21961000
H	6.93438200	2.49905200	-2.24896100
C	3.85819300	-1.49650200	1.34611300
H	4.92038400	-1.73745800	1.43996900
H	3.62279100	-0.70117500	2.06138000
H	3.29860900	-2.38319600	1.64103400

t3′

SCF Energy= -3016.268476

Thermal correction to Gibbs Free Energy= 0.376026

Charge = 0, Multiplicity = 1

C	3.61399700	-0.44469500	-0.40762800
C	0.75472500	0.86772200	-1.92705400
O	2.11539400	0.79256600	-1.82324200
O	0.19147100	-0.25035100	-1.40331800
O	0.16064100	1.78657600	-2.40793800
C	2.45311300	-0.33344300	-1.06904800
C	1.23958500	-1.22402400	-1.11670200
C	4.48515200	-4.42068900	-2.36029100
C	3.54425000	-3.24502800	-2.63039800

H	5.47280500	-4.25151800	-2.80260700
H	4.62325100	-4.57395200	-1.28273300
H	4.08594400	-5.35327400	-2.77745400
C	2.13961800	-3.47405000	-2.05673000
H	3.97492700	-2.32599100	-2.22107200
H	3.45618600	-3.08142100	-3.71324600
C	1.17771700	-2.28633300	-2.22276400
H	1.69890500	-4.34467900	-2.55853600
H	2.20708800	-3.75328300	-0.99601600
H	1.34777600	-1.79480800	-3.18919200
H	0.14300500	-2.64362600	-2.22305200
H	1.00679500	-1.66579100	-0.15010900
B	-1.76086300	0.23022700	0.73287400
C	-0.56696800	-0.13814200	1.68250500
C	-1.97830700	1.70359800	0.27546700
C	-2.76782100	-0.87208500	0.24891200
C	-0.61778300	-1.21580600	2.57939500
C	0.65425100	0.55432200	1.64978100
C	0.46276400	-1.60940800	3.36231500
C	1.75064500	0.19442100	2.42126700
C	1.65881600	-0.90269200	3.27179300
F	-1.74625200	-1.92650200	2.72412300
F	0.83804800	1.59117500	0.81824600
F	0.36520900	-2.65370000	4.19043300
F	2.90201800	0.86918300	2.33515000
F	2.72093700	-1.27806000	3.98515200
C	-1.72012300	2.79809600	1.11225500

C	-2.43016900	2.01645900	-1.01468400
C	-1.89081400	4.11442100	0.70912200
C	-2.59313700	3.32184300	-1.45958100
C	-2.32528500	4.37483300	-0.58989900
F	-1.30597700	2.59669200	2.37617600
F	-2.69701200	1.04143900	-1.89228600
F	-1.64658600	5.12870600	1.54659600
F	-3.00143300	3.57461100	-2.70535100
F	-2.48606900	5.63333600	-0.99572900
C	-2.38434400	-2.17715000	-0.08024400
C	-4.13276200	-0.59469800	0.08375500
C	-3.26206600	-3.13302700	-0.57291600
C	-5.04899100	-1.53098400	-0.38264700
C	-4.60813500	-2.80754100	-0.72072600
F	-1.10079100	-2.56989800	0.05053900
F	-4.62336600	0.61389300	0.39866300
F	-2.82868600	-4.35629400	-0.89728900
F	-6.34153900	-1.21744400	-0.51092700
F	-5.46886700	-3.71454900	-1.17929100
C	4.70247800	0.55567300	-0.52926100
C	4.98471000	1.17997300	-1.75635600
C	5.50888800	0.87078200	0.57735900
C	6.02660300	2.09753700	-1.86757600
H	4.38797800	0.93915600	-2.62813800
C	6.54787700	1.79217300	0.46546900
H	5.31184800	0.41251000	1.53957600
C	6.81231700	2.41011300	-0.75729800

H	6.22708800	2.56557800	-2.82713600
H	7.15078100	2.02820700	1.33781300
H	7.62431400	3.12622700	-0.84473700
C	3.86211100	-1.64180900	0.48121000
H	4.74088700	-2.20255500	0.14321800
H	4.05536800	-1.32805400	1.51198100
H	3.01512700	-2.32963400	0.50238300

P4′

SCF Energy= -808.020126

Thermal correction to Gibbs Free Energy= 0.257299

Charge = 0, Multiplicity = 1

C	0.62587100	-0.37014800	0.75808800
C	-0.55599100	2.83819500	-0.07318300
O	0.27517600	1.76542900	-0.29613700
O	-1.59075400	2.45727700	0.70916700
O	-0.37000800	3.93332600	-0.51064800
C	-0.15571700	0.68163500	0.46488800
C	-1.57578800	1.01466900	0.85820600
C	-4.11338500	-3.10253400	-0.85969600
C	-3.93791900	-1.58355000	-0.92469000
H	-4.90719500	-3.44197600	-1.53380500
H	-3.18859100	-3.61853300	-1.14476300
H	-4.37480400	-3.42675100	0.15496000
C	-2.83018500	-1.07740600	0.00594500
H	-3.70713600	-1.28184800	-1.95551500
H	-4.88425100	-1.08949400	-0.66541500

C	-2.65244200	0.43983100	-0.07273000
H	-3.06507100	-1.37327600	1.03857500
H	-1.88641400	-1.57209000	-0.25463300
H	-2.39693100	0.72922300	-1.10056700
H	-3.59492200	0.94436100	0.17329200
H	-1.79658700	0.79650200	1.90540500
C	1.99559600	-0.54656600	0.21658300
C	2.37588600	-0.03213600	-1.03735500
C	2.95127600	-1.28358600	0.93946500
C	3.66180800	-0.23093000	-1.53270500
H	1.65933500	0.52110800	-1.63029200
C	4.23936700	-1.47717600	0.44435500
H	2.69580300	-1.70457300	1.90559600
C	4.60296500	-0.95066700	-0.79474300
H	3.92678800	0.17586500	-2.50456500
H	4.95866700	-2.04257900	1.03029100
H	5.60574400	-1.10314900	-1.18333700
C	0.11383800	-1.42580300	1.71363900
H	-0.91808200	-1.25043600	2.01873800
H	0.16604200	-2.42411100	1.26454100
H	0.72121000	-1.44947800	2.62604000

TS3

SCF Energy= -3016.200981

Thermal correction to Gibbs Free Energy= 0.368499

Charge = 0, Multiplicity = 1

C	3.61467300	-1.54931700	-1.71149400

C	0.74405400	0.16666100	-1.43579900
O	2.07784800	0.15792700	-2.27424600
O	0.94947400	-0.19309000	-0.27368200
O	-0.19411400	0.52390400	-2.11660800
C	3.15074200	-0.21139900	-1.57322500
C	3.64830400	0.56416600	-0.53398600
C	4.72669100	5.38056300	0.56369900
C	3.65145800	4.30011100	0.43489700
H	4.29018000	6.33364100	0.88074900
H	5.48603900	5.09797100	1.30302900
H	5.23810100	5.54815700	-0.39197900
C	4.22333500	2.95007400	-0.01207600
H	3.13318600	4.17133900	1.39170200
H	2.88729700	4.62334000	-0.28357800
C	3.11286400	1.88242100	-0.13789200
H	4.73256500	3.06435200	-0.97831900
H	4.98232100	2.61178700	0.70710000
H	2.63102200	1.76490000	0.84311600
H	2.34440100	2.20954900	-0.84182000
H	4.45443600	0.15786400	0.06843400
B	-1.80978700	-0.00558700	0.29329800
C	-3.00652400	-0.24150500	-0.70851300
C	-1.45745400	-1.23234300	1.23496700
C	-1.26710200	1.42998500	0.58167100
C	-2.99455900	-1.10011100	-1.80763500
C	-4.22232100	0.38987300	-0.43660900
C	-4.11762800	-1.30043400	-2.60783800

C	-5.36612700	0.20155600	-1.20158600
C	-5.30868800	-0.65043700	-2.30154200
F	-1.88539700	-1.76604800	-2.14909300
F	-4.31058600	1.22407400	0.61880800
F	-4.06111800	-2.12165800	-3.66463600
F	-6.51053800	0.82670900	-0.89589400
F	-6.39444100	-0.84593600	-3.05618100
C	-0.77786100	-2.40263200	0.89969700
C	-1.94299600	-1.16706800	2.54186700
C	-0.55815900	-3.42547100	1.82020500
C	-1.75877000	-2.17275200	3.48247100
C	-1.05243800	-3.31458700	3.11511900
F	-0.28533500	-2.60743400	-0.33307900
F	-2.62238900	-0.06729800	2.92889200
F	0.12498600	-4.52313400	1.45994100
F	-2.24397200	-2.05303600	4.72476800
F	-0.85289200	-4.29823300	3.99923400
C	-0.28975700	1.68203300	1.55930800
C	-1.59634600	2.53332500	-0.22508200
C	0.31000400	2.92164400	1.73018600
C	-1.01056400	3.78782000	-0.07848400
C	-0.04613100	3.98148100	0.90344800
F	0.15883900	0.71306200	2.36511300
F	-2.48985800	2.43115000	-1.21138500
F	1.28075400	3.08665500	2.64794500
F	-1.35603000	4.80176000	-0.88061600
F	0.54604400	5.17064000	1.04355500

C	4.95546700	-1.94612500	-1.34576100
C	6.04160600	-1.04972700	-1.49048500
C	5.20942300	-3.24340800	-0.84164900
C	7.32524700	-1.42926400	-1.11326700
H	5.87056700	-0.08330400	-1.95033100
C	6.48930000	-3.60649500	-0.44889700
H	4.38772900	-3.93980200	-0.71534700
C	7.55006100	-2.70213900	-0.58520300
H	8.15258800	-0.73928800	-1.24576100
H	6.66724900	-4.59461200	-0.03658700
H	8.55315400	-2.99817900	-0.29320600
C	2.62926000	-2.52873700	-2.24465500
H	3.05682600	-3.51134400	-2.44197500
H	1.79059400	-2.60912300	-1.53707000
H	2.18803100	-2.11730000	-3.15984600

t4

SCF Energy= -3016.264522

Thermal correction to Gibbs Free Energy= 0.373108

Charge = 0, Multiplicity = 1

C	3.83509200	-1.99301000	-1.03833300
C	0.97366700	-0.49129400	-0.45549300
O	1.95813300	-0.63024500	-1.47752600
O	1.32236300	-0.53587500	0.70699400
O	-0.16324800	-0.32590300	-1.00822600
C	3.23263000	-0.71275800	-0.99878400
C	3.79498400	0.35424600	-0.32660000

C	4.50751700	5.35429500	-0.11543300
C	3.52544600	4.19175600	0.04052600
H	4.01930700	6.30824000	0.10841700
H	5.36232100	5.24788900	0.56369900
H	4.89834100	5.41060500	-1.13875700
C	4.17454400	2.83634400	-0.25784000
H	3.12003300	4.18480800	1.05927900
H	2.66659900	4.34152800	-0.62294100
C	3.16372400	1.67640700	-0.13874600
H	4.59995700	2.84522800	-1.27057800
H	5.01139900	2.66505200	0.43390200
H	2.72721300	1.68266100	0.87413700
H	2.32414700	1.80867500	-0.82790900
H	4.76122200	0.19525100	0.14285700
B	-1.38063900	-0.00184900	-0.09976500
C	-2.63715600	0.16109200	-1.12007000
C	-1.73399100	-1.26789900	0.86489800
C	-0.90811000	1.37181800	0.65517900
C	-2.87492900	-0.82397700	-2.08052200
C	-3.58839600	1.17818600	-1.06471800
C	-3.95421800	-0.79600100	-2.95846000
C	-4.68550000	1.24244100	-1.92170700
C	-4.86770400	0.25021200	-2.87836100
F	-2.04645400	-1.88537200	-2.17932700
F	-3.48781300	2.17120500	-0.15953500
F	-4.12819200	-1.76773000	-3.86901900
F	-5.56614800	2.25117800	-1.83280400

F	-5.91595700	0.29746700	-3.71176500
C	-1.19354300	-2.54830100	0.79222800
C	-2.77105600	-1.12305000	1.78734100
C	-1.61180200	-3.60416600	1.59986800
C	-3.22502500	-2.14525000	2.61154200
C	-2.63564800	-3.40333500	2.51667600
F	-0.20447200	-2.85725600	-0.08945800
F	-3.37615500	0.07661900	1.90901200
F	-1.03607200	-4.81458700	1.49200200
F	-4.21814500	-1.93796200	3.48861900
F	-3.05214100	-4.40833400	3.29938200
C	-0.55170000	1.48726500	1.99752000
C	-0.61212600	2.49000800	-0.12907400
C	0.05915900	2.62316300	2.53166100
C	-0.01220700	3.64356700	0.36283000
C	0.33498300	3.70723000	1.70762700
F	-0.73582800	0.47490300	2.86116900
F	-0.87148300	2.47499900	-1.45267000
F	0.40338400	2.67014700	3.82846900
F	0.27328400	4.67686400	-0.45227800
F	0.95513900	4.79377800	2.19648500
C	5.26508600	-2.16087300	-0.93753800
C	6.15052300	-1.19097000	-1.47043800
C	5.80894100	-3.30560800	-0.30659600
C	7.52539600	-1.34975400	-1.34734000
H	5.74710000	-0.35689800	-2.03300100
C	7.18171800	-3.44211700	-0.16616500

H	5.14669700	-4.05178400	0.11786100
C	8.04216200	-2.46768100	-0.68778300
H	8.19465800	-0.61276000	-1.77917200
H	7.58808600	-4.30760000	0.34694200
H	9.11672400	-2.59053800	-0.59278200
C	2.91946500	-3.15538300	-1.20367700
H	3.44120700	-4.11114100	-1.22162300
H	2.14404700	-3.14675300	-0.42594800
H	2.36807700	-3.02992800	-2.14532300

TS4

SCF Energy= -3016.251850

Thermal correction to Gibbs Free Energy= 0.373983

Charge = 0, Multiplicity = 1

C	3.80003800	-1.97987700	-1.50058200
C	0.91438000	-0.51981100	-0.62531600
O	1.83650000	-0.67912200	-1.66477200
O	1.34587900	-0.50586100	0.53407500
O	-0.26049500	-0.37478600	-1.06769000
C	3.09824000	-0.84697800	-1.14232000
C	3.43860000	0.04559800	-0.10371900
C	5.05567800	4.82166400	-0.20653500
C	3.87912900	3.86807400	0.00804000
H	5.45406300	4.73893400	-1.22501200
H	4.74789700	5.86092300	-0.05216800
H	5.87400000	4.60784200	0.49172700
C	4.27552000	2.39935300	-0.19453200

H	3.47279300	3.99683400	1.01867400
H	3.06142500	4.12186400	-0.67650500
C	3.04932300	1.47238500	-0.01148800
H	4.69377900	2.26413100	-1.20116400
H	5.06375800	2.12291900	0.51889900
H	2.62181600	1.65338700	0.98150800
H	2.28432800	1.72271700	-0.74979900
H	4.19139900	-0.29835700	0.60155500
B	-1.41875100	0.01558300	-0.08403100
C	-2.70133000	0.25144000	-1.05193900
C	-1.76703300	-1.24543600	0.88184600
C	-0.84297500	1.35945700	0.65050200
C	-3.04075300	-0.72367400	-1.99206100
C	-3.57730700	1.33249500	-0.97304200
C	-4.14856400	-0.63022100	-2.82872000
C	-4.69977000	1.46324800	-1.78855300
C	-4.98528700	0.47672200	-2.72574100
F	-2.28628800	-1.83625300	-2.11183400
F	-3.37495100	2.32379800	-0.08312000
F	-4.42207400	-1.59476500	-3.72110900
F	-5.50570900	2.52992800	-1.67786700
F	-6.05864200	0.58780400	-3.51896000
C	-2.79333600	-1.08648500	1.81420600
C	-1.23727800	-2.53101700	0.80499600
C	-3.25387900	-2.10303000	2.64082200
C	-1.66621200	-3.58203600	1.61454000
C	-2.68115800	-3.36849600	2.53845800

F	-3.37799500	0.12278600	1.94210800
F	-0.25352900	-2.84716400	-0.07590000
F	-4.23622300	-1.88398500	3.52646900
F	-1.10836400	-4.79906100	1.50298000
F	-3.10447200	-4.36832700	3.32283000
C	-0.49464300	1.47854300	1.99498600
C	-0.46967800	2.44277400	-0.14983500
C	0.18428400	2.58243400	2.51438200
C	0.20959200	3.55905900	0.32403700
C	0.54649400	3.62647800	1.67176100
F	-0.75024900	0.49661900	2.87527200
F	-0.71612800	2.41622800	-1.47600600
F	0.51320400	2.63329400	3.81416000
F	0.58675500	4.54545900	-0.51006500
F	1.23834600	4.67497300	2.14446700
C	5.19413000	-2.12162600	-1.11040000
C	5.70843700	-3.38641700	-0.74759800
C	6.05336200	-1.00058100	-1.05386100
C	7.01336400	-3.50916100	-0.29158600
H	5.06343100	-4.25799700	-0.77610000
C	7.36566200	-1.13399800	-0.60659400
H	5.70549500	-0.04505300	-1.43081300
C	7.84524800	-2.38452700	-0.21819500
H	7.38795800	-4.48184400	0.01123900
H	8.01722300	-0.26619600	-0.58280100
H	8.86981900	-2.49092200	0.12480200
C	3.09730100	-3.02912000	-2.30963800

H	3.73243300	-3.89525800	-2.49689000
H	2.17077200	-3.33876500	-1.81149900
H	2.79568500	-2.61032300	-3.27713900

t5

SCF Energy= -3016.280695

Thermal correction to Gibbs Free Energy= 0.375238

Charge = 0, Multiplicity = 1

C	3.98607900	-1.59694100	-1.88333400
C	0.81092100	-0.75558100	-0.74960300
O	1.66661100	-1.03947900	-1.72207900
O	1.38072100	-0.61758300	0.42371000
O	-0.39127400	-0.63535700	-0.99243500
C	2.96794000	-1.11863300	-1.16643800
C	2.84269800	-0.55692400	0.23258100
C	6.58530700	2.91978900	0.54899100
C	5.10210300	2.59945700	0.74481100
H	6.87416400	2.81769000	-0.50406300
H	6.81753900	3.94295400	0.86276900
H	7.21596000	2.23751500	1.13181600
C	4.75769900	1.16388500	0.33225000
H	4.82464100	2.74924900	1.79712700
H	4.48495900	3.30100000	0.16760800
C	3.25351900	0.90231500	0.42574600
H	5.09863300	0.98669800	-0.69304000
H	5.30964000	0.45464300	0.96339000
H	2.88300400	1.20017600	1.41411500

H	2.72200000	1.51508100	-0.31023000
H	3.27541900	-1.20047800	0.99688300
B	-1.56156300	-0.00812600	-0.04858000
C	-2.58877500	0.53513700	-1.17770900
C	-2.21051000	-1.24883800	0.76659300
C	-0.86358300	1.15038100	0.85211700
C	-3.03652400	-0.33861900	-2.17231000
C	-3.12497900	1.82120200	-1.22930300
C	-3.93193500	0.02982300	-3.17100000
C	-4.02695400	2.22953900	-2.21001300
C	-4.43084600	1.32887300	-3.18913400
F	-2.60168800	-1.61472400	-2.19116600
F	-2.80001700	2.74779200	-0.30670000
F	-4.32040500	-0.84909800	-4.10552100
F	-4.50883500	3.48008600	-2.21528000
F	-5.29363700	1.70616400	-4.13875900
C	-3.49061800	-1.09091600	1.30365400
C	-1.64379600	-2.50554300	0.96221500
C	-4.17586100	-2.09687000	1.97343500
C	-2.29477000	-3.54562600	1.62366700
C	-3.57192100	-3.34175400	2.13044500
F	-4.10636100	0.10399400	1.20815300
F	-0.39538800	-2.79595900	0.51634300
F	-5.40008200	-1.88131800	2.47147800
F	-1.69527300	-4.73564000	1.77536400
F	-4.21048500	-4.32661000	2.77135900
C	-1.05275400	1.32535000	2.22333600

C	0.00594300	2.07313300	0.26781900
C	-0.41624200	2.32520800	2.96171600
C	0.67793700	3.06694200	0.96333800
C	0.46173900	3.19868200	2.33170000
F	-1.86513400	0.51923000	2.92817800
F	0.29904400	1.97531400	-1.05489600
F	-0.63532200	2.43872300	4.27762100
F	1.56368600	3.86113600	0.33869000
F	1.10003500	4.14367600	3.02957700
C	5.33158800	-1.72448300	-1.26135500
C	5.51007100	-2.45621100	-0.07889200
C	6.44645600	-1.11191000	-1.85224900
C	6.76634900	-2.54198600	0.52086900
H	4.66353200	-2.97709200	0.35940000
C	7.70074500	-1.19381700	-1.25100300
H	6.32514600	-0.54542600	-2.77093200
C	7.86326900	-1.90304500	-0.05890100
H	6.88840800	-3.11427700	1.43575800
H	8.55154200	-0.70054500	-1.71158000
H	8.84112100	-1.96589700	0.40895500
C	3.82465800	-2.02088500	-3.32093400
H	4.11546100	-3.07151300	-3.43466500
H	2.79981700	-1.89638200	-3.67385300
H	4.48739000	-1.43509700	-3.96873600