

Mechanistic Studies on Nickel-Catalyzed Enantioselective [3+2] Annulation via Intermolecular C-C Activation of Cyclopropenones

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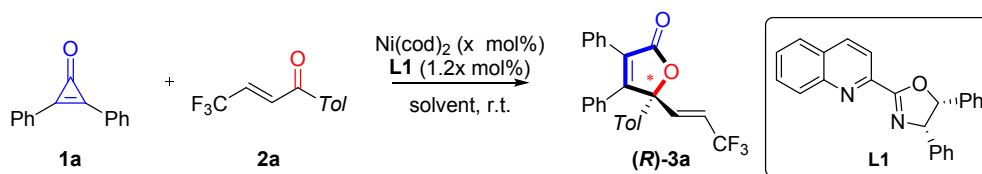
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1, General Information

All chemicals were obtained from commercial sources and were used as received unless otherwise noted. All the reactions were carried out in an argon-filled glove box. The ^1H NMR spectra were recorded on a 400 MHz or 600 MHz NMR spectrometer. The ^{13}C NMR spectra were recorded at 100 MHz or 150 MHz. The ^{19}F NMR spectra were recorded at 565 MHz. Chemical shifts were expressed in parts per million(δ) downfield from the internal standard tetramethylsilane, and were reported as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), dt (doublet of triplet), m (multiplet), br s (broad singlet), etc. The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale. High resolution mass spectra were obtained on an Agilent Q-TOF 6540 spectrometer. Column chromatography was performed on silica gel (300-400 mesh). Thin layer chromatography was performed on pre-coated glassbacked plates and visualized under UV light at 254 nm. Flash column chromatography was performed on silica gel. 1, 2-diones were purchased from commercial sources. Ligands **L1-L9** were prepared by following a literature procedure.¹ Cyclopropenones² and α , β -unsaturated ketones³ were prepared according to literature reports.

2, Coupling of Cyclopropenones with Enones or Diones

2.1 Table S1. The coupling of diphenylcyclopropenone **1a** and enone **2a** with Ni/L1 catalyst.^[a]

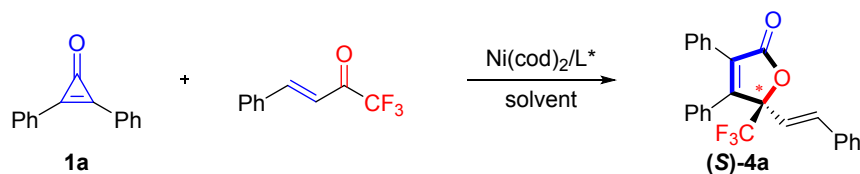


entry	Catalyst (x mol %)	Solvent	Time	yield(%)	ee (%)	TOF (h ⁻¹)
1	1.0	Toluene	5 min	99	95	1188
2	0.5	Toluene	5 min	51	95	1224
3	0.5	Dioxane	5 min	16	91	384
4	0.5	MeO'Bu	5 min	92	93	2208
5	0.5	THF	5 min	10	--	--
6	0.5	PhCl	5 min	0	--	--
7	0.5	PhCF ₃	5 min	0	--	--
8^b	5.0	MeO'Bu	3 h	SM	--	--
9^c	5.0	MeO'Bu	5 min	96	93	--
10^d	5.0	MeO'Bu	3 h	72	--	--

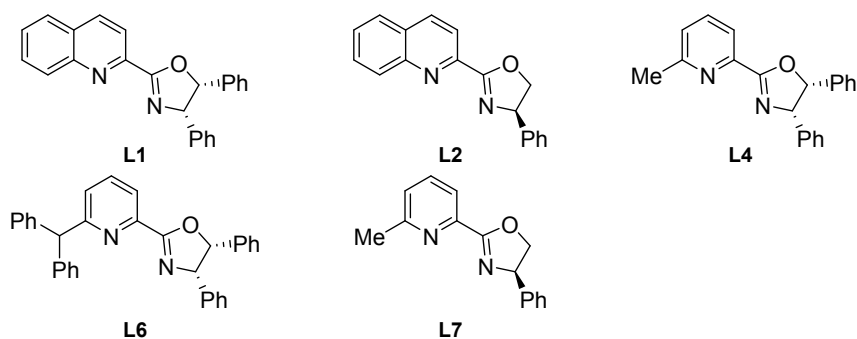
^[a] Reaction conditions: **1a** (0.2 mmol), enone **2a** (0.2 mmol), $\text{Ni}(\text{cod})_2$ (0.01 mmol) and chiral ligand (0.012 mmol) in solvent (2.0 mL) under Ar, isolated yield. The ee was determined by HPLC on a chiral stationary phase. ^[b] under O₂. ^[c]

10 eq H₂O was added. ^[d] PPh₃ was used as ligand instead of **L1**.

Table S2. Optimization Studies of Annulation of **1a** with α -Trifluoromethylated enone. ^a

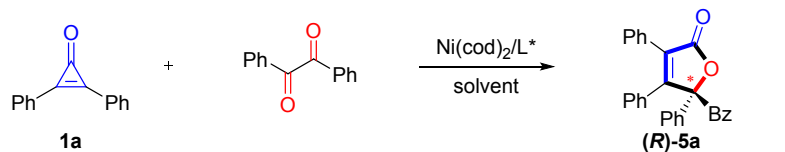


Entry	Catalyst (mol %)	L* (mol %)	Solvent	T (°C)	Yield (%)	ee (%)
1	Ni(cod) ₂ (5)	L1 (6)	toluene	r.t.	50	-98
2	Ni(cod) ₂ (5)	L2 (6)	toluene	r.t.	55	99
3	Ni(cod) ₂ (5)	L4 (6)	toluene	r.t.	50	-97
4	Ni(cod) ₂ (5)	L6 (6)	toluene	r.t.	11	-36
5	Ni(cod) ₂ (5)	L7 (6)	toluene	r.t.	44	-98
6	Ni(cod) ₂ (5)	L2 (6)	toluene	100	43	99
7	Ni(cod) ₂ (5)	L2 (6)	dioxane	r.t.	63	99
8	Ni(cod) ₂ (5)	L2 (6)	PhCl	r.t.	52	99
9	Ni(cod) ₂ (5)	L2 (6)	PhCF ₃	r.t.	50	98
10	Ni(cod) ₂ (5)	L2 (6)	DCE	r.t.	--	--
11	Ni(cod) ₂ (5)	L2 (6)	EtOH	r.t.	57	98
12	Ni(cod) ₂ (5)	L2 (6)	DMA	r.t.	77	98
13	Ni(cod) ₂ (5)	L2 (6)	MeO ^t Bu	r.t.	82	98
14	Ni(cod) ₂ (5)	L2 (6)	acetone	r.t.	66	98
15	Ni(cod) ₂ (5)	L2 (6)	THF	r.t.	59	92
16	--	L2 (6)	MeO ^t Bu	r.t.	--	--

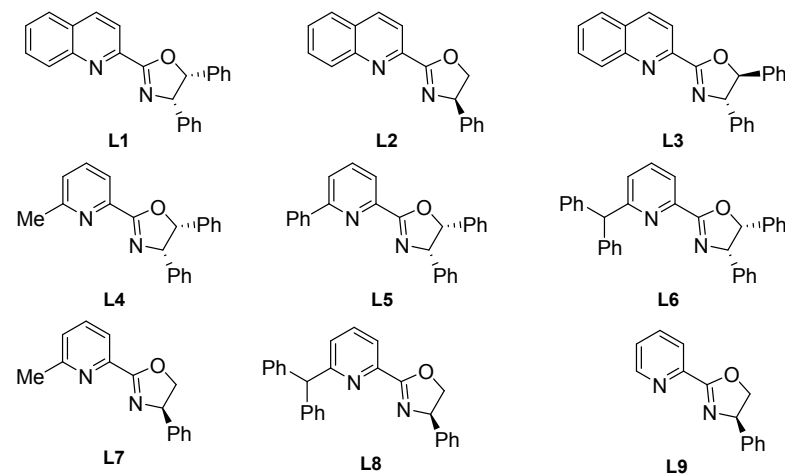


^aReaction conditions: **1** (0.20 mmol), **enone** (0.20 mmol), Ni(cod)₂ (0.01 mmol), **L*** (0.012 mmol), solvent (2.0 mL), 24 h under argon.

Table S3. Optimization Studies of Annulation of **1a** with 1, 2-dione.^a



Entry	Catalyst (mol %)	L* (mol %)	Solvent	T (°C)	Yield (%)	ee (%)
1	Ni(cod) ₂ (5)	L1 (6)	toluene	60	46	65
2	Ni(cod) ₂ (5)	L1 (6)	<i>i</i> PrOH	60	21	0
3	Ni(cod) ₂ (5)	L1 (6)	dioxane	60	43	53
4	Ni(cod) ₂ (5)	L1 (6)	THF	60	47	58
5	Ni(cod) ₂ (5)	L1 (6)	DCE	60	trace	--
6	Ni(cod) ₂ (5)	L1 (6)	PhCl	60	44	54
7	Ni(cod) ₂ (5)	L1 (6)	PhCF ₃	60	22	42
8	Ni(cod) ₂ (5)	L1 (6)	PhOMe	60	32	54
9	Ni(cod) ₂ (5)	L1 (6)	toluene	r.t.	41	66
10	Ni(cod) ₂ (5)	L2 (6)	toluene	r.t.	44	-41
11	Ni(cod) ₂ (5)	L3 (6)	toluene	r.t.	48	42
12	Ni(cod) ₂ (5)	L4 (6)	toluene	r.t.	49	76
13	Ni(cod) ₂ (5)	L5 (6)	toluene	r.t.	85	45
14	Ni(cod) ₂ (5)	L6 (6)	toluene	r.t.	77	80
15	Ni(cod) ₂ (5)	L6 (6)	toluene	0	76	90
16	Ni(cod) ₂ (5)	L7 (6)	toluene	0	38	72
17	Ni(cod) ₂ (5)	L8 (6)	toluene	0	27	20
18	Ni(cod) ₂ (5)	L9 (6)	toluene	0	16	4
19	Ni(cod) ₂ (5)	L6 (6)	toluene	-20	21	93
20	Ni(cod) ₂ (5)	L6 (6)	dioxane	12	95	86
21	Ni(cod) ₂ (5)	L6 (6)	THF	0	71	77
22	Ni(cod) ₂ (5)	L6 (6)	MeO ^t Bu	0	18	88
23	Ni(cod) ₂ (5)	L6 (6)	PhOPh	0	66	84
24	Ni(cod) ₂ (5)	L6 (6)	2-MeTHF	0	47	86
25	Ni(cod) ₂ (5)	L6 (6)	Tol:dioxane 1:1	0	67	92



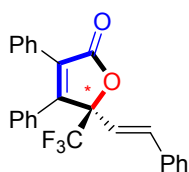
^aReaction conditions: **1** (0.20 mmol), **benzil** (0.20 mmol), Ni(cod)₂ (0.01 mmol), L* (0.012 mmol), solvent (2.0 mL), 24 h under argon.

3. General Synthetic Procedures

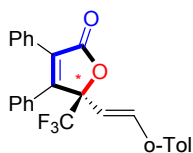
General procedure **A**: Ni(cod)₂ (2.75 mg, 0.01 mmol) and **L2** (4.2 mg, 0.012 mmol) in MeO^tBu (2.0 mL) were charged into a pressure tube under argon. The mixture was stirred for 10 min at room temperature, followed by addition of a cyclopropenone (0.200 mmol, 1.0 equiv) and α -CF₃ enone (0.200 mmol, 1.0 equiv). The reaction tube was then sealed and placed into an oil bath at room temperature. After reaction for 24 h, the reaction mixture was filtered through a pad of celite. The mixture was eluted with ethyl acetate, concentrated, and purified by silica gel chromatography (PE:EA = 10:1) to give the indicated product.

General procedure **B**: Ni(cod)₂ (2.75 mg, 0.01 mmol) and **L6** (5.6 mg, 0.012 mmol) in toluene (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 10 min at room temperature, followed by addition of a cyclopropenone (0.20 mmol, 1.0 equiv) and 1, 2-dione (0.20 mmol, 1.0 equiv). The reaction tube was then sealed and placed into an oil bath at 0 °C. After reaction for 24 h, the reaction mixture was filtered through a pad of celite. The mixture was eluted with ethyl acetate, concentrated, and purified by silica gel chromatography (PE:EA = 10:1) to give the indicated product.

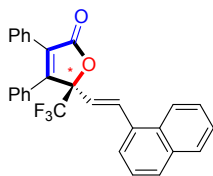
General procedure **C**: Ni(cod)₂ (2.75 mg, 0.01 mmol) and **L6** (5.6 mg, 0.012 mmol) in dioxane (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 10 min at room temperature, followed by addition of a cyclopropenone (0.200 mmol, 1.0 equiv) and 1, 2-dione (0.200 mmol, 1.0 equiv). The reaction tube was then sealed and placed in an oil bath 12 °C for 24 h. The reaction mixture was filtered through a pad of celite, eluted with ethyl acetate, concentrated, and purified by silica gel chromatography (PE:EA = 10:1) to give the indicated product.



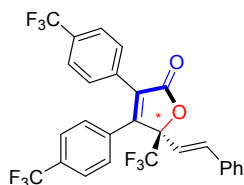
4a, General procedure **A**, white solid, mp: 118~120 °C. 65.8 mg (82% yield). ee: 98%, HPLC analysis on a Chiralcel OD-H column (hexane/isopropanol = 99/1, flow rate 1.0 mL/min): t_R = 6.9 min (major), t_R = 8.6 min (minor). $[\alpha]_D^{26}$ = 4.8 (c 0.9, CH₂Cl₂). ¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.32 (m, 5H), 7.32 – 7.22 (m, 5H), 7.22 – 7.12 (m, 5H), 7.07 (d, J = 16.0 Hz, 1H), 6.34 (d, J = 16.0 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 169.9, 157.1, 135.4, 135.0, 130.8, 129.9, 129.5, 129.4, 129.3, 129.2, 129.0, 128.5, 128.5, 128.4, 127.3, 122.8 (q, J = 285.9 Hz), 116.7, 86.2 (q, J = 30.8 Hz). ¹⁹F NMR (376



4g, General procedure **A**, yellow oil. 73.2 mg (87% yield). ee: 96%, HPLC analysis on a Chiralcel AS-H column (hexane/isopropanol = 95/5, flow rate 0.8 mL/min): $t_R = 7.0$ min (major), $t_R = 8.6$ min (minor). $[\alpha]_D^{26} = 18.7$ (c 1.1, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.38 – 7.33 (m, 4H), 7.32 – 7.27 (m, 3H), 7.21 – 7.16 (m, 5H), 7.15 – 7.09 (m, 3H), 6.23 (d, $J = 15.9$ Hz, 1H), 2.29 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 169.9, 157.0, 136.7, 134.3, 133.6, 130.8, 130.8, 129.9, 129.6, 129.5, 129.4, 129.2, 129.2, 128.6, 128.5, 128.5, 126.5, 126.1, 122.8 (q, $J = 286.2$ Hz), 118.2, 86.3 (q, $J = 30.7$ Hz), 19.9. ^{19}F NMR (565 MHz, CDCl_3) δ -74.95 (s). HRMS (ESI, m/z): calcd for $\text{C}_{26}\text{H}_{19}\text{F}_3\text{NaO}_2^+$ $[\text{M} + \text{Na}]^+$: 443.1229, found 443.1231.

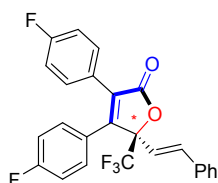


4h, General procedure **A**, yellow oil. 50.6 mg (55% yield). ee: 98%, HPLC analysis on a Chiralcel OD-H column (hexane/isopropanol = 99/1, flow rate 1.0 mL/min): $t_R = 9.3$ min (major), $t_R = 14.8$ min (minor). $[\alpha]_D^{27} = 20.4$ (c 0.57, CH_2Cl_2). ^1H NMR (600 MHz, CDCl_3) δ 7.77 – 7.73 (m, 4H), 7.53 – 7.52 (m, 1H), 7.44 – 7.40 (m, 2H), 7.39 – 7.29 (m, 5H), 7.25 – 7.14 (m, 6H), 6.45 (d, $J = 16.0$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 169.9, 157.0, 135.6, 133.8, 133.6, 132.4, 130.9, 130.0, 129.6, 129.5, 129.4, 129.2, 128.8, 128.6, 128.5, 128.4, 127.9, 127.0, 126.8, 123.3, 122.9 (q, $J = 286.1$ Hz), 117.0, 86.3 (q, $J = 30.8$ Hz). ^{19}F NMR (565 MHz, CDCl_3) δ -74.93 (s). HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{19}\text{F}_3\text{NaO}_2^+$ $[\text{M} + \text{Na}]^+$: 479.1229, found 479.1226.

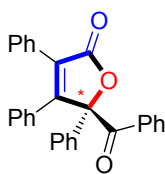


4i, General procedure **A**, mp: 179.5~180.1 °C. 22.8 mg (21% yield). ee: 99%, HPLC analysis on a Chiralcel OD-H column (hexane/isopropanol = 99/1, flow rate 1.0 mL/min): $t_R = 10.1$ min (major), $t_R = 7.8$ min (minor). $[\alpha]_D^{28} = 6.7$ (c 0.3, CH_2Cl_2). ^1H NMR (600 MHz, CDCl_3) δ 7.66 (d, $J = 8.2$ Hz, 2H),

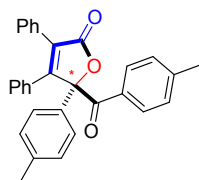
7.48 (d, $J = 8.2$ Hz, 2H), 7.42 – 7.37 (m, 4H), 7.36 – 7.29 (m, 5H), 7.10 (d, $J = 16.0$ Hz, 1H), 6.28 (d, $J = 16.0$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 168.8, 157.0, 136.5, 134.6, 134.0, 132.5 (dd, $J = 66.3$, 33.2 Hz), 131.9, 131.7, 131.4, 129.8, 129.7, 129.5, 129.2, 129.0, 127.4, 126.5 (dd, $J = 7.2$, 3.4 Hz), 125.7 (q, $J = 3.8$ Hz), 124.6 (q, $J = 16.5$ Hz), 122.8 (q, $J = 16.9$ Hz), 121.7, 115.5, 86.4 (q, $J = 30.8$ Hz). ^{19}F NMR (565 MHz, CDCl_3) δ -63.02 (s, 3F), -63.09 (s, 3F), -74.91 (s, 3F). HRMS (ESI, m/z): calcd for $\text{C}_{27}\text{H}_{15}\text{F}_9\text{NaO}_2^+$ [$\text{M} + \text{Na}$] $^+$: 565.0821, found 565.0794.



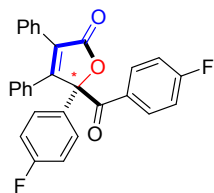
4j, General procedure **A**, mp: 112~114 °C. 53.1 mg (60% yield). ee: 98%, HPLC analysis on a Chiralcel AS-H column (hexane/isopropanol = 95/5, flow rate 0.8 mL/min): $t_{\text{R}} = 9.3$ min (major), $t_{\text{R}} = 11.3$ min (minor). $[\alpha]_{\text{D}}^{25} = 7.2$ (c 0.3, CH_2Cl_2). ^1H NMR (600 MHz, CDCl_3) δ 7.41 – 7.35 (m, 2H), 7.34 – 7.26 (m, 5H), 7.20 – 7.14 (m, 2H), 7.10 – 7.03 (m, 3H), 6.93 – 6.87 (m, 2H), 6.30 (d, $J = 16.0$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 169.6, 163.6 (d, $J = 248.1$ Hz), 163.3 (d, $J = 254.2$ Hz), 155.7, 135.9, 134.8, 131.4 (d, $J = 8.2$ Hz), 130.7 (d, $J = 8.5$ Hz), 129.6, 129.1, 129.0, 127.3, 126.6 (d, $J = 3.2$ Hz), 124.3 (d, $J = 3.3$ Hz), 122.8 (q, $J = 286.0$ Hz), 116.8 (d, $J = 21.9$ Hz), 116.3, 115.9 (d, $J = 21.9$ Hz), 86.2 (q, $J = 31.1$ Hz). ^{19}F NMR (565 MHz, CDCl_3) δ -75.03 (s, 3F), -109.56 – -109.62 (m, 1F), -109.98 – -110.04 (m, 1F). HRMS (ESI, m/z): calcd for $\text{C}_{25}\text{H}_{15}\text{F}_5\text{NaO}_2^+$ [$\text{M} + \text{Na}$] $^+$: 465.0884, found 465.0869.



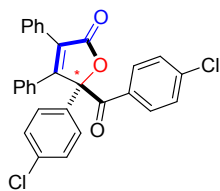
5a, General procedure **B**, yellow oil. 63.3 mg (76% yield). ee: 90%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_{\text{R}} = 9.7$ min (major), $t_{\text{R}} = 12.4$ min (minor). $[\alpha]_{\text{D}}^{24} = -53.2$ (c 0.7, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.94 – 7.92 (m, 2H), 7.49 – 7.46 (m, 1H), 7.39 – 7.29 (m, 7H), 7.26 – 7.17 (m, 8H), 6.88 – 6.83 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.4, 171.3, 163.8, 134.9, 134.3, 133.6, 132.5, 131.0, 129.5, 129.4, 129.2, 129.0, 128.9, 128.4, 128.3, 128.1, 127.5, 126.1, 93.5. HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{21}\text{O}_3^+$ [$\text{M} + \text{H}$] $^+$: 417.1485, found 417.1484.



5b, General procedure **B**, yellow oil. 46.2 mg (52% yield). ee: 84.0%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_R = 17.4$ min (major), $t_R = 20.6$ min (minor). $[\alpha]_D^{27} = -95.1$ (c 1.4, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.77 – 7.75 (m, 2H), 7.26 – 7.24 (m, 2H), 7.18 – 7.08 (m, 6H), 7.05 – 7.04 (m, 6H), 6.84 – 6.71 (m, 2H), 2.27 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.2, 171.4, 164.0, 144.6, 139.3, 132.8, 132.1, 132.0, 131.2, 129.7, 129.6, 129.5, 129.1, 128.9, 128.8, 128.3, 128.1, 127.4, 126.1, 93.6, 21.8, 21.4. HRMS (ESI, m/z): calcd for $\text{C}_{31}\text{H}_{24}\text{NaO}_3^+$ $[\text{M} + \text{Na}]^+$: 467.1618, found 467.1604.

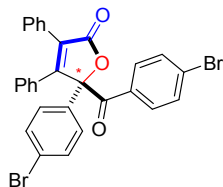


5c, General procedure **C**, yellow oil. 80.2 mg (89% yield). ee: 90.0%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_R = 9.5$ min (major), $t_R = 16.1$ min (minor). $[\alpha]_D^{28} = -96.2$ (c 2.6, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.90 – 7.87 (m, 2H), 7.27 – 7.25 (m, 2H), 7.24 – 7.10 (m, 8H), 6.99 – 6.91 (m, 4H), 6.81 – 6.79 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 191.8, 170.9, 160.0 (d, $J = 257.2$ Hz), 163.5, 163.2 (d, $J = 250.0$ Hz), 133.8 (d, $J = 9.5$ Hz), 132.3, 130.7 (d, $J = 3.4$ Hz), 130.6 (d, $J = 3.0$ Hz), 129.5, 129.4, 129.2, 129.1, 129.0, 128.4, 128.3, 128.0 (d, $J = 8.5$ Hz), 127.7, 116.3 (d, $J = 21.9$ Hz), 115.8 (d, $J = 21.9$ Hz), 92.9. ^{19}F NMR (377 MHz, CDCl_3) δ -103.13 – -103.22 (m, 1F), -111.08 – -111.17 (m, 1F). HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{19}\text{F}_2\text{O}_3^+$ $[\text{M} + \text{H}]^+$: 453.1297, found 453.1286.

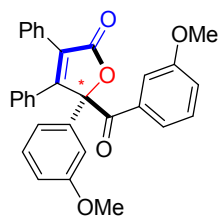


5d, General procedure **C**, yellow oil. 62.1 mg (64% yield). ee: 92%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_R = 11.7$ min (major), $t_R = 17.8$ min (minor). $[\alpha]_D^{27} = -55.0$ (c 3.7, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.77 (d, $J = 8.6$ Hz, 2H), 7.29 –

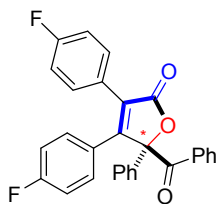
7.20 (m, 6H), 7.20 – 7.13 (m, 6H), 7.09 (d, $J = 8.6$ Hz, 2H), 6.82 (d, $J = 7.4$ Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 192.0, 170.7, 163.1, 140.5, 135.7, 133.3, 132.5, 132.3, 132.1, 129.5, 129.5, 129.4, 129.3, 129.1, 128.9, 128.4, 128.4, 127.9, 127.4, 92.7. HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{19}\text{Cl}_2\text{O}_3^+$ [$\text{M} + \text{H}$] $^+$: 485.0706, found 485.0702.



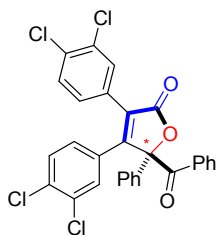
5e, General procedure C, yellow oil. 100.5 mg (88 % yield). ee: 92.0%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_{\text{R}} = 13.5$ min (major), $t_{\text{R}} = 20.2$ min (minor). $[\alpha]_{\text{D}}^{27} = -62.3$ (c 2.5, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.70 – 7.68 (m, 2H), 7.44 – 7.36 (m, 4H), 7.29 – 7.10 (m, 8H), 7.03 – 7.01 (m, 2H), 6.84 – 6.78 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 192.2, 170.7, 163.0, 133.9, 132.9, 132.6, 132.3, 132.1, 132.0, 131.4, 129.5, 129.5, 129.4, 129.3, 129.2, 128.9, 128.4, 128.4, 127.9, 127.6, 123.9, 92.8. HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{18}\text{Br}_2\text{NaO}_3^+$ [$\text{M} + \text{Na}$] $^+$: 594.9515, found 594.9511.



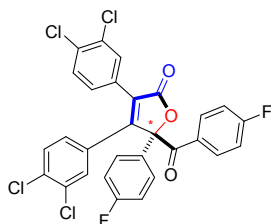
5g, General procedure C, room temperature, yellow oil. 67.4 mg (71% yield). ee: 78.0%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_{\text{R}} = 18.0$ min (major), $t_{\text{R}} = 16.3$ min (minor). $[\alpha]_{\text{D}}^{27} = -99.4$ (c 1.5, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.47 – 7.37 (m, 2H), 7.27 – 7.25 (m, 2H), 7.22 – 7.09 (m, 8H), 6.96 – 6.93 (m, 1H), 6.84 – 6.79 (m, 3H), 6.74 – 6.70 (m, 2H), 3.65 (s, 3H), 3.59 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.1, 171.1, 163.7, 160.0, 159.5, 136.4, 135.6, 132.6, 130.0, 129.6, 129.5, 129.4, 129.3, 129.0, 128.9, 128.3, 128.1, 127.6, 123.9, 120.5, 120.1, 118.5, 115.1, 114.8, 113.4, 111.3, 93.4, 83.7, 55.5, 29.8. HRMS (ESI, m/z): calcd for $\text{C}_{31}\text{H}_{24}\text{NaO}_5^+$ [$\text{M} + \text{Na}$] $^+$: 499.1516, found 499.1509.



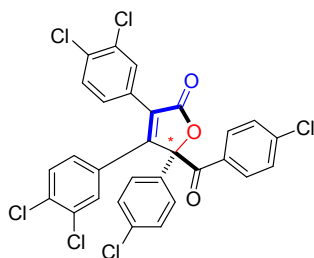
5h, General procedure C, yellow oil. 71.2 mg (79% yield). ee: 90.0%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): t_R = 8.8 min (major), t_R = 11.9 min (minor). $[\alpha]_D^{26}$ = -95.1 (c 1.1, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.86 – 7.83 (m, 2H), 7.44 – 7.40 (m, 1H), 7.33 – 7.21 (m, 7H), 7.19 – 7.12 (m, 2H), 6.93 – 6.80 (m, 4H), 6.80 – 6.73 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 193.4, 171.0, 163.1 (d, J = 249.9 Hz), 163.0 (d, J = 250.3 Hz), 162.8, 134.6, 134.1, 133.8, 131.5 (d, J = 4.0 Hz), 131.4 (d, J = 3.4 Hz), 131.1, 129.6, 129.2, 128.5, 128.3 (d, J = 3.5 Hz), 126.9, 125.9, 125.1 (d, J = 3.2 Hz), 115.7 (d, J = 6.5 Hz), 115.5 (d, J = 6.5 Hz), 93.5. ^{19}F NMR (565 MHz, CDCl_3) δ -111.12 – -111.21 (m, 1F), -111.31 – -111.40 (m, 1F). HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{18}\text{F}_2\text{NaO}_3^+$ $[\text{M} + \text{Na}]^+$: 475.1116, found 475.1115.



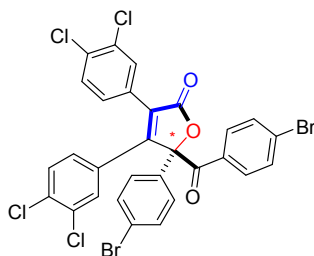
5i, General procedure C, yellow oil. 90.4 mg (82% yield). ee: 90.0%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): t_R = 7.4 min (major), t_R = 11.1 min (minor). $[\alpha]_D^{25}$ = -84.4 (c 1.6, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.86 – 7.83 (m, 2H), 7.45 – 7.40 (m, 1H), 7.33 – 7.26 (m, 5H), 7.22 – 7.13 (m, 4H), 7.10 – 7.06 (m, 2H), 6.74 (m, 1H), 6.69 – 6.60 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.1, 170.3, 163.3, 134.5, 134.3, 134.0, 133.9, 131.1, 130.6, 129.8, 129.7, 129.6, 129.5, 129.4, 129.3, 129.2, 128.5, 127.8, 127.6, 127.0, 125.9, 93.6. HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{16}\text{Cl}_4\text{NaO}_3^+$ $[\text{M} + \text{Na}]^+$: 574.9746, found 574.9751.



5j, General procedure B, yellow oil. 94.3 mg (68% yield). ee: 88%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_R = 7.8$ min (major), $t_R = 14.2$ min (minor). $[\alpha]_D^{23} = -113.8$ (c 3.9, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.92 – 7.76 (m, 2H), 7.32 – 7.31 (m, 1H), 7.22 – 7.15 (m, 2H), 7.14 – 7.09 (m, 2H), 7.08 – 7.06 (m, 2H), 7.02 – 6.89 (m, 4H), 6.83 – 6.82 (m, 1H), 6.65 – 6.63 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 191.4, 169.9, 166.0 (d, $J = 257.8$ Hz), 163.3 (d, $J = 250.8$ Hz), 162.9, 134.4 (d, $J = 8.8$ Hz), 133.9 (d, $J = 9.5$ Hz), 133.5, 130.2, 130.0 (d, $J = 2.9$ Hz), 129.9 (d, $J = 3.2$ Hz), 129.7, 129.6, 129.5, 129.4, 129.2, 127.8, 127.7, 127.7, 127.6, 127.1, 116.5 (d, $J = 22.1$ Hz), 115.8 (d, $J = 22.0$ Hz), 92.8. ^{19}F NMR (376 MHz, CDCl_3) δ -102.46 – -102.50 (m), -110.28 – -110.35 (m). HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{15}\text{Cl}_4\text{F}_2\text{O}_3^+$ $[\text{M} + \text{H}]^+$: 588.9738, found 588.9741.



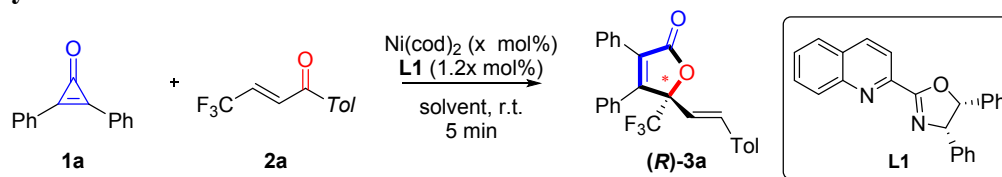
5k, General procedure B, yellow oil. 119.1 mg (87.8% yield). ee: 90%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_R = 8.9$ min (major), $t_R = 16.6$ min (minor). $[\alpha]_D^{23} = -109.3$ (c 2.8, CH_2Cl_2). ^1H NMR (400 MHz, Acetone- d_6) δ 7.80 – 7.78 (m, 2H), 7.43 – 7.30 (m, 5H), 7.25 (s, 2H), 7.19 – 7.15 (m, 2H), 7.13 – 7.11 (m, 1H), 6.94 (s, 1H), 6.77 – 6.75 (m, 1H). ^{13}C NMR (101 MHz, Acetone- d_6) δ 192.7, 170.0, 162.6, 140.7, 136.2, 134.7, 134.5, 134.5, 133.9, 133.6, 133.2, 131.9, 130.8, 130.8, 130.2, 130.2, 130.1, 130.0, 130.0, 130.0, 128.9, 128.9, 128.7, 128.7, 93.5. HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{15}\text{Cl}_6\text{O}_3^+$ $[\text{M} + \text{H}]^+$: 620.9147, found 620.9145.



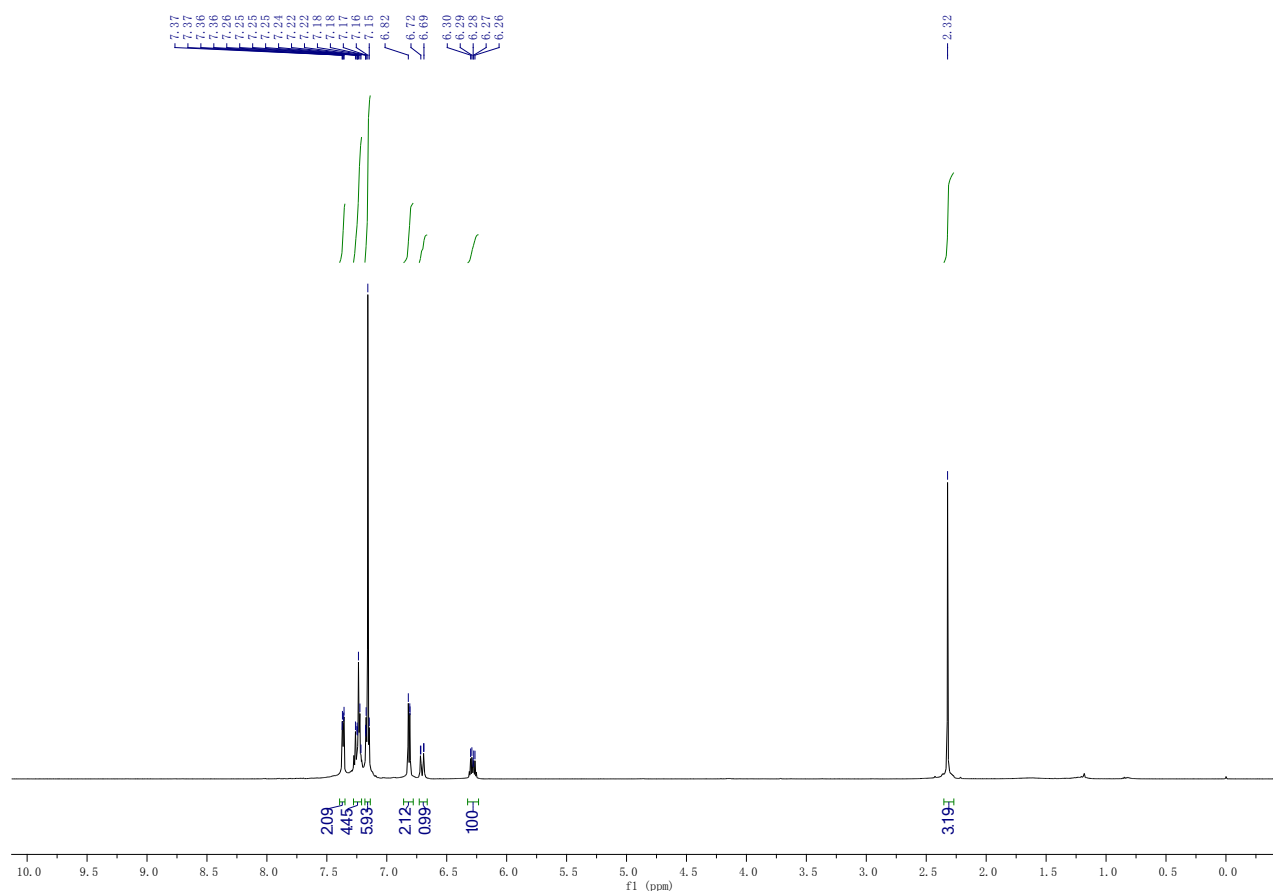
5l, General procedure C, yellow oil. 115.5 mg (81% yield). ee: 86%, HPLC analysis on a Chiralcel AD-H column (hexane/isopropanol = 95/5, flow rate 1.0 mL/min): $t_R = 10.1$ min (major), $t_R = 18.8$ min (minor). $[\alpha]_D^{24} = -90.5$ (c 2.6, CH_2Cl_2). ^1H NMR (400 MHz, Acetone- d_6) δ 7.77 – 7.64 (m, 2H), 7.56 – 7.48 (m, 4H), 7.34 – 7.33 (m, 1H), 7.27 – 7.24 (m, 1H), 7.21 – 7.17 (m, 2H), 7.16 – 7.16 (m, 1H), 7.14 –

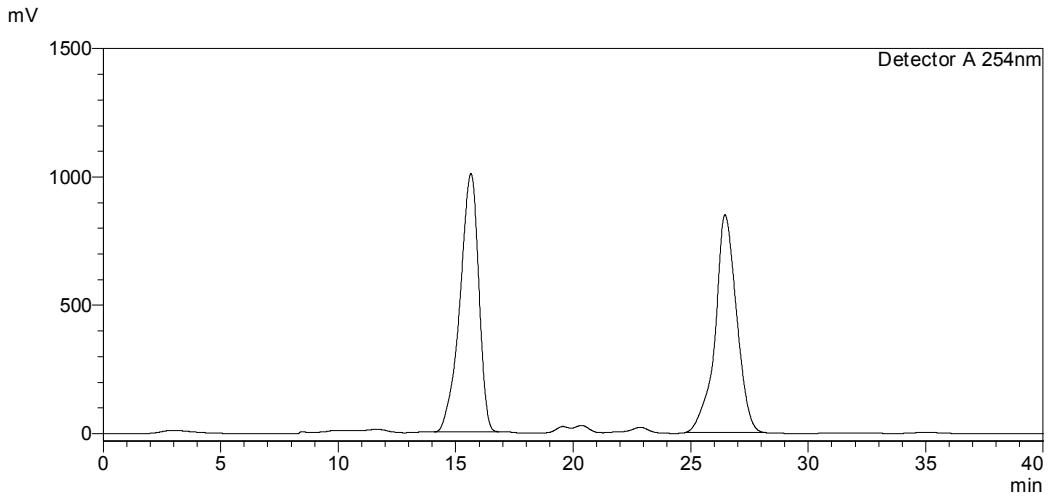
7.10 (m, 1H), 6.95 – 6.94 (m, 1H), 6.77 – 6.75 (m, 1H). ^{13}C NMR (101 MHz, Acetone- d_6) δ 192.9, 167.0, 162.5, 134.7, 134.5, 134.5, 134.4, 133.9, 133.3, 133.2, 132.7, 131.9, 130.9, 130.8, 130.2, 130.1, 130.0, 130.0, 129.5, 128.9, 128.7, 124.4, 93.5. HRMS (ESI, m/z): calcd for $\text{C}_{29}\text{H}_{15}\text{Br}_2\text{Cl}_4\text{O}_3^+$ [M + H] $^+$: 708.8137, found 708.8140.

4. TOF Study.

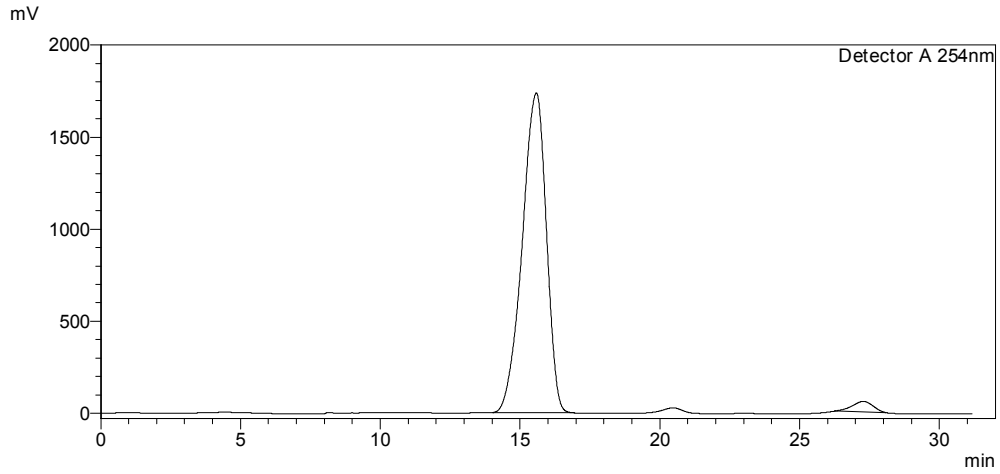


To a solution of the chiral catalyst $\text{Ni}(\text{cod})_2/\text{L1}$ (0.20 μmol : 0.04 mL of a 5×10^{-3} mmol/mL stock solution in MeOtBu) in MeO'Bu (2.0 mL) under the argon atmosphere. cyclopropenone **1a** (42 mg, 0.2 mmol, 1.00 equiv) and α, β -unsaturated ketone **2a** (42 mg, 0.2 mmol, 1.0 equiv) was added. The reaction vessel was then sealed and placed in an oil bath at room temperature for 5 min, The reaction mixture was filtered through a pad of celite, eluted with ethyl acetate, concentrated, and purified by silica gel chromatography (PE : EA = 10:1) to give the indicated product **3a** (75.6 mg, yield 91%, ee 93%). HPLC analysis on a Chiralcel OD-H column (hexane/isopropanol = 99/1, flow rate 0.5 mL/min): $t_R = 15.6$ min (major), $t_R = 27.3$ min (minor). ^1H NMR (600 MHz, CDCl_3): δ 7.36 (dd, $J = 7.6, 1.8$ Hz, 2H), 7.29 – 7.19 (m, 4H), 7.19 – 7.09 (m, 6H), 6.81 (d, $J = 7.4$ Hz, 2H), 6.70 (dd, $J = 15.6, 1.9$ Hz, 1H), 6.28 (m, 1H), 2.32 (s, 3H).





Peak#	Ret. Time	Area	Height	Conc.
1	15.650	55917962	1006967	50.856
2	26.461	54035576	848978	49.144

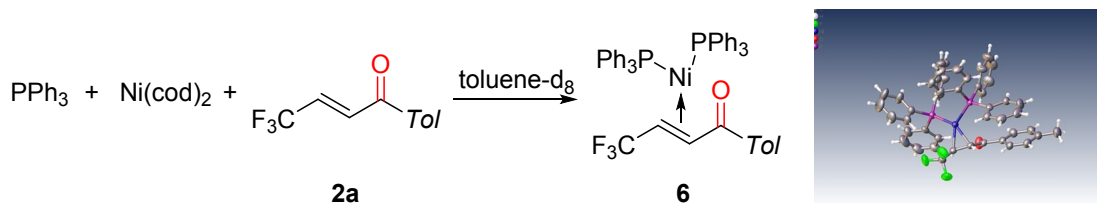


Peak#	Ret. Time	Area	Height	Conc.
1	15.581	104151757	1737350	97.244
2	27.279	2952283	57071	2.756

5. Mechanistic Studies

5.1 Identify of Reaction Intermediate

5.1.1 Characterization of the olfine-Ni complex **6**

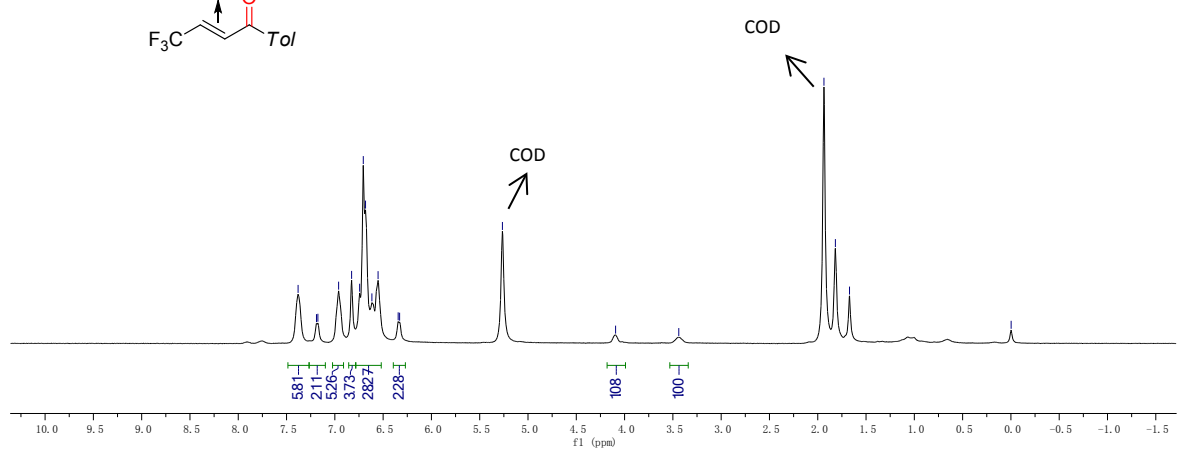
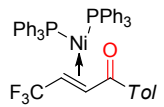
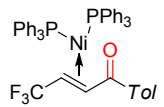
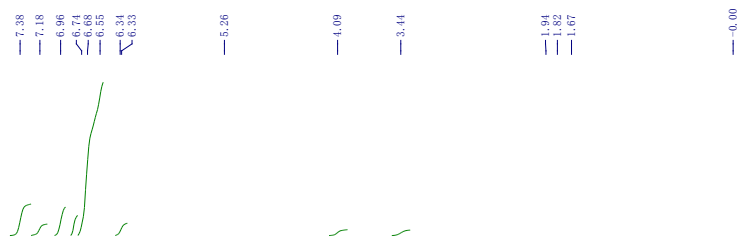


Ni(cod)₂ (3.5 mg, 0.0125 mmol, 1.0 equiv) and PPh₃ (6.6 mg, 0.025 mmol, 2.0 equiv) in toluene-*d*₈ (1.0 mL) were charged into a 25 mL pressure tube under the argon atmosphere. The mixture was stirred for 10 min at room temperature, followed by addition of α, β-unsaturated ketone **2a** (2.7 mg, 0.0125 mmol, 1.00 equiv). The reaction stirred for 8 h providing a deep red solution. The reaction mixture was transferred to the NMR tube directly in the dry box. ¹H NMR (600 MHz, toluene-*d*₈): δ 7.72 (m, 5H), 7.53 (d, *J* = 5.8 Hz, 2H), 7.30 (m, 6H), 7.11 – 6.83 (m, 18H), 6.68 (d, *J* = 6.0 Hz, 2H), 4.60-4.40 (m, 1H), 3.85-3.75 (m, 1H), 2.02 (s, 3H). ¹⁹F NMR (565 MHz, toluene-*d*₈) δ -52.73 (d, *J* = 9.2 Hz). ³¹P NMR (243 MHz, toluene-*d*₈) δ 36.03 (d, *J* = 20.7 Hz, 1P), 28.92-29.02 (m, 1P). ¹³C NMR (151 MHz, toluene-*d*₈) δ 191.4, 140.0, 134.9, 134.7, 134.7, 134.4, 133.9 (d, *J* = 12.8 Hz), 133.7 (d, *J* = 13.0 Hz), 55.3 (d, *J* = 13.0 Hz), 49.8-49.2 (m), 20.9.

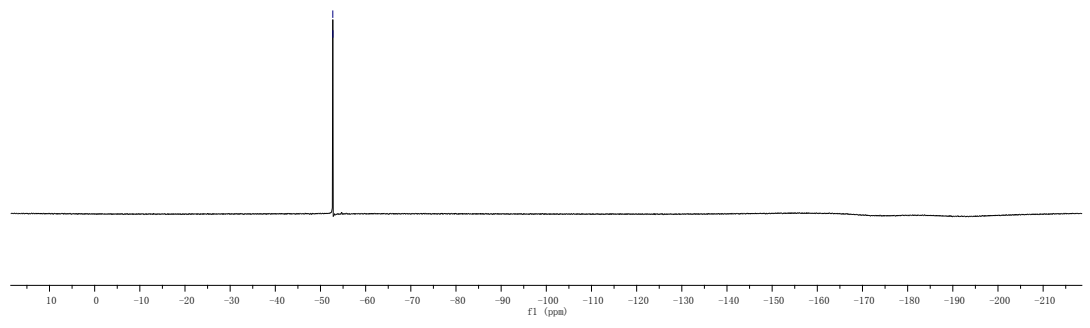
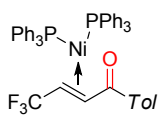
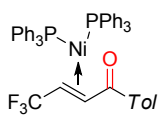
Toluene-*d*₈ and 1,5-Cyclooctadiene (cod) was removed using reduced pressure in the dry-box. ¹H NMR (400 MHz, C₆D₆) δ 7.90 (m, 6H), 7.74 (d, *J* = 7.3 Hz, 2H), 7.55 – 7.42 (m, 6H), 7.24 – 6.92 (m, 18H), 6.83 (d, *J* = 7.4 Hz, 2H), 4.75-4.60 (m, 1H), 4.20-4.00 (m, 1H), 2.11 (s, 3H). ¹⁹F NMR (376 MHz, C₆D₆) δ -52.69 (t, *J* = 9.8 Hz).

The X-ray of **6** was obtained with the toluene-*d*₈/hexane (2/1) in the dry box under the argon atmosphere.

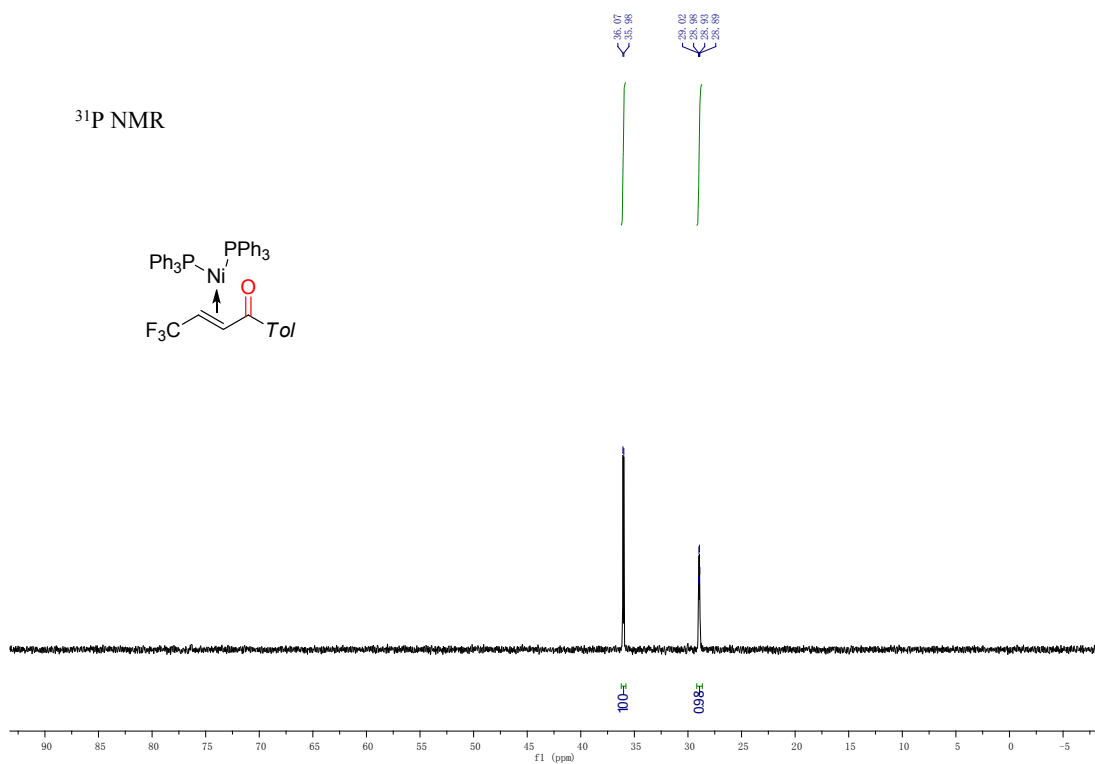
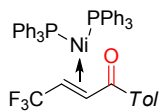
¹H NMR



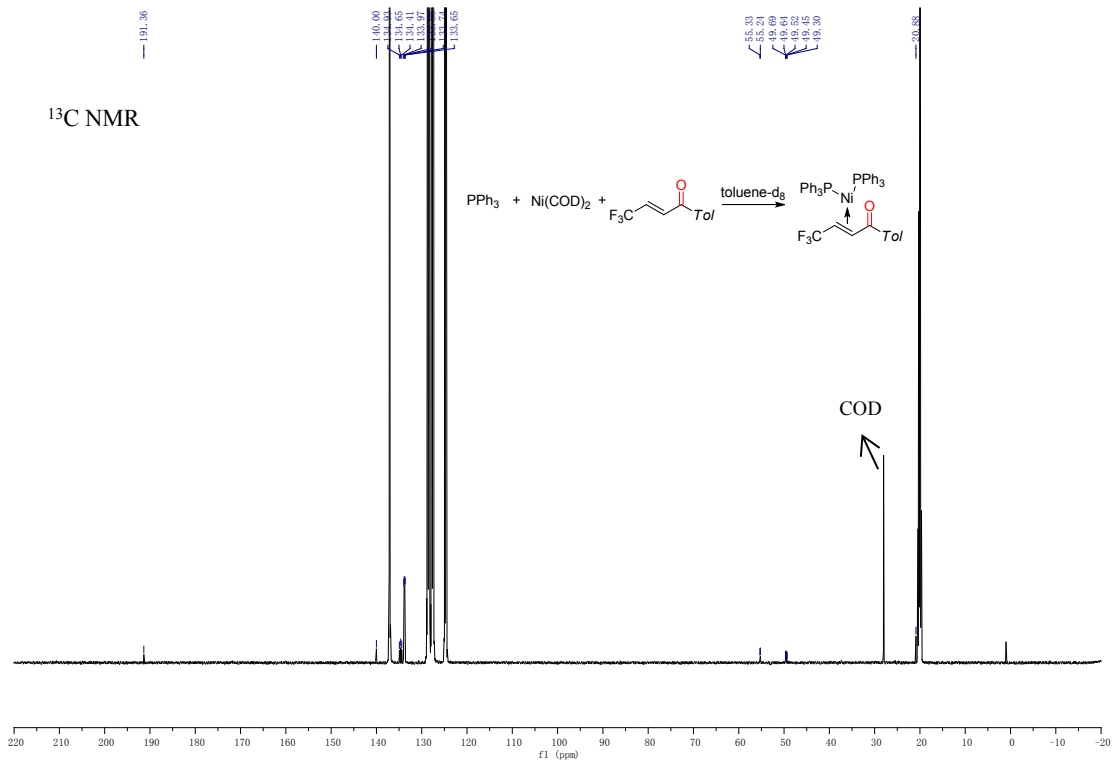
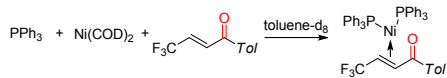
¹⁹F NMR

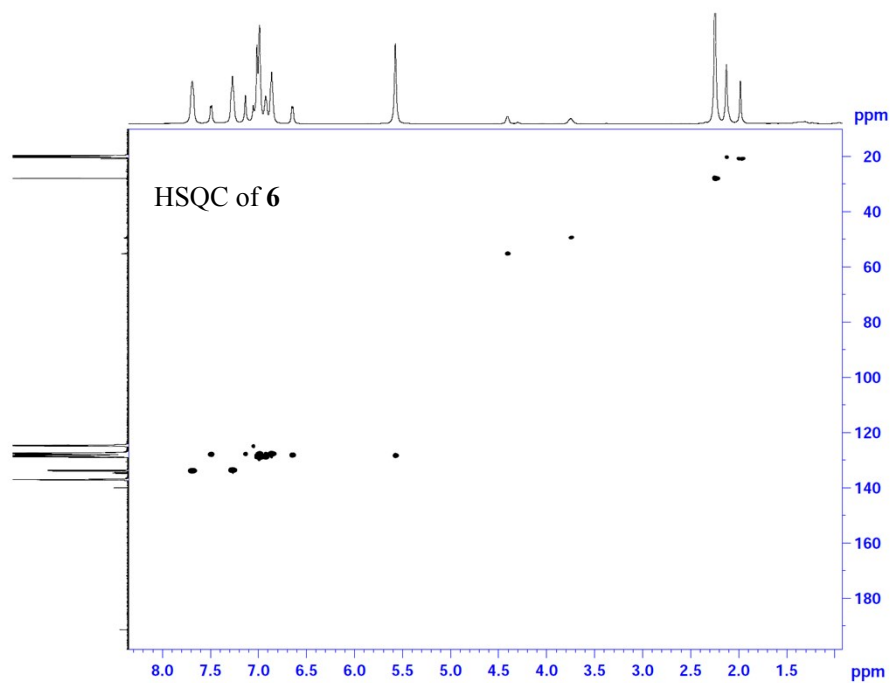
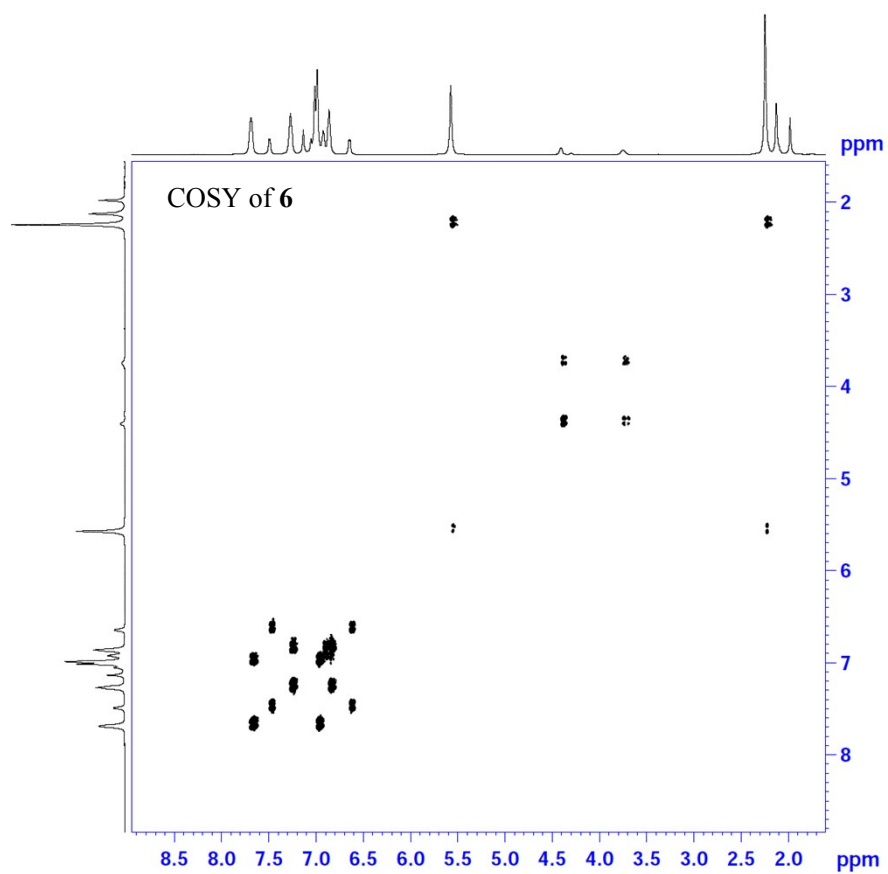


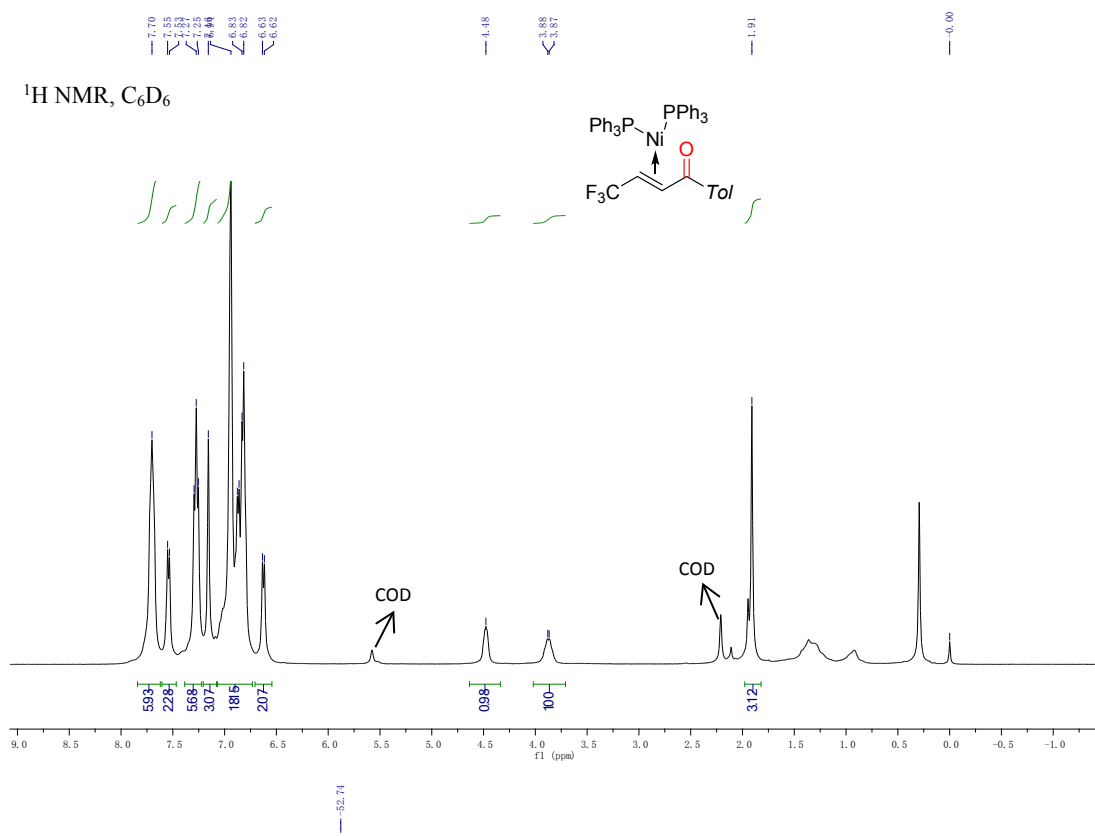
^{31}P NMR



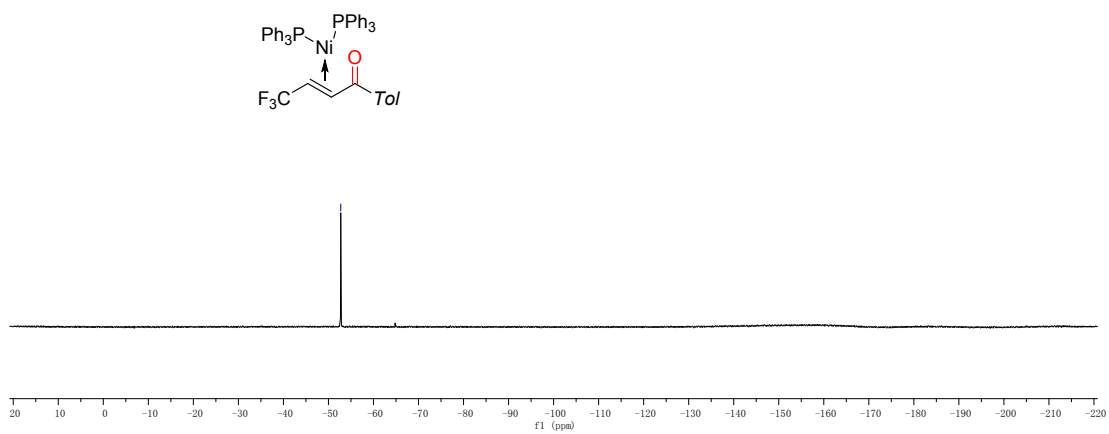
^{13}C NMR



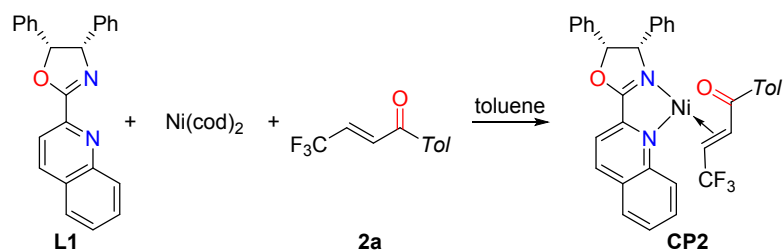




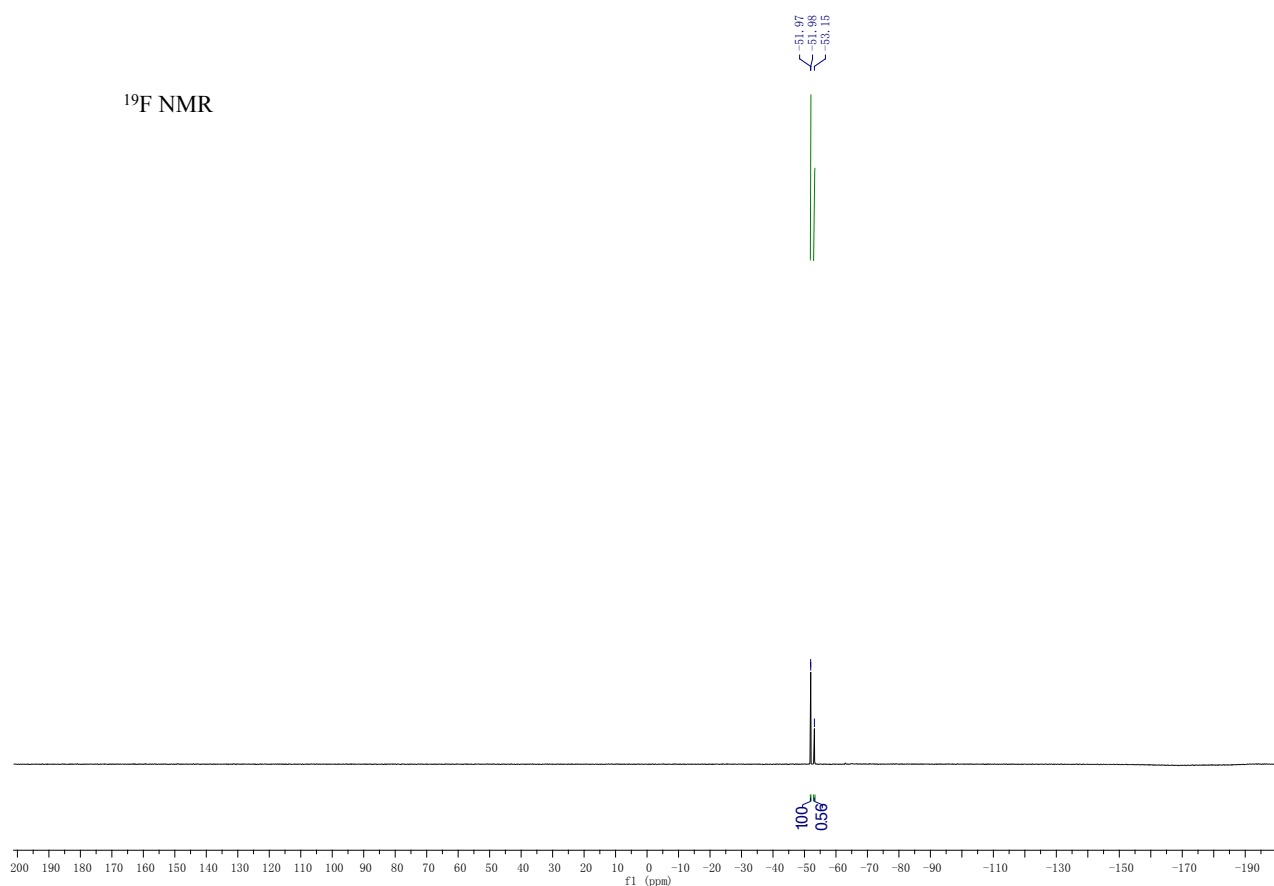
¹⁹F NMR, C₆D₆

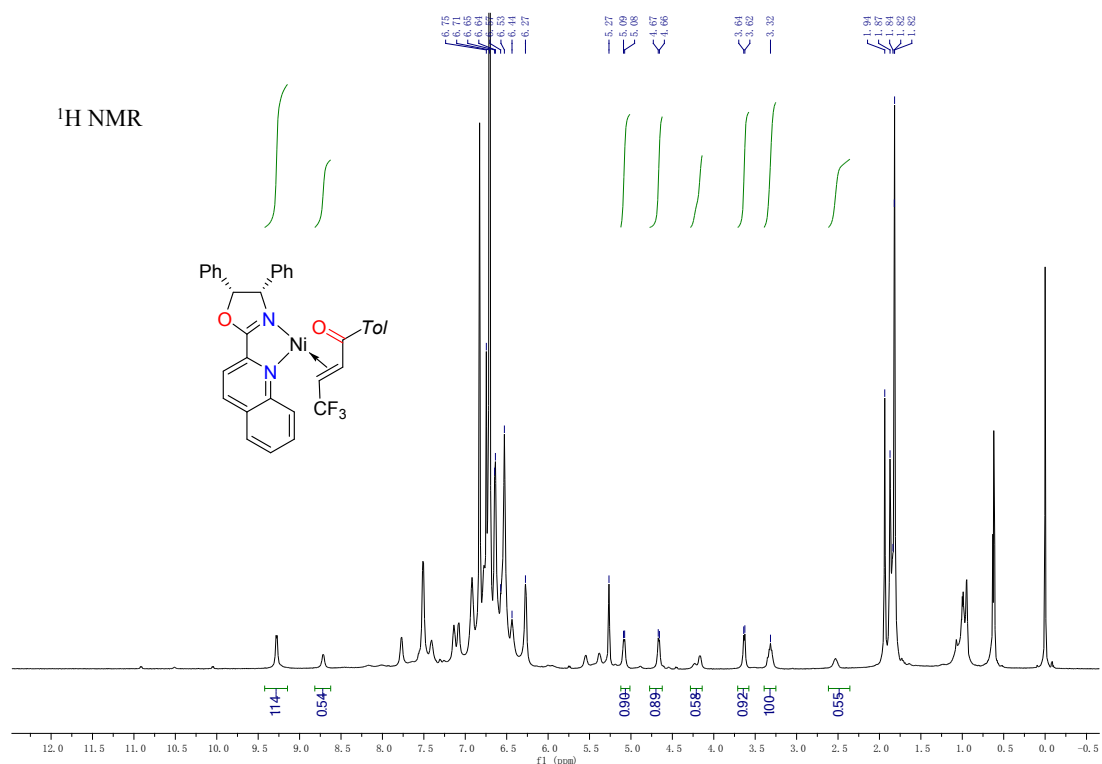


5.1.2 Capture of the CP2 in the reaction system

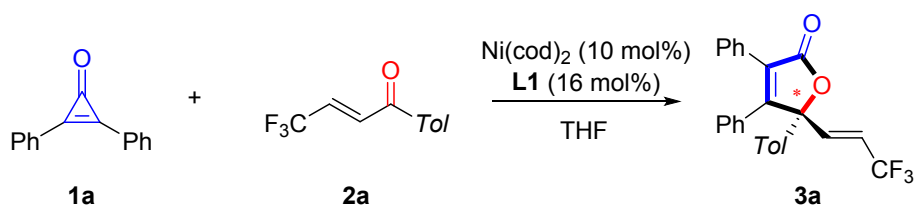


Ni(cod)₂ (3.5 mg, 0.0125 mmol, 1.0 equiv) and **L1** (5.6 mg, 0.016 mmol, 1.3 equiv) in toluene (1.0 mL) were charged into a 25 mL pressure tube under the argon atmosphere. The mixture was stirred for 10 min at room temperature, followed by addition of α, β-unsaturated ketone **2a** (2.7 mg, 0.0125 mmol, 1.00 equiv). The reaction stirred for 1h providing a deep green solution. toluene and 1,5-Cyclooctadiene (cod) was removed using reduced pressure in the dry-box. ¹H NMR (400 MHz, toluene-*d*₈) δ (major diastereomer) 5.15-5.05 (m, 1H), 4.68-4.62 (m, 1H), 3.68-3.61(m, 1H), 3.35-3.25 (m, 1H). δ (minor diastereomer) 4.20-4.12 (m, 1H), 2.58-2.48 (m, 1H), ¹⁹F NMR (565 MHz, toluene-*d*₈) δ (major diastereomer) -52.01 (m), δ (minor diastereomer) -53.19 (m).

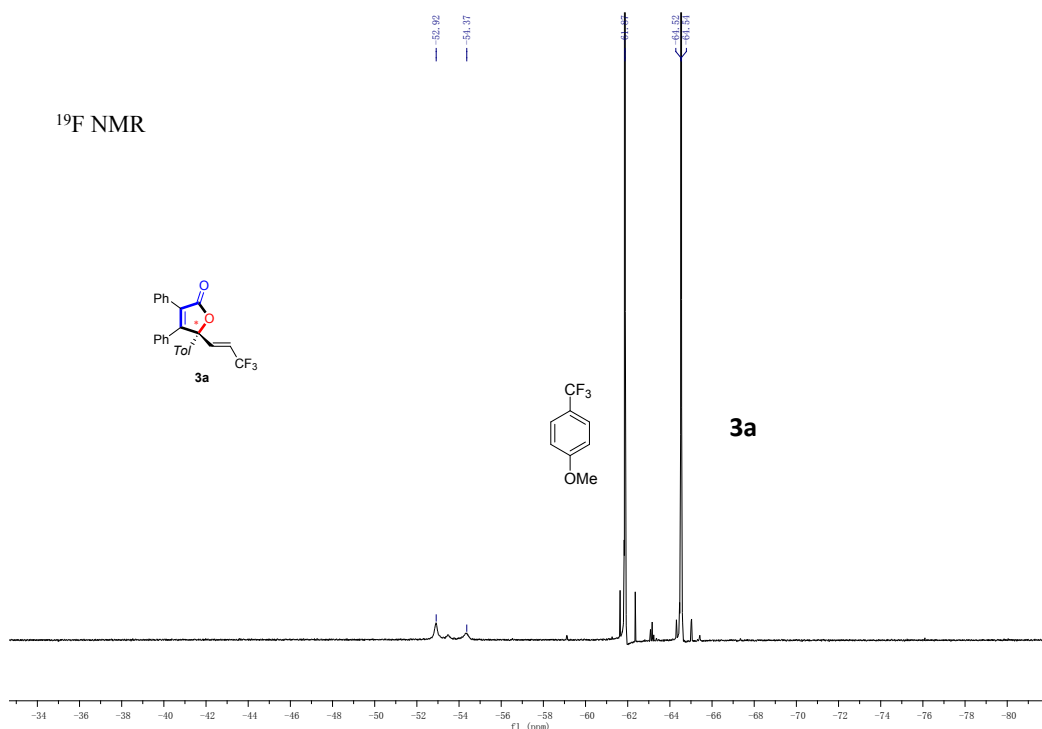




The reaction proceeded very quickly and transformed completed within 5 min following the general procedures (0.1 M of **1a**), The ¹⁹F NMR peak of the **CP2** peak could not be obtained with 1.0 mmol % or 10 mmol% catalysis using toluene as solvent. When the solvent was changed to THF and the concentration decreased to 0.025 M, the ¹⁹F NMR peak of **CP2** and the **3a** was observed within 5 min, When the concentration decreased to 0.005 M, the **CP2** could be observed in the first 10 min, and the reaction completed within 15 min and the ¹⁹F NMR peak of the **CP2** disappeared.

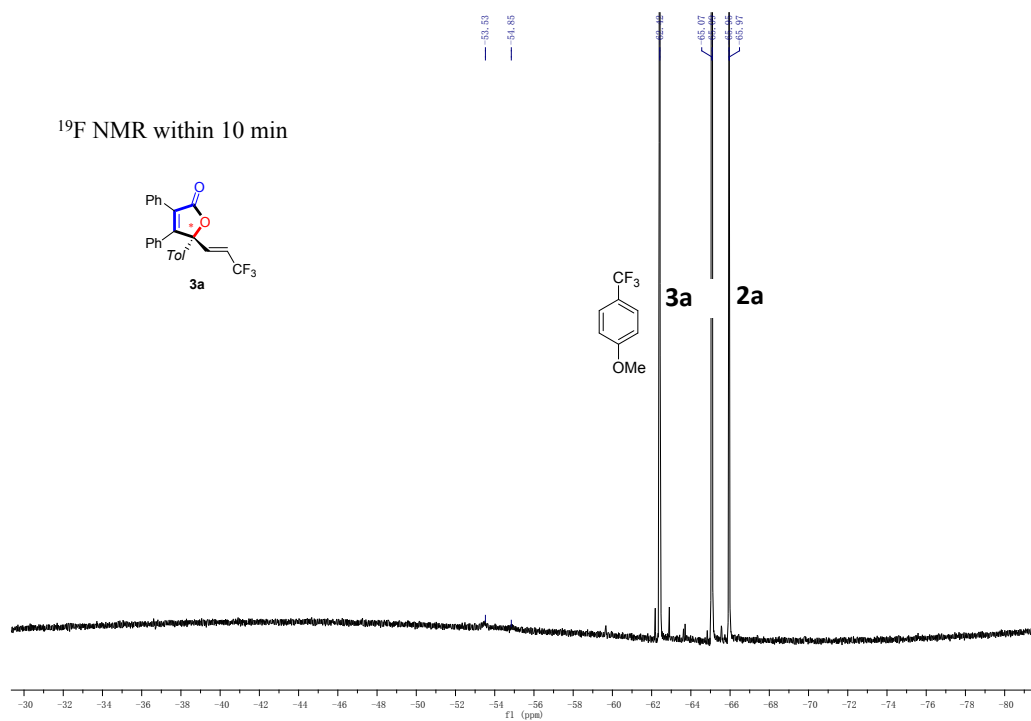
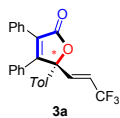


Procedures: Ni(cod)₂ (2.75 mg, 0.01 mmol, 0.01 equiv) and **L1** (6.2 mg, 0.016 mmol, 0.017 equiv) in THF (4.0 mL) were charged into pressure tube under the argon atmosphere. The mixture was stirred for 10 min at room temperature, followed by addition of cyclopropanone **1a** (21 mg, 0.1 mmol, 1.00 equiv), α , β -unsaturated ketone **2a** (21 mg, 0.1 mmol, 1.0 equiv) and 4-(trifluoromethyl)anisole (17.6 mg, 0.1 mmol, 1.00 equiv). The reaction mixture was transferred to the NMR tube immediately, and ¹⁹F NMR was obtained as quickly as possible.

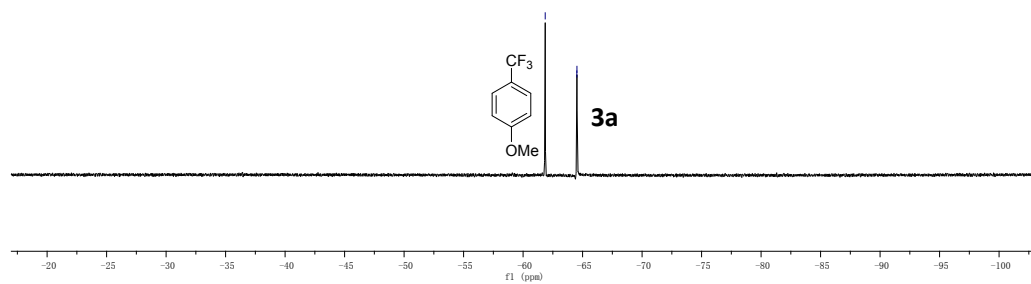
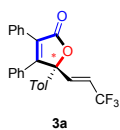


Ni(cod)₂ (2.75 mg, 0.01 mmol, 0.01 equiv) and **L1** (6.2 mg, 0.016 mmol, 0.016 equiv) in THF (20.0 mL) were charged into pressure tube under the argon atmosphere. The mixture was stirred for 10 min at room temperature, followed by addition of cyclopropenone **1a** (21 mg, 0.1 mmol, 1.00 equiv), α , β -unsaturated ketone **2a** (21 g, 0.1 mmol, 1.0 equiv) and 4-(trifluoromethyl)anisole (17.6 mg, 0.1 mmol, 1.00 equiv). The reaction mixture was transfer to the NMR tube immediately, and ¹⁹F NMR of **CP2** was obtained in the first 10 min.

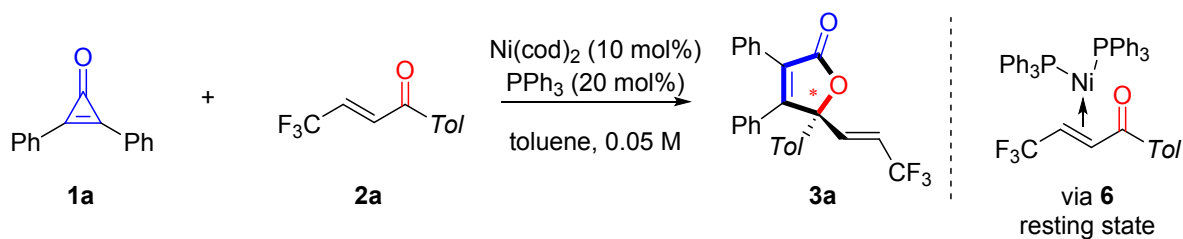
¹⁹F NMR within 10 min



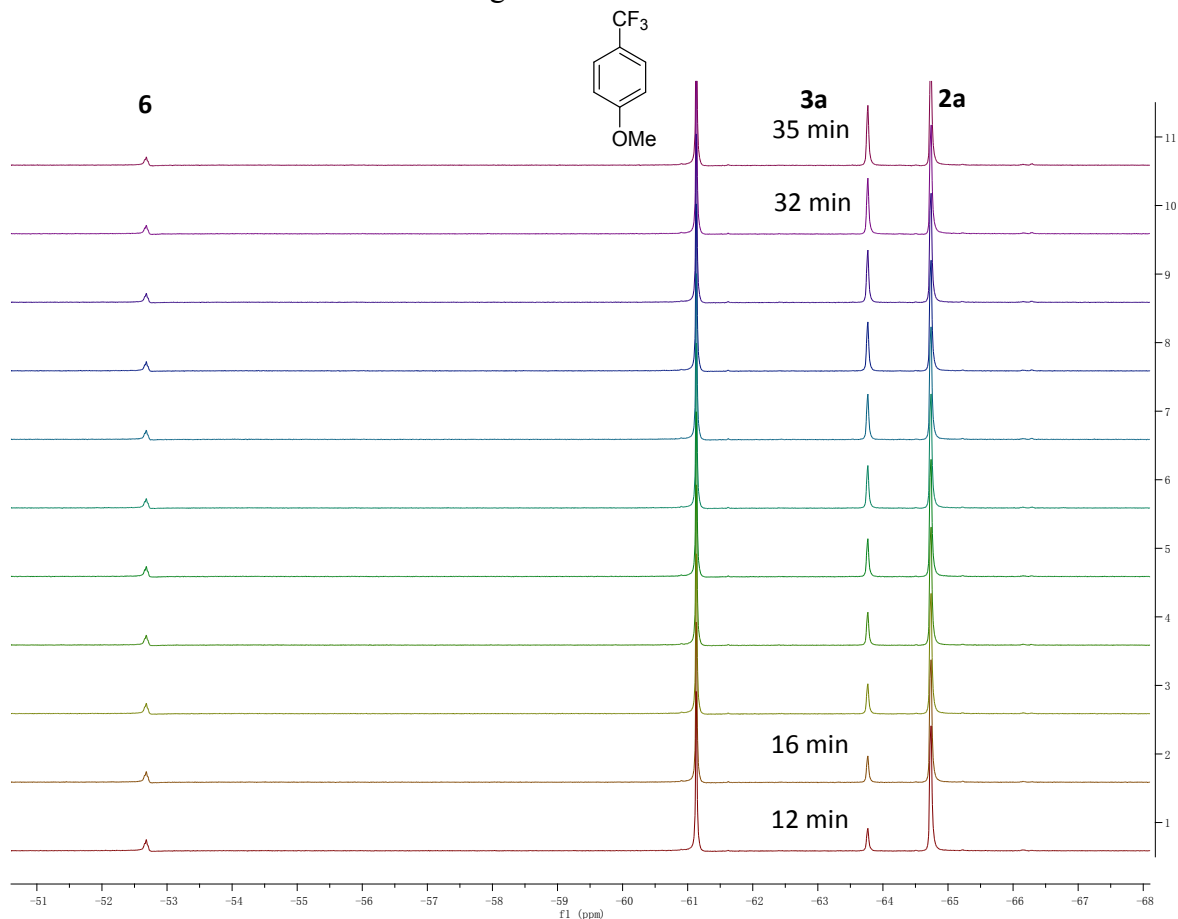
¹⁹F NMR after 15 min



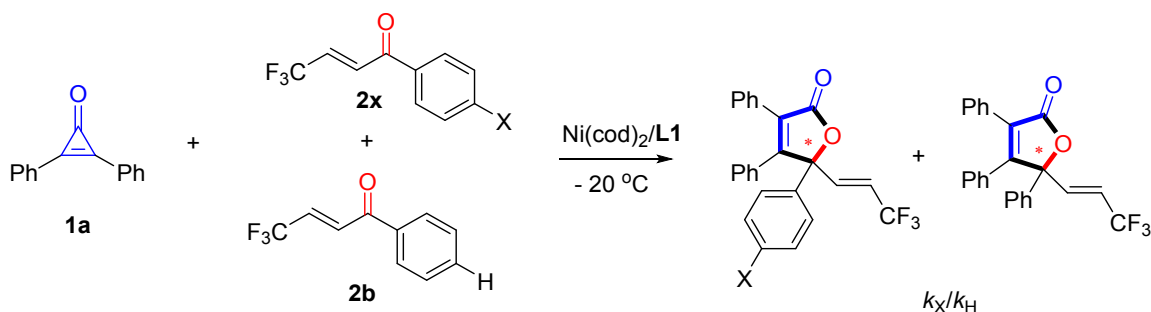
5.2 Resting state study



$\text{Ni}(\text{cod})_2$ (4.5 mg, 0.016 mmol, 0.08 equiv) and PPh_3 (8.4 mg, 0.032 mmol, 0.016 equiv) in toluene (4.0 mL) were charged into a 25 mL pressure tube under the argon atmosphere. The mixture was stirred for 10 min at room temperature, followed by addition of α, β -unsaturated ketone **2a** (42.0 mg, 0.2 mmol), and cyclopropenone **1a** (42.0 mg, 0.2 mmol) under argon. The conversion was measured by ^{19}F NMR spectroscopy at the room temperature using 4-(trifluoromethyl)anisole as an internal standard. The concentration of the **6** didn't changed at the first 35 min.



5.3 General procedure for the Hammett equation



$\text{Ni}(\text{cod})_2$ (1.2 mg, 0.004 mmol, 0.02 equiv) and **L1** (2.7 mg, 0.008 mmol, 0.04 equiv) in toluene (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 10 min at room temperature, followed by addition of cyclopropenone **1a** (0.200 mmol, 1.0 equiv), α, β -unsaturated ketone **2b** (0.10 mmol, 0.5 equiv), and a *para*-substituted α, β -unsaturated ketone **2x** (0.10 mmol, 0.5 equiv). The reaction tube was then sealed and stirred at $-20\text{ }^\circ\text{C}$ for 15 min. The reaction mixture was quickly filtered through a pad of celite and eluted with ethyl acetate. After the solvent was removed under reduced pressure, the residue sample was analyzed by GC/MS to determine ratio of k_X/k_H (all the reaction was purified and the yield of all the reaction was below 5%)

X	σ_p	k_X/k_H	$\text{Log}(k_X/k_H)$
Me	-0.17	39/61	-0.194
MeO	-0.27	27/73	-0.431
Cl	0.23	75/25	0.495
F	0.06	53/47	0.042
H	0	1	0

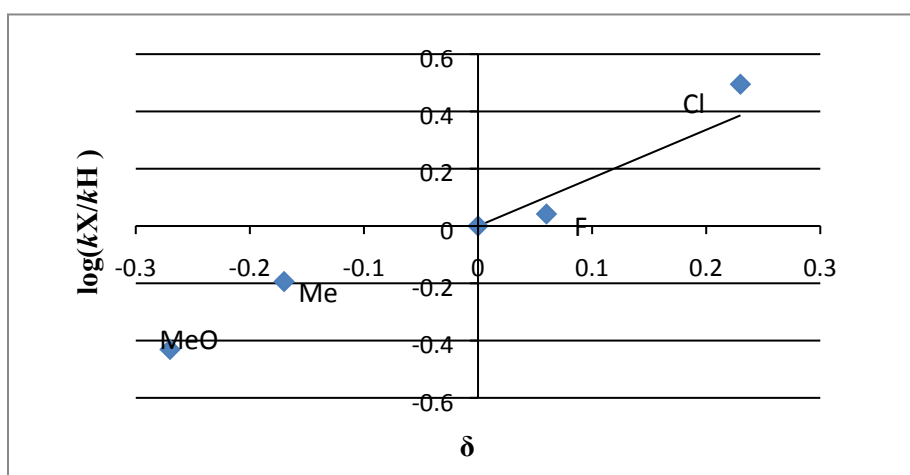


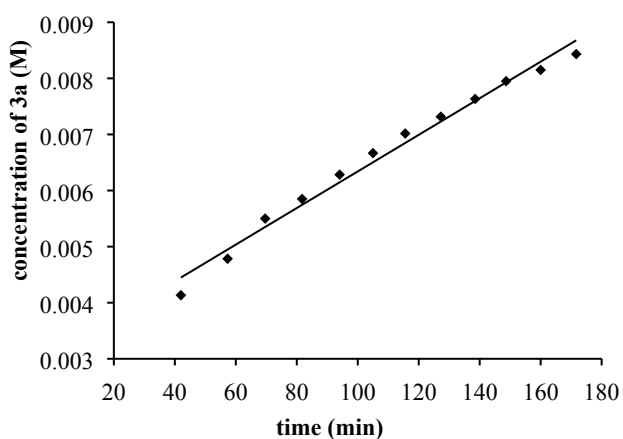
Figure S1. Hammett Plot

5.4 Kinetic Studies (Initial Rates)

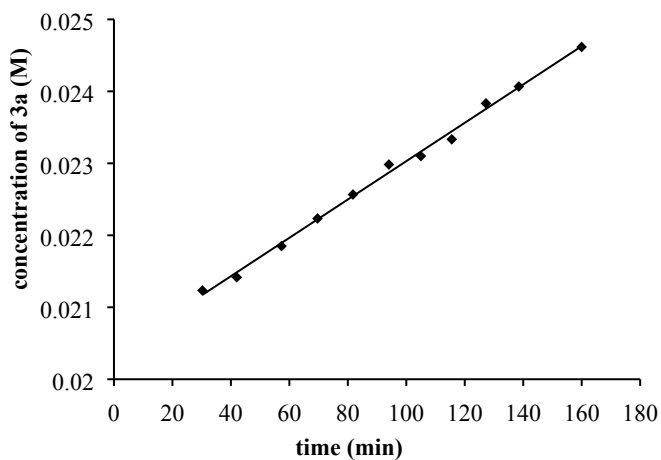
Plot of initial yield versus time under different [2a].

To a J-Young NMR tube were added the chiral catalyst Ni(cod)₂/L1 (0.150 μmol: 0.03 mL of a 5 × 10⁻³ mmol/mL stock solution in toluene) in toluene (0.6 mL), α, β-unsaturated ketone **2a** (2.1 mg, 0.01 mmol), and cyclopropenone **1a** (21.0 mg, 0.1 mmol) under argon. The NMR tube was shaken to ensure thorough mixing. The conversion was measured by ¹⁹F NMR spectroscopy at the room temperature using 4-(trifluoromethyl)anisole as an internal standard. The concentrations of the products were plotted to yield the initial rates for the formation of **3a** (Figure S2). The same experimental procedure was repeated using 0.02, 0.03, 0.034, 0.04, 0.05, 0.06 mmol of **2a** under otherwise identical conditions, and their corresponding conversions were measured over time (Figure S2).

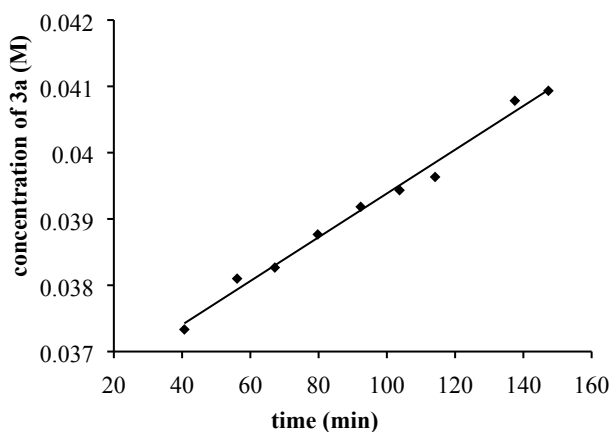
(a) Initial Rate = 2.36*10⁻⁵M·min⁻¹



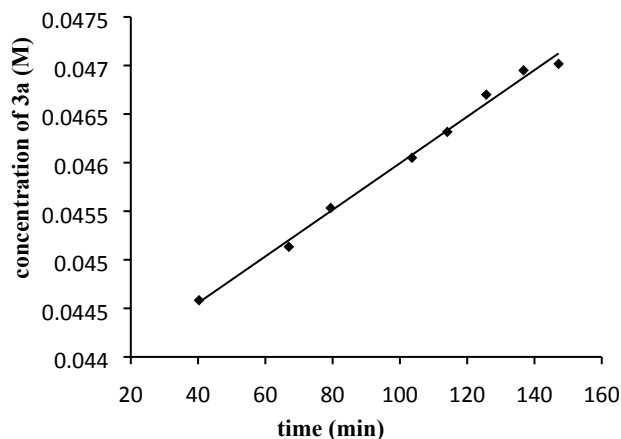
(b) Initial Rate = 2.66*10⁻⁵M·min⁻¹



(c) Initial Rate = 3.30*10⁻⁵M·min⁻¹

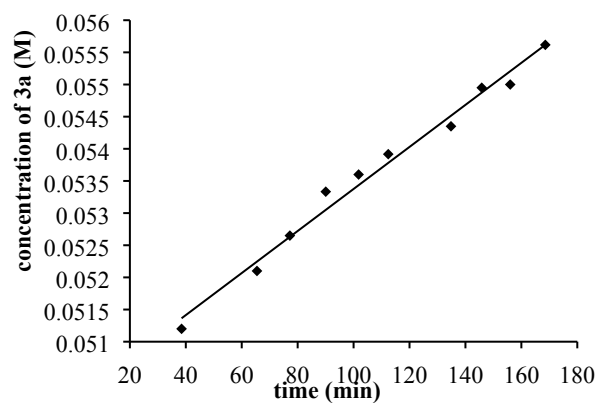
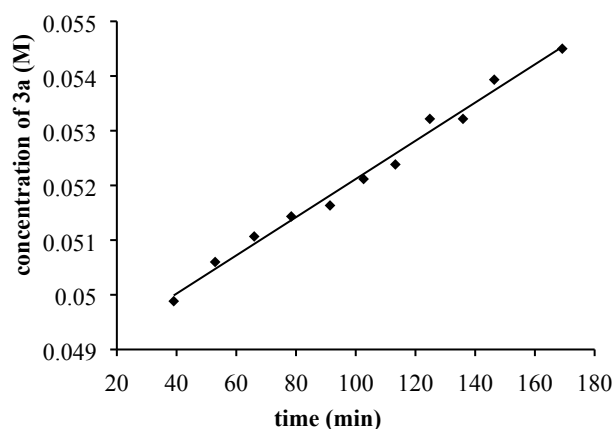


(d) Initial Rate = 2.40*10⁻⁵M·min⁻¹

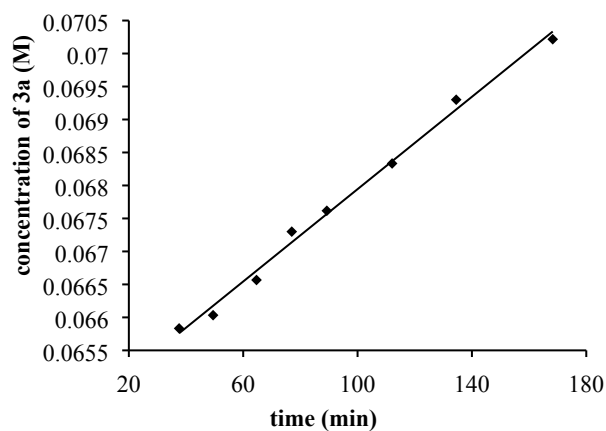


(e) Initial Rate = 3.49*10⁻⁵M·min⁻¹

(f) Initial Rate = 3.27*10⁻⁵M·min⁻¹



(g) Initial Rate = $3.50 \times 10^{-5} \text{ M} \cdot \text{min}^{-1}$



(h) Plot of Initial Rate vs [2a]

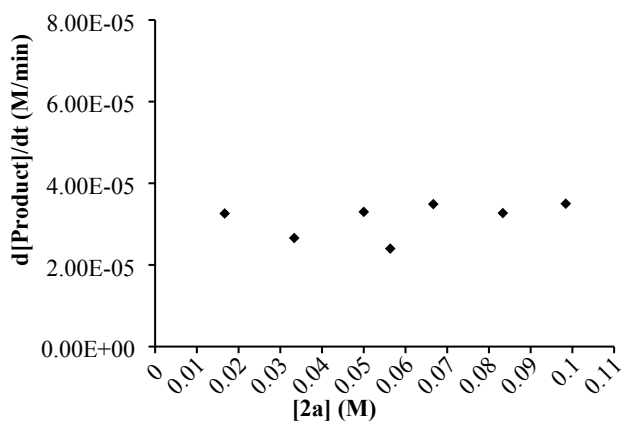


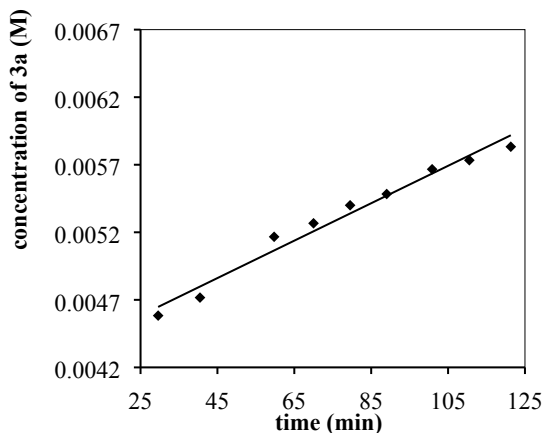
Figure S2. (a), (b), (c), (d), (e), (f), (g) initial rate for the formation of **3a** using 0.01, 0.02, 0.03, 0.034, 0.04, 0.05, 0.06 mmol of [**2a**], respectively. (h) plot of yield versus time with different [**2a**].

Plot of initial yield versus time with different [1a].

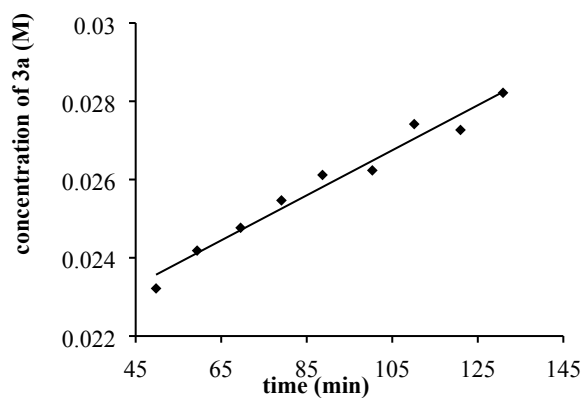
To a J-Young NMR tube were added under argon chiral catalyst $\text{Ni}(\text{cod})_2/\text{L1}$ (0.20 μmol , 0.04 mL of a 5×10^{-3} mmol/mL stock solution in toluene, Ni:L1 = 4:7) in toluene (0.6 mL), α , β -unsaturated ketone **2a** (21.0 mg, 0.1 mmol), and cyclopropanone **1a** (2.1 mg, 0.1 mmol). The NMR tube was shaken to ensure thorough mixing. The conversion was then measured by ^{19}F NMR spectroscopy at room temperature using 4-(trifluoromethyl)anisole as an internal standard. The concentrations of the products were plotted to give the initial rates for the formation of **3a** (Figure S3). The same experimental procedure was repeated using 0.02, 0.034, 0.04, 0.05 mmol of **1a** under otherwise identical conditions, and their corresponding conversions were measured over time (Figure S3).

(a) Initial Rate = $1.38 \times 10^{-5} \text{ M} \cdot \text{min}^{-1}$

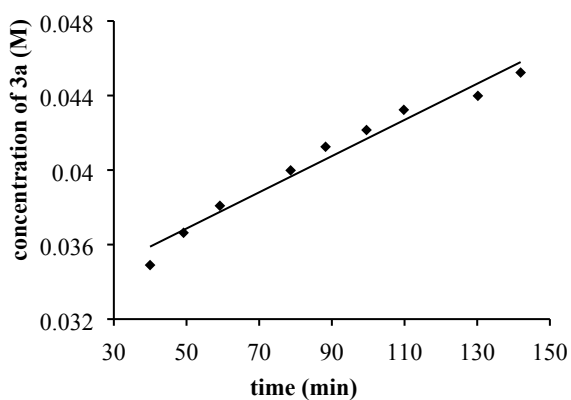
(b) Initial Rate = $5.76 \times 10^{-5} \text{ M} \cdot \text{min}^{-1}$



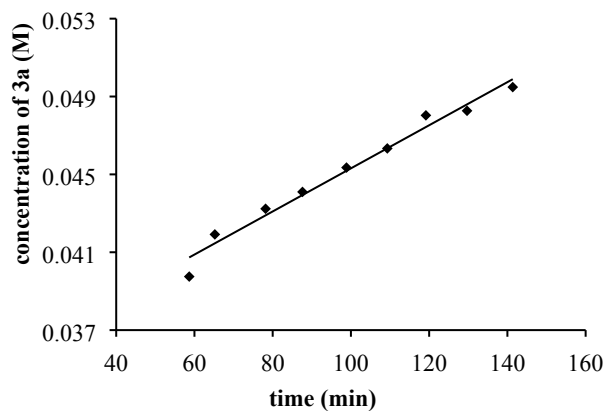
(c) Initial Rate = $9.71 \times 10^{-5} \text{M} \cdot \text{min}^{-1}$



(d) Initial Rate = $1.11 \times 10^{-4} \text{M} \cdot \text{min}^{-1}$



(e) Initial Rate = $1.68 \times 10^{-4} \text{M} \cdot \text{min}^{-1}$



(f) Plot of Initial Rate vs $[\mathbf{1a}]$

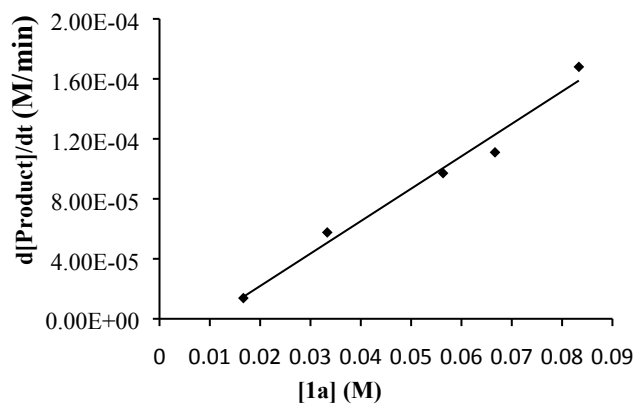
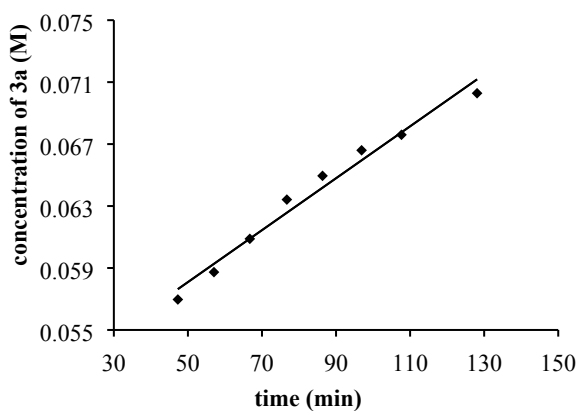


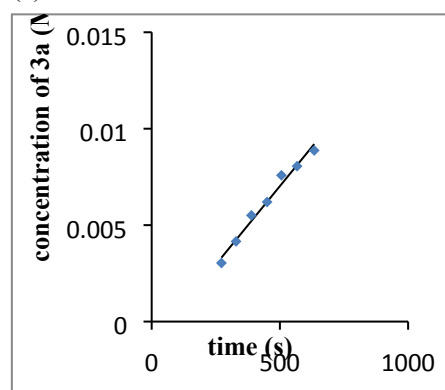
Figure S3. (a), (b), (c), (d), (e) initial rates for the formation of **3a** using 0.01, 0.02, 0.034, 0.04, 0.05 mmol of **[1a]**, respectively. (f) plot of yield versus time with different **[1a]**.

5.5 Kinetic Studies (Initial Rates) using PPh₃ as ligand.

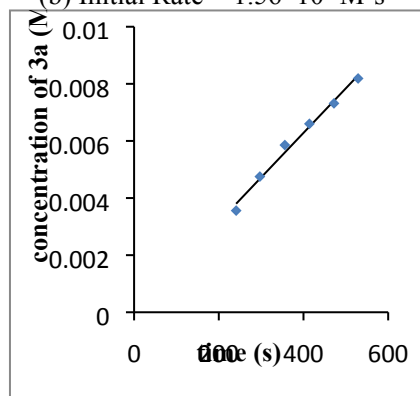
Plot of initial yield versus time under different [2a] using PPh₃ as ligand.

To a J-Young NMR tube were added the catalyst Ni(cod)₂/PPh₃ (0.6 μmol: 0.03 mL of a 2 x 10⁻² mmol/mL stock solution in toluene, Ni/PPh₃ = 1/2) in toluene (0.5 mL), α, β-unsaturated ketone **2a** (5.3 mg, 0.025 mmol), and cyclopropenone **1a** (21.0 mg, 0.1 mmol) under argon. The NMR tube was shaken to ensure thorough mixing. The conversion was measured by ¹⁹F NMR spectroscopy at the room temperature using 4-(trifluoromethyl)anisole as an internal standard. The concentrations of the products were plotted to yield the initial rates for the formation of **3a** (Figure S4). The same experimental procedure was repeated using 0.025, 0.03, 0.034, 0.04, 0.05 mmol of **2a** under otherwise identical conditions, and their corresponding conversions were measured over time (Figure S4).

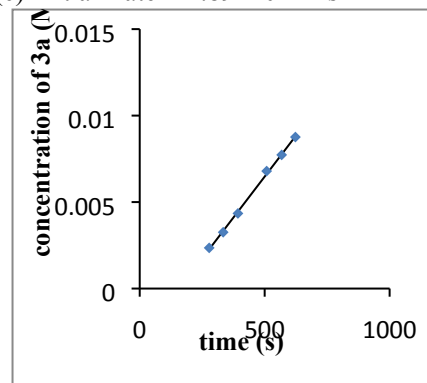
(a) Initial Rate = 1.63*10⁻⁵M·s⁻¹



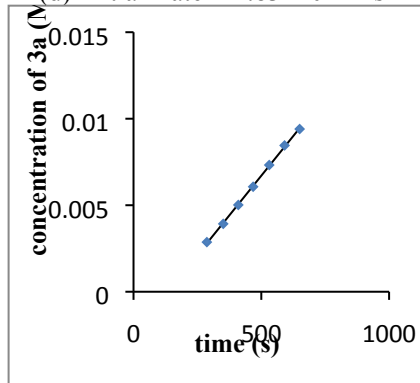
(b) Initial Rate = 1.56*10⁻⁵M·s⁻¹



(c) Initial Rate = 1.89*10⁻⁵M·s⁻¹



(d) Initial Rate = 1.83*10⁻⁵M·s⁻¹



(e) Initial Rate = 1.99*10⁻⁵M·s⁻¹

(f) Plot of Initial Rate vs [2a]

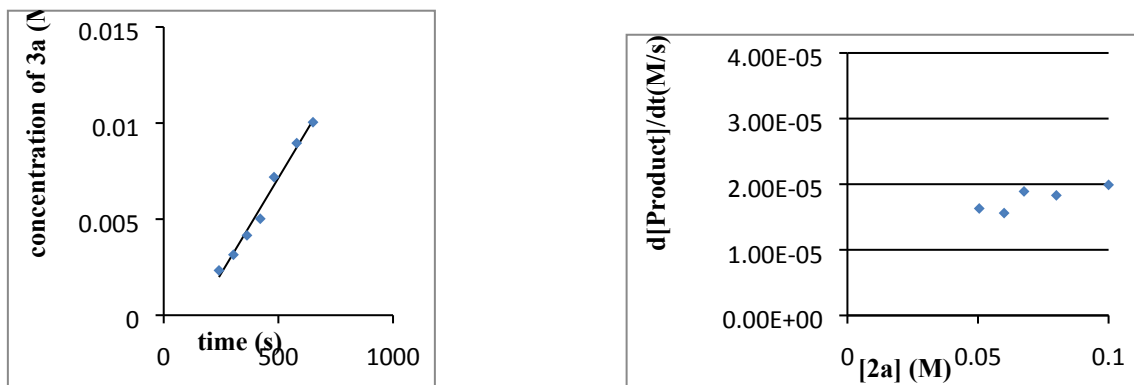
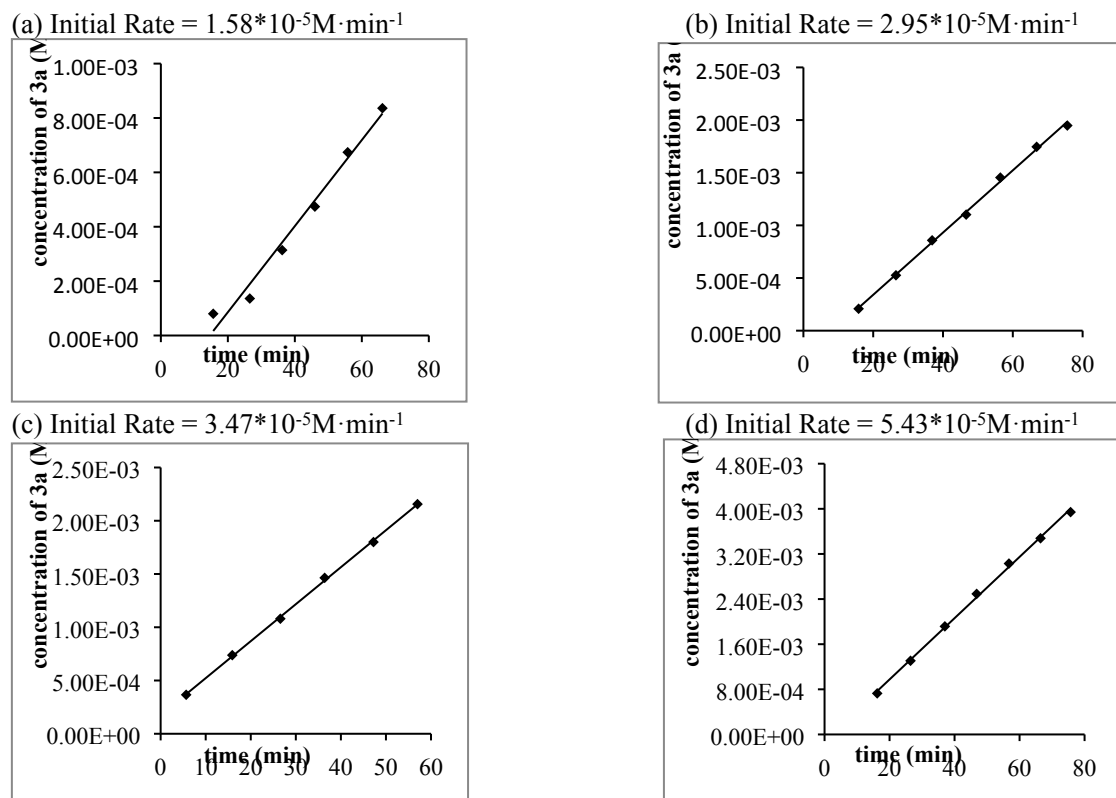


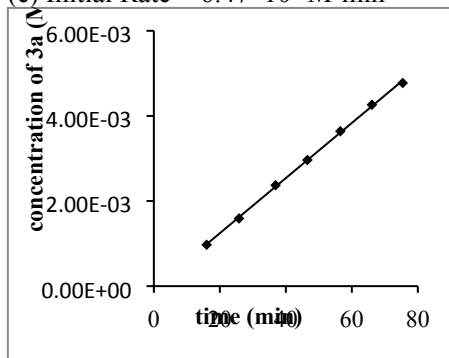
Figure S4. (a), (b), (c), (d), (e) initial rates for the formation of **3a** using 0.025, 0.03, 0.034, 0.04, 0.05 mmol of **2a**, respectively. (f) plot of yield versus time with different **2a**.

Plot of initial yield versus time under different **1a** using PPh_3 as ligand.

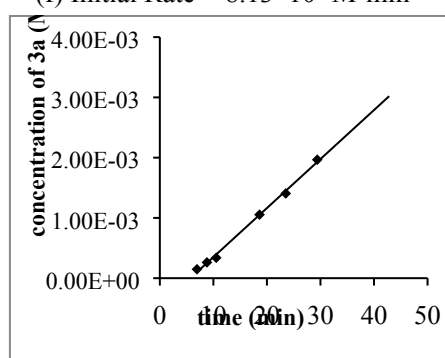
To a J-Young NMR tube were added the catalyst $\text{Ni}(\text{cod})_2/\text{PPh}_3$ (1.2 μmol : 0.06 mL of a 2×10^{-2} mmol/mL stock solution in toluene, $\text{Ni}/\text{PPh}_3 = 1/2$) in toluene (0.5 mL), α , β -unsaturated ketone **2a** (21.0 mg, 0.1 mmol), and cyclopropenone **1a** (2.1 mg, 0.01 mmol) under argon. The NMR tube was shaken to ensure thorough mixing. The conversion was measured by ^{19}F NMR spectroscopy at the room temperature using 4-(trifluoromethyl)anisole as an internal standard. The concentrations of the products were plotted to yield the initial rates for the formation of **3a** (Figure S5). The same experimental procedure was repeated using 0.01, 0.02, 0.025, 0.03, 0.034, 0.04 mmol of **1a** under otherwise identical conditions, and their corresponding conversions were measured over time (Figure S5).



(e) Initial Rate = $6.47 \times 10^{-5} \text{ M} \cdot \text{min}^{-1}$



(f) Initial Rate = $8.13 \times 10^{-5} \text{ M} \cdot \text{min}^{-1}$



(g) Plot of Initial Rate vs [1a]

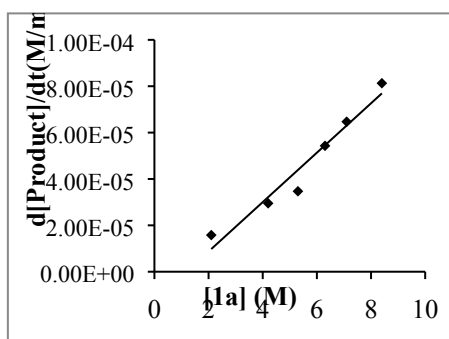


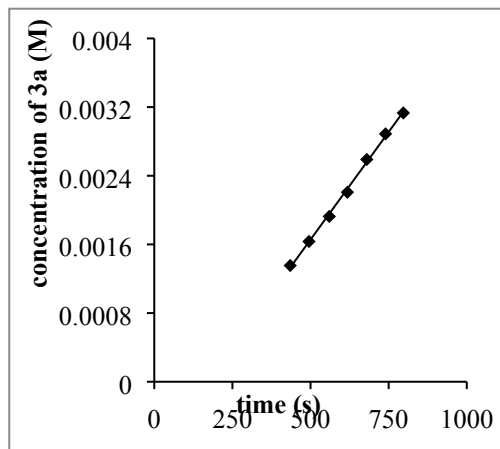
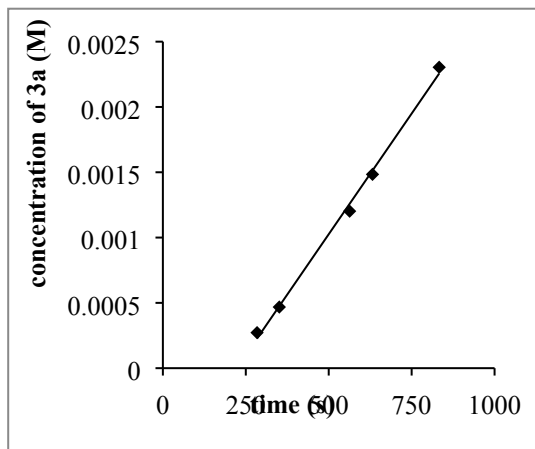
Figure S5. (a), (b), (c), (d), (e), (f) initial rate for the formation of **3a** using 0.01, 0.02, 0.025, 0.03, 0.034, 0.04 mmol of [**1a**], respectively. (h) plot of yield versus time with different [**1a**].

Plot of initial yield versus time under different [cat].

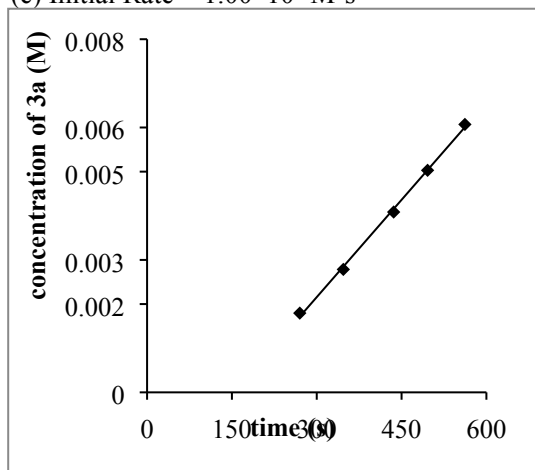
To a J-Young NMR tube were added the catalyst $\text{Ni}(\text{cod})_2/\text{PPh}_3$ ($x \times 2 \times 10^{-2} \mu\text{mol}$: $x \times 2 \times 10^{-2}$ mL of a 2×10^{-2} mmol/mL stock solution in toluene, $\text{Ni}/\text{PPh}_3 = 1/2$) in toluene (0.5 mL), α , β -unsaturated ketone **1a** (10.5 mg, 0.05 mmol), and cyclopropenone **1a** (10.5 mg, 0.05 mmol) under argon. The NMR tube was shaken to ensure thorough mixing. The conversion was measured by ^{19}F NMR spectroscopy at the room temperature using benzotrifluoride as an internal standard. The concentrations of the products were plotted to yield the initial rates for the formation of **3a** (Figure S6). The same experimental procedure was repeated using 30, 50, 60, 70, 80 μL of *cat* under otherwise identical conditions, and their corresponding conversions were measured over time (Figure S6).

(a) Initial Rate = $3.69 \times 10^{-6} \text{ M} \cdot \text{s}^{-1}$

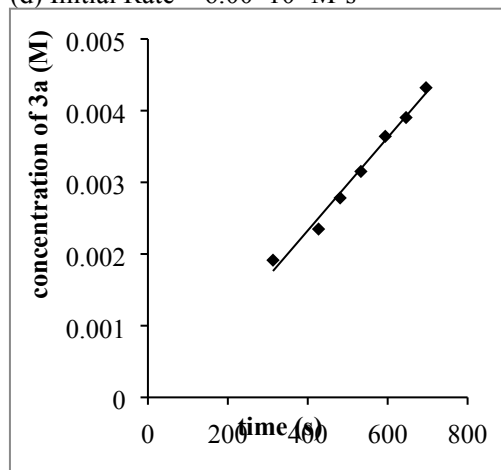
(b) Initial Rate = $5.00 \times 10^{-6} \text{ M} \cdot \text{s}^{-1}$



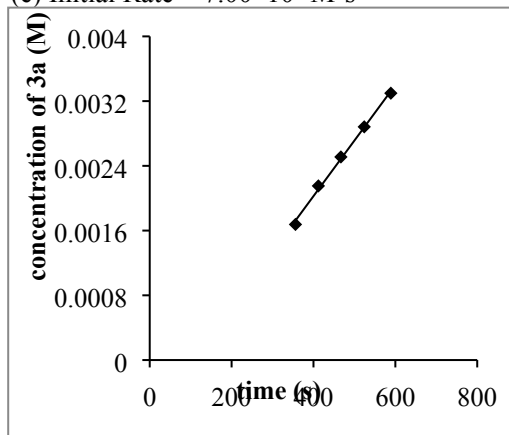
(c) Initial Rate = $1.00 \cdot 10^{-5} \text{M} \cdot \text{s}^{-1}$



(d) Initial Rate = $6.00 \cdot 10^{-6} \text{M} \cdot \text{s}^{-1}$



(e) Initial Rate = $7.00 \cdot 10^{-6} \text{M} \cdot \text{s}^{-1}$



(f) Plot of Initial Rate vs [cat]

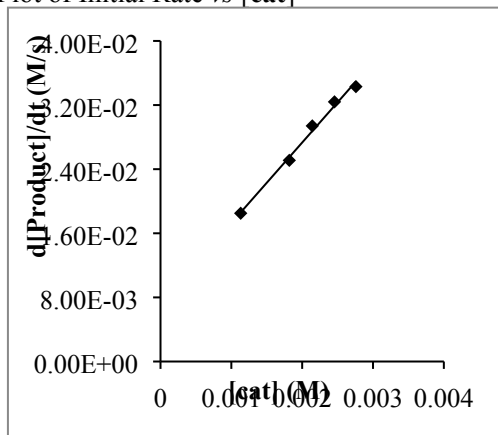


Figure S6. (a), (b), (c), (d), (e) initial rates for the formation of *cat* using $1.13 \cdot 10^{-3}$, $1.82 \cdot 10^{-3}$, $2.14 \cdot 10^{-3}$, $2.46 \cdot 10^{-3}$, $2.76 \cdot 10^{-3}$ M of [cat]; 0.6, 1.0, 1.2, 1.4, 1.6 μmol of [cat], respectively. (f) plot of yield versus time with different [cat].

6. Crystal structure details for **6** (CDCC 1962621)

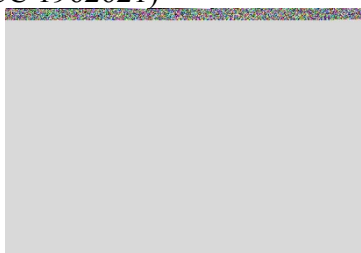


Table 1 Crystal data and structure refinement for **6**

Identification code	6
Empirical formula	C ₄₇ H ₃₉ F ₃ NiOP ₂
Formula weight	797.43
Temperature/K	284(1)
Crystal system	orthorhombic
Space group	Pca2 ₁
a/Å	28.4714(13)
b/Å	11.5708(5)
c/Å	12.0356(6)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	3965.0(3)
Z	4
ρ _{calc} /cm ³	1.336
μ/mm ⁻¹	0.620
F(000)	1656.0
Crystal size/mm ³	0.32 × 0.26 × 0.25
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	6.65 to 58.086
Index ranges	-38 ≤ h ≤ 37, -13 ≤ k ≤ 14, -13 ≤ l ≤ 16
Reflections collected	20527
Independent reflections	8151 [R _{int} = 0.0340, R _{sigma} = 0.0486]
Data/restraints/parameters	8151/1/488
Goodness-of-fit on F ²	1.033
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0380, wR ₂ = 0.0691
Final R indexes [all data]	R ₁ = 0.0498, wR ₂ = 0.0752
Largest diff. peak/hole / e Å ⁻³	0.35/-0.23
Flack parameter	0.002(7)

Crystal structure details for **4c** (CDCC 2034194)

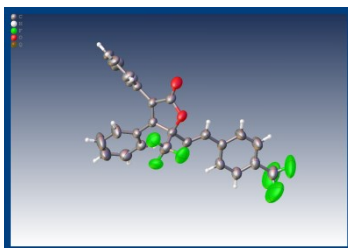


Table 1 Crystal data and structure refinement for **4c**.

Identification code	4c
Empirical formula	C ₂₆ H ₁₆ F ₆ O ₂
Formula weight	474.39
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	10.26200(10)
b/Å	10.3101(2)
c/Å	22.0678(3)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	2334.82(6)
Z	4
ρ _{calc} /cm ³	1.350
μ/mm ⁻¹	1.018
F(000)	968.0
Crystal size/mm ³	0.13 × 0.05 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	8.012 to 142.992
Index ranges	-12 ≤ h ≤ 12, -12 ≤ k ≤ 12, -27 ≤ l ≤ 27
Reflections collected	32602
Independent reflections	4522 [R _{int} = 0.0665, R _{sigma} = 0.0297]
Data/restraints/parameters	4522/42/335
Goodness-of-fit on F ²	1.251
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0720, wR ₂ = 0.1840
Final R indexes [all data]	R ₁ = 0.0760, wR ₂ = 0.1867
Largest diff. peak/hole / e Å ⁻³	0.27/-0.46
Flack parameter	0.01(6)

7. Computational Studies

We also considered the possibility of coordination of another enone molecule into Ni(0) center in **CP2**. As shown in Figure S7, the coordination of another enone **1a** onto Ni(0) center gives complex **CP15** with 7.0 kcal/mol endergonicity. Therefore, **CP15** is not a constructive intermediate in the reaction pathway and won't kinetically affect the outcome in Figure 1.

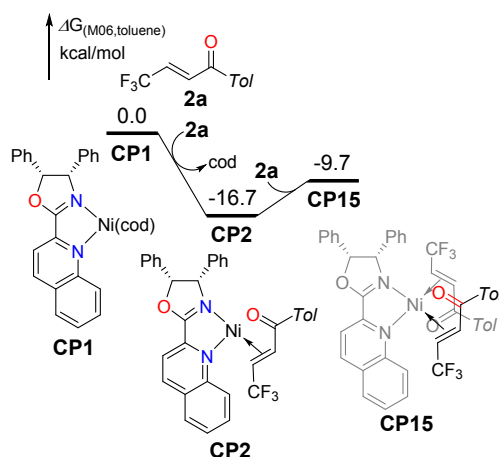


Figure S7. Free energy profile for the coordination of another molecular enone onto Ni(0) center in **CP2**.

A detailed computational study was performed to investigate the mechanism with PPh_3 as ligand. The calculated Gibbs energy profiles for the pathway are given in Figure S8, where $(\text{PPh}_3)_2\text{-Ni}(0)$ species **CP16** was set as the relative energy zero point. Ligand exchange of enone with cyclooctadiene in **CP16** gives olefin complex **CP17** with 17.6 kcal/mol exergonic. The cyclopropenone **1a** then coordinated to Ni(0) center to give **CP18** with 7.2 kcal/mol endergonic. The subsequent oxidative addition of cyclopropenone onto Ni(0) occurs via transition state **TS10** with an energy barrier of 17.1 kcal/mol, where the four-membered nickelacycle **CP19** was generated. The following 4,1-insertion of enone into the Ni-acyl bond gives the tethered allyl-Ni(II) intermediate **CP21** via transition state **TS11** with an overall activation free energy of 9.0 kcal/mol. The calculated results are consistent with kinetic studies and other experimental observations.

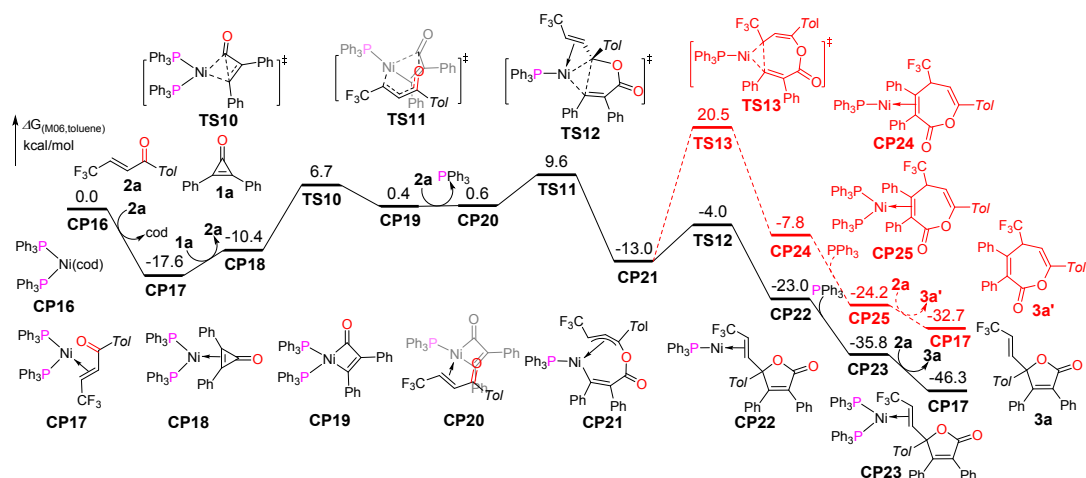


Figure S8. Free energy profiles for oxidation addition, 4,1-insertion and reductive elimination pathway of the Ni(0)-catalyzed [3+2] annulation reaction using PPh₃ as ligand.

Using PPh₃ as liand, the alternative oxidative cyclization pathway is ligand exchange of enone with PPh₃ give TS14 (Figure S9), while the energy barrier this pathway is higher than Figure S8, Therefore, this pathway can be excluded.

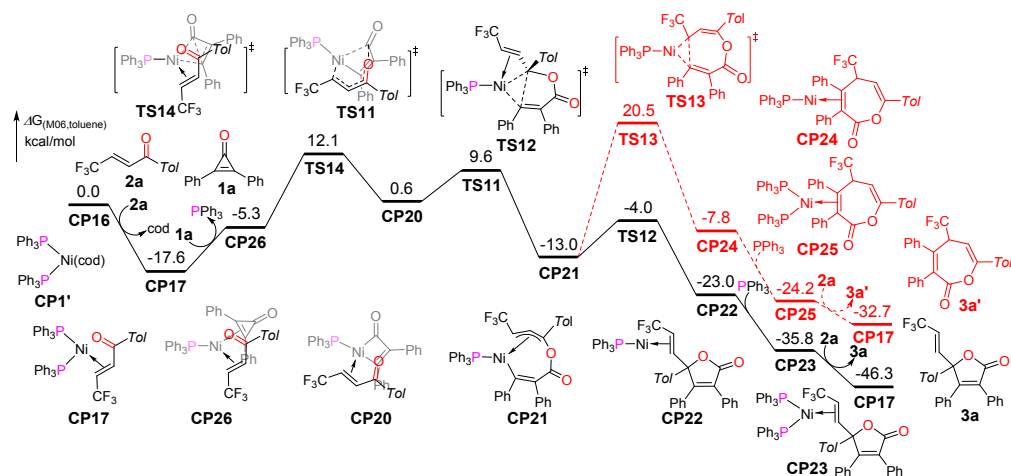


Figure S9. Free energy profiles for oxidation addition, 4,1-insertion and reductive elimination pathway of the Ni(0)-catalyzed [3+2] annulation reaction using PPh₃ as ligand.

7.1. Complete reference for Gaussian 09

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.;

Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, **2013**.

7.2. Computational Methods.

All DFT calculations were carried out with the GAUSSIAN 09 series of programs. Density functional B3-LYP⁴ with a standard 6-31G(d) basis set (LANL08⁵ basis set for Ni) was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. All minima have zero imaginary frequency and all transition states have only one imaginary frequency. The solvent effects were considered by single point calculations on the gas-phase stationary points with a continuum solvation model SMD.⁶ The DFT method M06⁷ functional with the 6-311+G(d) (LANL08 basis set for Ni) basis set was used to calculate the single point energies with toluene as solvent and provide highly accurate energy information. The energies given in this report are the M06 calculated Gibbs free energies in toluene solvent. The optimized structures were displayed using CYLview.⁸

7.3. B3LYP and M06 absolute calculation energies, enthalpies, and free energies.

Geometry	E(elec- B3LYP)1	H(corr- B3LYP)2	G(corr- B3LYP)3	E(solv-M06)4	IF5
CP1	-1591.501073	0.574479	0.480789	-1590.824693	-
2a	-799.318288	0.191592	0.132404	-799.096300	-
CP2	-2078.824198	0.577876	0.464814	-2078.103638	-
cod	-312.024465	0.189565	0.149672	-311.845208	-
1a	-652.765930	0.214776	0.162705	-652.457266	-
CP3	-2731.579896	0.795298	0.649953	-2730.563073	-

TS1	-2731.565424	0.793823	0.649065	-2730.549716	-104.8
CP4	-2731.594310	0.794985	0.649644	-2730.570399	-
TS2	-2731.575377	0.793249	0.651285	-2730.548575	-329.5
CP5	-2731.606188	0.795426	0.652157	-2730.588284	-
TS3	-2731.582320	0.793736	0.653302	-2730.566445	-281.2
CP6	-2731.652565	0.797056	0.657274	-2730.625804	-
3a	-1452.156178	0.411056	0.322259	-1451.626350	-
TS4	-2731.545376	0.793785	0.652404	-2730.518093	-249.2
CP7	-2731.622611	0.797135	0.655742	-2730.600821	-
3a'	-1452.138380	0.409965	0.325111	-1451.607624	-
TS2-R-exo	-2731.557674	0.793076	0.649718	-2730.521715	-408.9
TS2-S-endo	-2731.573145	0.793199	0.650816	-2730.542833	-312.3
TS2-S-exo	-2731.556964	0.793185	0.650424	-2730.518359	-410.5
CP8	-1932.258321	0.601723	0.490907	-1931.448877	-
TS5	-1932.226200	0.599336	0.488894	-1931.407488	-161.3
CP9	-1932.27174	0.602373	0.491509	-1931.444811	-
CP10	-2731.558382	0.794842	0.646199	-2730.527527	-
TS6	-2731.550473	0.793657	0.648321	-2730.511897	-236.9
CP11	-2731.557742	0.793948	0.651175	-2730.527085	-
TS7	-2731.542213	0.793807	0.652650	-2730.499212	-29.9
TS8	-2078.786293	0.575338	0.46473	-2078.058717	-219.7
CP12	-2078.808108	0.577472	0.465551	-2078.077425	-
CP13	-2078.821815	0.577650	0.465144	-2078.103358	-
TS9	-2078.785117	0.575851	0.465864	-2078.054453	-158.0

CP14	-2078.810141	0.577495	0.465794	-2078.077051	-
CP15	-2878.150680	0.771728	0.624646	-2877.216269	-
CP16	-2553.958637	0.777486	0.658102	-2553.079283	-
CP17	-3041.295449	0.781818	0.641735	-3040.359378	-
CP18	-2894.720005	0.805109	0.666769	-2893.703602	-
TS10	-2894.696661	0.803291	0.664912	-2893.674485	-172.0
CP19	-2894.718710	0.805217	0.667288	-2893.686891	-
CP20	-2657.765912	0.704562	0.568609	-2656.886888	-
PPh₃	-1036.281644	0.291202	0.227665	-1035.892574	-
TS11	-2657.750428	0.703039	0.570775	-2656.874641	-286.6
CP21	-2657.783243	0.705544	0.576499	-2656.916396	-
TS12	-2657.764546	0.703673	0.573897	-2656.899466	-269.6
CP22	-2657.805825	0.705632	0.573223	-2656.929144	-
CP23	-3694.112605	1.000851	0.832901	-3692.874036	-
TS13	-2657.729598	0.703204	0.566240	-2656.852755	-305.3
CP24	-2657.781041	0.705706	0.574571	-2656.906265	-
CP25	-3694.088738	1.000635	0.829299	-3692.851992	-
CP26	-2657.758307	0.705145	0.569638	-2656.897261	-
TS14	-2657.741679	0.704135	0.572645	-2656.872611	-70.5

¹The electronic energy calculated by B3LYP in gas phase. ²The thermal correction to enthalpy calculated by B3LYP in gas phase. ³The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ⁴The electronic energy calculated by M06 in toluene solvent. ⁵The B3LYP calculated imaginary frequencies for the transition states.

7.4. B3LYP geometries for all the optimized compounds and transition states

CP1				C	-4.69239100	-3.54492300	0.58078100
C	-5.54494600	-1.30256100	0.83862400	C	-5.75211300	-2.69738400	0.83678900
C	-4.29345500	-0.77780400	0.57783500	H	-6.37496000	-0.63374300	1.05039700
C	-3.19137800	-1.61896400	0.30011500	H	-4.12227900	0.28956900	0.58488300
C	-3.39893800	-3.03711100	0.31299800	C	-2.28586500	-3.89382400	0.06388400

H	-4.83542700	-4.62307500	0.58247000	H	2.60757400	1.60239500	0.14931300
H	-6.73958800	-3.10171500	1.04114100	C	1.18845900	0.05657800	-0.03992700
C	-1.06029300	-3.33775300	-0.17574400	H	1.03044800	-1.00952300	-0.15146600
C	-0.92788700	-1.92638400	-0.18047800	C	3.65225600	-0.32600800	-0.00590300
H	-2.42725500	-4.97113600	0.06902700	F	3.36516400	-1.63481900	-0.16971600
H	-0.18111200	-3.94228400	-0.37177600	F	4.46187200	0.04405100	-1.02262300
N	-1.95289000	-1.05526800	0.04185800	F	4.36711900	-0.20635600	1.13512500
C	2.39734200	-1.00357300	-1.21436900	C	0.01784300	0.99147500	0.01307600
C	1.79576300	0.37621800	-0.73383900	O	0.20887200	2.20267800	0.06086800
C	0.31665600	-1.27661300	-0.45206000	C	-1.36629500	0.43363300	0.00317500
N	0.38041200	0.02271200	-0.52985800	C	-1.66111900	-0.93759400	0.04505700
O	1.47260100	-1.97079200	-0.65178600	C	-2.43619200	1.34696800	-0.03750400
H	2.27626300	-1.05042500	-2.30542200	C	-2.98421700	-1.37816000	0.04469100
H	1.87772300	1.09710600	-1.55300000	H	-0.87001100	-1.67849600	0.08926000
C	2.43943000	0.98140600	0.50392500	C	-3.74983200	0.90166300	-0.04209600
C	2.07556100	0.58230900	1.79658500	H	-2.20365900	2.40629400	-0.06456800
C	3.44671200	1.94297500	0.35484900	C	-4.04968200	-0.47157100	-0.00156300
C	2.71035700	1.12958700	2.91270400	H	-3.19135900	-2.44473100	0.08174000
H	1.27907400	-0.14327300	1.93054500	H	-4.56198000	1.62440400	-0.07613900
C	4.08465500	2.48978600	1.46899500	C	-5.48267700	-0.94547600	-0.01176100
H	3.73539600	2.26611100	-0.64297300	H	-5.54807100	-2.03309400	0.08849100
C	3.71784400	2.08337800	2.75310400	H	-6.05542400	-0.49519800	0.80811900
H	2.41258300	0.81334400	3.90902100	H	-5.98543200	-0.66381700	-0.94561700
H	4.86256500	3.23650700	1.33330200				
H	4.20872300	2.51119200	3.62310800	CP2			
C	3.82002600	-1.33612000	-0.85554200	C	-6.09475500	-0.47175400	-0.27620200
C	4.84547700	-0.97704300	-1.73924100	C	-4.73331200	-0.29162400	-0.17329500
C	4.14967400	-1.97606400	0.34525500	C	-3.84460100	-1.30116100	-0.61930500
C	6.17979300	-1.23455100	-1.42290300	C	-4.38774200	-2.51444200	-1.16773500
H	4.59821800	-0.49802200	-2.68466300	C	-5.79591900	-2.66246100	-1.25961900
C	5.48287500	-2.24373400	0.65653100	C	-6.63379500	-1.66073100	-0.82559600
H	3.35909100	-2.27438700	1.02520800	H	-6.76396700	0.30929600	0.07263900
C	6.50184100	-1.87007500	-0.22241900	H	-4.31527900	0.60515000	0.26039700
H	6.96442800	-0.94968800	-2.11872400	C	-3.49216100	-3.52325000	-1.59654700
H	5.72582900	-2.74621100	1.58901000	H	-6.19700600	-3.58151700	-1.67913600
H	7.53942900	-2.07969800	0.02320300	H	-7.71088500	-1.78051300	-0.89952300
Ni	-1.40199100	0.88695300	-0.28631100	C	-2.13798400	-3.31754900	-1.48531600
C	-0.85792200	2.72088700	0.51328600	C	-1.68797800	-2.09589900	-0.94475100
C	-2.03684300	2.30696500	1.13208500	H	-3.88511100	-4.44737400	-2.01195100
C	-3.41400500	2.83220000	0.76736700	H	-1.41068300	-4.05498100	-1.80527700
C	-3.70190000	2.78207600	-0.75941700	N	-2.48933900	-1.10725700	-0.51591700
C	-2.91151800	1.70012600	-1.49056000	C	1.94221400	-1.92024200	-1.10824200
C	-1.66706200	1.90184000	-2.08564000	C	1.56528900	-0.62548500	-0.28044500
C	-0.84506500	3.17500300	-2.00694800	C	-0.26942700	-1.77612600	-0.82113300
C	-0.79345800	3.78206700	-0.57947900	N	0.09744900	-0.61370400	-0.40763100
H	0.07495200	2.51435200	1.03176000	O	0.68170100	-2.67478800	-1.12610000
H	-1.95554400	1.82159700	2.10426700	H	2.11649400	-1.61550000	-2.14661700
H	-3.55111300	3.86212800	1.13660200	H	1.97244400	0.24997200	-0.79280400
H	-4.16233400	2.23417700	1.30063200	C	2.02073100	-0.58859300	1.16977000
H	-4.77407800	2.61322100	-0.91907300	C	1.21618700	-1.05277900	2.21719600
H	-3.48853400	3.75761500	-1.21120700	C	3.29621600	-0.08849500	1.46641200
H	-3.48368800	0.84010800	-1.83446900	C	1.68160700	-1.02402500	3.53383500
H	-1.36285700	1.19852600	-2.86029600	H	0.21382000	-1.41464100	2.01116000
H	-1.20765400	3.93052100	-2.72423400	C	3.76447700	-0.06656600	2.77967400
H	0.17648100	2.92984300	-2.32467600	H	3.92366300	0.29038500	0.66355000
H	0.13267600	4.35980800	-0.47075700	C	2.95690200	-0.53509100	3.81867800
H	-1.60853400	4.50340600	-0.44873800	H	1.04057700	-1.37741000	4.33687200
				H	4.75631300	0.32332800	2.99238900
2a				H	3.31659500	-0.51041200	4.84371300
C	2.43137700	0.53590000	0.04089600	C	3.07728700	-2.78781500	-0.64125100

C	4.33026400	-2.65027200	-1.25030100	H	-5.28546100	0.75903600	-0.00001000
C	2.92055000	-3.71500600	0.39699700	H	-3.27357400	-3.04710400	0.00001600
C	5.41666700	-3.41336300	-0.81966600	H	-5.37747500	-1.72544600	0.00000500
H	4.45678100	-1.94487200	-2.06891500				
C	4.00277800	-4.48606700	0.81869300	CP3			
H	1.95037300	-3.83723100	0.86694000	C	-0.37836100	6.09980600	1.44101500
C	5.25403800	-4.33472000	0.21568900	C	-0.40803600	4.73703500	1.24983300
H	6.38367800	-3.29555600	-1.30083200	C	-1.41875200	4.16134600	0.43089800
H	3.86899600	-5.20573100	1.62165900	C	-2.40847600	5.01223500	-0.16906800
H	6.09567200	-4.93634800	0.54781300	C	-2.34038800	6.41273800	0.04733800
Ni	-1.41490000	0.56327500	0.00794200	C	-1.34265900	6.94423400	0.83304900
C	-2.29142400	2.21869300	0.52076300	H	0.39029300	6.53712200	2.07199000
H	-2.94593100	2.66425800	-0.22838400	H	0.30136400	4.07609400	1.73740500
C	-0.86954000	2.39525100	0.33242700	C	-3.41705600	4.39739900	-0.95034900
H	-0.23221500	2.48579000	1.20841700	H	-3.08803000	7.05391500	-0.41329500
C	-2.82231100	2.35140100	1.90293100	H	-1.29449300	8.01736300	0.99688100
F	-2.82008700	3.63187000	2.36759800	C	-3.42337000	3.03210100	-1.10618100
F	-4.12038500	1.93389000	2.00096200	C	-2.39112500	2.28187800	-0.48447700
F	-2.11515500	1.62735400	2.81442900	H	-4.18140000	5.01322900	-1.41817700
C	-0.38100600	2.94771200	-0.94423400	H	-4.18110100	2.52469000	-1.69113500
O	-1.13515500	3.15925000	-1.89874100	N	-1.42633300	2.81324800	0.25025500
C	1.09345800	3.24121300	-1.11189300	C	-3.03168300	-1.14527900	-1.46487400
C	2.05340700	3.07719600	-0.10291700	C	-1.90180500	-1.35450500	-0.40394700
C	1.52211300	3.72369800	-2.35949900	C	-2.35869200	0.81456800	-0.62589000
C	3.39501300	3.38684900	-0.33790900	N	-1.39934000	0.03488300	-0.25868600
H	1.76921000	2.70039400	0.87371800	O	-3.44202700	0.23300100	-1.18755600
C	2.85842600	4.03046300	-2.58910500	H	-2.55036200	-1.12726100	-2.45022800
H	0.77434800	3.85053200	-3.13551400	H	-1.11891500	-1.97719400	-0.83638300
C	3.82173400	3.87244900	-1.57972700	C	-2.36967800	-1.94474600	0.91679800
H	4.11987400	3.25529100	0.46284800	C	-2.94224500	-1.16357000	1.92884700
H	3.16425000	4.40213900	-3.56526200	C	-2.29603000	-3.33192100	1.09742600
C	5.26657400	4.24065000	-1.82294800	C	-3.44749000	-1.76062700	3.08512400
H	5.92707000	3.79877400	-1.06953100	H	-2.97958500	-0.08342000	1.82796700
H	5.60606300	3.90681600	-2.81046200	C	-2.80108000	-3.93001500	2.25139500
H	5.40972000	5.32890900	-1.78620000	H	-1.84396300	-3.94860800	0.32428300
				C	-3.38407500	-3.14512700	3.24783900
1a				H	-3.88549000	-1.13936100	3.86197100
C	0.68597200	0.81873500	-0.00000300	H	-2.73463600	-5.00779600	2.37342700
C	-0.68597200	0.81873500	-0.00000300	H	-3.77707600	-3.60855500	4.14891300
C	0.00000000	2.07497600	-0.00000200	C	-4.21432900	-2.07116200	-1.48797000
O	0.00000000	3.29281100	0.00000400	C	-4.19422200	-3.16570500	-2.36162900
C	1.93801000	0.09238400	-0.00000200	C	-5.32468600	-1.88271700	-0.65556300
C	3.13613400	0.83246700	0.00000600	C	-5.25699100	-4.06945100	-2.39186300
C	2.00143800	-1.31341400	-0.00000900	H	-3.34338200	-3.30816400	-3.02453700
C	4.36625600	0.17998300	0.00000700	C	-6.39188200	-2.77954300	-0.69487900
H	3.08265800	1.91725900	0.00001100	H	-5.35299700	-1.03087800	0.01500400
C	3.23339800	-1.96126500	-0.00000800	C	-6.36023400	-3.87677000	-1.55871200
H	1.08364700	-1.89310500	-0.00001600	H	-5.22751100	-4.91461800	-3.07423700
C	4.41724700	-1.21669200	0.00000000	H	-7.25046000	-2.62078300	-0.04796400
H	5.28546100	0.75903600	0.00001400	H	-7.19356900	-4.57366600	-1.58659400
H	3.27357400	-3.04710400	-0.00001400	Ni	0.54669300	0.65102100	-0.03114300
H	5.37747500	-1.72544600	0.00000100	C	1.00325000	0.10055300	1.87207500
C	-1.93801000	0.09238400	-0.00000100	C	1.99398000	0.98370400	1.21781400
C	-3.13613400	0.83246700	-0.00000700	C	1.09701800	1.46008900	2.27964000
C	-2.00143800	-1.31341400	0.00000700	O	0.83602600	2.33870600	3.08269400
C	-4.36625600	0.17998300	-0.00000500	C	0.92988300	-1.21785700	2.50830000
H	-3.08265800	1.91725900	-0.00001300	C	1.45104800	-2.36807300	1.88753900
C	-3.23339800	-1.96126500	0.00000900	C	0.36184000	-1.33701600	3.78905800
H	-1.08364700	-1.89310500	0.00001300	C	1.41779800	-3.59977400	2.53886100
C	-4.41724700	-1.21669200	0.00000300	H	1.89077500	-2.28876500	0.89706100

C	0.33222400	-2.57070800	4.43679600	C	-2.16730100	-1.40675900	-0.82565100
H	-0.04018400	-0.45021100	4.26995700	C	-2.79209800	0.66198300	-0.21428900
C	0.86095900	-3.70525700	3.81625800	N	-1.73746600	-0.03854100	-0.44145800
H	1.83022000	-4.47850400	2.04939900	O	-3.98224700	0.05458300	-0.44080300
H	-0.10412500	-2.64669200	5.42926600	H	-3.73050900	-0.88639400	-2.24347300
H	0.83797000	-4.66596500	4.32401000	H	-1.62306400	-1.70260200	-1.72511800
C	3.46497900	1.00722200	1.07602000	C	-1.89154400	-2.44277900	0.24971600
C	4.10809800	2.07523200	0.42376100	C	-2.14225000	-2.19871700	1.60644400
C	4.25901800	-0.00904500	1.63833500	C	-1.42071600	-3.70348500	-0.13812700
C	5.49916900	2.11704400	0.32786900	C	-1.94591200	-3.20788400	2.55010000
H	3.50936700	2.86736700	-0.01156200	H	-2.44928800	-1.21197000	1.93640700
C	5.65069500	0.04243300	1.55035900	C	-1.22573200	-4.71240800	0.80603800
H	3.78057400	-0.83755900	2.15067500	H	-1.19310200	-3.89089200	-1.18431400
C	6.27739900	1.10208400	0.89039800	C	-1.49471600	-4.46854200	2.15346400
H	5.97615800	2.94981100	-0.18253800	H	-2.14256200	-3.00434700	3.59959600
H	6.24550900	-0.74810000	2.00126700	H	-0.85685900	-5.68413100	0.48868000
H	7.36127200	1.14031000	0.82040300	H	-1.34159700	-5.25149900	2.89155800
C	0.66553700	1.30943500	-1.96960500	C	-4.68371100	-2.24390400	-0.89882000
H	-0.20117900	0.95624600	-2.51923200	C	-4.93585900	-3.20357800	-1.88712300
C	1.68277400	0.38718500	-1.69631400	C	-5.36344100	-2.32682600	0.32172500
H	2.69027400	0.73974600	-1.51273500	C	-5.83966300	-4.24043000	-1.65518300
C	0.95068900	2.76396100	-2.18078700	H	-4.42517600	-3.13738800	-2.84561100
F	1.53353400	3.37265100	-1.11805000	C	-6.27629100	-3.35714500	0.54901700
F	1.78446600	2.96665800	-3.23474800	H	-5.18431300	-1.57801700	1.08554500
F	-0.18642400	3.44575200	-2.45345100	C	-6.51369600	-4.31877000	-0.43503700
C	1.49307300	-1.03388400	-2.11837700	H	-6.02426300	-4.97895300	-2.43057400
O	0.40008900	-1.42099600	-2.54316800	H	-6.80238600	-3.40820900	1.49849000
C	2.64452100	-1.98635300	-2.05253500	H	-7.22438200	-5.12077800	-0.25476900
C	3.91181600	-1.65210600	-1.55032900	Ni	0.16425000	0.50485800	-0.48224700
C	2.44187400	-3.29069100	-2.54112500	C	1.41325400	-0.39726600	1.55531900
C	4.93807900	-2.59648300	-1.53591300	C	1.60465300	0.77346700	0.79895900
H	4.11353400	-0.66564000	-1.15119300	C	0.22077800	0.32937000	1.64340600
C	3.46986600	-4.22286500	-2.52871000	O	-0.69912600	0.64700100	2.38174600
H	1.46174300	-3.54555500	-2.93000100	C	2.11238300	-1.42361400	2.31567600
C	4.74101200	-3.89193500	-2.02761500	C	3.36063200	-1.93235400	1.91021200
H	5.90747000	-2.31642900	-1.13157900	C	1.49862900	-1.94737600	3.46992900
H	3.29135500	-5.22509800	-2.91237800	C	3.98385500	-2.93173500	2.65406100
C	5.86138700	-4.90368100	-2.03986200	H	3.82813000	-1.54996700	1.00807800
H	5.51800700	-5.88556500	-1.69415800	C	2.13360800	-2.93857500	4.21405100
H	6.25686600	-5.04102000	-3.05505100	H	0.53003300	-1.55981800	3.76919800
H	6.69328900	-4.58973000	-1.40182100	C	3.37630200	-3.43400200	3.80875700
				H	4.94481300	-3.32242100	2.33014600
				H	1.65750900	-3.32935300	5.10943800
				H	3.86716800	-4.21229600	4.38718400
				C	2.73254600	1.72600200	0.79633600
				C	2.72458400	2.85156400	-0.04894600
				C	3.81661900	1.57268600	1.68376300
				C	3.77056300	3.77402200	-0.02741500
				H	1.89080300	2.99319000	-0.72624700
				C	4.85672400	2.49960900	1.71021700
				H	3.83809600	0.72546300	2.36078100
				C	4.84290500	3.60161400	0.85091800
				H	3.74433200	4.63140900	-0.69512400
				H	5.68102200	2.36103500	2.40520000
				H	5.65643400	4.32193500	0.87082600
				C	0.08057600	0.66563500	-2.47113600
				H	-0.51967200	-0.14212900	-2.88030500
				C	1.40102900	0.36419800	-2.09383500
				H	2.15896300	1.13683100	-2.10526600
				C	-0.31929500	1.99770800	-3.00802800
TS1							
C	-0.51534000	6.03437600	1.27787600				
C	-0.52586300	4.73499500	0.82618500				
C	-1.74685900	4.01037200	0.75431600				
C	-2.96237900	4.65464000	1.16267500				
C	-2.91648300	5.99749300	1.61949000				
C	-1.71825700	6.67286800	1.67506700				
H	0.42261100	6.57961200	1.33530700				
H	0.38453100	4.22818700	0.52840700				
C	-4.15850200	3.90059200	1.08298400				
H	-3.84122000	6.48053600	1.92606000				
H	-1.68884600	7.70016600	2.02763800				
C	-4.11563600	2.60396800	0.63293900				
C	-2.85686900	2.05891000	0.25938200				
H	-5.10038200	4.35557600	1.37977500				
H	-5.00962300	1.99707400	0.55723000				
N	-1.71952400	2.72871200	0.30441900				
C	-3.67739200	-1.16180200	-1.18211500				

C	2.32108800	-2.85314200	-1.32334600	C	1.29059900	0.92117000	-1.98797000
C	0.94300900	-3.19739100	-1.31351000	C	0.49893700	0.32960500	-2.99149100
C	0.51808600	-4.41690800	-1.93867400	C	2.55562500	1.42329300	-2.36079200
C	1.49130300	-5.26371500	-2.52966100	C	0.93587000	0.27290500	-4.31437500
C	2.82231000	-4.91172000	-2.51260100	H	-0.46969600	-0.07918000	-2.72145300
H	4.28871300	-3.42584700	-1.92247000	C	2.99844200	1.34600300	-3.68024100
H	2.61620300	-1.91008100	-0.87682100	H	3.19010700	1.86937500	-1.60062600
C	-0.86864200	-4.71215700	-1.93692600	C	2.18968400	0.77767000	-4.66771400
H	1.16743800	-6.19001100	-2.99762700	H	0.29735300	-0.17601200	-5.07187500
H	3.56248500	-5.56321800	-2.96843300	H	3.97923100	1.73812700	-3.93914600
C	-1.75428400	-3.83495700	-1.35756000	H	2.53406000	0.72362900	-5.69711800
C	-1.23529800	-2.66075400	-0.75977900	C	0.47087100	-1.27257900	2.46011900
H	-1.21934800	-5.63150600	-2.39903100	H	0.05411600	-0.57283700	3.18150300
H	-2.82183200	-4.02160300	-1.33785100	C	1.79145000	-1.03243700	1.95657000
N	0.05582500	-2.35322300	-0.72204900	H	2.35245200	-1.88031300	1.57943100
C	-3.92314100	-0.89867600	0.91573600	C	0.04352200	-2.67022300	2.73387100
C	-2.80639400	0.20779200	0.88061200	F	0.61113300	-3.58233900	1.90235000
C	-2.10175700	-1.66654900	-0.11881300	F	0.33706500	-3.07861500	3.99850800
N	-1.64806400	-0.58203500	0.40633900	F	-1.30933000	-2.81993600	2.60953600
O	-3.43105300	-1.88036900	-0.05636000	C	2.47022600	0.21582700	2.02928500
H	-3.86238800	-1.39752800	1.89028400	O	1.88016900	1.30858300	2.38355800
H	-2.60004200	0.55161600	1.89484800	C	3.90760300	0.32449800	1.67895600
C	-3.07366000	1.41734000	0.00215400	C	4.78806200	-0.76931900	1.73929400
C	-3.05414200	1.33532200	-1.39610700	C	4.42579500	1.57825200	1.30900100
C	-3.37176800	2.64610800	0.60166800	C	6.13508300	-0.61422000	1.42293000
C	-3.33537900	2.45568900	-2.17776100	H	4.42983700	-1.74031800	2.06741300
H	-2.80873700	0.39514300	-1.88162900	C	5.77139800	1.72266200	0.98771200
C	-3.65614800	3.76814600	-0.17781400	H	3.75699600	2.43107300	1.27630200
H	-3.36230900	2.72919000	1.68481700	C	6.65065500	0.63033900	1.03364900
C	-3.63962000	3.67568200	-1.56994600	H	6.80152900	-1.47116200	1.49016900
H	-3.31035300	2.37662500	-3.26135900	H	6.14973500	2.70081900	0.69929900
H	-3.87680400	4.71654800	0.30413000	C	8.10498700	0.78782100	0.65938300
H	-3.85256100	4.55056300	-2.17824500	H	8.24847700	0.67382600	-0.42376500
C	-5.34711400	-0.50992000	0.63186600	H	8.48427600	1.77837600	0.93261500
C	-6.15768800	-0.10993700	1.70182000	H	8.73046300	0.03557600	1.15141900
C	-5.88103700	-0.51957200	-0.66186000				
C	-7.47479400	0.29328500	1.48217200	CP5			
H	-5.75712500	-0.11697800	2.71334900	C	-2.00147100	-5.08091300	2.19614600
C	-7.20217000	-0.12797300	-0.87956700	C	-1.45986400	-3.93205500	1.66754700
H	-5.26533700	-0.84515500	-1.49310300	C	-0.05866900	-3.84088000	1.44449200
C	-8.00079000	0.28420000	0.18898100	C	0.78085300	-4.95119400	1.79232100
H	-8.09119800	0.60312800	2.32155400	C	0.18808300	-6.12262100	2.33113000
H	-7.60773800	-0.14453800	-1.88757700	C	-1.17361400	-6.18559700	2.52564400
H	-9.02896100	0.59003700	0.01583000	H	-3.07187700	-5.14686600	2.36896700
Ni	0.30059500	-0.44015200	0.65925900	H	-2.06763200	-3.06617800	1.42612600
C	0.74454200	2.04691500	0.21172900	C	2.17415900	-4.80706900	1.57746400
C	0.85531700	0.95517600	-0.58754400	H	0.82530600	-6.96490400	2.58910400
C	0.29892700	1.56781600	1.54317400	H	-1.62178500	-7.08470200	2.93906600
O	-0.55671100	1.83731000	2.33287100	C	2.66749500	-3.63462000	1.05681100
C	0.91114700	3.50632500	-0.00736700	C	1.74694100	-2.60063000	0.73691800
C	1.32285900	4.34335500	1.04570500	H	2.84226500	-5.62763600	1.82702800
C	0.64407100	4.08812600	-1.25973200	H	3.72584200	-3.48954600	0.87689100
C	1.47829700	5.71540300	0.84743700	N	0.44004700	-2.69451100	0.91582000
H	1.52774900	3.91072800	2.02063500	C	3.76977800	-0.07735200	-0.88078800
C	0.80470800	5.45871900	-1.45426800	C	2.43025200	0.72148700	-0.72300700
H	0.29965200	3.46167000	-2.07524500	C	2.23327600	-1.33535900	0.15503400
C	1.22379400	6.27981400	-0.40385500	N	1.50770900	-0.35797700	-0.27193200
H	1.79992300	6.34379700	1.67434400	O	3.57174400	-1.19573600	0.03679300
H	0.59244300	5.88911000	-2.42997500	H	3.77400300	-0.51949700	-1.88410200
H	1.34451500	7.34893400	-0.55843200	H	2.10392800	1.06516600	-1.70717100

C	2.45256800	1.91197100	0.21669700	C	-3.94609900	-1.11451800	-0.84248700
C	2.67172600	1.76456400	1.59313700	C	-4.33068400	0.80311100	-2.24547700
C	2.29435000	3.19964400	-0.30798900	C	-5.30724200	-1.17808300	-0.55957300
C	2.74675200	2.88325000	2.42263600	H	-3.26799100	-1.82723800	-0.38119500
H	2.78399900	0.77365200	2.02398700	C	-5.69246900	0.73651500	-1.95037100
C	2.36915500	4.32091600	0.51994900	H	-3.96188800	1.56695500	-2.92232900
H	2.09351300	3.32876900	-1.36862500	C	-6.20847000	-0.25095900	-1.10333500
C	2.60161000	4.16535800	1.88669300	H	-5.67604600	-1.95378800	0.10829900
H	2.91671500	2.75307500	3.48803000	H	-6.36688500	1.46486900	-2.39532800
H	2.23173900	5.31156100	0.09664400	C	-7.67911300	-0.30156100	-0.76081700
H	2.65768300	5.03652400	2.53365400	H	-7.88296500	0.19185000	0.19922400
C	5.07653100	0.62362600	-0.62956300	H	-8.28448900	0.20342000	-1.52085500
C	5.63942700	1.37624500	-1.66866300	H	-8.03659300	-1.33394800	-0.67476100
C	5.74262600	0.55136200	0.59841600				
C	6.83828600	2.06230700	-1.47794300	TS3			
H	5.13965000	1.42336900	-2.63398700	C	2.05283000	5.12529600	2.34551200
C	6.94880600	1.22853500	0.78479200	C	1.47126900	3.97153900	1.87156100
H	5.32459800	-0.04688000	1.40066100	C	0.13078400	3.98831000	1.39846100
C	7.49721700	1.98926400	-0.24884300	C	-0.60626800	5.21798200	1.43198400
H	7.26141800	2.64463000	-2.29174000	C	0.02423100	6.38905600	1.92596000
H	7.46017100	1.16011800	1.74115300	C	1.32640500	6.34335200	2.37161600
H	8.43551100	2.51666900	-0.10072400	H	3.07822700	5.10817700	2.70398400
Ni	-0.35100600	-0.40837300	-0.86602800	H	2.00728800	3.02804700	1.84996000
C	-1.48092000	2.11690400	-0.38335400	C	-1.94489500	5.19053200	0.96600900
C	-1.19787000	0.92803000	0.22357100	H	-0.53665600	7.32025100	1.94548200
C	-1.34789200	2.25208800	-1.86381800	H	1.80445400	7.24380700	2.74680300
O	-1.11152400	3.27099500	-2.46877900	C	-2.48228300	4.01380700	0.50436800
C	-1.88260000	3.37951700	0.31076500	C	-1.66470600	2.85173500	0.50485000
C	-2.92402500	4.18134500	-0.18785000	H	-2.53372400	6.10433400	0.97545100
C	-1.23004400	3.79843300	1.48163000	H	-3.49895600	3.95464100	0.13487400
C	-3.31156100	5.34758600	0.47021400	N	-0.41254900	2.83001000	0.93807200
H	-3.43536700	3.88779300	-1.09968300	C	-3.72987600	0.32425700	-1.04756600
C	-1.61693800	4.96502900	2.14073200	C	-2.48184400	-0.53984400	-0.65467800
H	-0.40886400	3.20719400	1.87199800	C	-2.19570000	1.58017400	-0.00988500
C	-2.66113800	5.74493200	1.64048000	N	-1.50697700	0.52043100	-0.28976800
H	-4.12342200	5.94758400	0.06643600	O	-3.52826700	1.52018600	-0.23537500
H	-1.09406200	5.26808200	3.04462500	H	-3.60195800	0.64078400	-2.09072500
H	-2.96143600	6.65550300	2.15279200	H	-2.11725300	-1.07580900	-1.53360700
C	-1.54518000	0.63913600	1.62913500	C	-2.72238500	-1.52974700	0.47321200
C	-0.62153800	0.08241500	2.53366400	C	-2.60262100	-1.17097100	1.82156600
C	-2.86471800	0.84849500	2.08371100	C	-3.15585300	-2.82322100	0.15374900
C	-0.98784100	-0.21614800	3.84497200	C	-2.92611700	-2.08325800	2.82874400
H	0.39087200	-0.10380800	2.19778600	H	-2.24203900	-0.18311700	2.09001100
C	-3.23596000	0.52508400	3.38769200	C	-3.48662100	-3.73192900	1.15770300
H	-3.59584800	1.26734200	1.40014200	H	-3.23832300	-3.11978000	-0.88884700
C	-2.29827000	-0.00120700	4.27923400	C	-3.37725300	-3.36251900	2.50002400
H	-0.24931200	-0.62852700	4.52865900	H	-2.82391200	-1.79118900	3.87060100
H	-4.26043200	0.69394300	3.71063300	H	-3.81917200	-4.73110700	0.89104900
H	-2.58578300	-0.24465200	5.29889900	H	-3.63278700	-4.07032300	3.28409000
C	0.05452600	-1.28945400	-2.73102000	C	-5.11051100	-0.23764900	-0.85516900
H	0.50356100	-0.44228200	-3.24486800	C	-5.73704900	-0.87458900	-1.93354900
C	-1.31246500	-1.27675500	-2.42032400	C	-5.77847700	-0.15755200	0.37294100
H	-1.82046700	-2.21324700	-2.20875900	C	-7.00357400	-1.44102800	-1.78433500
C	0.76752300	-2.57325400	-2.95922600	H	-5.23348200	-0.92467200	-2.89674400
F	0.24221500	-3.59932400	-2.24940900	C	-7.04941700	-0.71291800	0.51789100
F	0.76834300	-2.95944700	-4.26005300	H	-5.30470400	0.34623100	1.20841500
F	2.08464100	-2.47770200	-2.60384500	C	-7.66347400	-1.35980800	-0.55707500
C	-1.99021400	-0.08377300	-2.05899700	H	-7.47716400	-1.93366000	-2.62904800
O	-1.54828800	1.10548800	-2.65375300	H	-7.56109100	-0.64067600	1.47379700
C	-3.43440600	-0.12485500	-1.69641800	H	-8.65349500	-1.79221800	-0.44041400

Ni	0.38498400	0.54697000	-0.69930400	H	1.87635900	1.68737900	-1.81406300
C	1.10597700	-2.31914400	-0.68964100	C	-1.01468000	5.06923600	-0.66192400
C	1.36205800	-1.12285800	-0.06323800	H	1.16489400	6.58680100	-1.21780600
C	1.17486800	-2.22049800	-2.16496200	H	3.35053000	5.74059900	-2.02169600
O	0.77020900	-2.99065100	-3.00594800	C	-2.02391500	4.15361800	-0.48525400
C	0.86183700	-3.64484100	-0.07892400	C	-1.73866900	2.78926200	-0.70215700
C	1.27592300	-4.82707700	-0.72561900	H	-1.19046000	6.13095200	-0.51066500
C	0.22774900	-3.76423900	1.17223300	H	-3.02907900	4.44582000	-0.20312700
C	1.08527400	-6.07254400	-0.12990500	N	-0.52793700	2.30863500	-1.03022200
H	1.74515200	-4.76834900	-1.70033500	C	-4.79983200	0.83218200	-0.70097400
C	0.03771900	-5.01090800	1.76347500	C	-3.67983100	-0.27349000	-0.86053700
H	-0.12906900	-2.87418400	1.67722500	C	-2.76657600	1.75568100	-0.67582400
C	0.46970000	-6.17240200	1.11928400	N	-2.47732000	0.55824500	-1.05473300
H	1.42065100	-6.96839100	-0.64632300	O	-4.03183900	2.02139800	-0.30576000
H	-0.46010500	-5.07260300	2.72737200	H	-5.19558500	1.05670200	-1.69880400
H	0.32079100	-7.14486300	1.58168000	H	-3.86486100	-0.83632700	-1.77885700
C	1.81668700	-1.00069800	1.34456900	C	-3.52940200	-1.25735800	0.28728500
C	1.31772400	0.00077200	2.19710000	C	-2.71382200	-0.99279100	1.39326400
C	2.82161700	-1.85492100	1.84303300	C	-4.24630200	-2.46092300	0.24476300
C	1.77853900	0.12021500	3.50986700	C	-2.61803400	-1.91320400	2.43852400
H	0.56515700	0.69008800	1.82521400	H	-2.11493300	-0.09022800	1.43994200
C	3.28962200	-1.72558600	3.14829600	C	-4.16158400	-3.37555700	1.29394400
H	3.23744100	-2.61819400	1.19392200	H	-4.87313000	-2.68404400	-0.61592000
C	2.76555500	-0.74172700	3.99128600	C	-3.34569000	-3.10275300	2.39513600
H	1.36886300	0.89525600	4.15311500	H	-1.95389500	-1.69379900	3.26899000
H	4.06690600	-2.39484800	3.50797200	H	-4.72325000	-4.30481700	1.24594800
H	3.12997400	-0.64348500	5.01068100	H	-3.26884200	-3.82105600	3.20722800
C	0.76837300	1.52247000	-2.47587000	C	-5.94016000	0.59244100	0.24808700
H	0.35589000	0.86653800	-3.23783000	C	-7.16743900	0.15485500	-0.26381100
C	1.91622900	1.15196300	-1.75109000	C	-5.80321900	0.77783100	1.62985000
H	2.53100100	1.91986000	-1.29201500	C	-8.23908100	-0.11109700	0.58989400
C	0.45600800	2.95730000	-2.70304700	H	-7.28737100	0.02438400	-1.33734500
F	0.97973100	3.77383700	-1.75425000	C	-6.87755500	0.52389900	2.48122100
F	0.90996800	3.42020000	-3.89868800	H	-4.85862900	1.12447000	2.03488500
F	-0.89030200	3.17518600	-2.71356700	C	-8.09599500	0.07504000	1.96544500
C	2.30747800	-0.24116200	-1.53413900	H	-9.18545400	-0.45169400	0.17876500
O	1.85564700	-1.08358900	-2.56571400	H	-6.76143100	0.67418900	3.55101200
C	3.75185000	-0.46895800	-1.16353800	H	-8.93044600	-0.12363400	2.63252300
C	4.40168300	0.33783400	-0.21741900	Ni	-0.55306000	0.27619200	-1.26955300
C	4.48563900	-1.49381500	-1.77490700	C	-0.23237900	-1.54979100	-1.64561500
C	5.74304300	0.13113100	0.09421600	H	-0.68795800	-2.24897800	-0.94519600
H	3.85508000	1.12046100	0.29982000	C	1.02100000	-0.91007900	-1.29763500
C	5.82901000	-1.69322200	-1.45623900	H	1.75321200	-0.74896100	-2.09018000
H	4.01226600	-2.12446000	-2.51896200	C	-0.52645700	-1.90788600	-3.05748700
C	6.48597300	-0.88518500	-0.52123800	F	-1.86225300	-2.06637200	-3.27421400
H	6.21873200	0.76783100	0.83699800	F	-0.09036500	-0.97638200	-3.94703900
H	6.37679500	-2.49178600	-1.95190800	F	0.04455300	-3.08909600	-3.45879700
C	7.94966300	-1.08367400	-0.20351100	C	1.65552300	-1.26235600	0.04848300
H	8.16754300	-0.85590700	0.84587900	O	0.63472900	-1.05788900	1.07563900
H	8.26603400	-2.11384300	-0.39890800	C	2.11429100	-2.72962800	0.21854000
H	8.58314200	-0.42704600	-0.81530600	C	2.06713300	-3.66190300	-0.82221200
				C	2.59840800	-3.15857900	1.46520600
				C	2.49423600	-4.97819400	-0.62084500
				H	1.68695700	-3.37563900	-1.79460100
				C	3.01737600	-4.47036200	1.66079800
				H	2.64735100	-2.46052700	2.29570800
				C	2.97382900	-5.40925300	0.61876500
				H	2.44388500	-5.68123700	-1.44946400
				H	3.38549400	-4.77192400	2.63942900
				C	3.41182300	-6.83797300	0.84202000
CP6							
C	2.74406600	3.65706300	-1.97862200				
C	1.74008300	2.75636900	-1.69734000				
C	0.47537600	3.21580600	-1.25396200				
C	0.26448200	4.62588600	-1.08059700				
C	1.33011400	5.52113400	-1.35458000				
C	2.54291000	5.04798100	-1.80245800				
H	3.70426500	3.29245400	-2.32970800				

H	3.52448500	-7.37438100	-0.10566100	C	3.61012100	1.09076000	0.04097500
H	4.36950900	-6.88689200	1.37393400	C	3.87994400	-0.66981800	-1.59713800
H	2.67994000	-7.38883500	1.44758700	C	4.99302500	1.24001000	0.10923300
C	2.39211100	0.34490700	1.60822700	H	2.96855100	1.72998300	0.63916000
C	2.76602400	-0.28357800	0.46242400	C	5.26455000	-0.52099400	-1.52011600
C	1.00833500	-0.08814600	1.94419500	H	3.44865400	-1.39503000	-2.27684100
O	0.27021900	0.31105300	2.82251300	C	5.82632200	0.43084300	-0.66781900
C	3.12436400	1.25878500	2.50901400	H	5.42058500	1.99331400	0.76548000
C	4.45272400	0.99017600	2.88485900	H	5.90488600	-1.14854100	-2.13403800
C	2.48558200	2.38432200	3.05695700	H	6.90538900	0.54787600	-0.61423300
C	5.12896600	1.83412200	3.76303900	C	0.78082700	0.18708600	1.52988700
H	4.95077100	0.11053500	2.48823200	C	1.70070800	-0.66056100	2.17741000
C	3.16732900	3.23027900	3.93233200	C	0.01678000	1.07094800	2.31367300
H	1.45060200	2.58320600	2.80342000	C	1.85518600	-0.62004500	3.56054000
C	4.49010500	2.96115100	4.28725100	H	2.28490200	-1.35916000	1.58735600
H	6.15390000	1.60714600	4.04473400	C	0.18165900	1.11350600	3.69886800
H	2.65878800	4.09858400	4.34318100	H	-0.69325700	1.73827200	1.83910700
H	5.01747600	3.61848000	4.97357200	C	1.09800700	0.26978100	4.32731300
C	3.99601000	-0.07865100	-0.33171700	H	2.56483700	-1.28801000	4.04080900
C	4.61821700	1.18684900	-0.35865500	H	-0.41063500	1.80991400	4.28611700
C	4.57370500	-1.10935100	-1.09842600	H	1.21995100	0.30161500	5.40650500
C	5.77318600	1.40564800	-1.10505400				
H	4.18223000	2.00503200	0.20138500				
C	5.73213000	-0.88713000	-1.84362000	TS4			
H	4.12812400	-2.09570800	-1.09988000	C	-1.67478600	5.79521100	0.82849800
C	6.33997500	0.36799600	-1.85025500	C	-1.47578000	4.45880800	0.55950500
H	6.23255300	2.39094000	-1.10342200	C	-2.49176700	3.69901300	-0.07374800
H	6.15875700	-1.70378500	-2.41966900	C	-3.72293800	4.34364400	-0.43142200
H	7.24269900	0.53847600	-2.43071400	C	-3.88981100	5.72239400	-0.14464300
				C	-2.88679600	6.43540300	0.47385900
3a				H	-0.89093600	6.36629600	1.31781100
C	-1.83299900	-2.34484000	-0.70949600	H	-0.54901100	3.96467800	0.82615600
H	-1.67675500	-2.41395800	-1.78094100	C	-4.72797300	3.56771000	-1.06465200
C	-1.46220500	-1.27634100	-0.00792100	H	-4.82518400	6.20334900	-0.41957400
H	-1.63503000	-1.24033900	1.06392300	H	-3.02232900	7.49099900	0.69129000
C	-2.49483700	-3.53113000	-0.08557500	C	-4.50850600	2.23255400	-1.29842200
F	-3.70695500	-3.75639800	-0.64357300	C	-3.27262000	1.67276400	-0.90270400
F	-1.76364400	-4.65338500	-0.27406700	H	-5.66371700	4.03879900	-1.35388000
F	-2.68334100	-3.39045300	1.24460000	H	-5.24957100	1.59884900	-1.77224000
C	-0.76777300	-0.06666500	-0.59434800	N	-2.27975500	2.36927200	-0.32859900
O	-0.46400200	-0.31683100	-1.98251100	C	-3.11246800	-1.83881300	-1.80997200
C	-1.62537700	1.20604400	-0.53410000	C	-1.97283800	-1.71345500	-0.72892500
C	-2.97421900	1.17504500	-0.17302300	C	-2.97420400	0.25486400	-1.04850800
C	-1.06157800	2.43656400	-0.90575800	N	-1.88939900	-0.24720800	-0.55949100
C	-3.73721100	2.34592800	-0.16972200	O	-3.84535600	-0.57816200	-1.65672800
H	-3.44508400	0.23513800	0.09679600	H	-2.63874400	-1.78947300	-2.79835800
C	-1.82710200	3.59731100	-0.90529400	H	-1.03463800	-2.08642900	-1.14162100
H	-0.01724700	2.48579800	-1.20051700	C	-2.22548200	-2.41956600	0.59317000
C	-3.18095000	3.57579900	-0.53228700	C	-3.01543800	-1.85720800	1.60447800
H	-4.78554200	2.29510500	0.11455900	C	-1.67295000	-3.69084800	0.79524800
H	-1.36801800	4.53792600	-1.20145900	C	-3.25566900	-2.55698000	2.78881500
C	-3.99958800	4.84527200	-0.52215600	H	-3.43216400	-0.86220900	1.47674900
H	-5.05677400	4.63814100	-0.32946400	C	-1.91659700	-4.39275800	1.97597700
H	-3.64975300	5.53931800	0.25293600	H	-1.03911300	-4.12264900	0.02594800
H	-3.92887200	5.37291600	-1.48075000	C	-2.70993000	-3.82819600	2.97643600
C	1.56804700	-0.02252600	-0.89227300	H	-3.86787600	-2.10619100	3.56576400
C	0.61443000	0.08515100	0.06447100	H	-1.47736600	-5.37643600	2.11847000
C	0.89220900	-0.31475000	-2.18951900	H	-2.89434800	-4.37121400	3.89951900
O	1.36751700	-0.53278900	-3.27657400	C	-4.04466700	-3.01738300	-1.75863900
C	3.03311600	0.12742400	-0.80656900	C	-3.72655000	-4.16143100	-2.50113000
				C	-5.20645200	-3.01257700	-0.97735100

C	-4.54583000	-5.28963400	-2.45236700	CP7			
H	-2.83346700	-4.16937500	-3.12234600	C	-1.18130600	5.21203600	-0.97741800
C	-6.03183200	-4.13627700	-0.93863400	C	-0.64695300	3.96564300	-0.74512500
H	-5.46765300	-2.12511900	-0.41096800	C	0.41941700	3.80788300	0.17527600
C	-5.70272400	-5.27877200	-1.67129300	C	0.93727200	4.96966500	0.84671600
H	-4.28527100	-6.17074000	-3.03236700	C	0.34388800	6.23494900	0.60035000
H	-6.93409900	-4.11918700	-0.33315300	C	-0.69440700	6.35377000	-0.29449200
H	-6.34710900	-6.15309500	-1.63784800	H	-1.99562000	5.31793800	-1.68789900
Ni	-0.60037500	1.18243800	0.01342700	H	-1.02282600	3.09220000	-1.25694900
C	1.60427500	-0.83882600	0.42934800	C	2.04345000	4.80965800	1.71434000
C	1.02673800	0.42011700	0.46198500	H	0.73458600	7.10536200	1.12119400
C	1.74302600	-1.56301100	-0.86587900	H	-1.14087100	7.32572800	-0.48482300
O	1.12998300	-2.55340100	-1.21301100	C	2.62169500	3.57045400	1.85622500
C	2.18585600	-1.55732700	1.59261500	C	2.05477900	2.48676000	1.15430900
C	2.04059500	-2.95331500	1.73531200	H	2.43863400	5.67353900	2.24239000
C	2.95542400	-0.88253200	2.56416700	H	3.49136500	3.40382800	2.48137000
C	2.61736100	-3.63250900	2.80780100	N	0.96658700	2.56698300	0.37551300
H	1.46293500	-3.50153600	0.99984900	C	4.07946700	-0.48983300	1.66547300
C	3.52145000	-1.56366900	3.63839100	C	3.11709700	-0.91845700	0.49409400
H	3.12146500	0.18454300	2.46595400	C	2.66390000	1.15853000	1.15339500
C	3.35642700	-2.94499400	3.77164200	N	2.12489500	0.17718700	0.51352000
H	2.48115300	-4.70833000	2.89118700	O	3.85110100	0.95659100	1.75165300
H	4.11030700	-1.01217200	4.36761500	H	3.67802500	-0.90989600	2.59533300
H	3.80281700	-3.47572400	4.60841900	H	2.63197300	-1.85350400	0.76768800
C	0.78266300	1.18436100	1.72351900	C	3.75502500	-1.08466600	-0.87744100
C	-0.15065700	0.65327300	2.64989800	C	3.84323800	-0.03179300	-1.79618900
C	1.40369800	2.41499200	2.04194200	C	4.28364400	-2.33452200	-1.22983200
C	-0.44840900	1.33197500	3.83329300	C	4.45625900	-0.22286300	-3.03650800
H	-0.60755500	-0.30824600	2.44380800	H	3.41090700	0.93420400	-1.55463800
C	1.10948900	3.07730700	3.23083600	C	4.89993400	-2.52529400	-2.46612600
H	2.12466300	2.84064100	1.35603100	H	4.21229600	-3.16402200	-0.53017600
C	0.17858000	2.54283200	4.12896200	C	4.98830800	-1.46774400	-3.37433700
H	-1.16592000	0.90384000	4.52828300	H	4.51004400	0.60252000	-3.74140300
H	1.60815300	4.01606900	3.45901800	H	5.30442500	-3.50084100	-2.72206700
H	-0.05010900	3.06622000	5.05354100	H	5.46138700	-1.61622000	-4.34120300
C	1.53403700	1.36985300	-1.13589900	C	5.54710100	-0.79662800	1.56410700
H	1.07954700	0.73881600	-1.90390600	C	6.04998100	-1.92686800	2.21983800
C	3.00662900	1.14366100	-1.11846300	C	6.42029300	0.00501300	0.81788500
H	3.65120200	1.96933100	-0.83774100	C	7.40071200	-2.26352000	2.11931900
C	1.28524800	2.79656300	-1.59521600	H	5.38260000	-2.54495800	2.81678000
F	1.66977700	3.73630700	-0.68911300	C	7.77202200	-0.32449200	0.72798900
F	1.98975600	3.06934100	-2.72667100	H	6.04148300	0.88984800	0.31723500
F	-0.00758000	3.05151300	-1.90792500	C	8.26536300	-1.46094900	1.37381900
C	3.55283100	-0.04822200	-1.40900100	H	7.77711500	-3.14374100	2.63317100
O	2.71427700	-1.11688200	-1.74371400	H	8.44170000	0.30753000	0.15117300
C	4.98461400	-0.38040000	-1.47934000	H	9.31924100	-1.71529700	1.30115000
C	5.96956600	0.62095300	-1.56972000	Ni	0.24863400	0.63127500	0.01649100
C	5.40861900	-1.71889100	-1.45795300	C	-1.66613000	0.46325900	-0.34166200
C	7.31952000	0.29277200	-1.60925900	C	-1.00076700	-0.83472800	-0.10483900
H	5.67756600	1.66555700	-1.62607400	C	-2.46618500	1.15738500	0.72669700
C	6.76458000	-2.03803700	-1.50304000	O	-2.45257400	2.35230400	0.92506700
H	4.67056800	-2.51092700	-1.39970100	C	-2.07613400	0.89655800	-1.72575300
C	7.74648500	-1.04391300	-1.57810500	C	-1.18233300	0.84669200	-2.81423000
H	8.05818100	1.08870800	-1.67779500	C	-3.37750700	1.36728700	-1.98470700
H	7.06383400	-3.08347700	-1.47625700	C	-1.57156900	1.23940200	-4.09371400
C	9.21419600	-1.39230400	-1.65579500	H	-0.16904500	0.49404200	-2.64891900
H	9.58397800	-1.33586900	-2.68869800	C	-3.76638700	1.76933700	-3.26344000
H	9.82288300	-0.70377000	-1.05838400	H	-4.10240100	1.42097500	-1.17725500
H	9.40330200	-2.40920800	-1.29653600	C	-2.86685000	1.70656900	-4.32807800
				H	-0.85492200	1.18446800	-4.90949700

H	-4.78070000	2.12618600	-3.42492600	H	-3.71433200	-1.56587700	-0.77247000
H	-3.16907400	2.01737100	-5.32472800	C	-4.18847400	-1.12396900	2.56584700
C	-0.92237600	-1.84665300	-1.22993500	H	-2.74569800	-0.25332600	3.91338900
C	-2.08863300	-2.32974600	-1.85094900	H	-5.40946500	-1.93448000	0.98303100
C	0.30620700	-2.35908500	-1.66853500	H	-4.93331300	-1.29246100	3.33884800
C	-2.02520200	-3.29143700	-2.85938300	C	-0.33078000	-1.57874300	-1.00011100
H	-3.05337400	-1.93697200	-1.54605000	H	-0.20054200	-1.45043800	-2.08228800
C	0.37627900	-3.31914100	-2.67976200	C	1.00991500	-1.43822700	-0.32100100
H	1.22169700	-1.98648700	-1.22500400	H	1.26790800	-2.11893700	0.48043100
C	-0.79110800	-3.79333600	-3.27851200	C	-0.85643300	-2.99794300	-0.85471200
H	-2.94321700	-3.64328100	-3.32407900	F	0.02855200	-3.86615900	-1.39339000
H	1.34750100	-3.68876600	-2.99996000	F	-1.03881400	-3.36564200	0.42943700
H	-0.74114400	-4.53914700	-4.06792100	F	-2.02677000	-3.16938200	-1.50867800
C	-1.36283500	-1.45822500	1.27612400	C	1.82747900	-0.42833700	-0.65478600
H	-1.19456500	-0.69365400	2.04429800	O	1.46971500	0.46801900	-1.65059600
C	-2.82368900	-1.83271900	1.29875300	C	3.16888700	-0.15800600	-0.10405600
H	-3.11039500	-2.86969200	1.17584900	C	3.86521500	-1.13155400	0.63578300
C	-0.53247700	-2.63798900	1.74906500	C	3.78630000	1.08571500	-0.30543000
F	-0.88252500	-2.97290300	3.01578500	C	5.11637700	-0.85638600	1.17288600
F	-0.68527100	-3.74939300	1.00066600	H	3.43586400	-2.11911500	0.77527000
F	0.79728100	-2.36125200	1.78589400	C	5.04465200	1.35062700	0.23409900
C	-3.74659600	-0.86576900	1.37941100	H	3.28140400	1.84343700	-0.89417500
O	-3.34105100	0.45236400	1.55614000	C	5.73171100	0.39229000	0.98651900
C	-5.21525000	-1.01830300	1.37885500	H	5.63400300	-1.62918400	1.73689400
C	-5.82963600	-2.27585500	1.22579700	H	5.50066400	2.32277100	0.06240800
C	-6.04580100	0.10291800	1.53269500	C	7.08911300	0.68091100	1.58198000
C	-7.21327100	-2.39844300	1.22134400	H	7.81013000	-0.10776000	1.33566900
H	-5.22357200	-3.16871200	1.10599800	H	7.49246600	1.63104100	1.21805500
C	-7.43439100	-0.03130000	1.52905200	H	7.03931500	0.73920300	2.67718300
H	-5.59604300	1.08031500	1.66487400				
C	-8.04691600	-1.27808800	1.37120900	TS2-R-exo			
H	-7.65829600	-3.38376800	1.09903200	Ni	-0.92855400	0.07832200	0.19949900
H	-8.05204700	0.85548800	1.65307600	C	-1.82857600	2.11365200	-0.93794400
C	-9.55033100	-1.42260600	1.34967700	C	-2.43150300	1.18819500	-0.13358700
H	-9.88913300	-2.20313600	2.04180800	C	-0.41850200	1.68998400	-0.95044700
H	-10.04522200	-0.48728700	1.63011700	O	0.40717700	1.53812800	-1.82314200
H	-9.91156100	-1.70149700	0.35090200	C	-2.34268800	3.25699300	-1.72324700
				C	-1.63440400	3.71727600	-2.84946000
3a'				C	-3.52569200	3.92653900	-1.35718500
C	-0.88452100	0.81823700	-0.86830300	C	-2.10488400	4.79829300	-3.59330500
C	-1.21435700	-0.43645800	-0.47180900	H	-0.71344200	3.22028800	-3.13541700
C	0.23299100	1.07434800	-1.83608100	C	-3.99065000	5.00709000	-2.10375300
O	0.14659400	1.84322000	-2.76040500	H	-4.07429700	3.60477200	-0.47908100
C	-1.60996900	2.05877800	-0.46378900	C	-3.28607700	5.44650700	-3.22746500
C	-2.99791400	2.18445600	-0.61939100	H	-1.54428200	5.13604400	-4.46138000
C	-0.89139100	3.14458200	0.06212000	H	-4.90440000	5.51266400	-1.80156800
C	-3.65128000	3.35771900	-0.24311500	H	-3.65124700	6.29020700	-3.80731500
H	-3.56466600	1.36334700	-1.04502300	C	-3.86935000	1.04544100	0.14309500
C	-1.54476300	4.31524700	0.44277300	C	-4.75203700	0.65609800	-0.88395000
H	0.18713700	3.06962000	0.17749700	C	-4.40393200	1.27762700	1.42468500
C	-2.92882700	4.42525100	0.29243000	C	-6.11715500	0.51505300	-0.64020800
H	-4.72684500	3.43856000	-0.37545000	H	-4.35518400	0.47499400	-1.87900700
H	-0.97205000	5.14241000	0.85340300	C	-5.77201600	1.14232500	1.66331000
H	-3.43918000	5.33913900	0.58422200	H	-3.74216600	1.56542800	2.23446300
C	-2.26389400	-0.68751700	0.56337700	C	-6.63581300	0.75989200	0.63379800
C	-2.00877600	-0.32008400	1.89412500	H	-6.77878000	0.21818900	-1.45021900
C	-3.49858900	-1.27658200	0.25022400	H	-6.16349800	1.33964700	2.65827400
C	-2.96156200	-0.54153200	2.88812900	H	-7.70132800	0.65694400	0.82162600
H	-1.05897300	0.14327500	2.14404700	C	-0.48141900	0.93722300	2.01325000
C	-4.45461000	-1.48623600	1.24408200	H	-1.15539400	1.78958900	1.98162400

C	0.90155900	1.26716000	1.94957500	H	4.22788300	-0.72342400	-3.47389500
H	1.63969500	0.64685700	2.44436000	C	5.26945500	-4.07015100	-1.82534500
C	-0.88420200	-0.05598300	3.06656000	H	3.30638100	-4.07051200	-0.93961300
F	-0.24284500	-1.24466800	2.94274900	C	6.17039400	-3.39130100	-2.64940000
F	-2.21854000	-0.32421000	3.03882000	H	6.48594100	-1.65166900	-3.88644400
F	-0.62078000	0.39266400	4.31916300	H	5.55397100	-5.01459500	-1.36947000
C	1.28466300	2.33003900	1.12169200	H	7.15715100	-3.80596800	-2.83686400
O	0.41896600	2.86928900	0.32810100				
C	2.67831000	2.84156200	1.07347300				
C	3.58077400	2.67462700	2.13706100				
C	3.11358500	3.53783800	-0.06654000				
C	4.87838000	3.17306300	2.05287100				
H	3.25981000	2.16587300	3.04136200				
C	4.41493200	4.02596400	-0.14651200				
H	2.41313800	3.67689700	-0.88326500				
C	5.32083200	3.85750000	0.91125400				
H	5.55873400	3.03670700	2.89107700				
H	4.73522400	4.55231900	-1.04348700				
C	6.71798100	4.42795500	0.83931800				
H	7.07739700	4.48064400	-0.19420800				
H	7.42907700	3.82605100	1.41599200				
H	6.75268600	5.44776000	1.24654100				
C	-5.23331800	-2.91785800	1.21412600				
C	-3.99963300	-2.33752100	1.02809200				
C	-3.08812600	-2.89036800	0.09054900				
C	-3.46429300	-4.06672800	-0.64426300				
C	-4.74691800	-4.63452000	-0.42958500				
C	-5.61304800	-4.06965500	0.47923800				
H	-5.92701600	-2.48419600	1.92782200				
H	-3.69279600	-1.46267800	1.58541700				
C	-2.52012900	-4.61072500	-1.54840200				
H	-5.02921100	-5.52218000	-0.99019100				
H	-6.59345200	-4.50911500	0.64039900				
C	-1.28637800	-4.01940500	-1.68476800				
C	-1.01114900	-2.86273400	-0.91540800				
H	-2.77788100	-5.49722600	-2.12242700				
H	-0.53144600	-4.40839900	-2.35770300				
N	-1.87070500	-2.30091900	-0.07392500				
C	2.27754100	-1.70598800	-1.91010400				
C	2.04422600	-0.86472700	-0.60625000				
C	0.29877200	-2.19768800	-0.99819200				
N	0.60992300	-1.12817400	-0.34918900				
O	1.23283500	-2.73544700	-1.80074700				
H	1.98581000	-1.08153900	-2.76232700				
H	2.16614900	0.19356100	-0.84007000				
C	2.92337100	-1.23989300	0.57657800				
C	2.56133500	-2.23234100	1.49584900				
C	4.16031000	-0.59833100	0.72667000				
C	3.42319500	-2.58254900	2.53734400				
H	1.59271000	-2.71496500	1.41927800				
C	5.02391100	-0.95152200	1.76319900				
H	4.44569600	0.18817700	0.03349700				
C	4.65869000	-1.94722300	2.67166400				
H	3.12257300	-3.34763600	3.24823800				
H	5.97623400	-0.43874700	1.86595200				
H	5.32778600	-2.21874200	3.48386200				
C	3.62084100	-2.32718700	-2.16625500				
C	4.52309400	-1.65835800	-3.00256800				
C	4.00296500	-3.54074900	-1.58056400				
C	5.79517500	-2.18226200	-3.23692300				
				TS2-S-endo			
				Ni	-0.25650300	0.22558100	-0.40707400
				C	-0.96223800	-2.09265600	0.47388200
				C	-1.04707500	-0.85134900	1.01550200
				C	-0.31533800	-1.93335500	-0.85365800
				O	0.60000400	-2.42566400	-1.43782200
				C	-1.31514100	-3.45383900	0.95094900
				C	-1.53682700	-4.49639800	0.03149500
				C	-1.42564200	-3.74235200	2.32429800
				C	-1.86993700	-5.77772700	0.47042300
				H	-1.45368800	-4.29723600	-1.03239500
				C	-1.76155100	-5.02373400	2.75746400
				H	-1.24290000	-2.95999300	3.05237400
				C	-1.98707200	-6.04855900	1.83486200
				H	-2.03846100	-6.56616400	-0.25889100
				H	-1.84118600	-5.22332800	3.82331600
				H	-2.24629000	-7.04726200	2.17644000
				C	-1.59862300	-0.47417000	2.32091700
				C	-0.78008300	0.04032100	3.34554300
				C	-2.98501000	-0.56016400	2.56625100
				C	-1.32036700	0.43070900	4.57055700
				H	0.29051100	0.12026500	3.17661400
				C	-3.52273500	-0.15633400	3.78751700
				H	-3.63479200	-0.94887300	1.78699500
				C	-2.69533300	0.33804300	4.79909700
				H	-0.66388300	0.81264000	5.34897400
				H	-4.59501600	-0.23407000	3.95139900
				H	-3.11642600	0.64876300	5.75148700
				C	-0.21925800	0.75389400	-2.31706500
				H	0.28322200	-0.03570900	-2.87166700
				C	-1.59447100	0.57980800	-1.93168500
				H	-2.18188000	1.47959500	-1.79516500
				C	0.18881200	2.11619000	-2.76937500
				F	-0.59950100	3.10652400	-2.27419200
				F	0.15684900	2.24664900	-4.12335500
				F	1.46615400	2.44447300	-2.40711500
				C	-2.32361100	-0.64524100	-1.91715100
				O	-1.75967800	-1.79905500	-1.94703600
				C	-3.80459200	-0.63747700	-1.81782500
				C	-4.58579300	0.44581000	-2.25593000
				C	-4.46055300	-1.76913600	-1.30134900
				C	-5.97408000	0.40201600	-2.16329900
				H	-4.11083300	1.31359500	-2.70356800
				C	-5.84781900	-1.80010400	-1.20370100
				H	-3.86655400	-2.61635500	-0.97650400
				C	-6.63046300	-0.71585700	-1.62839100
				H	-6.56043200	1.24493700	-2.52198400
				H	-6.33509300	-2.68211000	-0.79433500
				C	-8.13446100	-0.74532200	-1.49778900
				H	-8.45281000	-0.36909100	-0.51599100
				H	-8.52532600	-1.76359300	-1.59630400
				H	-8.61590000	-0.11991100	-2.25698800

C	-3.09452900	4.27340700	0.83184500	H	-1.63820100	-6.32871500	-0.61333800
C	-2.22886100	3.22652600	0.61214700	H	0.47913300	-4.99319000	-0.50358800
C	-0.84100100	3.38297200	0.86842900	N	-1.71469900	-2.49932900	0.13770600
C	-0.36247600	4.63076200	1.38978500	C	2.82286700	-1.89220900	-0.17308900
C	-1.28161300	5.69261600	1.59261300	C	2.07450900	-0.68158400	0.47454700
C	-2.61870400	5.51876300	1.31479900	C	0.64044100	-2.33093900	0.02843500
H	-4.15613700	4.14539100	0.64066900	N	0.66337700	-1.05426900	0.20978700
H	-2.57759400	2.26091800	0.26548900	O	1.82615800	-2.96302700	-0.05109900
C	1.01699100	4.73301500	1.69957400	H	2.91397200	-1.69528000	-1.24843400
H	-0.91293000	6.63950600	1.97909800	H	2.31354400	0.23197600	-0.06949000
H	-3.31826200	6.33397800	1.47628000	C	2.34902700	-0.46596300	1.95445300
C	1.83920100	3.64784300	1.51597000	C	1.67172700	-1.17109500	2.95571800
C	1.27623200	2.46681100	0.97266200	C	3.34926600	0.44152900	2.32568900
H	1.40784600	5.66644900	2.09658000	C	1.99405600	-0.97868800	4.30093700
H	2.89318400	3.67370000	1.76728600	H	0.87260500	-1.85853800	2.69442800
N	-0.00202900	2.33523800	0.63794100	C	3.67613600	0.63036200	3.66723400
C	3.68250400	-0.21268800	1.29744200	H	3.86409600	1.01333900	1.55790800
C	2.72536000	-0.80905700	0.19377400	C	2.99948800	-0.08096300	4.66072500
C	2.08015800	1.25589300	0.77707600	H	1.45298400	-1.52813900	5.06690100
N	1.64105400	0.20297600	0.17927600	H	4.45158000	1.34207600	3.93762300
O	3.32056900	1.20648300	1.30344900	H	3.24793000	0.07104600	5.70771400
H	3.35801100	-0.60332000	2.27006100	C	4.15527900	-2.31586900	0.37651100
H	2.31007200	-1.75141700	0.55663100	C	5.31442800	-1.76588400	-0.18549300
C	3.36485000	-1.05727700	-1.16138100	C	4.27109500	-3.21997500	1.43872900
C	3.45630300	-0.06479300	-2.14128100	C	6.57187100	-2.10316200	0.31590000
C	3.93008700	-2.31380400	-1.41347800	H	5.23208700	-1.06859200	-1.01680400
C	4.10357400	-0.32442300	-3.35185200	C	5.52976600	-3.56625300	1.93023900
H	2.99519300	0.90097700	-1.97855800	H	3.37752900	-3.65592700	1.87229800
C	4.58424900	-2.57113700	-2.61670100	C	6.68226300	-3.00712600	1.37406600
H	3.84934700	-3.09959400	-0.66643800	H	7.46346200	-1.66776400	-0.12691300
C	4.67319700	-1.57499000	-3.59188500	H	5.60941600	-4.27324000	2.75157800
H	4.15437200	0.45412800	-4.10856100	H	7.66112100	-3.27800500	1.76033600
H	5.01303500	-3.55314300	-2.79772400	Ni	-0.94728700	0.11520800	-0.08726000
H	5.17448100	-1.77669900	-4.53482500	C	-1.69498400	2.41344700	0.58330600
C	5.16914000	-0.38761800	1.16166800	C	-2.39594000	1.30995200	0.18572600
C	5.79837800	-1.41488800	1.87478700	C	-0.28922300	1.98421100	0.51861000
C	5.93787000	0.43900700	0.33262800	O	0.64514000	2.02385400	1.27588900
C	7.17201900	-1.62760600	1.74999000	C	-2.10604700	3.74886500	1.06889500
H	5.21136000	-2.05112900	2.53385700	C	-1.26363400	4.48781400	1.92028800
C	7.31204600	0.23409100	0.21750800	C	-3.32742600	4.32320900	0.66965400
H	5.45882500	1.24283100	-0.21588500	C	-1.64140100	5.75187100	2.37093400
C	7.93217100	-0.80136800	0.92120000	H	-0.31308600	4.06300000	2.22600100
H	7.64701500	-2.42989700	2.30791500	C	-3.69947400	5.58705200	1.12240000
H	7.89969400	0.88337500	-0.42569300	H	-3.98019900	3.77992900	-0.00480200
H	9.00317700	-0.95930100	0.82764400	C	-2.86091500	6.30653700	1.97766200
				H	-0.97844400	6.30557300	3.03095200
				H	-4.64542400	6.01463600	0.79971100
				H	-3.15307000	7.29289400	2.32850600
				C	-3.85641100	1.13084100	0.22049100
				C	-4.53081500	1.12098300	1.45895100
				C	-4.61434700	0.93323500	-0.94904200
				C	-5.91025300	0.92722400	1.52200600
				H	-3.95995300	1.27046900	2.37102100
				C	-5.99578000	0.75135500	-0.88276200
				H	-4.11510900	0.91611400	-1.91111900
				C	-6.65152500	0.74484600	0.35116200
				H	-6.40788500	0.92556300	2.48860500
				H	-6.56076000	0.61027700	-1.80070200
				H	-7.72787500	0.60218400	0.39985800
				C	-0.82606700	0.48696400	-2.10341000
TS2-S-exo							
C	-5.29328200	-3.21677900	0.26671700				
C	-4.10409100	-2.52597900	0.31069200				
C	-2.87757500	-3.20440000	0.08290700				
C	-2.89753400	-4.61539600	-0.18710400				
C	-4.14260300	-5.29521800	-0.22460300				
C	-5.31532800	-4.60921100	-0.00261400				
H	-6.22532500	-2.68640600	0.43719600				
H	-4.07413100	-1.46261700	0.51217900				
C	-1.65659800	-5.26238200	-0.40236400				
H	-4.15241700	-6.36264400	-0.43070000				
H	-6.26592700	-5.13433900	-0.03343900				
C	-0.49058700	-4.53740000	-0.34302700				
C	-0.57878500	-3.14955800	-0.06825400				

C	5.96882000	-0.56626900	-0.98788700	H	-2.93899700	-2.13033800	-0.03289100
H	4.18123500	0.62619200	-1.00275200	C	0.57434700	-5.07467400	-0.39432800
C	6.56845900	-1.76595900	-0.59354200	H	-1.43789200	-6.88190400	-0.14540700
H	6.26032700	-3.64497100	0.42360600	H	-3.84226300	-6.33972600	0.10961500
H	6.54099800	0.16805300	-1.55024700	C	1.45186500	-4.02511600	-0.52001100
H	7.60822300	-1.96785700	-0.83614600	C	0.93587500	-2.71021200	-0.45936800
C	4.38481600	3.26794900	1.12489500	H	0.92540600	-6.10285100	-0.42947700
C	3.34211400	2.41342700	0.82909200	H	2.51560900	-4.17364600	-0.66622600
C	2.22317300	2.87517700	0.09632900	N	-0.35241000	-2.40742500	-0.28351000
C	2.17063200	4.25457800	-0.29451700	C	3.60119800	-0.34639800	-1.17414600
C	3.26666400	5.09843200	0.01057100	C	2.43747400	0.60100900	-0.70039200
C	4.35809500	4.61622000	0.70258800	C	1.79772200	-1.54092500	-0.61540900
H	5.23294100	2.89808400	1.69379700	N	1.30949100	-0.34998200	-0.63130300
H	3.34552000	1.38200300	1.16153800	O	3.12880500	-1.67677600	-0.76183300
C	1.00555900	4.73136600	-0.95804100	H	3.59562300	-0.36218200	-2.27093500
H	3.22229400	6.13998000	-0.29817600	H	2.20853400	1.33968500	-1.46933600
H	5.18971600	5.27418700	0.93790900	C	2.64264300	1.33011200	0.61612100
C	-0.05527900	3.88326600	-1.14999800	C	2.49340600	0.69137900	1.85380100
C	0.06709000	2.53786200	-0.73985700	C	3.00859500	2.68095500	0.59276700
H	0.95735500	5.77001800	-1.27326500	C	2.72046800	1.38609000	3.04269700
H	-0.98464400	4.21213800	-1.60208000	H	2.18084500	-0.34827400	1.89470400
N	1.19788000	2.00582200	-0.20877200	C	3.24044700	3.37615400	1.77963200
C	-2.91543400	0.57937300	-1.42932000	H	3.09554400	3.19391300	-0.36099800
C	-2.12667300	-0.32065000	-0.38254200	C	3.09846300	2.72958000	3.00872500
C	-1.01795500	1.59081400	-0.78915100	H	2.59533500	0.87842700	3.99551100
N	-0.88047400	0.43758700	-0.20678300	H	3.51908200	4.42582200	1.74371700
O	-2.19340000	1.85142600	-1.39664700	H	3.27067300	3.27189100	3.93458200
H	-2.74178800	0.16144600	-2.42745200	C	4.99939100	-0.09114400	-0.68344900
H	-1.89339300	-1.27589400	-0.86323800	C	5.84391800	0.71972700	-1.45179700
C	-2.82332100	-0.61362300	0.93555100	C	5.47365500	-0.62071700	0.52241600
C	-2.65190700	0.20070300	2.06053300	C	7.13580300	1.01366800	-1.01489600
C	-3.66882900	-1.72701500	1.02662000	H	5.49010000	1.12229700	-2.39858800
C	-3.32233400	-0.08765100	3.25054400	C	6.76993800	-0.33738000	0.95251100
H	-1.97223000	1.04581200	2.01333500	H	4.83142400	-1.26238500	1.11585100
C	-4.34461200	-2.01228900	2.21262500	C	7.60257800	0.48368200	0.18915700
H	-3.79738600	-2.37601900	0.16319600	H	7.77900500	1.64654700	-1.62013000
C	-4.17298400	-1.19112000	3.32913400	H	7.12913500	-0.75823600	1.88772400
H	-3.17005500	0.54635000	4.11974800	H	8.61114600	0.70426500	0.52792900
H	-4.99649800	-2.88008900	2.26753700	Ni	-0.58410600	-0.09137300	-0.41042500
H	-4.69084600	-1.41674500	4.25743200	C	-2.05302200	1.90539800	-0.53793900
C	-4.38992100	0.80231200	-1.23080300	C	-2.34531100	0.62387700	-0.11121300
C	-5.30140100	0.01951200	-1.94883700	C	-0.65927800	1.70879300	-0.93277000
C	-4.87356100	1.76138600	-0.33220700	O	0.17075100	2.43685400	-1.45825500
C	-6.67542500	0.17797400	-1.76197800	C	-2.81751100	3.16966500	-0.59085300
H	-4.93486800	-0.71569100	-2.66233100	C	-2.37415900	4.21398100	-1.42693500
C	-6.24623700	1.92795500	-0.15377800	C	-3.96746000	3.38855200	0.19271600
H	-4.17405900	2.38256400	0.21738700	C	-3.07040700	5.42015400	-1.49266600
C	-7.15071200	1.13444700	-0.86374900	H	-1.47252000	4.06919800	-2.01153000
H	-7.37162900	-0.43680100	-2.32591000	C	-4.65790400	4.59707600	0.12540300
H	-6.61054800	2.67837600	0.54253000	H	-4.31514400	2.61166900	0.86417500
H	-8.21995200	1.26571700	-0.72164700	C	-4.21730000	5.61779400	-0.72109800
				H	-2.71225400	6.21068500	-2.14786400
				H	-5.54219200	4.74388000	0.74099500
				H	-4.75851900	6.55923700	-0.77249700
				C	-3.64507100	0.14163400	0.38214200
				C	-3.79198000	-0.29263700	1.71433800
				C	-4.76264600	0.04632400	-0.47155700
				C	-5.01257700	-0.78187200	2.17969500
				H	-2.93540300	-0.23771800	2.38142000
				C	-5.97573600	-0.46408100	-0.00947100
CP9							
C	-3.53218800	-4.19161600	0.05224600				
C	-2.62233800	-3.16350900	-0.05154100				
C	-1.23927900	-3.44338600	-0.18850300				
C	-0.80777100	-4.81450600	-0.23029600				
C	-1.77294300	-5.84811200	-0.11562800				
C	-3.10826400	-5.54346700	0.02408200				
H	-4.58737300	-3.95839800	0.15882700				

H	-4.66784900	0.37588000	-1.50260500	C	-0.88522800	4.58098700	-0.22020500
C	-6.10999900	-0.87660700	1.31938100	C	1.38026900	5.63609200	-1.42573600
H	-5.10457700	-1.09765200	3.21616500	H	1.57128900	3.74294200	-2.40758300
H	-6.82286600	-0.53019300	-0.68805900	C	-0.49293300	5.88854900	0.05205900
H	-7.05852400	-1.26567200	1.68023600	H	-1.77547500	4.15729300	0.23234300
CP10				C	0.64731900	6.44394700	-0.54604500
C	-3.23327300	-4.36482800	1.68896500	H	2.26286300	6.04417600	-1.91532500
C	-2.25844000	-3.46468100	1.31016900	H	-1.08224400	6.49366100	0.73921900
C	-0.99275400	-3.91386800	0.85961400	C	1.05004900	7.87637500	-0.28125300
C	-0.72707100	-5.32541200	0.85827300	H	0.54320400	8.56921700	-0.96737800
C	-1.75505000	-6.22345200	1.23765500	H	0.78955100	8.18549700	0.73751900
C	-2.98892200	-5.75538400	1.63918700	H	2.12792600	8.02279300	-0.41349800
H	-4.19713900	-4.00085200	2.03388100	C	-4.21849100	0.06598800	0.01760900
H	-2.43379900	-2.39944000	1.36140200	C	-3.20655900	0.48835600	0.84923000
C	0.57992500	-5.76756900	0.51447600	C	-2.91786400	-0.41504100	-0.18676000
H	-1.54826000	-7.29064900	1.21525500	O	-2.15561900	-1.18372600	-0.80859300
H	-3.76889900	-6.45279900	1.93134200	C	-5.59796800	0.12742600	-0.40599900
C	1.54726200	-4.83946100	0.21593900	C	-6.02965300	-0.72290200	-1.44141300
C	1.19562100	-3.47342500	0.21032300	C	-6.51300300	1.01901200	0.18329100
H	0.80144900	-6.83121400	0.50930000	C	-7.35399300	-0.68715500	-1.86913600
H	2.56394200	-5.12438300	-0.03235300	H	-5.31675800	-1.40142300	-1.90074600
N	-0.03750600	-2.99374300	0.49433800	C	-7.83468600	1.05250200	-0.25155600
C	4.02126000	-1.41273500	-0.74193000	H	-6.17639900	1.69453400	0.96358400
C	2.86813700	-0.36240800	-0.56771900	C	-8.25783600	0.19815900	-1.27474200
C	2.12916300	-2.42997900	-0.15393500	H	-7.68152100	-1.34533800	-2.66873400
N	1.69949300	-1.26485200	-0.53044100	H	-8.53584300	1.74674400	0.20290100
O	3.46240500	-2.60771600	-0.09813400	H	-9.29050700	0.22644300	-1.61147800
H	4.08270800	-1.64968000	-1.81101700	C	-2.77836500	1.26342700	1.98953900
H	2.81982300	0.25901800	-1.45927900	C	-1.40350900	1.46774200	2.20752700
C	2.95581500	0.53162800	0.65812200	C	-3.71290600	1.79349300	2.89742600
C	2.56850200	0.09534000	1.93220000	C	-0.97687400	2.19995000	3.31162500
C	3.47301500	1.82630100	0.51935800	H	-0.68826100	1.07663600	1.49165600
C	2.71575300	0.92879500	3.04329700	C	-3.27868500	2.51576500	4.00560000
H	2.13798400	-0.89311500	2.06125800	H	-4.77336400	1.62018300	2.73967300
C	3.61827000	2.66159000	1.62631600	C	-1.91127900	2.72246500	4.21121800
H	3.75899900	2.18620800	-0.46563800	H	0.08531000	2.36616700	3.46265400
C	3.24431100	2.21292500	2.89477500	H	-4.00363600	2.92015100	4.70651200
H	2.41525700	0.57187500	4.02512400	H	-1.57441600	3.29368500	5.07224700
H	4.01340200	3.66503000	1.49568700	H	-1.28479600	0.05492000	-2.44605700
H	3.35898800	2.86135900	3.75942200	C	0.48782800	-0.59577600	-3.40276400
C	5.38883400	-1.09567200	-0.20695900	F	0.09476900	-0.12704400	-4.61508400
C	6.32941500	-0.51440600	-1.06656200	F	1.84993500	-0.46178800	-3.38301800
C	5.74359400	-1.34602600	1.12429600	F	0.24413900	-1.93568700	-3.42592500
C	7.59908000	-0.17053300	-0.60135500	TS6			
H	6.06850800	-0.33410700	-2.10729100	C	2.21058800	5.14764400	1.07987400
C	7.01718200	-1.01367600	1.58553200	C	1.45854300	4.04560100	0.73702300
H	5.02559000	-1.81029100	1.79144800	C	0.04711600	4.15290300	0.63159300
C	7.94630000	-0.42141300	0.72720000	C	-0.57867500	5.42234000	0.88256500
H	8.31825300	0.28089400	-1.27932100	C	0.22952500	6.53293000	1.23586200
H	7.28422800	-1.21820400	2.61884100	C	1.59655600	6.39833700	1.33528000
H	8.93744400	-0.16328100	1.09023300	H	3.29108700	5.05920400	1.15047300
Ni	-0.21275100	-1.14618800	-0.66896000	H	1.90982900	3.08861800	0.50573400
C	-0.21015700	0.10450000	-2.27298300	C	-1.98985500	5.50795600	0.77482700
C	0.24113000	1.42156100	-1.94397500	H	-0.25000200	7.49054600	1.42276800
H	1.26863800	1.69884700	-2.14710200	H	2.20948900	7.25392200	1.60453800
C	-0.63359500	2.36093000	-1.33733100	C	-2.71341300	4.38990300	0.43616200
O	-1.81203600	2.07294800	-0.98370700	C	-2.01397800	3.18281600	0.21293800
C	-0.14481600	3.76573300	-1.09086800	H	-2.48405100	6.45820200	0.95931200
C	0.99279200	4.32435700	-1.69582800	H	-3.79269300	4.40771200	0.33462800

N	-0.68701800	3.04208900	0.31354400	H	6.25174700	-0.25888800	1.40638300
C	-4.36462500	0.56815500	-0.68768900	C	7.92529000	1.26503800	-1.13515400
C	-3.00513200	-0.20952500	-0.63232600	H	7.00008000	2.18291900	-2.85517400
C	-2.69670000	1.95001200	-0.16102800	H	8.55910400	0.26577600	0.66995500
N	-2.04999400	0.92448100	-0.61256700	H	8.93772400	1.48977000	-1.45982300
O	-4.02791700	1.83185100	-0.01785300	C	2.80093900	-0.70952300	2.27661500
H	-4.55045400	0.82853400	-1.73693200	C	1.54297400	-1.29127900	2.51773000
H	-2.87777700	-0.77274400	-1.55262000	C	3.78534900	-0.76066400	3.28158200
C	-2.82239900	-1.14103400	0.55362800	C	1.28623500	-1.92446600	3.73188200
C	-2.50251100	-0.67321700	1.83487800	H	0.78543700	-1.26115000	1.74051800
C	-3.03041200	-2.51428100	0.37087600	C	3.51708000	-1.38061100	4.49868500
C	-2.41680600	-1.55761700	2.91198100	H	4.75181800	-0.29707200	3.10665900
H	-2.30949300	0.38294500	1.99773400	C	2.26866400	-1.96889900	4.72438400
C	-2.94051100	-3.40043200	1.44385400	H	0.31730000	-2.38553600	3.89779600
H	-3.26409900	-2.89283400	-0.62110300	H	4.28153300	-1.41060100	5.27046900
C	-2.63872000	-2.92308200	2.72063000	H	2.06419900	-2.46154100	5.67132600
H	-2.17301200	-1.17675800	3.90020800	H	1.08901800	0.41671700	-2.68062100
H	-3.09897800	-4.46264300	1.28065000	C	-0.83527700	0.38577900	-3.52266400
H	-2.57103800	-3.61135600	3.55888300	F	-0.34537600	0.05774400	-4.74456900
C	-5.59294900	-0.05709100	-0.08981800	F	-2.06182900	-0.22145600	-3.45026200
C	-6.42810800	-0.81852000	-0.91718200	F	-1.08414000	1.72365500	-3.56600000
C	-5.91444200	0.07950700	1.26601400				
C	-7.55737900	-1.45044700	-0.39579800	CP11			
H	-6.19575500	-0.91480900	-1.97566300	Ni	0.22465900	-0.66567000	-0.28316800
C	-7.05047900	-0.54247500	1.78384500	C	-0.04084300	0.74088600	-1.60535000
H	-5.28123400	0.68062800	1.90936600	C	-0.13522800	1.99860400	-0.84217800
C	-7.87164800	-1.31241300	0.95729200	H	0.75483200	2.61545500	-0.81185300
H	-8.19568600	-2.03939300	-1.04862700	C	-1.20964000	2.41485700	-0.12756000
H	-7.29401500	-0.42516100	2.83628900	O	-2.40478000	1.76224800	-0.06827900
H	-8.75538300	-1.79636200	1.36405500	C	-1.24063300	3.68454800	0.63719900
Ni	-0.15073600	1.10305000	-0.80678900	C	-0.07428700	4.40575600	0.95690400
C	0.10964700	0.00996100	-2.41823100	C	-2.46872900	4.21799600	1.06555700
C	0.18980400	-1.39294800	-2.06704000	C	-0.14155800	5.60862000	1.65222500
H	-0.69400600	-2.01423900	-2.15854000	H	0.90074300	4.01744900	0.67971200
C	1.36365900	-1.92622500	-1.54968600	C	-2.52657600	5.42481100	1.76070900
O	2.43514300	-1.22363600	-1.33036300	H	-3.38107800	3.67898100	0.83904300
C	1.45319100	-3.38629500	-1.22113800	C	-1.36819700	6.14657000	2.06894400
C	0.57097100	-4.35101500	-1.73704300	H	0.78051500	6.13885900	1.88370400
C	2.48417600	-3.83482100	-0.37952000	H	-3.49544600	5.81378700	2.06821000
C	0.70045900	-5.69725600	-1.40243400	C	-1.42849300	7.43981400	2.84802900
H	-0.21157000	-4.05354900	-2.42867400	H	-0.69897100	8.16863200	2.47571200
C	2.60808100	-5.18066400	-0.04448200	H	-2.42192200	7.89725800	2.78757600
H	3.18619400	-3.10183200	0.00201100	H	-1.20811300	7.27986400	3.91274900
C	1.71963900	-6.14046100	-0.54847700	C	-3.50709700	-0.10014800	-1.31178500
H	0.00380700	-6.42105700	-1.82200600	C	-3.94141900	-0.11973900	-0.05745300
H	3.41193300	-5.49470100	0.61936800	C	-2.54312800	0.31716900	-0.23505000
C	1.87896000	-7.60577600	-0.21449600	O	-1.52434400	-0.41626900	0.24155100
H	2.60258600	-8.09448600	-0.88177700	C	-3.80321400	-0.37142200	-2.70838400
H	2.24139500	-7.74756200	0.81026400	C	-3.12408000	0.29247600	-3.74686900
H	0.93103000	-8.14623200	-0.31472700	C	-4.79005700	-1.31883400	-3.04777600
C	3.95482100	0.40749200	0.10532200	C	-3.42944100	0.01996800	-5.07965000
C	3.06093400	-0.07932500	1.00057800	H	-2.36416100	1.02889200	-3.51024200
C	2.56745100	0.46649900	-0.22793000	C	-5.08660500	-1.59262400	-4.38031100
O	1.74149900	1.30949300	-0.71743200	H	-5.30532800	-1.85260200	-2.25422100
C	5.31325600	0.68381700	-0.29586600	C	-4.40876600	-0.92169700	-5.40262400
C	5.53803000	1.36739300	-1.50616200	H	-2.89654100	0.54521100	-5.86769300
C	6.41712300	0.28895400	0.48346400	H	-5.84618900	-2.33138400	-4.62323100
C	6.83598200	1.65639500	-1.91903800	H	-4.64149400	-1.13379700	-6.44280100
H	4.68406600	1.65830100	-2.11047600	C	-4.97667500	-0.35056100	0.92639700
C	7.71262200	0.57828900	0.06438500	C	-4.68964500	-0.15054600	2.29075800

C	-6.27194200	-0.76545300	0.56074700	TS7			
C	-5.66668300	-0.37215300	3.25984700	C	-3.62989300	-4.18685100	-1.59015100
H	-3.69582600	0.18530200	2.57249000	C	-2.59457300	-3.28000100	-1.53080700
C	-7.24597300	-0.98154500	1.53239600	C	-1.33832200	-3.66825000	-0.99570800
H	-6.50890400	-0.90364000	-0.49005300	C	-1.17258500	-5.01694400	-0.52233900
C	-6.94686300	-0.79000400	2.88497200	C	-2.26419200	-5.91915700	-0.59790300
H	-5.43162900	-0.21186700	4.30891000	C	-3.47038500	-5.51350900	-1.12216800
H	-8.24240000	-1.29886200	1.23569800	H	-4.58766900	-3.87629300	-1.99767000
H	-7.70875600	-0.96039300	3.64103200	H	-2.71157700	-2.25848900	-1.86721800
H	-1.00063100	0.39727100	-1.98702800	C	0.08713300	-5.40122600	0.00021500
C	0.82691600	0.84287100	-2.82674600	H	-2.12699000	-6.93479500	-0.23560700
F	1.25288300	-0.36483500	-3.28662700	H	-4.30312200	-6.20884500	-1.17672900
F	1.95197600	1.60118300	-2.65542100	C	1.11573700	-4.49206700	0.02765400
F	0.16471400	1.42142200	-3.86875700	C	0.86778600	-3.19131900	-0.46217700
C	-2.75375200	-3.64653900	2.49919200	H	0.22776800	-6.41532000	0.36483400
C	-1.83256500	-2.87071600	1.83149300	H	2.10120100	-4.74037600	0.40392800
C	-0.53118200	-3.37672200	1.57676700	N	-0.30442400	-2.76674800	-0.94370700
C	-0.19318000	-4.69984000	2.03120100	C	3.99752100	-1.35246200	-0.46754700
C	-1.17287900	-5.47016300	2.70939400	C	2.96084600	-0.22327500	-0.84428200
C	-2.42787800	-4.95394600	2.93907400	C	1.91935500	-2.18230900	-0.51458200
H	-3.74543100	-3.24664900	2.69122900	N	1.72037200	-1.01352100	-1.02929700
H	-2.05314600	-1.87287500	1.46863900	O	3.13750300	-2.45917000	-0.03454700
C	1.11730500	-5.17922300	1.79518800	H	4.47148700	-1.69751200	-1.39373600
H	-0.91031900	-6.46993500	3.04613700	H	3.25362500	0.19435000	-1.80448600
H	-3.17291100	-5.54789200	3.46125000	C	2.79883500	0.91295900	0.14652300
C	2.02877400	-4.37491900	1.15553600	C	2.00006700	0.80133700	1.29079700
C	1.60815700	-3.09074200	0.74302800	C	3.50292800	2.10298700	-0.07903800
H	1.39048400	-6.17707600	2.12870100	C	1.91913800	1.85837400	2.19900400
H	3.04604700	-4.69250000	0.95843100	H	1.41730500	-0.09670200	1.47124300
N	0.38526800	-2.59167000	0.92631800	C	3.42482600	3.15793900	0.82975000
C	4.42192700	-1.41614900	-0.82431600	H	4.11066000	2.20600600	-0.97470500
C	3.32615000	-0.28833400	-0.81927500	C	2.63281600	3.03645600	1.97314000
C	2.51956900	-2.16602900	0.07721100	H	1.28691500	1.75467300	3.07544200
N	2.11459300	-1.05482000	-0.44208500	H	3.97427500	4.07606700	0.63962300
O	3.83271500	-2.44021500	0.04212300	H	2.56342300	3.86036200	2.67826600
H	4.44504700	-1.85624600	-1.82840100	C	5.05680200	-1.06358000	0.55971500
H	3.21826300	0.08251500	-1.83395900	C	6.32834100	-0.67031200	0.12570300
C	3.56224200	0.89062900	0.10996100	C	4.80278000	-1.16323600	1.93326000
C	3.17432900	0.87314700	1.45551200	C	7.32899900	-0.36294700	1.04831700
C	4.20113300	2.03102800	-0.39442900	H	6.53879100	-0.60698400	-0.93987700
C	3.43064500	1.96913800	2.28161000	C	5.80730400	-0.86882400	2.85457300
H	2.64559400	0.01507900	1.85909900	H	3.82452200	-1.47925800	2.27931800
C	4.46337900	3.12424000	0.43084600	C	7.07011300	-0.46362300	2.41601400
H	4.48683000	2.06632100	-1.44228500	H	8.31091000	-0.05701900	0.69798800
C	4.07899400	3.09587400	1.77341200	H	5.60121200	-0.95363300	3.91795500
H	3.11311300	1.94437700	3.32038900	H	7.84957800	-0.23291900	3.13703000
H	4.95809000	4.00125100	0.02238900	Ni	-0.08925200	-0.67463100	-1.57596600
H	4.27481200	3.94982400	2.41616200	C	0.10753300	0.86240000	-2.78252000
C	5.82080900	-1.07779300	-0.38987000	C	-0.08372000	2.11294300	-2.02832900
C	6.77191200	-0.75889200	-1.36656900	H	0.74829200	2.81033500	-2.03861200
C	6.19185900	-1.05146900	0.96010400	C	-1.12612100	2.52499300	-1.26900500
C	8.07053800	-0.40141400	-1.00191200	O	-2.23103500	1.76284400	-0.89438200
H	6.49658000	-0.79297200	-2.41857000	C	-1.21785200	3.87232700	-0.66757600
C	7.49340300	-0.70709600	1.32334500	C	-0.57452400	4.97844500	-1.25122600
H	5.46491800	-1.30962600	1.72284100	C	-1.96176600	4.09143500	0.50476900
C	8.43437800	-0.37654500	0.34526500	C	-0.64343800	6.23874800	-0.66536600
H	8.79813700	-0.15449200	-1.77007000	H	-0.03210800	4.85486700	-2.18381000
H	7.77242600	-0.69512100	2.37338500	C	-2.03176800	5.35817100	1.07968600
H	9.44713200	-0.10672200	0.63179900	H	-2.48019300	3.25858900	0.96650500
				C	-1.37486300	6.45662900	0.51061600

H	7.29822600	0.15177700	-0.13714800	F	2.78166300	-1.46029700	2.01431300
H	7.50769800	-2.25041700	-0.71298000				
C	3.76063700	2.15951300	-0.23435100	CP13			
C	2.65409100	1.32273500	-0.47323400	C	5.83592000	-0.33592000	-1.53134900
H	5.88198800	2.18286300	0.09137100	C	4.53628800	-0.16547700	-1.11079900
H	3.60441800	3.22760200	-0.13583200	C	3.83692400	-1.24010900	-0.50653800
N	2.72393300	-0.01667100	-0.58376000	C	4.49704000	-2.50700600	-0.35294900
C	-0.32816000	3.26072600	-1.21022700	C	5.84257400	-2.63952600	-0.78346400
C	-0.89886000	1.79135800	-1.05006900	C	6.49885600	-1.57634400	-1.36082800
C	1.30474300	1.83499700	-0.68502200	H	6.36218100	0.49292900	-1.99546300
N	0.35035200	1.01472700	-0.95463000	H	4.01898300	0.77725700	-1.22518200
O	1.03113400	3.14729500	-0.65279700	C	3.76911100	-3.58340800	0.21086000
H	-0.18611800	3.45237100	-2.28032700	H	6.33968000	-3.59772900	-0.65612500
H	-1.41300300	1.51475700	-1.97411000	H	7.52775800	-1.68596600	-1.69128900
C	-1.84895400	1.56464200	0.11342900	C	2.45201700	-3.40339400	0.56197100
C	-1.40557000	1.17423100	1.38096400	C	1.87717400	-2.13043800	0.37189300
C	-3.21666600	1.78823000	-0.08886000	H	4.25572600	-4.54568500	0.34546400
C	-2.31526200	1.01506000	2.42768200	H	1.84713100	-4.20295000	0.97444300
H	-0.35868000	0.94937000	1.55048700	N	2.53675900	-1.06293000	-0.10762000
C	-4.12508000	1.63692500	0.95775400	C	-1.61833800	-2.10010400	1.38960400
H	-3.57483700	2.07998600	-1.07375500	C	-1.46634800	-0.73901100	0.60027600
C	-3.67528900	1.24975200	2.22165600	C	0.46959100	-1.84808900	0.63882700
H	-1.95697700	0.68976500	3.40034500	N	-0.00481100	-0.66948600	0.42175300
H	-5.18358900	1.80952700	0.78273800	O	-0.37284900	-2.80631500	1.06359300
H	-4.38230500	1.11870400	3.03636500	H	-1.55679100	-1.87514500	2.46116600
C	-1.06255600	4.41409900	-0.58795700	H	-1.79146400	0.08247800	1.24313100
C	-1.87036800	5.21948200	-1.39943700	C	-2.20635800	-0.63718700	-0.72347000
C	-0.97226600	4.69637400	0.78127600	C	-1.66563800	-1.13217400	-1.91663600
C	-2.59278600	6.28094200	-0.85217700	C	-3.47813900	-0.05194600	-0.74817100
H	-1.93317300	5.01793400	-2.46680800	C	-2.38898900	-1.05369600	-3.10775600
C	-1.68387800	5.76436000	1.32539100	H	-0.66723100	-1.55883300	-1.92486700
H	-0.34233500	4.08349300	1.41697800	C	-4.20358600	0.02291900	-1.93667600
C	-2.49905200	6.55618900	0.51251800	H	-3.89627600	0.36450700	0.16438000
H	-3.21741000	6.89663100	-1.49346200	C	-3.66151700	-0.48062000	-3.12046300
H	-1.60399400	5.97680600	2.38789100	H	-1.95208700	-1.43298900	-4.02759400
H	-3.05409800	7.38629300	0.94087300	H	-5.18592800	0.48702400	-1.93920300
Ni	0.91523200	-0.86318400	-0.55281500	H	-4.22169300	-0.41534400	-4.04931600
C	1.24635000	-2.49086700	0.49293600	C	-2.81670800	-2.96801900	1.12536900
C	-0.02629600	-3.28415000	0.41542400	C	-3.93741100	-2.84166800	1.95519300
H	-0.11047000	-4.26684200	0.86956900	C	-2.85245600	-3.87945500	0.06308200
C	-1.03193900	-2.66744200	-0.24272500	C	-5.08477500	-3.59949200	1.71826200
O	-0.77615300	-1.46360400	-0.78504200	H	-3.91175600	-2.14859100	2.79351000
C	-2.40360300	-3.18658200	-0.45335200	C	-3.99471900	-4.64603400	-0.16563700
C	-2.88679900	-4.32473300	0.21688500	H	-1.98318400	-3.99357800	-0.57554600
C	-3.26825800	-2.53866700	-1.34748700	C	-5.11479400	-4.50536900	0.65688800
C	-4.17401300	-4.79836300	-0.01267000	H	-5.94784700	-3.49031000	2.36917200
H	-2.25352000	-4.83494300	0.93650900	H	-4.01008500	-5.35412200	-0.98963400
C	-4.55911200	-3.01727800	-1.57162900	H	-6.00362600	-5.10327500	0.47504700
H	-2.91229700	-1.65296200	-1.86166500	Ni	1.43722500	0.62325500	0.08875200
C	-5.03693700	-4.15657100	-0.91510900	C	2.36368500	2.31382200	0.13760900
H	-4.52136100	-5.67947200	0.52398100	H	2.70773900	2.69585800	-0.82415300
H	-5.20861200	-2.49476200	-2.27174200	C	0.96032300	2.47732600	0.43462100
C	-6.42737800	-4.69013100	-1.17189200	H	0.66842200	2.61905600	1.47198300
H	-6.94760200	-4.92769300	-0.23582700	C	3.34513000	2.53866800	1.23300800
H	-7.03854800	-3.96548100	-1.72046500	F	2.95034600	1.98613500	2.41466900
H	-6.40114700	-5.61392900	-1.76592500	F	4.56855400	2.01097100	0.94924700
C	1.56359600	-2.07245900	1.90728500	F	3.56870400	3.85676600	1.49599100
H	2.11176900	-3.08695500	0.17813400	C	0.04153300	2.95782400	-0.61041600
F	0.65964200	-1.20041000	2.43416700	O	0.40273700	3.12866300	-1.77834700
F	1.61080000	-3.12373600	2.77326800	C	-1.39992100	3.23791900	-0.24602100

C	-1.93418200	3.08821400	1.04224900	Ni	-1.37955200	0.30743200	-0.39104800
C	-2.25144100	3.69488000	-1.26356500	C	-2.42191200	1.81550100	0.18130800
C	-3.27381800	3.38547000	1.29997300	C	-1.19555400	2.38001200	0.78132600
H	-1.31049100	2.74113900	1.85988100	H	-1.18388700	2.76487400	1.79616700
C	-3.58463600	3.99222800	-1.00340100	C	-0.10050600	2.45643600	-0.08370100
H	-1.83391200	3.80741700	-2.25863200	O	-0.12838900	1.69578600	-1.14448200
C	-4.12178100	3.84744600	0.28526800	C	1.05627900	3.35950100	0.10627900
H	-3.66358000	3.26714200	2.30920800	C	1.06504700	4.37542500	1.07839000
H	-4.22344700	4.34516400	-1.81073400	C	2.17696900	3.23038100	-0.72785400
C	-5.56059000	4.20844300	0.57218300	C	2.16403200	5.21585300	1.21903200
H	-5.92247200	3.72601500	1.48640300	H	0.19427800	4.52328400	1.70969400
H	-5.67839100	5.29220800	0.70657600	C	3.26917200	4.08342600	-0.59049800
H	-6.22094700	3.91443100	-0.25170700	H	2.17063400	2.45301800	-1.48315800
				C	3.28810900	5.08560700	0.38816200
				H	2.14633800	5.99847800	1.97482300
				H	4.12503300	3.96995400	-1.25283200
				C	4.48474400	5.99172800	0.55801200
				H		5.11585000	5.66730400
TS9				1.39689600			
C	-6.09450500	-0.43737400	0.30301800	H	5.11263300	5.99911500	-0.33917400
C	-4.76167700	-0.36435800	-0.04884300	H	4.18079200	7.02403500	0.76653400
C	-3.85959100	-1.39321900	0.31504000	C	-3.06661300	2.61302200	-0.94505100
C	-4.38912000	-2.56103100	0.96711400	H	-3.19706100	1.59046800	0.91595200
C	-5.75782500	-2.59175800	1.33469900	F	-4.20842600	3.22686000	-0.51100100
C	-6.59566600	-1.54270900	1.02490600	F	-2.29418000	3.57516300	-1.47540200
H	-6.76597500	0.36279100	0.00558000	F	-3.46854400	1.82591200	-1.99302200
H	-4.40010800	0.44994000	-0.65530300				
C	-3.53578400	-3.67392600	1.17851400				
H	-6.13590900	-3.47204500	1.84836700				
H	-7.64448800	-1.57845500	1.30513800				
C	-2.23886500	-3.61530800	0.73349800				
C	-1.76970400	-2.41271300	0.17135100	CP14			
H	-3.92691000	-4.56659900	1.65850400	Ni	1.15592100	0.44323900	-0.22192400
H	-1.55627600	-4.45313000	0.82163200	C	2.46683000	1.85599800	0.14434000
N	-2.51595500	-1.29306600	0.00039200	C	1.68274500	3.13897500	0.14014600
C	1.57256100	-2.78820700	-1.17651700	H	2.16765600	4.10248400	0.26647900
C	1.45651200	-1.22201300	-0.96158300	C	0.35082500	2.98242000	-0.01013400
C	-0.39973700	-2.26074700	-0.27690100	O	-0.11653100	1.73291900	-0.19135300
N	0.04398600	-1.09204300	-0.58239100	C	-0.67475500	4.05096800	-0.01457900
O	0.43095700	-3.31096000	-0.41408200	C	-0.41180900	5.34286200	0.47480800
H	1.34291400	-2.99711600	-2.22804600	C	-1.95894000	3.78784200	-0.51430800
H	1.61595600	-0.72112300	-1.91982700	C	-1.38998000	6.33112900	0.44748000
C	2.40410800	-0.61974300	0.06280700	H	0.56316400	5.56759300	0.89721200
C	2.05365900	-0.47746600	1.40978100	C	-2.93605900	4.78344500	-0.53653800
C	3.68577300	-0.23017900	-0.34766700	H	-2.17793100	2.79385900	-0.88978900
C	2.96977400	0.03919100	2.32842900	C	-2.67269000	6.07298100	-0.06170700
H	1.05527100	-0.74786200	1.73895700	H	-1.15897800	7.32090000	0.83739800
C	4.60374800	0.27915400	0.56939000	H	-3.92323000	4.55397700	-0.93387000
H	3.96765900	-0.32886100	-1.39355600	C	-3.72478100	7.15739800	-0.09815500
C	4.24741400	0.41504300	1.91272400	H	-3.83426400	7.64689500	0.87773500
H	2.67945400	0.15375100	3.36941900	H	-4.70309700	6.75525300	-0.38204300
H	5.59304700	0.57799700	0.23357700	H	-3.46891000	7.94296200	-0.82191000
H	4.95794300	0.82029200	2.62801300	C	3.07803900	1.58731600	1.49696300
C	2.83971000	-3.49820500	-0.79043700	H	3.31109200	1.89483300	-0.55594200
C	3.77469800	-3.80674500	-1.78573800	F	2.15399800	1.32457800	2.46062400
C	3.11678300	-3.84684700	0.53764400	F	3.81801100	2.63195000	1.96494100
C	4.97659000	-4.43746000	-1.46071900	F	3.92961700	0.51678300	1.48869000
H	3.55981300	-3.55650800	-2.82257600	C	5.46019500	-0.59111900	-2.07930700
C	4.31201800	-4.48748500	0.86076300	C	4.17759500	-0.41038400	-1.61174400
H	2.39258800	-3.62356500	1.31383100	C	3.57911000	-1.38246600	-0.77063800
C	5.24696900	-4.78037700	-0.13535900	C	4.31173900	-2.57962500	-0.46432600
H	5.69317700	-4.67031600	-2.24356100	C	5.64196700	-2.71681900	-0.93955000
H	4.51455000	-4.75769700	1.89353600	C	6.20890400	-1.73974900	-1.72516700
H	6.17805900	-5.27883000	0.12016700	H	5.90187500	0.15551500	-2.73271700

H	3.59203600	0.45289400	-1.89702300	O	2.69555900	-2.61083600	-0.77834800
C	3.66522800	-3.59864600	0.27606500	H	3.37146700	-1.35906900	-2.25201300
H	6.19512800	-3.61718900	-0.68560800	H	2.83285400	0.57439900	-1.15536700
H	7.22461300	-1.85506700	-2.09186700	C	3.43942300	0.18815600	0.85660400
C	2.34393900	-3.44915700	0.62683200	C	3.70927700	-0.70520000	1.90219800
C	1.69944700	-2.24240600	0.29749000	C	3.75815800	1.54075500	1.02775700
H	4.21121500	-4.50285300	0.53082400	C	4.28640900	-0.25655700	3.08810200
H	1.78921900	-4.22067800	1.14859300	H	3.45977100	-1.75632700	1.79664200
N	2.30053700	-1.20133600	-0.30859400	C	4.33199400	1.99418900	2.21770100
C	-1.78138900	-2.15516800	1.39930900	H	3.55221200	2.24680000	0.22760000
C	-1.67371100	-0.91084900	0.41613400	C	4.59998200	1.09540700	3.24989700
C	0.27895700	-2.00150400	0.53715700	H	4.48750600	-0.96235800	3.88949600
N	-0.24389700	-0.91542500	0.09167600	H	4.56763900	3.04864500	2.33376200
O	-0.50893300	-2.87201900	1.18304400	H	5.04785300	1.44410200	4.17672300
H	-1.72846400	-1.78101700	2.42691600	C	4.99590100	-1.75637600	-0.92007300
H	-1.88917700	0.00476400	0.97139600	C	5.94133400	-0.85817900	-1.43426700
C	-2.54840600	-0.93395800	-0.82458300	C	5.43690600	-2.88290700	-0.21916900
C	-2.12965200	-1.53344000	-2.01787300	C	7.30359000	-1.07436300	-1.23472000
C	-3.81807300	-0.34531100	-0.77214400	H	5.61008600	0.01377100	-1.99377000
C	-2.96756700	-1.55059900	-3.13420100	C	6.80270500	-3.10155000	-0.02525800
H	-1.13623000	-1.96729100	-2.08413600	H	4.71180300	-3.59136500	0.16644400
C	-4.65920200	-0.36681300	-1.88450300	C	7.73912300	-2.19836400	-0.52828000
H	-4.14773600	0.13975500	0.14361500	H	8.02511200	-0.76359800	-1.63536200
C	-4.23568800	-0.97099100	-3.06994100	H	7.13268200	-3.98206800	0.51959700
H	-2.62506200	-2.01161800	-4.05685000	H	8.80122300	-2.36990900	-0.37627400
H	-5.64009500	0.09729300	-1.82796000	Ni	-0.53065100	-0.11289200	-0.23472200
H	-4.88608400	-0.98137700	-3.94035600	C	-0.88723200	0.25955600	-2.23053400
C	-2.94724300	-3.09483100	1.26489400	H	-0.11231400	-0.20292300	-2.83688800
C	-4.04544000	-2.93593000	2.11840700	C	-0.56067600	1.46152800	-1.57756100
C	-2.97448700	-4.10835600	0.29885300	H	-1.34518500	2.13027800	-1.24154600
C	-5.16241600	-3.76403400	1.99968000	C	-2.25263300	0.00957900	-2.76772300
H	-4.02587500	-2.16257400	2.88329500	F	-3.24923600	0.46958400	-1.96390600
C	-4.08504800	-4.94400200	0.18864200	F	-2.43334000	0.61478700	-3.97145700
H	-2.12209600	-4.24909400	-0.35751800	F	-2.48741300	-1.31108300	-2.97755700
C	-5.18357800	-4.77150000	1.03427800	C	0.78002900	2.06109700	-1.83919600
H	-6.00810900	-3.62861000	2.66815000	O	1.58700400	1.48785900	-2.58008800
H	-4.09319900	-5.73079100	-0.56069900	C	1.14097300	3.38573200	-1.24810100
H	-6.04829700	-5.42325300	0.94468300	C	0.40808700	4.00208900	-0.22309700
				C	2.28584000	4.03583500	-1.74536500
				C	0.82159000	5.23195100	0.29035700
				H	-0.47622000	3.52714300	0.18839200
				C	2.68369400	5.26394000	-1.23255200
				H	2.84700400	3.55632000	-2.54091800
				C	1.95638700	5.88641800	-0.20345600
				H	0.24691400	5.69056100	1.09175200
				H	3.56879300	5.75374800	-1.63339900
				C	2.37724300	7.23395600	0.33253600
				H		3.46663700	7.30511600
					0.42987800		
				H	2.06104900	8.04251700	-0.34030100
				H	1.93342900	7.43214500	1.31345000
				C	-0.66629200	0.47934800	1.69469500
				H	-0.20410500	1.45566700	1.81999400
				C	-1.97245400	0.39774600	1.15513400
				H	-2.50621100	-0.52184600	1.36369700
				C	-0.28664900	-0.48538100	2.77041200
				F	-0.75272500	-1.74539800	2.54792600
				F	1.04725000	-0.58526700	2.94361000
				F	-0.79637700	-0.10929000	3.97699300
				C	-2.82124200	1.58045100	0.88649200
CP15							
C	-4.40281500	-3.18663100	-0.19009000				
C	-3.25620100	-2.43104900	-0.29100100				
C	-1.97966200	-3.04990300	-0.24973100				
C	-1.91631600	-4.48119900	-0.15059500				
C	-3.11800000	-5.22829200	-0.04113100				
C	-4.33884300	-4.59429700	-0.05107500				
H	-5.36880000	-2.69147400	-0.22682700				
H	-3.31557500	-1.36309400	-0.43957700				
C	-0.64449000	-5.10152900	-0.19230500				
H	-3.05260900	-6.31015000	0.04179100				
H	-5.25539800	-5.17140300	0.03055300				
C	0.48013000	-4.32801100	-0.32940300				
C	0.32948200	-2.92235400	-0.37313800				
H	-0.57443500	-6.18431400	-0.12962400				
H	1.47324600	-4.75640300	-0.39166700				
N	-0.84201200	-2.28697500	-0.32259600				
C	3.53730300	-1.48016700	-1.17324300				
C	2.84722800	-0.26645700	-0.46479500				
C	1.50221500	-2.05182600	-0.48110500				
N	1.44626200	-0.77643500	-0.33629700				

O	-2.35550300	2.71054300	0.71998000	H	-1.84503800	0.25950300	4.93149500
C	-4.31251300	1.40167900	0.83218900	H	-4.07864200	1.34267300	5.11252400
C	-4.99541300	0.32563800	1.41740900	C	-3.35649400	-0.53386300	-0.89857800
C	-5.06892200	2.40486400	0.20189700	C	-3.72391600	-0.18949200	-2.20770900
C	-6.38845400	0.25278100	1.36199300	C	-4.15062500	-1.47771100	-0.22039800
H	-4.45444000	-0.45019900	1.94927800	C	-4.83964900	-0.76881100	-2.81889600
C	-6.45323500	2.31901000	0.13590500	H	-3.15487700	0.55139100	-2.75778800
H	-4.54286600	3.24854400	-0.23203000	C	-5.26660800	-2.05284900	-0.82751200
C	-7.14091400	1.23894400	0.71415200	H	-3.90201700	-1.76111300	0.79782000
H	-6.89849300	-0.58107700	1.83922900	C	-5.61553700	-1.70344400	-2.13415000
H	-7.01603700	3.10197100	-0.36789300	H	-5.10412600	-0.47749700	-3.83242800
C	-8.64610100	1.15048100	0.63094500	H	-5.86422600	-2.77498400	-0.27677500
H	-9.03642800	0.34016600	1.25470600	H	-6.48450800	-2.15085500	-2.60922300
H	-9.11943600	2.08487300	0.95543000	P	1.81317100	0.10815700	0.05373500
H	-8.97582400	0.96591500	-0.39980300	C	1.63357900	1.79699800	0.82494900
				C	1.90878600	2.99908200	0.15566400
				C	1.14290300	1.87567400	2.14027900
CP16				C	1.72419900	4.23062700	0.78881900
Ni	0.00001500	-1.25034700	0.00007400	H	2.25889400	2.98470400	-0.86964800
C	0.93136800	-2.77638700	-1.24056100	C	0.97060400	3.10372900	2.77916600
C	-0.40242100	-2.65421000	-1.59598600	H	0.88535600	0.96561500	2.67133900
C	-1.49872900	-3.59809700	-1.14367100	C	1.26435100	4.28981500	2.10407700
C	-1.48169600	-3.90569900	0.37787300	H	1.94107200	5.14674200	0.24533900
C	-0.93068000	-2.77660300	1.24076400	H	0.59524700	3.13106400	3.79885800
C	0.40306100	-2.65381400	1.59620000	H	1.12589700	5.24945300	2.59525500
C	1.49965200	-3.59747200	1.14407300	C	2.56945600	0.52608400	-1.60301500
C	1.48307000	-3.90503500	-0.37751900	C	3.83540500	1.12738400	-1.72267400
H	1.65919700	-2.25620100	-1.85617400	C	1.86865800	0.22065400	-2.77657400
H	-0.64519500	-2.05347600	-2.47244500	C	4.37163200	1.42417000	-2.97555400
H	-1.44312000	-4.54544600	-1.70655000	H	4.40802500	1.36135300	-0.83008800
H	-2.46143600	-3.15138300	-1.40468600	C	2.40415800	0.51225700	-4.03467200
H	-2.50631400	-4.13119200	0.69877600	H	0.90038700	-0.26149700	-2.69577300
H	-0.90636700	-4.81926200	0.56854800	C	3.65622900	1.11762000	-4.13673100
H	-1.65880400	-2.25664500	1.85621500	H	5.35087200	1.89095100	-3.04583300
H	0.64561900	-2.05282000	2.47254000	H	1.84416900	0.25971600	-4.93156800
H	1.44406000	-4.54485900	1.70687800	H	4.07732000	1.34374100	-5.11294800
H	2.46222500	-3.15061900	1.40534000	C	3.35669700	-0.53358000	0.89810300
H	2.50791800	-4.12969900	-0.69825100	C	3.72405000	-0.18966100	2.20736900
H	0.90851300	-4.81906000	-0.56832400	C	4.15102700	-1.47698800	0.21954400
P	-1.81320600	0.10793400	-	C	4.83990600	-0.76899100	2.81832300
0.05382800				H	3.15484400	0.55087700	2.75774100
C	-1.63370500	1.79698800	-0.82461100	C	5.26713500	-2.05213200	0.82642200
C	-1.90900200	2.99884000	-0.15493100	H	3.90247300	-1.76007600	-0.79876500
C	-1.14302800	1.87614100	-2.13990300	C	5.61599200	-1.70318300	2.13320100
C	-1.72451600	4.23060400	-0.78768500	H	5.10431900	-0.47803300	3.83197300
H	-2.25910500	2.98413300	0.87037700	H	5.86490600	-2.77391600	0.27538900
C	-0.97084600	3.10442100	-2.77839700	H	6.48505100	-2.15060900	2.60809900
H	-0.88533600	0.96630100	-2.67126300				
C	-1.26469400	4.29026300	-2.10293600	CP17			
H	-1.94145900	5.14651900	-0.24389700	C	-0.00571700	-2.57767700	-0.68561300
H	-0.59549500	3.13210000	-3.79808200	H	-0.29232900	-3.26760000	0.10394600
H	-1.12634300	5.25006800	-2.59381600	C	1.31030300	-2.01454600	-0.63685700
C	-2.56993200	0.52550100	1.60282600	H	1.82660000	-1.80270900	-1.56650000
C	-3.83610100	1.12637800	1.72228800	C	-0.55426300	-2.96766700	-2.01269000
C	-1.86919700	0.22038200	2.77650300	F	0.03615200	-4.07782700	-2.53028600
C	-4.37263500	1.42298100	2.97507800	F	-1.88535700	-3.25037400	-1.95853200
H	-4.40865600	1.36017900	0.82961500	F	-0.40486600	-1.99523100	-2.96092400
C	-2.40499800	0.51180700	4.03451300	C	2.11310400	-2.23572900	0.57469000
H	-0.90072400	-0.26137700	2.69587200	O	1.58692800	-2.59638300	1.63899000
C	-3.65731100	1.11670100	4.13637700	C	3.60379200	-2.03155100	0.53386100
H	-5.35205400	1.88941200	3.04518800				

C	4.29520800	-1.48998500	-0.55966200	H	-2.39593600	6.00132900	-1.13172600
C	4.34589500	-2.42073500	1.66178300	C	2.08484000	1.40718200	-1.60034600
C	5.68151300	-1.34091700	-0.51971600	C	3.30826100	2.08848500	-1.52879100
H	3.76283600	-1.16265400	-1.44575600	C	1.75478500	0.73614700	-2.79092600
C	5.72792000	-2.27965300	1.69192800	C	4.17575600	2.10613200	-2.62341100
H	3.80669900	-2.83706900	2.50632500	H	3.59781600	2.59629600	-0.61533400
C	6.42347200	-1.73800900	0.59909500	C	2.61725700	0.76555700	-3.88851400
H	6.19400900	-0.90701700	-1.37530300	H	0.82965300	0.17057500	-2.85204900
H	6.28132200	-2.59292700	2.57501800	C	3.83197900	1.45036100	-3.80668200
C	7.92840600	-1.61159700	0.62447400	H	5.12317900	2.63352400	-2.54764800
H	8.28374300	-0.89214700	-0.12056300	H	2.34339100	0.24267100	-4.80097500
H	8.28777300	-1.28824800	1.60811400	H	4.50863600	1.46635800	-4.65698300
H	8.41044200	-2.57422100	0.40640900	C	1.82101400	1.82735700	1.29457100
Ni	-0.15028300	-0.69629100	-0.19474200	C	2.25798800	3.14626100	1.51459200
P		-2.31264100	-0.48019100	C	2.12510400	0.84811500	2.25285000
0.32539200				C	2.99072600	3.47132500	2.65608200
C	-3.29954300	0.33682800	-1.00604800	H	2.01420700	3.92543400	0.79872500
C	-3.74229800	1.66431600	-0.90576200	C	2.85920100	1.17655000	3.39578300
C	-3.50783600	-0.35280000	-2.21560800	H	1.78856200	-0.17404700	2.11479500
C	-4.39729200	2.27898600	-1.97547300	C	3.29455000	2.48578300	3.59913900
H	-3.56898600	2.23131300	0.00160100	H	3.32116400	4.49526200	2.81031900
C	-4.16906900	0.26305100	-3.27808100	H	3.08731500	0.40304400	4.12380400
H	-3.15289800	-1.37083800	-2.33069600	H	3.86395700	2.74070100	4.48914800
C	-4.61943600	1.58013800	-3.16154600				
H	-4.72802000	3.30934800	-1.87665600	CP18			
H	-4.32800400	-0.28954600	-4.20039800	Ni	0.06434500	0.53001600	-0.14097000
H	-5.13226300	2.05854500	-3.99184800	P	1.80235400	-0.87966100	0.00481900
C	-2.70151200	0.45694200	1.87781700	C	1.57003500	-2.16027200	-1.30883800
C	-4.01571700	0.79689100	2.24022300	C	1.71496100	-3.53941800	-1.11031200
C	-1.66243800	0.73435500	2.77619600	C	1.20463700	-1.69275600	-2.58600800
C	-4.27524700	1.42908400	3.45552700	C	1.51952300	-4.43148300	-2.16737100
H	-4.84008100	0.56319400	1.57279400	H	1.96731000	-3.92708600	-0.12951700
C	-1.92299100	1.35833600	3.99965700	C	1.02497500	-2.58668100	-3.64237400
H	-0.64493000	0.45474300	2.52209500	H	1.06717900	-0.62797700	-2.76205100
C	-3.22865700	1.71350100	4.33793200	C	1.18306800	-3.95901400	-3.43607900
H	-5.29660400	1.69149100	3.71897600	H	1.63010000	-5.49872600	-1.99417700
H	-1.10325400	1.56308300	4.68308700	H	0.75554200	-2.20711200	-4.62439300
H	-3.43414400	2.20064600	5.28750800	H	1.03702700	-4.65546000	-4.25763500
C	-3.23135200	-2.04295000	0.71094900	C	2.08154500	-1.76996800	1.60136000
C	-4.52790600	-2.32225400	0.25963300	C	3.16143400	-2.64709300	1.80361800
C	-2.59904400	-2.95669000	1.57055200	C	1.22819400	-1.49450300	2.67954400
C	-5.17460500	-3.49757000	0.65022700	C	3.35692000	-3.25846200	3.04190300
H	-5.03618600	-1.62990900	-0.40391200	H	3.86174300	-2.83859400	0.99576500
C	-3.25067100	-4.12427100	1.96640800	C	1.43029000	-2.09755900	3.92415400
H	-1.59246200	-2.75576600	1.92887300	H	0.40645800	-0.79652300	2.54338500
C	-4.53954600	-4.40029800	1.50350200	C	2.49047600	-2.98616900	4.10465600
H	-6.17752300	-3.70445000	0.28545200	H	4.19341200	-3.93821700	3.18132000
H	-2.74673600	-4.82162900	2.63029900	H	0.76172000	-1.86763200	4.74957400
H	-5.04413700	-5.31438300	1.80508700	H	2.65032400	-3.45631400	5.07139900
P	0.85970600	1.33208300	-0.20841900	C	3.52325700	-0.26279400	-0.32683900
C	-0.15862300	2.85835400	-0.52279900	C	4.16223200	-0.42132500	-1.56443500
C	-0.31475100	3.38967500	-1.81159500	C	4.19703700	0.42823800	0.69425400
C	-0.83843800	3.47542300	0.54201200	C	5.44498600	0.09206600	-1.77248000
C	-1.12029000	4.50990000	-2.02906400	H	3.66862700	-0.95251900	-2.37070600
H	0.19991800	2.93784000	-2.65301200	C	5.47694500	0.93834700	0.48521600
C	-1.63507100	4.60011500	0.32453700	H	3.72257100	0.56938100	1.66044100
H	-0.73966000	3.08617500	1.54992500	C	6.10693700	0.77047400	-0.74996500
C	-1.77874400	5.12276000	-0.96291500	H	5.92515000	-0.04541400	-2.73790400
H	-1.22314300	4.90679600	-3.03559400	H	5.97784500	1.47422300	1.28658200
H	-2.14088300	5.06843600	1.16505100	H	7.10485100	1.16869800	-0.91351100

P	-1.84561000	-0.65745600	H	-4.34596000	5.77960800	0.86076700	
0.13479900							
C	-1.83316700	-2.51485800	0.03181800	TS10			
C	-2.21677700	-3.18535000	-1.13930300	Ni	0.12617800	0.40230000	-0.49633600
C	-1.38445300	-3.27996800	1.12238300	C	0.13435800	2.67607800	-0.56263900
C	-2.16105300	-4.57873500	-1.21483500	C	1.27037000	1.87440400	-0.87667900
H	-2.56745400	-2.62280200	-1.99780800	C	-0.29069900	1.97569200	-1.68965900
C	-1.33568900	-4.67201900	1.04777400	O	-0.87695800	2.01198200	-2.76596200
H	-1.08044100	-2.79315300	2.04277600	C	-0.21896600	3.85344300	0.22825100
C	-1.72559100	-5.32768600	-0.12178600	C	-1.41825900	4.53922700	-0.03670700
H	-2.46551700	-5.07633300	-2.13178000	C	0.60692500	4.30110100	1.27599400
H	-0.99409600	-5.24256400	1.90765700	C	-1.77414600	5.65269400	0.72245000
H	-1.69050000	-6.41248300	-0.17922600	H	-2.06222700	4.18778900	-0.83733700
C	-3.12083700	-0.22757400	-1.13934400	C	0.24660000	5.41461900	2.03096600
C	-4.50026400	-0.26999000	-0.88705900	H	1.53436700	3.77396500	1.48221400
C	-2.67827300	0.11893100	-2.42638800	C	-0.94452300	6.09451000	1.75638800
C	-5.41569000	0.01882700	-1.90039800	H	-2.70263800	6.17528300	0.50806200
H	-4.86673000	-0.51699700	0.10395500	H	0.89464800	5.75572400	2.83437200
C	-3.59646700	0.39401400	-3.44243900	H	-1.22456900	6.96254500	2.34753800
H	-1.61753800	0.20656900	-2.63684000	C	2.65488400	2.33836000	-1.04276300
C	-4.96701500	0.34479400	-3.18205200	C	2.90178700	3.69917500	-1.33831100
H	-6.48086300	-0.00964700	-1.68569600	C	3.76763500	1.47818800	-0.98464300
H	-3.23311800	0.66506700	-4.42988500	C	4.19402200	4.17191900	-1.54771200
H	-5.68161500	0.56876300	-3.96979400	H	2.06327300	4.38463100	-1.41498100
C	-2.68183500	-0.36616800	1.76094000	C	5.06233300	1.95439200	-1.18494000
C	-3.63815300	-1.24041600	2.30601400	H	3.61923400	0.42882000	-0.77015300
C	-2.34612600	0.79355200	2.47633400	C	5.28597900	3.30305500	-1.46752900
C	-4.24604200	-0.95484700	3.52923000	H	4.34871400	5.22330400	-1.77779700
H	-3.89977100	-2.15365600	1.78069600	H	5.89986800	1.26389800	-1.12275700
C	-2.95730600	1.08020300	3.69869400	H	6.29538600	3.67170800	-1.63017400
H	-1.61241000	1.47959100	2.06630600	P	-2.03735300	-0.27079000	-0.24537100
C	-3.90800600	0.20674600	4.22800800	C	-2.31173300	-0.95726400	1.45102800
H	-4.98327900	-1.64164400	3.93692500	C	-3.02530200	-2.12753300	1.73885400
H	-2.68960200	1.98769600	4.23308900	C	-1.76384600	-0.22289400	2.51834200
H	-4.38241100	0.42731200	5.18063400	C	-3.20269700	-2.54289900	3.06103700
C	0.90915100	2.19736900	-0.70706200	H	-3.43826600	-2.72656900	0.93465800
C	-0.58522300	2.28809000	-0.74880800	C	-1.95540600	-0.62944000	3.83872600
C	0.19202400	2.11030500	-1.95258300	H	-1.18977300	0.67688300	2.30956000
O	0.22623400	2.04694000	-3.17730200	C	-2.67853100	-1.79251700	4.11359500
C	2.03049900	2.99849400	-0.20202600	H	-3.75416600	-3.45691400	3.26518000
C	2.94982000	3.56342100	-1.10369700	H	-1.53479200	-0.04140200	4.65033900
C	2.20406400	3.24304400	1.17217300	H	-2.82500100	-2.11493100	5.14113000
C	3.99928300	4.35777700	-0.64381400	C	-2.66694900	-1.53047100	-1.44093800
H	2.82377900	3.37694200	-2.16625700	C	-4.01260400	-1.93523100	-1.47676900
C	3.25266100	4.03877900	1.63060700	C	-1.77985400	-2.05142800	-2.39379100
H	1.50966500	2.79528000	1.87908600	C	-4.44796400	-2.86690000	-2.41887700
C	4.15456600	4.60135700	0.72326000	H	-4.72519100	-1.50775500	-0.77710700
H	4.69762100	4.79025200	-1.35592500	C	-2.21769200	-2.97918500	-3.34245900
H	3.36616900	4.22188200	2.69648900	H	-0.74789000	-1.71242000	-2.40343500
H	4.97101000	5.22459300	1.07892100	C	-3.54978000	-3.39363500	-3.35147100
C	-1.61547700	3.23325200	-0.29585100	H	-5.49076200	-3.17300300	-2.43299400
C	-1.46915100	3.95664000	0.90322700	H	-1.51858200	-3.36751600	-4.07823900
C	-2.76578700	3.46132100	-1.07382800	H	-3.89251400	-4.11284500	-4.09076600
C	-2.44245700	4.86617100	1.31467700	C	-3.38508600	1.00965400	-0.35917400
H	-0.57378500	3.81687500	1.50155900	C	-4.10929600	1.45558000	0.75633100
C	-3.73990600	4.36737500	-0.65707200	C	-3.68001600	1.56126300	-1.61932600
H	-2.88641700	2.92203600	-2.00723600	C	-5.10268200	2.42893500	0.61833400
C	-3.58605100	5.07206000	0.53943500	H	-3.90979000	1.04407900	1.73936600
H	-2.30428300	5.42047700	2.23997500	C	-4.67460900	2.53009600	-1.75237100
H	-4.62134100	4.52718900	-1.27307200	H	-3.11539000	1.25630300	-2.49230000

C	-5.39032700	2.96795500	-0.63501900	H	1.29741500	-0.51801400	-2.41311800
H	-5.65287500	2.75907900	1.49581800	C	2.95053800	-3.23135500	-3.61896500
H	-4.88629200	2.94466800	-2.73450400	H	2.98102900	-5.17439200	-2.67928100
H	-6.16552100	3.72242400	-0.74216300	H	2.69817200	-1.20751400	-4.32628500
P	1.40836900	-1.31064600	0.21614800	H	3.56600400	-3.53899600	-4.46020300
C	0.69941400	-2.83520100	1.00950700	C	-0.99869500	-3.27463400	-0.17947700
C	0.77707000	-3.05255900	2.39323700	C	-1.10582600	-4.28248500	0.78819800
C	0.02802200	-3.78508900	0.22033600	C	-1.81562100	-3.34016300	-1.31966100
C	0.21358100	-4.19337100	2.96858200	C	-2.00710400	-5.33676000	0.61495400
H	1.28560400	-2.33467600	3.02794300	H	-0.48682300	-4.25266800	1.67875200
C	-0.53095200	-4.92590600	0.79576700	C	-2.71081400	-4.39312000	-1.49176000
H	-0.05135500	-3.64356200	-0.85236500	H	-1.75492700	-2.56063500	-2.07408700
C	-0.43695300	-5.13663800	2.17295600	C	-2.80845600	-5.39670900	-0.52423400
H	0.29007300	-4.34400800	4.04224300	H	-2.07712900	-6.11203000	1.37386200
H	-1.03721400	-5.65135100	0.16412400	H	-3.33988900	-4.42468800	-2.37687900
H	-0.86807100	-6.02792900	2.62134300	H	-3.50884900	-6.21693200	-0.65763900
C	2.70894900	-0.83135900	1.44981700	P	1.62702800	1.44704900	-0.00826100
C	3.91719700	-1.52275900	1.62783400	C	3.14502500	0.60570800	0.66804300
C	2.44054600	0.27691600	2.26747100	C	3.49418800	0.70502500	2.02373500
C	4.83101000	-1.11498400	2.60061200	C	3.96111100	-0.16904700	-0.17486300
H	4.15759000	-2.37397200	0.99942900	C	4.62931100	0.05963100	2.51862500
C	3.34800600	0.67586400	3.25072400	H	2.88775700	1.29864100	2.69882300
H		1.52150700	0.83639100	C	5.09748200	-0.80917100	0.32007700
2.11674300				H	3.72300100	-0.26275300	-1.22847600
C	4.54678200	-0.01848800	3.41788700	C	5.43810900	-0.69523200	1.66930500
H	5.76660900	-1.65533200	2.71947300	H	4.88252900	0.15674500	3.57104100
H	3.12309000	1.53616900	3.87562900	H	5.71903500	-1.39269400	-0.35429100
H	5.25985100	0.29662800	4.17503900	H	6.32718800	-1.18849300	2.05359100
C	2.31696300	-2.05794000	-1.22046400	C	1.41789000	2.83753600	1.19575800
C	2.95830000	-3.30805700	-1.15800200	C	2.07902300	4.06658000	1.07908500
C	2.33602700	-1.35198100	-2.43463800	C	0.57414400	2.62305000	2.29633800
C	3.62108200	-3.82381500	-2.27197800	C	1.90342300	5.05763000	2.04636700
H	2.91974200	-3.89424500	-0.24494900	H	2.71645600	4.26496300	0.22420800
C	2.99621800	-1.87241100	-3.55065100	C	0.40765300	3.61053800	3.26849600
H	1.82988900	-0.39259000	-2.50141300	H	0.03108900	1.68555900	2.38234000
C	3.64335400	-3.10574500	-3.47054500	C	1.07213400	4.83182100	3.14472500
H	4.11329000	-4.79069100	-2.20570300	H		2.41314900	6.01116500
H	3.00003500	-1.31056300	-4.48065600	1.93558700			
H	4.15627900	-3.51122300	-4.33878000	H	-0.25214400	3.42951700	4.11290700
CP19				H	0.93531200	5.60645100	3.89459300
Ni	-0.44490400	0.39443000	-0.21913400	C	2.29455800	2.20229800	-1.56082900
P	0.22484800	-1.88423900	-0.07933200	C	3.61375800	2.67863800	-1.65344100
C	1.07052500	-2.22664100	1.52832600	C	1.46686300	2.28926400	-2.69089400
C	2.26479600	-2.94271400	1.68448900	C	4.08798400	3.23567300	-2.84211000
C	0.43148900	-1.72487500	2.67688800	H	4.28020000	2.60224100	-0.80004200
C	2.79468600	-3.16813400	2.95727300	C	1.94575000	2.83871000	-3.88159500
H	2.79499600	-3.31633100	0.81588500	H	0.44192300	1.94371100	-2.63022800
C	0.95557600	-1.96014100	3.94780200	C	3.25496700	3.31569800	-3.95981700
H	-0.48342800	-1.14668900	2.57208400	H	5.11001900	3.60179300	-2.89425000
C	2.13954600	-2.68690500	4.09125000	H	1.28965600	2.89873700	-4.74581100
H	3.72480300	-3.72087000	3.05888600	H	3.62561000	3.74591400	-4.88658500
H	0.44203800	-1.57161700	4.82336200	C	-2.60949500	1.68446700	-0.28435700
H	2.55246500	-2.86913600	5.07986400	C	-2.38835900	0.32776200	-0.15403200
C	1.35940900	-2.43835200	-1.43661700	C	-1.24057600	2.12023800	-0.52967400
C	1.82426400	-3.76109600	-1.54252600	O	-0.79199800	3.20641600	-0.87475600
C	1.67687900	-1.53362400	-2.45935800	C	-3.81616300	2.53834900	-0.20780000
C	2.62433000	-4.14961800	-2.61658600	C	-3.80997100	3.80595000	-0.82383900
H	1.54113100	-4.49611000	-0.79496700	C	-4.96839700	2.15091000	0.50406700
C	2.46689500	-1.92535300	-3.54390300	C	-4.92510600	4.64010400	-0.75071800
				H	-2.91638500	4.12985100	-1.34500000

C	-6.07843400	2.99005800	0.57726200	C	-2.28305100	2.35257600	-0.96790900
H	-4.99047400	1.19064200	1.00714300	C	-2.82402300	2.36323500	-2.26602800
C	-6.06589000	4.23653300	-0.05436400	C	-2.53735500	3.45094700	-0.12651800
H	-4.89957100	5.61228100	-1.23716500	C	-3.61039300	3.42947400	-2.70057300
H	-6.95646000	2.66992200	1.13317300	H	-2.62502700	1.53107900	-2.93466900
H	-6.93400300	4.88850500	0.00282800	C	-3.32614600	4.51326400	-0.56378700
C	-3.45688000	-0.67689100	-0.02584500	H	-2.11197000	3.47111500	0.87160000
C	-3.57545500	-1.49037800	1.11502200	C	-3.86844400	4.50739300	-1.85160800
C	-4.41404300	-0.83178700	-1.04900700	H	-4.02237700	3.41618800	-3.70619000
C	-4.62233200	-2.40309700	1.24182100	H	-3.51188600	5.35257700	0.10171900
H	-2.84574500	-1.39225000	1.91428100	H	-4.48181900	5.33773800	-2.19101000
C	-5.44932400	-1.75668100	-0.92962000	C	-1.56703000	0.86588900	2.01606700
H	-4.34109400	-0.20785000	-1.93568200	C	-0.69627500	0.70821300	3.11449500
C	-5.56356800	-2.54318600	0.21985600	C	-2.92114600	1.17207600	2.27811500
H	-4.69746700	-3.01303800	2.13854900	C	-1.14711800	0.89557300	4.41998800
H	-6.17692400	-1.85515300	-1.73182400	H	0.34215100	0.44726100	2.93023700
H	-6.37528100	-3.25943700	0.31650500	C	-3.37463500	1.32635000	3.58569200
PPh₃				H	-3.61405300	1.26998200	1.44892400
P	0.00005200	-0.00069200	-1.20788900	C	-2.48860700	1.20102900	4.66077200
C	1.01941400	-1.32334000	-0.40353300	H	-0.45424200	0.78762100	5.25020000
C	0.64741600	-2.02401300	0.75431500	H	-4.42218700	1.55192000	3.76808700
C	2.23257600	-1.65822000	-1.02951100	H	-2.84481600	1.33198900	5.67906100
C	1.47141100	-3.02424000	1.27607500	C	0.46336700	-2.65580500	-0.53618200
H	-0.29087100	-1.79067800	1.24840600	H	0.68778200	-2.77148400	-1.59318700
C	3.06113500	-2.64887900	-0.50222700	C	-0.88740700	-2.43505300	-0.16538400
H	2.52642100	-1.14089900	-1.94009300	H	-1.19174800	-2.68012800	0.84893600
C	2.68068200	-3.33673500	0.65242900	C	1.34140300	-3.45930000	0.35570400
H	1.16684600	-3.55904400	2.17226700	F	1.06003700	-3.24753900	1.68161100
H	3.99744000	-2.89105300	-0.99840000	F	1.20846700	-4.79397100	0.15756200
H	3.31973200	-4.11597600	1.05945700	F	2.65925500	-3.18441200	0.19426300
C	-1.65571800	-0.22112300	-0.40418900	C	-1.95243100	-2.38949900	-1.20384600
C	-2.07325500	0.44727300	0.75723100	O	-1.67549800	-2.49439100	-2.39714000
C	-2.55603100	-1.09782500	-1.03387500	C	-3.38348500	-2.24028200	-0.77627000
C	-3.35170100	0.23584800	1.27908200	C	-3.78319200	-1.97496000	0.54080300
H	-1.39954800	1.13856600	1.25445600	C	-4.37727000	-2.37645300	-1.76065700
C	-3.82884100	-1.31760900	-0.50690600	C	-5.13578400	-1.85220200	0.86090800
H	-2.25712100	-1.60796200	-1.94683500	H	-3.04695000	-1.83941800	1.32546100
C	-4.23077300	-0.64874500	0.65163600	C	-5.72226100	-2.25834200	-1.43519400
H	-3.65982300	0.76377400	2.17812400	H	-4.06282900	-2.57775300	-2.77946900
H	-4.50969800	-2.00225000	-1.00610100	C	-6.12793200	-1.99522900	-0.11599900
H	-5.22544200	-0.81097300	1.05855600	H	-5.42233500	-1.63914800	1.88817500
C	0.63659300	1.54309200	-0.40335600	H	-6.47494100	-2.37069400	-2.21289700
C	1.41323400	1.57128000	0.76555400	C	-7.59322500	-1.87742500	0.23022400
C	0.33647200	2.76028500	-1.03881500	H	-8.09519900	-1.13700400	-0.40458400
C	1.86734800	2.78429000	1.28881000	H	-8.11467900	-2.83184500	0.08179400
H	1.66773500	0.64236300	1.26699100	H	-7.73695100	-1.57940400	1.27360400
C	0.78034200	3.97267900	-0.51041300	P	2.30156500	0.24405600	-0.12178300
H	-0.24598200	2.75562300	-1.95738100	C	2.24249500	2.01352600	-0.65358000
C	1.54963500	3.98715000	0.65533600	C	2.85555200	2.47630700	-1.82643800
H	2.47002400	2.78798500	2.19363300	C	1.52199600	2.92469600	0.13868400
H	0.53490200	4.90415900	-1.01400800	C	2.75247200	3.81974000	-2.19653600
H	1.90497600	4.92974500	1.06340500	H	3.41397300	1.79166100	-2.45556500
CP20				C	1.42667700	4.26559900	-0.22961200
Ni	0.16266900	-0.71715200	0.00279600	H	1.03823100	2.58656800	1.05048800
C	-1.43138200	1.22392400	-0.53268700	C	2.03998000	4.71671300	-1.40115300
C	-1.06881900	0.62844500	0.66338700	H	3.23250900	4.16136000	-3.10967300
C	-0.61826300	0.43210400	-1.40542700	H	0.86612100	4.95620600	0.39431000
O	-0.27391500	0.28568300	-2.53880100	H	1.95925000	5.76054400	-1.69204800
				C	3.47508500	-0.53302800	-1.31360500
				C	4.83765200	-0.71081700	-1.03614200

C	2.9660000	-0.9659390	-2.5501110	C	-3.7864070	-3.1828740	0.0978380
C	5.6760640	-1.3108880	-1.9781320	C	-4.4477830	-1.1342380	-0.9896680
H	5.2476150	-0.3907050	-0.0837320	C	-5.1058040	-3.3991410	0.4833330
C	3.8105470	-1.5527470	-3.4928820	H	-3.0348870	-3.9252440	0.3473810
H	1.9109620	-0.8409130	-2.7762220	C	-5.7631900	-1.3523080	-0.5931220
C	5.1662580	-1.7307530	-3.2074640	H	-4.1901760	-0.2567890	-1.5709690
H	6.7288560	-1.4507210	-1.7473090	C	-6.1172650	-2.4849690	0.1540670
H	3.4042430	-1.8798330	-4.4461330	H	-5.3579080	-4.2966530	1.0434490
H	5.8206750	-2.1988030	-3.9379930	H	-6.5312340	-0.6333000	-0.8693030
C	3.2308400	0.3383940	1.4736740	C	-7.5405010	-2.7054070	0.6070490
C	4.1153830	1.3943550	1.7523110	H	-7.7045970	-2.2850410	1.6086240
C	3.0604700	-0.6722150	2.4339780	H	-8.2558120	-2.2245150	-0.0683690
C	4.8132730	1.4353650	2.9600640	H	-7.7846260	-3.7718220	0.6601840
H	4.2563040	2.1890080	1.0267330	P	2.2486690	0.1820070	-0.0039240
C	3.7610130	-0.6276390	3.6414110	C	3.4777100	-0.5234200	-1.1893320
H	2.3924540	-1.5029700	2.2413750	C	4.7831490	-0.8619040	-0.8073770
C	4.6373310	0.4251250	3.9081160	C	3.0847090	-0.7278380	-2.5230910
H	5.4937290	2.2590120	3.1593140	C	5.6768670	-1.3950040	-1.7387620
H	3.6179280	-1.4189030	4.3723350	H	5.1057270	-0.7194430	0.2186330
H	5.1793930	0.4598650	4.8493530	C	3.9839290	-1.2495640	-3.4530240
TS11				H	2.0779150	-0.4734130	-2.8400200
Ni	0.2055960	-0.7227190	-0.0016770	C	5.2814240	-1.5889410	-3.0624040
C	-1.3904210	1.2537200	-0.7250680	H	6.6831170	-1.6600940	-1.4251120
C	-0.9907430	0.7039970	0.4695350	H	3.6658110	-1.3987490	-4.4813660
C	-0.7500040	0.5590470	-1.8253370	H	5.9778070	-2.0055520	-3.7851880
O	-0.0882790	0.6647880	-2.7868850	C	3.0463260	0.0044400	1.6533280
C	-2.2529840	2.4035040	-1.1244900	C	3.9469750	0.9568830	2.1578690
C	-3.0384600	2.3369870	-2.2887090	C	2.7468960	-1.1269440	2.4303650
C	-2.2592650	3.5959910	-0.3796400	C	4.5360580	0.7790780	3.4108260
C	-3.8191190	3.4228560	-2.6866510	H	4.1859420	1.8402320	1.5742790
H	-3.0372270	1.4263880	-2.8823090	C	3.3400530	-1.3017340	3.6819770
C	-3.0476870	4.6746720	-0.7748200	H	2.0590100	-1.8774330	2.0565580
H	-1.6415460	3.6730420	0.5084280	C	4.2334820	-0.3494940	4.1756360
C	-3.8316270	4.5948590	-1.9292530	H	5.2305400	1.5248010	3.7886280
H	-4.4194210	3.3492230	-3.5897530	H	3.0988730	-2.1826000	4.2706830
H	-3.0406010	5.5871300	-0.1839660	H	4.6908090	-0.4846800	5.1521790
H	-4.4404650	5.4405300	-2.2373620	C	2.3583320	2.0026710	-0.3330180
C	-1.4913480	1.0946790	1.7968440	C	3.1094790	2.5330200	-1.3916790
C	-0.6429640	1.0322910	2.9210150	C	1.6523650	2.8868020	0.5012610
C	-2.8433950	1.4375490	2.0160040	C	3.1520760	3.9124580	-1.6116670
C	-1.1042410	1.3599880	4.1952800	H	3.6645960	1.8743080	-2.0501310
H	0.3864760	0.7142360	2.7868620	C	1.7073270	4.2630760	0.2875100
C	-3.3108320	1.7315070	3.2947810	H	1.0600250	2.5018910	1.3248580
H	-3.5308580	1.4522630	1.1769500	C	2.4545750	4.7809700	-0.7735880
C	-2.4417380	1.7105640	4.3895200	H	3.7364010	4.3035340	-2.4403000
H	-0.4216930	1.3192710	5.0403630	H	1.1608000	4.9309900	0.9479960
H	-4.3591380	1.9819400	3.4372270	H	2.4900550	5.8534720	-0.9448300
H	-2.8077910	1.9493910	5.3845380	CP21			
C	0.4114560	-2.4665250	-0.8788060	Ni	-0.2395940	-0.9217220	-0.0067130
H	0.5883990	-2.3304170	-1.9448710	C	1.7718470	0.7887380	0.9072120
C	-0.9421070	-2.3687530	-0.3914380	C	1.1791540	0.3523880	-0.2471580
H	-1.1858550	-2.9161710	0.5132650	C	1.5382430	0.0447890	2.1766530
C	1.2402480	-3.5642580	-0.3065900	O	1.6237400	0.4850890	3.2977610
F	1.0433740	-3.7135980	1.0401770	C	2.6277570	2.0025450	1.0757850
F	0.9661600	-4.7799890	-0.8532920	C	3.8549810	1.9396720	1.7580360
F	2.5668720	-3.3649770	-0.4834710	C	2.2163620	3.2426550	0.5611330
C	-2.0387700	-1.7791770	-1.0920210	C	4.6529790	3.0740160	1.9024220
O	-1.8870430	-0.9929240	-2.0932970	H	4.1875840	0.9933510	2.1743760
C	-3.4318240	-2.0395370	-0.6396000	C	3.0135230	4.3774770	0.7069830

H	1.26418200	3.31347800	0.04629000	H	-6.20325200	-0.31145400	2.64108600
C	4.23677800	4.29883900	1.37586000	H	-2.51983000	-0.17991900	4.86339800
H	5.60083900	3.00075800	2.42971700	H	-4.99866600	-0.43122900	4.81402200
H	2.67225000	5.32744600	0.30313900	C	-3.19091600	0.22489200	-1.43436500
H	4.85682700	5.18401100	1.49207000	C	-4.17619500	1.18357500	-1.73054700
C	1.57397400	0.73569000	-1.61663100	C	-3.10039000	-0.92336600	-2.23524200
C	0.68584200	0.52771300	-2.69416500	C	-5.05237600	0.99143700	-2.79839900
C	2.87834100	1.17563600	-1.93830900	H	-4.25383500	2.08502100	-1.13046900
C	1.05035100	0.80150600	-4.01135700	C	-3.97761600	-1.11180900	-3.30565600
H	-0.30307200	0.12887500	-2.48892600	H	-2.35093800	-1.67670100	-2.02055900
C	3.24958100	1.43442900	-3.25518000	C	-4.95400400	-0.15662800	-3.58893100
H	3.60790900	1.30074200	-1.14769000	H	-5.80924400	1.74050000	-3.01507700
C	2.33609000	1.26323500	-4.29909900	H	-3.89408300	-2.00679500	-3.91592400
H	0.33457500	0.63833600	-4.81321600	H	-5.63464100	-0.30295300	-4.42332400
H	4.26197300	1.76831600	-3.46817600				
H	2.62935000	1.46973300	-5.32508800				
C	-1.05950300	-2.62554000	0.83074100	TS12			
H	-1.29758800	-2.28532700	1.83511900	Ni	0.26868800	-0.92409200	-0.03586100
C	0.28658300	-2.83009300	0.45171100	C	-1.63552200	1.08298900	-1.03101300
H	0.50798800	-3.50532900	-0.37003200	C	-1.38603000	0.27130400	0.04676300
C	-2.09988000	-3.52111900	0.25204700	C	-1.54711400	0.36334700	-2.32280500
F	-1.84155600	-3.83529700	-1.05005000	O	-1.46352300	0.81298700	-3.44237200
F	-2.20582800	-4.70331000	0.91011700	C	-1.98446200	2.52058100	-1.05591800
F	-3.32974200	-2.95579100	0.28640200	C	-2.86122900	3.03568600	-2.03067600
C	1.34411100	-1.99337600	0.86465500	C	-1.44380400	3.41249800	-0.11116300
O	1.21719900	-1.33205400	2.08579200	C	-3.19965100	4.38778600	-2.04235300
C	2.73432100	-2.23771100	0.39611900	H	-3.27446000	2.37515900	-2.78403800
C	3.01645400	-2.54941100	-0.94294900	C	-1.78037800	4.76374300	-0.12926400
C	3.79464000	-2.22126600	1.31427800	H	-0.74601100	3.04477700	0.63211200
C	4.31564500	-2.84642100	-1.34338300	C	-2.66351000	5.25867500	-1.09185200
H	2.21866700	-2.53349300	-1.68010400	H	-3.88334500	4.76105800	-2.80035400
C	5.09355700	-2.51732900	0.90222600	H	-1.34053400	5.43196500	0.60621700
H	3.59571500	-1.99948000	2.35792900	H	-2.92434900	6.31369900	-1.10643900
C	5.38072900	-2.83417000	-0.43073500	C	-1.80426400	0.51625300	1.44312400
H	4.50890800	-3.08015100	-2.38797300	C	-1.05480900	-0.00596700	2.51464600
H	5.89729000	-2.50847900	1.63505600	C	-3.00835400	1.18399300	1.74607400
C	6.79370500	-3.12346400	-0.88017100	C	-1.46125700	0.16904400	3.83758900
H	7.27634000	-2.22211500	-1.28168500	H	-0.14091500	-0.55780400	2.29625700
H	7.41237800	-3.48139000	-0.05049200	C	-3.42030800	1.35111800	3.06557600
H	6.81615600	-3.88114400	-1.67128200	H	-3.62221100	1.56500700	0.93737000
P	-2.02325800	0.43854600	-0.02331900	C	-2.64613200	0.85233500	4.11759500
C	-1.74027700	2.27278100	-0.02366600	H	-0.85899900	-0.23751700	4.64584600
C	-1.82863600	3.03958200	1.14743500	H	-4.35280500	1.86881700	3.27433000
C	-1.39999800	2.91879700	-1.22529100	H	-2.97151600	0.98418700	5.14611300
C	-1.58828800	4.41545100	1.11760400	C	0.44742100	-2.67850800	-1.08812200
H	-2.09427500	2.57321600	2.08936000	H	0.63677600	-2.32846300	-2.09974600
C	-1.16690800	4.29360300	-1.25352100	C	-0.81018100	-2.51280500	-0.48284700
H	-1.32019900	2.35351300	-2.14741300	H	-1.08006200	-3.15196900	0.35242200
C	-1.26060200	5.04772600	-0.08122800	C	1.30610300	-3.82895500	-0.69223500
H	-1.66185000	4.98984000	2.03688700	F	1.14262200	-4.17532400	0.61700300
H	-0.91050500	4.77332400	-2.19426000	F	1.05301700	-4.95100600	-1.41313400
H	-1.07895900	6.11883900	-0.10368000	F	2.62001400	-3.55347900	-0.86759500
C	-3.02525400	0.16624700	1.50567900	C	-1.75817300	-1.45752000	-0.83017800
C	-4.41900000	0.02119900	1.48726100	O	-1.60869300	-1.01109700	-2.15260600
C	-2.35013200	0.08106600	2.73692600	C	-3.19373400	-1.69622000	-0.43053100
C	-5.12334700	-0.19444900	2.67391300	C	-3.53026900	-2.20613200	0.83284200
H	-4.96063800	0.06515000	0.54866500	C	-4.22860100	-1.43560500	-1.33799800
C	-3.05854800	-0.12262400	3.92174200	C	-4.85885500	-2.45109400	1.16948800
H	-1.26833000	0.17374200	2.78077700	H	-2.75701000	-2.40168400	1.56922900
C	-4.44783000	-0.26305600	3.89265400	C	-5.55630000	-1.68640200	-0.99146300
				H	-3.99621000	-1.06475400	-2.32990500

C	-5.89949000	-2.19481000	0.26622600	H	-4.35046500	0.28180800	-1.79936700
H	-5.09022800	-2.84745000	2.15565200	C	-5.96241000	-2.68682400	-1.32565000
H	-6.33867600	-1.48962000	-1.72104000	H	-5.12424900	-4.35317200	-0.25275000
C	-7.34040200	-2.44030300	0.64803200	H	-6.46726200	-0.84466300	-2.33280200
H	-7.44561600	-3.34421500	1.25844500	C	-7.26663100	-3.37322500	-1.65819000
H	-7.74520800	-1.60501400	1.23534200	H	-7.29754700	-4.38970800	-1.25354400
H	-7.97515800	-2.55434100	-0.23684900	H	-8.12443500	-2.82399400	-1.24989300
P	2.13950700	0.22860200	0.14374800	H	-7.41668700	-3.44050900	-2.74301200
C	2.12183300	2.03848500	0.54614000	C	-1.91027600	1.65966000	-0.73552400
C	2.51644900	3.03075800	-0.36160200	C	-2.38363300	0.75142600	0.15396500
C	1.67418400	2.42988300	1.82077300	C	-1.33744400	0.91490700	-1.89041200
C	2.46825400	4.38094800	-0.00300300	O	-0.73537000	1.33505800	-2.85469500
H	2.86649300	2.75535200	-1.35086200	C	-1.91502900	3.13488800	-0.69535400
C	1.63695800	3.77652300	2.18051900	C	-3.03292100	3.83682900	-0.20974600
H	1.35324000	1.68056200	2.53886500	C	-0.81355000	3.86715600	-1.17178700
C	2.03404700	4.75791500	1.26742200	C	-3.04345600	5.22951600	-0.18685900
H	2.77622000	5.13626200	-0.72102300	H	-3.89866200	3.28424800	0.14225300
H	1.29494100	4.05864200	3.17283100	C	-0.82638000	5.26163400	-1.14142700
H	2.00455600	5.80786200	1.54629900	H	0.04529900	3.34035600	-1.57064500
C	3.05103000	0.14308600	-1.46141600	C	-1.93791700	5.94804200	-0.64980900
C	4.41147500	-0.18216000	-1.55617000	H	-3.91873800	5.75448200	0.18662100
C	2.32673800	0.38330100	-2.64288200	H	0.03614000	5.81158200	-1.50825900
C	5.03500700	-0.25809000	-2.80381500	H	-1.94711700	7.03475300	-0.63331800
H	4.98663700	-0.38647800	-0.65929400	C	-2.87000800	0.98382800	1.52984600
C	2.95521800	0.31833100	-3.88648500	C	-2.16675500	1.86920700	2.37017700
H	1.26845900	0.62404300	-2.59991400	C	-3.99170300	0.31473400	2.05157500
C	4.31155600	-0.00528700	-3.96989100	C	-2.57485600	2.08025000	3.68470000
H	6.08870200	-0.51823100	-2.86097400	H	-1.29225800	2.38345600	1.98448500
H	2.37904300	0.51115400	-4.78711600	C	-4.40264100	0.53710800	3.36664500
H	4.79936200	-0.06624700	-4.93902700	H	-4.55068500	-0.36951000	1.42415700
C	3.32382400	-0.40667800	1.41420200	C	-3.69745400	1.41723200	4.18803800
C	4.40633200	0.36561700	1.87013900	H	-2.01419100	2.76194500	4.31866000
C	3.14222700	-1.69463000	1.94005400	H	-5.27684300	0.01655400	3.74813800
C	5.28860900	-0.14343800	2.82307600	H	-4.01659700	1.58370900	5.21331000
H	4.55621000	1.36927800	1.48383400	P	2.74775700	-0.21645500	-0.01130700
C	4.02603500	-2.20136500	2.89567600	C	2.88545400	1.60781700	0.25059000
H	2.31437000	-2.30613000	1.59978200	C	3.50748300	2.47737700	-0.65615600
C	5.09965100	-1.42835100	3.33866000	C	2.29421500	2.14287600	1.40932100
H	6.12136900	0.46521800	3.16555200	C	3.54369100	3.85179100	-0.40482200
H	3.87156200	-3.20134800	3.29184000	H	3.96032500	2.08369500	-1.56067200
H	5.78562000	-1.82235800	4.08388200	C	2.33650200	3.51378200	1.66053000
CP22				H	1.80383500	1.48037300	2.12016200
Ni	0.63448800	-0.81919000	0.34248700	C	2.96069400	4.37217100	0.75137800
C	-0.33994000	-2.42101600	-0.05970300	H	4.02912000	4.51455100	-1.11638300
H	-0.33641400	-2.64622100	-1.12526100	H	1.87781600	3.91265200	2.56126500
C	-1.21332700	-1.42479600	0.45910200	H	2.98807000	5.44140900	0.94277700
H	-1.53326600	-1.50387300	1.49840700	C	3.35057400	-0.49322700	-1.73076800
C	0.04610800	-3.59352500	0.77682100	C	4.66711900	-0.88212400	-2.02082400
F	1.21496500	-4.15198000	0.36076700	C	2.44091000	-0.30858700	-2.78650300
F	0.19762200	-3.28803400	2.08881900	C	5.06799900	-1.07865600	-3.34402300
F	-0.88118000	-4.59398700	0.72518400	H	5.37902500	-1.03658200	-1.21609600
C	-2.19396300	-0.66011300	-0.41839800	C	2.85048500	-0.49514600	-4.10704400
O	-1.56691000	-0.41609200	-1.71042300	H	1.41429600	-0.01428600	-2.58722700
C	-3.51693400	-1.38672600	-0.70879500	C	4.16235800	-0.88390000	-4.38835800
C	-3.75661700	-2.69627600	-0.28571600	H	6.08890800	-1.38536600	-3.55620700
C	-4.51487100	-0.73430900	-1.45152300	H	2.13711600	-0.34279600	-4.91206100
C	-4.96405300	-3.33203400	-0.59125000	H	4.47644000	-1.03871000	-5.41726600
H	-2.99932900	-3.23825700	0.26893600	C	4.06335700	-0.91989800	1.07262000
C	-5.71268600	-1.37264100	-1.75340700	C	5.17924500	-0.17820400	1.49031200
				C	3.93204600	-2.25408500	1.49102700

C	6.14765300	-0.76206300	2.30913600	Ni	0.77130000	0.27132200	-0.43731900
H	5.28987700	0.85682500	1.18085100	P	0.85374400	-1.99722000	-0.52054200
C	4.90599200	-2.83568700	2.30385500	C	0.91629500	-2.94908600	1.06356500
H	3.06929100	-2.83589300	1.18218800	C	2.13777800	-3.35786600	1.62350500
C	6.01314100	-2.09109100	2.71626000	C	-0.25911600	-3.15267500	1.80647300
H	7.00573500	-0.17708900	2.62980200	C	2.17858400	-3.98030600	2.87213600
H	4.79324100	-3.86871400	2.62146400	H	3.06388700	-3.19432400	1.08228900
H	6.76636700	-2.54307500	3.35617700	C	-0.21765200	-3.78452300	3.04991400
CP23				H	-1.21665500	-2.82394400	1.41380400
C	0.05831600	1.86586000	-1.29453700	C	1.00117800	-4.20364000	3.58645900
H	0.08643900	2.78716000	-0.71797200	H	3.13498500	-4.29002700	3.28495100
C	-1.00527700	0.93175000	-1.08957600	H	-1.14172000	-3.94665900	3.59766300
H	-1.41788000	0.39319600	-1.94050500	H	1.03265900	-4.69406100	4.55564300
C	0.60760700	2.06915300	-2.66229900	C	2.32050600	-2.62034400	-1.47537300
F	1.77072200	2.77441400	-2.64837500	C	2.68125700	-3.97874600	-1.49000600
F	0.86799800	0.90257300	-3.32527000	C	3.00651800	-1.73164900	-2.31256100
F	-0.23088400	2.76734600	-3.48480700	C	3.72222400	-4.42742200	-2.30102100
C	-2.03512600	1.25236900	0.00081700	H	2.14508000	-4.69045400	-0.86924600
O	-1.38196300	1.16066500	1.30289900	C	4.04255900	-2.18400600	-3.13401200
C	-2.64029700	2.67006900	-0.09755300	H	2.72222400	-0.68555900	-2.33288800
C	-2.73508400	3.34602900	-1.31968600	C	4.40668600	-3.52957500	-3.12535900
C	-3.17813600	3.28728200	1.04157900	H	3.99293300	-5.48022700	-2.29678700
C	-3.34346400	4.60043400	-1.39607700	H	4.56718100	-1.47761700	-2.77046600
H	-2.32259300	2.90318800	-2.21780000	H	5.21533700	-3.88146200	-3.76078400
C	-3.78001700	4.54096400	0.95912800	C	-0.44464300	-2.86419000	-1.53752000
H	-3.12131200	2.79291800	2.00571700	C	-1.02799500	-4.09723900	-1.21226500
C	-3.87428000	5.22417200	-0.26171100	C	-0.74186000	-2.28672800	-2.78422800
H	-3.39930900	5.10236200	-2.35951200	C	-1.89045500	-4.73402800	-2.10999400
H	-4.18350200	4.99652200	1.86105500	H	-0.80542900	-4.57515600	-0.26428900
C	-4.50075800	6.59669100	-0.34045100	C	-1.58744700	-2.93204000	-3.68555800
H	-4.84767700	6.82129300	-1.35453600	H	-0.29354300	-1.33631300	-3.05753300
H	-5.35583000	6.68781300	0.33883700	C	-2.16649000	-4.15870900	-3.35092000
H	-3.78183500	7.37867500	-0.06110400	H	-2.33405800	-5.68900500	-1.83981500
C	-3.16393400	-0.32567800	1.35555100	H	-1.79755500	-2.47265100	-4.64764100
C	-3.16426600	0.22106900	0.11435300	H	-2.82449800	-4.66351900	-4.05358600
C	-1.99776300	0.23704100	2.09403400	P	2.66421000	1.07878300	0.55749300
O	-1.58423400	-0.01779400	3.20497900	C	4.29759400	0.74177400	-0.24357800
C	-4.11706000	-1.25978800	1.99255600	C	5.20633800	-0.19744000	0.26774300
C	-5.46279600	-1.32298500	1.58249100	C	4.59414300	1.35972800	-1.47268700
C	-3.70848800	-2.08759100	3.05608400	C	6.39188300	-0.48709700	-0.41191200
C	-6.35646200	-2.19935800	2.19337900	H	4.99427600	-0.70371700	1.20360300
H	-5.81547200	-0.67382500	0.78992200	C	5.78422400	1.07693300	-2.14361700
C	-4.60713100	-2.96535600	3.66252300	H	3.88973800	2.05912200	-1.91089100
H	-2.69149800	-2.01690500	3.42017500	C	6.69043800	0.15512200	-1.61340600
C	-5.93260700	-3.03132800	3.23225800	H	7.08315300	-1.21537400	0.00422300
H	-7.39059700	-2.22598000	1.86000600	H	6.00027800	1.57679400	-3.08447600
H	-4.26887900	-3.59448500	4.48206800	H	7.61723300	-0.06485900	-2.13662300
H	-6.63146600	-3.71447300	3.70774800	C	2.87751000	0.56748100	2.32419400
C	-4.08032100	-0.08899100	-1.00999800	C	4.01750200	0.90957400	3.07361900
C	-4.08407400	-1.38280700	-1.55858900	C	1.80279700	-0.05296000	2.97246900
C	-4.97603500	0.86569400	-1.52503900	C	4.08860300	0.60272500	4.43095200
C	-4.95423700	-1.71029200	-2.59769900	H	4.84678700	1.42504200	2.59764300
H	-3.40023200	-2.13016800	-1.17010500	C	1.86669500	-0.34263000	4.33815500
C	-5.84973300	0.52939600	-2.55980900	H	0.90022700	-0.29302900	2.42343500
H	-5.00530300	1.86240900	-1.10153200	C	3.01172600	-0.02500100	5.06637400
C	-5.84068800	-0.75696100	-3.10170400	H	4.97809200	0.86700700	4.99736600
H	-4.93368100	-2.71412000	-3.01147100	H	1.01261900	-0.80922600	4.81905500
H	-6.54101000	1.27719600	-2.93929600	H	3.06507500	-0.25185200	6.12822000
H	-6.52109500	-1.01484000	-3.90898300	C	2.65934300	2.92123500	0.81570000
				C	3.74389400	3.76919000	0.55631200

C	1.49198200	3.47002000	1.37528400	H	8.33140000	-3.64404600	0.92393700
C	3.65714700	5.13691000	0.83234300	H	8.54805600	-3.74777100	-0.83026800
H	4.66312400	3.37149000	0.13995100	P	-2.65986600	-0.63969800	0.16053200
C	1.41084900	4.83323700	1.65659200	C	-4.05989800	-0.15997900	-0.94489400
H	0.64545000	2.82621300	1.59867900	C	-5.36099400	0.06747200	-0.46934800
C	2.49239800	5.67343500	1.38020200	C	-3.80673500	-0.02967100	-2.31999900
H	4.50733000	5.78041100	0.62017000	C	-6.38644800	0.41006800	-1.35253100
H	0.49890700	5.23760600	2.08782900	H	-5.57364300	-0.01769700	0.59177000
H	2.42767000	6.73718400	1.59350600	C	-4.83520800	0.30621900	-3.20153200
TS13				H	-2.80058400	-0.17598300	-2.69826800
Ni	-0.62890600	0.13522800	-0.40747000	C	-6.12679600	0.52753000	-2.71965800
C	1.36085200	0.71218100	0.84885200	H	-7.38841300	0.58698800	-0.97039200
C	0.82077800	1.23197100	-0.31369700	H	-4.62294700	0.40411500	-4.26274200
C	1.32057400	-0.76215800	1.12799500	H	-6.92616600	0.79667800	-3.40495100
O	0.88967500	-1.24144500	2.15775200	C	-3.19854000	-0.05447600	1.82695600
C	1.87651300	1.52951100	1.98632200	C	-3.93976100	-0.85049600	2.71256300
C	1.23155500	2.70078000	2.41613700	C	-2.85263900	1.25058000	2.21141700
C	3.04207500	1.12491600	2.66115400	C	-4.33260000	-0.34610500	3.95419500
C	1.74396900	3.45125000	3.47293500	H	-4.20337400	-1.86721100	2.43740400
H	0.32189700	3.02048800	1.91896100	C	-3.25121200	1.75483200	3.44897700
C	3.55540500	1.87677200	3.71658100	H	-2.26133600	1.86852600	1.54025800
H	3.55593200	0.21922000	2.34980000	C	-3.99156600	0.95613800	4.32345800
C	2.90935300	3.04482500	4.12633500	H	-4.90164300	-0.97446700	4.63424000
H	1.22680900	4.35283200	3.79100200	H	-2.97299900	2.76544100	3.73517200
H	4.46130500	1.54818800	4.21910500	H	-4.29378200	1.34459100	5.29229700
H	3.30692600	3.62968400	4.95149600	C	-2.77182000	-2.47972800	0.27706000
C	0.94699200	2.62994700	-0.76602800	C	-3.81342800	-3.21891500	-0.30225200
C	-0.18367000	3.36086200	-1.17217700	C	-1.74676700	-3.15713300	0.96203200
C	2.20631200	3.25539100	-0.81873500	C	-3.83262600	-4.61208600	-0.19667000
C	-0.06235700	4.68296700	-1.59592600	H	-4.61019400	-2.71187600	-0.83702600
H	-1.15892200	2.88280100	-1.15006600	C	-1.77772600	-4.54720000	1.07139000
C	2.32699100	4.57330900	-1.25340100	H	-0.92647400	-2.60531300	1.41427200
H	3.08677200	2.69775100	-0.51445600	C	-2.81734200	-5.27820500	0.49045100
C	1.19345000	5.29335600	-1.63986200	H	-4.64355000	-5.17376100	-0.65310200
H	-0.94837500	5.23540100	-1.89769100	H	-0.98127000	-5.05817300	1.60542400
H	3.30774300	5.04022100	-1.28974700	H	-2.83326000	-6.36199100	0.57023200
H	1.28903100	6.32195100	-1.97731700	CP24			
C	0.82621900	-0.12428500	-1.86608100	Ni	-0.69361200	0.04885100	-0.31525600
H	0.19897000	-1.03696600	-1.79389100	C	1.16869500	0.37999700	-0.79134500
C	2.25686900	-0.50015300	-1.79149200	C	0.90294700	0.75149000	0.57642900
H	2.91637700	-0.13880100	-2.57204400	C	1.59375900	-1.01222500	-1.15265100
C	0.47730300	0.52995700	-3.18072200	O	1.11763700	-1.63713300	-2.07901600
F	1.31514500	1.53487600	-3.51124200	C	1.29454900	1.34975400	-1.92971800
F	0.53558700	-0.36778700	-4.20085200	C	0.37938100	2.39961900	-2.12871500
F	-0.78345500	1.03510700	-3.19480900	C	2.35707900	1.22809700	-2.84353700
C	2.75453700	-1.23739000	-0.78621100	C	0.52295300	3.28988700	-3.19202800
O	1.87933600	-1.65462300	0.22198500	H	-0.45116600	2.51653200	-1.44050200
C	4.13495100	-1.71036400	-0.60653200	C	2.50054900	2.11638900	-3.90840900
C	5.12824800	-1.49672200	-1.58340200	H	3.08528500	0.43101400	-2.71930000
C	4.50367800	-2.39964100	0.56106500	C	1.58364800	3.15324000	-4.08913600
C	6.42979000	-1.93780700	-1.38657500	H	-0.20153100	4.08993500	-3.32077800
H	4.88209400	-0.98615400	-2.50966400	H	3.33370800	1.99725100	-4.59625200
C	5.81428500	-2.84049800	0.74708700	H	1.69343800	3.84519100	-4.91986600
H	3.75460400	-2.59963300	1.31923900	C	0.94367700	2.19901000	0.99431900
C	6.80352400	-2.61827200	-0.21535900	C	2.11914700	2.94839600	0.81851500
H	7.17347700	-1.75601800	-2.15973400	C	-0.16105600	2.82689800	1.58937100
H	6.06851700	-3.37163400	1.66162900	C	2.18750900	4.28091100	1.22487400
C	8.22401000	-3.09000900	-0.01397500	H	2.98116700	2.48125600	0.35160500
H	8.92620700	-2.24677400	0.01509500	C	-0.09486000	4.16139800	1.99325700

H	-1.07777200	2.26493800	1.73481700	H	-6.92003500	0.88483800	2.33901100
C	1.07955500	4.89390900	1.81340800	H	-4.46884500	4.00693700	0.67649500
H	3.10711200	4.84147400	1.07714900	H	-6.48575300	3.30219400	1.95275500
H	-0.96443800	4.62740300	2.45005900				
H	1.13118300	5.93316800	2.12748000	CP25			
C	1.37978600	-0.28556200	1.63048000	Ni	0.65826600	0.02050600	0.02890900
H	0.93298500	-1.25461800	1.37995700	P	1.94995000	1.67396100	-0.86720600
C	2.87937900	-0.42428700	1.54894100	C	3.57112300	1.23399400	-1.67448800
H	3.50049800	0.05439900	2.29589700	C	4.64511600	0.86585000	-0.84463400
C	0.93514100	-0.03238300	3.06063900	C	3.76793900	1.22324700	-3.06367700
F	1.22322900	-1.10622700	3.83370700	C	5.87428800	0.49531500	-1.38773600
F	1.53714200	1.03082400	3.63042100	H	4.52349800	0.87447000	0.23354700
F	-0.40531800	0.16533700	3.15240700	C	4.99971500	0.84468900	-3.60701000
C	3.42461800	-1.06574300	0.50550000	H	2.96451000	1.51718600	-3.73005800
O	2.59601400	-1.66146600	-0.44476000	C	6.05573000	0.47891200	-2.77307700
C	4.85712300	-1.29732600	0.23881200	H	6.68823400	0.21479900	-0.72472300
C	5.84942500	-0.93177800	1.16807500	H	5.13106700	0.84646300	-4.68621600
C	5.26970900	-1.89606700	-0.96183400	H	7.01279600	0.18626100	-3.19684200
C	7.19473600	-1.14188600	0.89390300	C	2.46440000	3.14588000	0.13002500
H	5.57039100	-0.48771300	2.11876600	C	3.43921500	4.05329300	-0.32006700
C	6.62313800	-2.10600100	-1.22601300	C	1.86756400	3.36038600	1.37954000
H	4.52400100	-2.20828100	-1.68407900	C	3.79927700	5.15112600	0.46115800
C	7.61172200	-1.73085200	-0.311108200	H	3.92056500	3.89866200	-1.28115000
H	7.93870300	-0.85006400	1.63206100	C	2.22740500	4.46144500	2.16076100
H	6.91278100	-2.57424800	-2.16396300	H	1.11359600	2.67032000	1.74084500
C	9.07855700	-1.94041300	-0.60327800	C	3.19381600	5.35762300	1.70412400
H	9.59441200	-2.40510200	0.24547700	H	4.55410700	5.84497400	0.10016800
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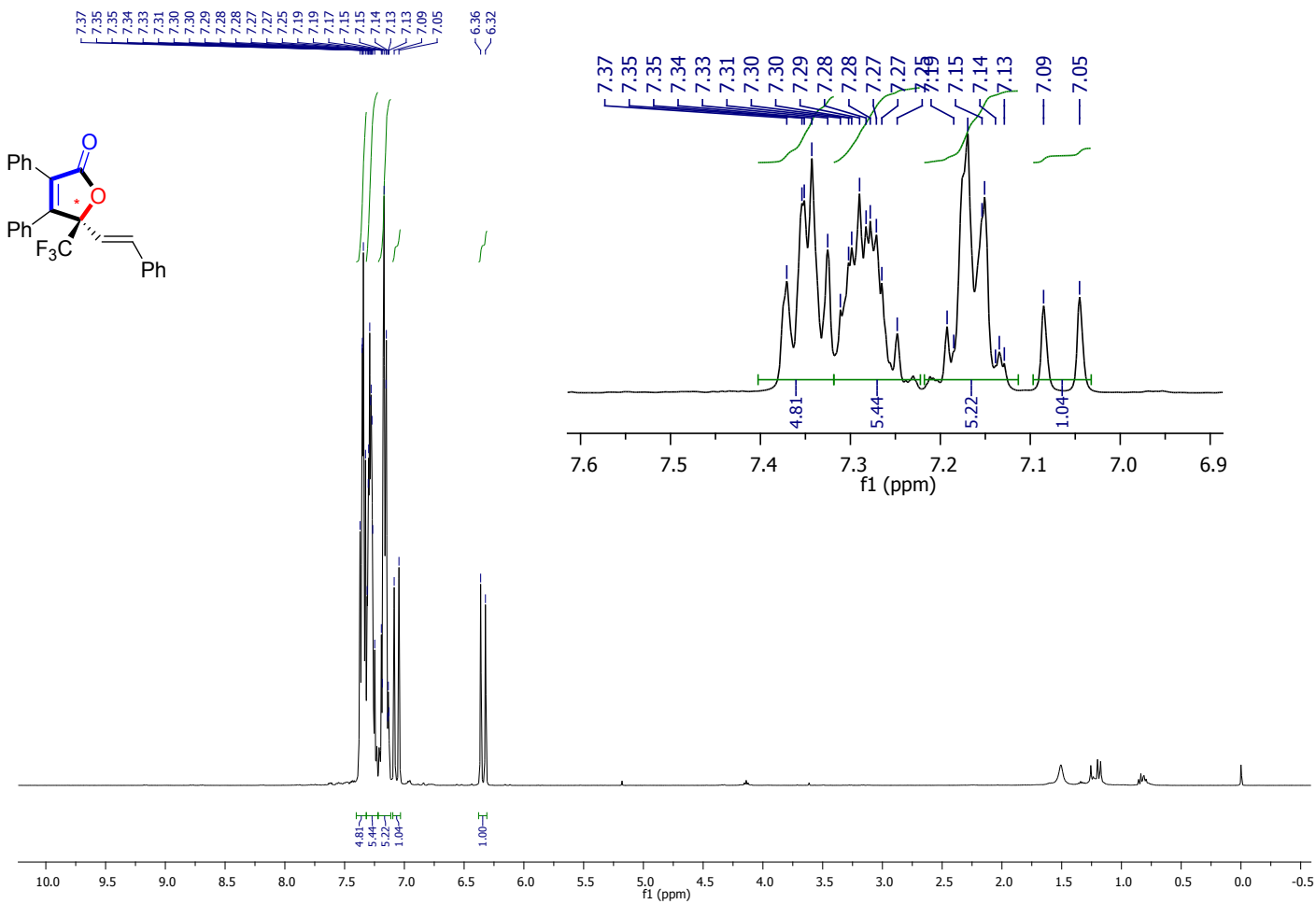
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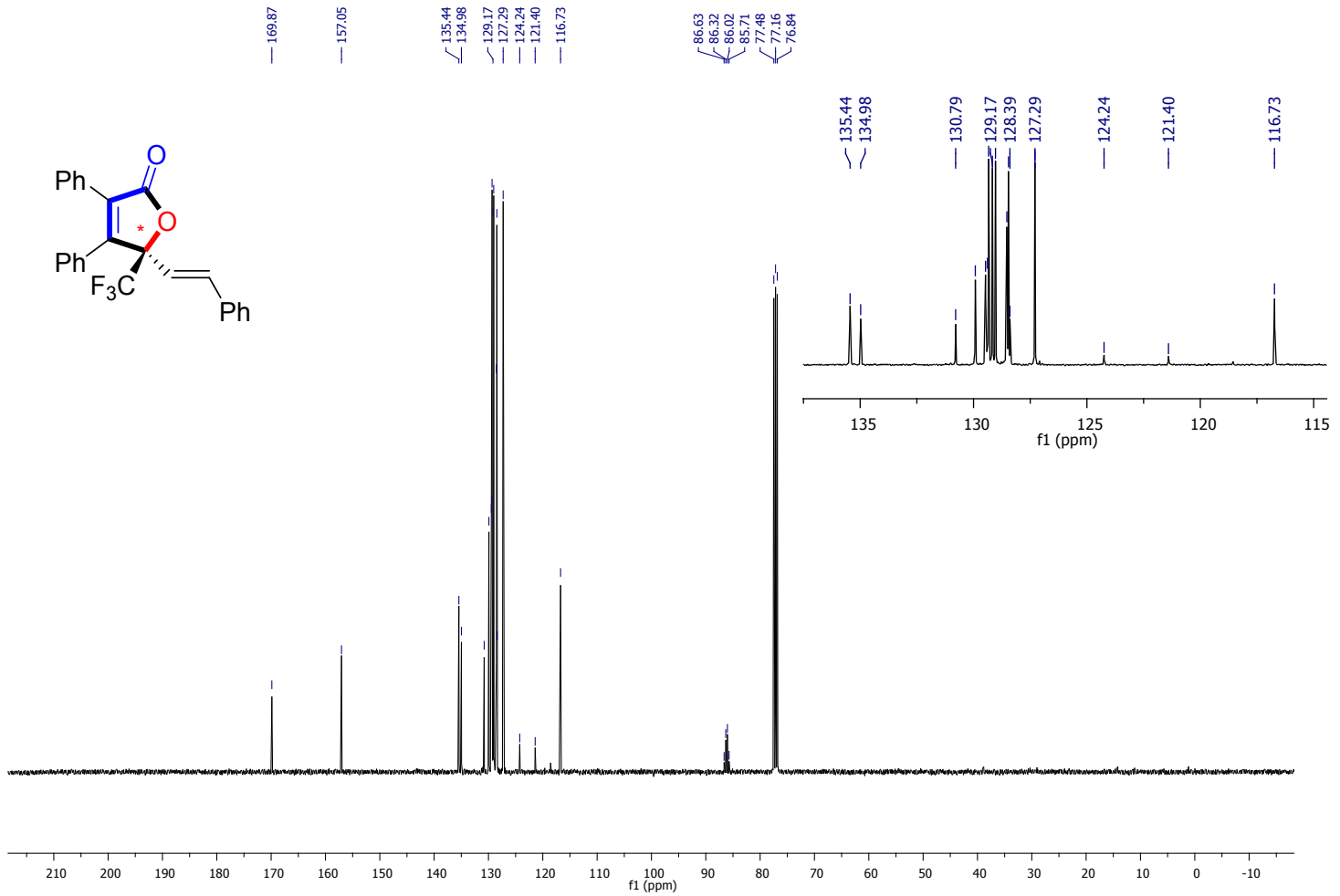
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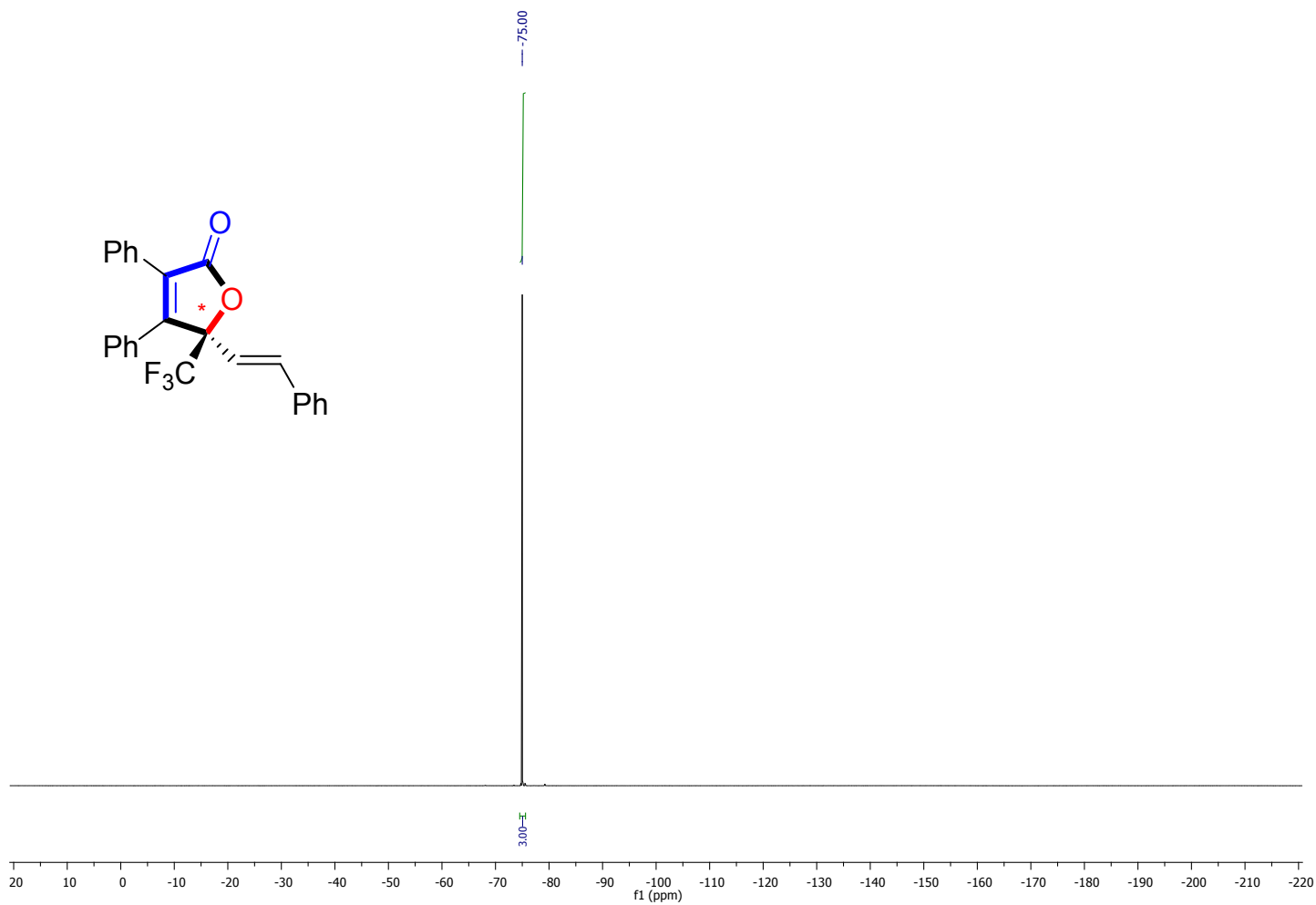
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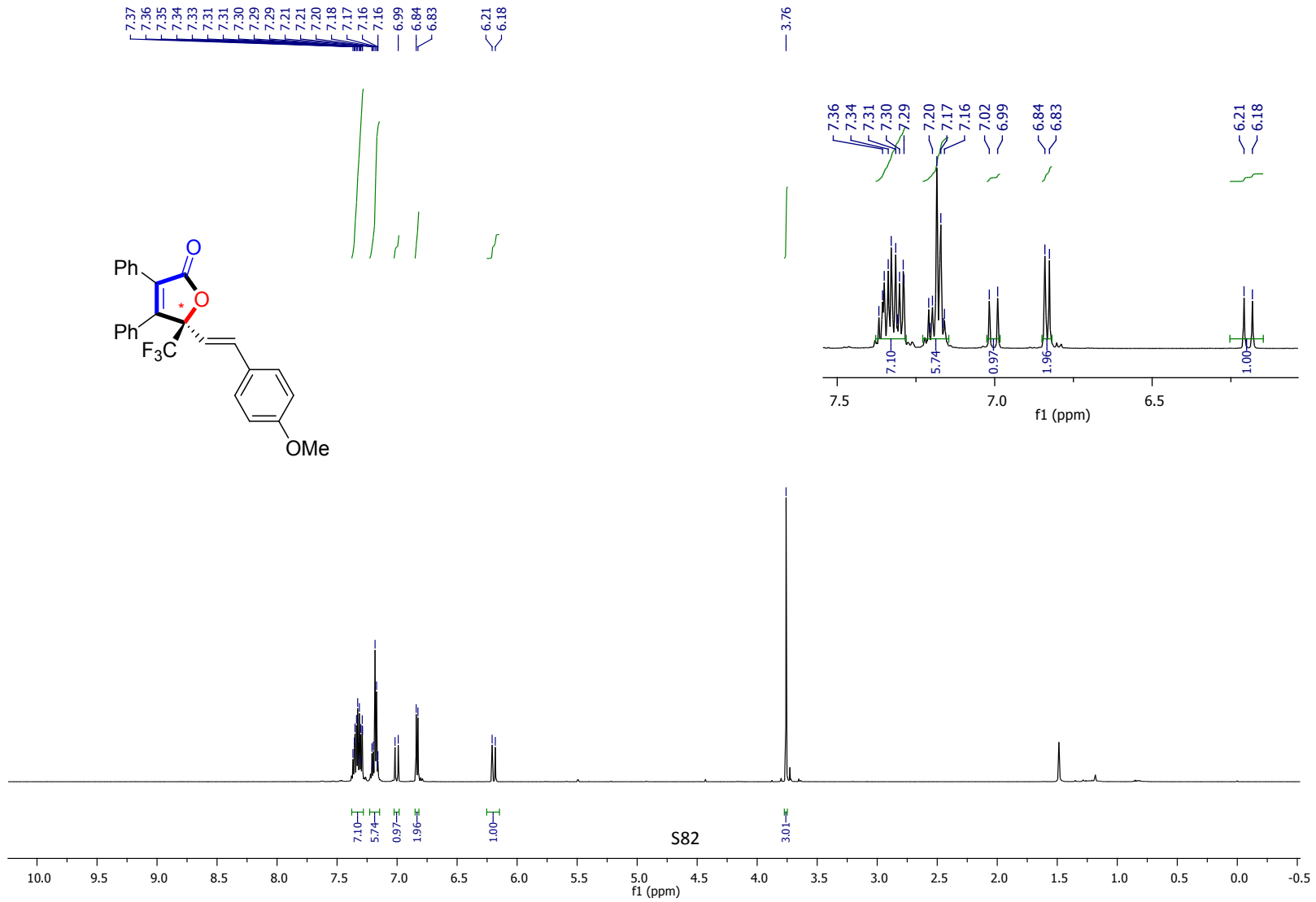
9. NMR Spectra

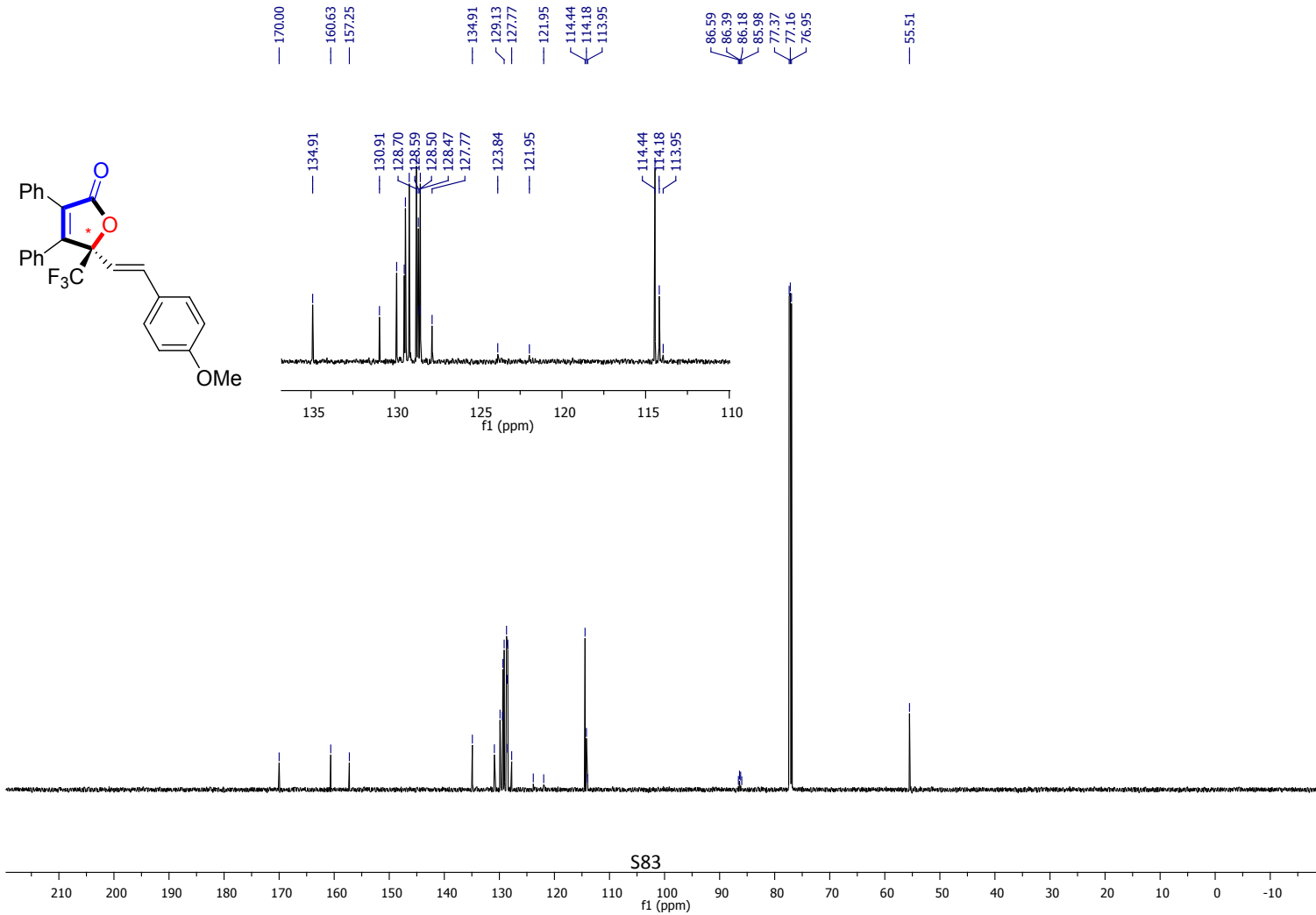


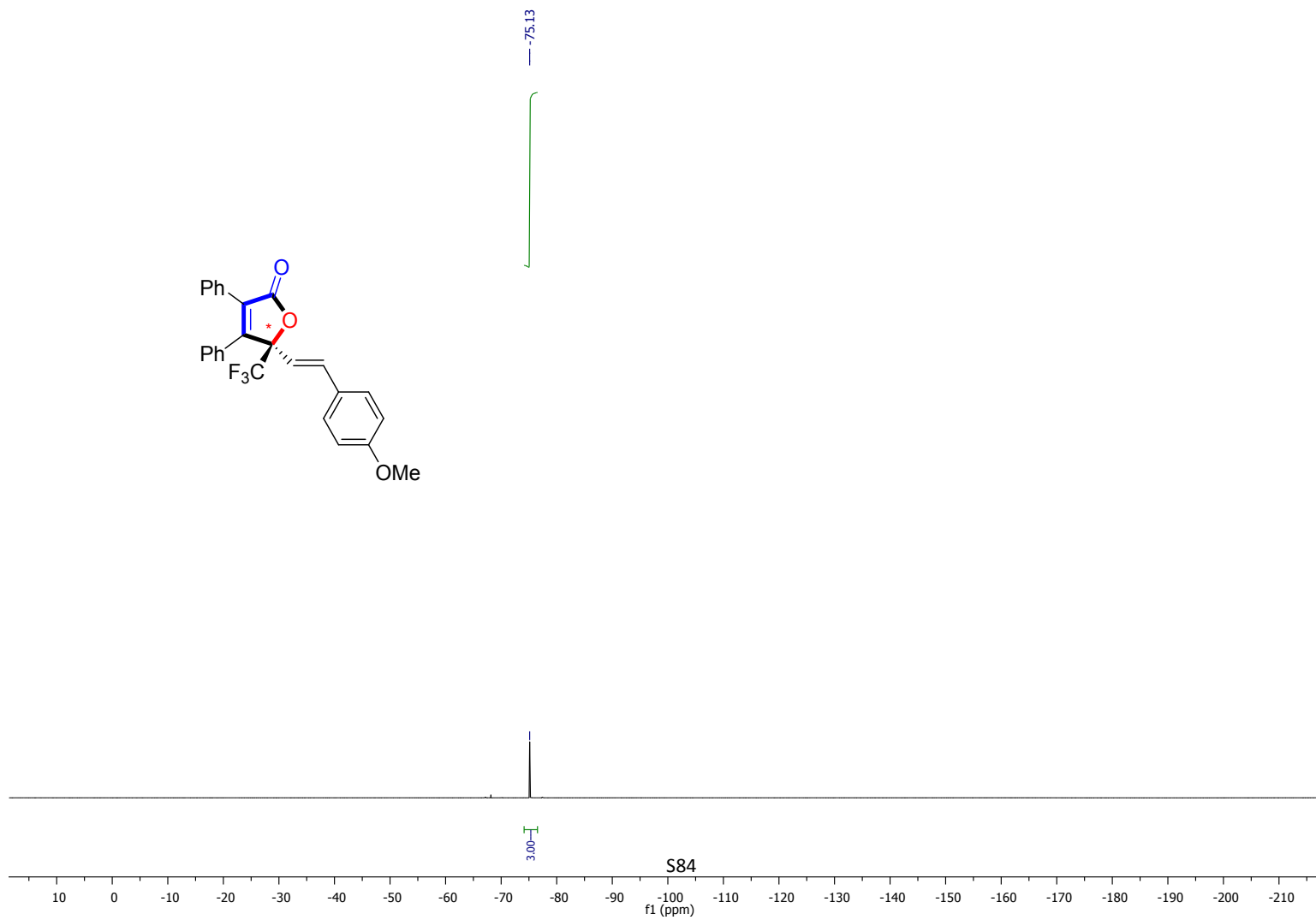
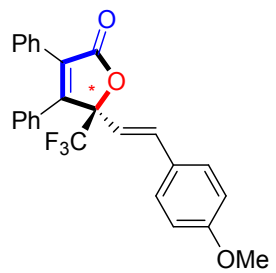




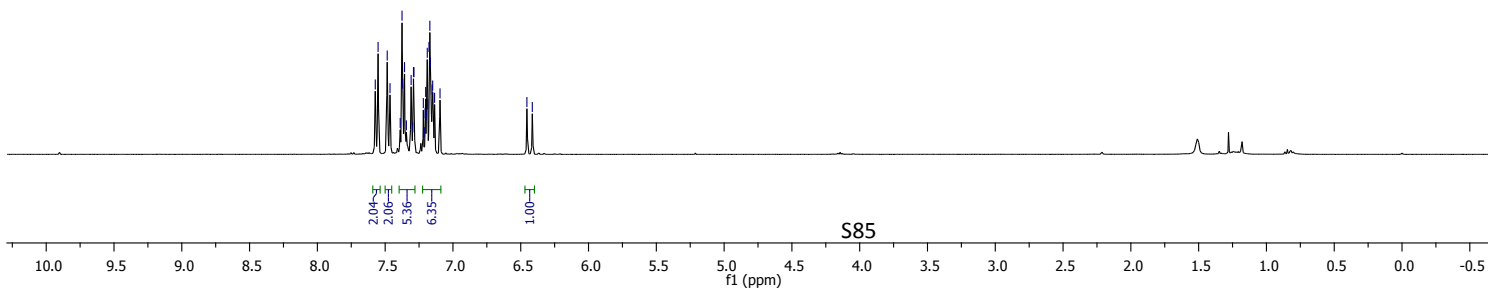
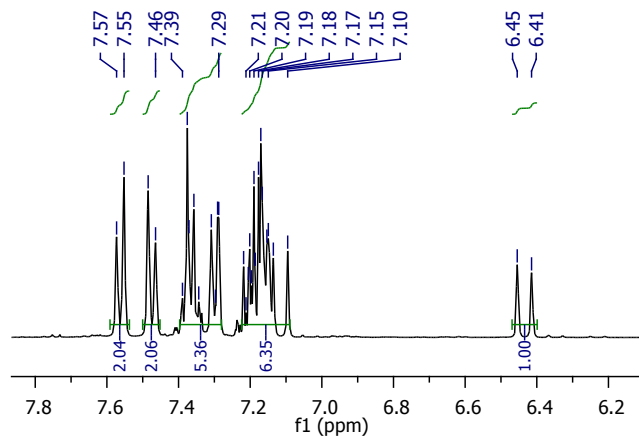
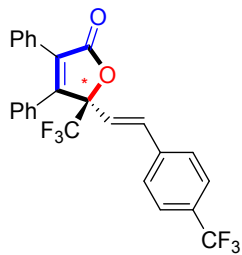
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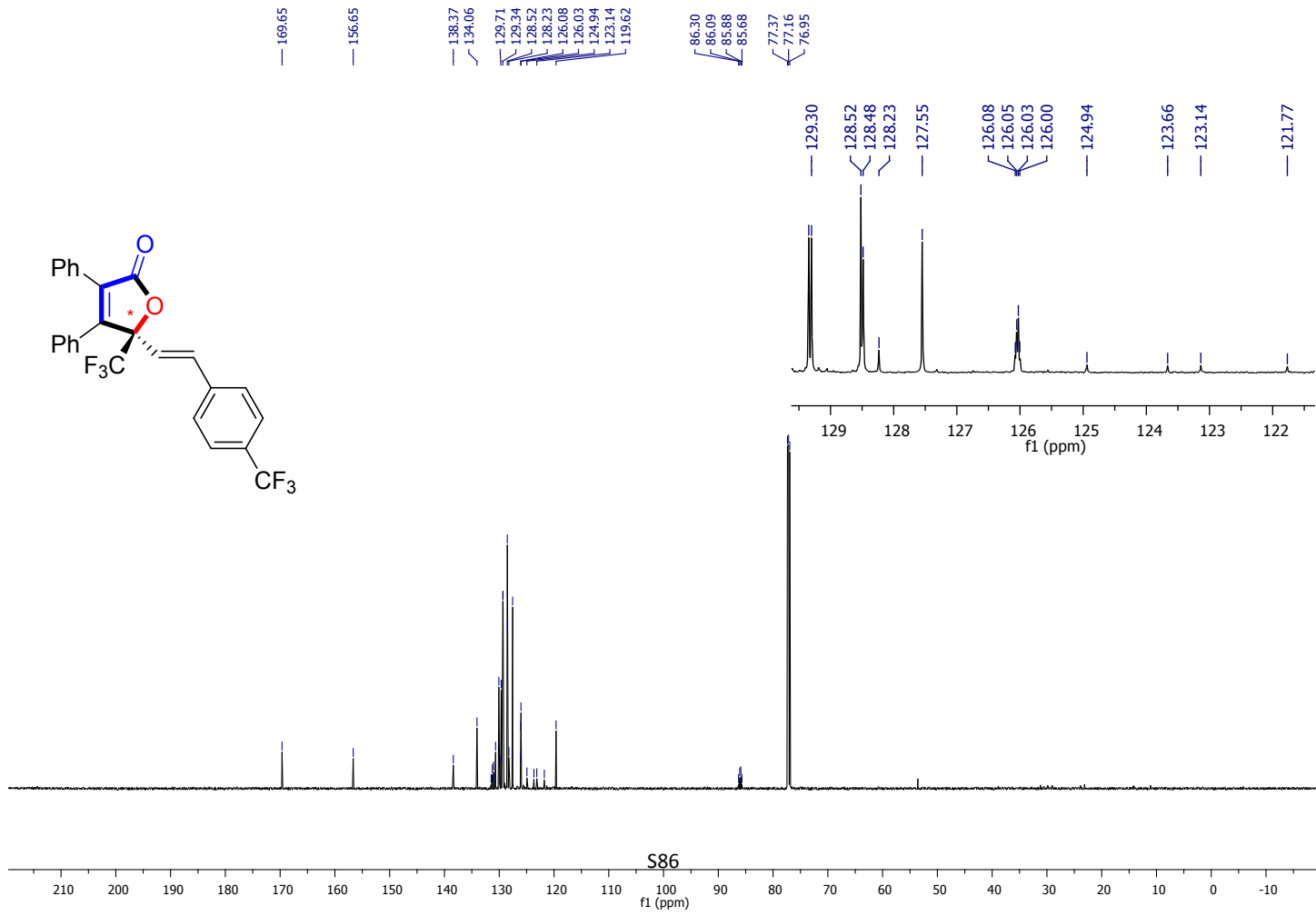




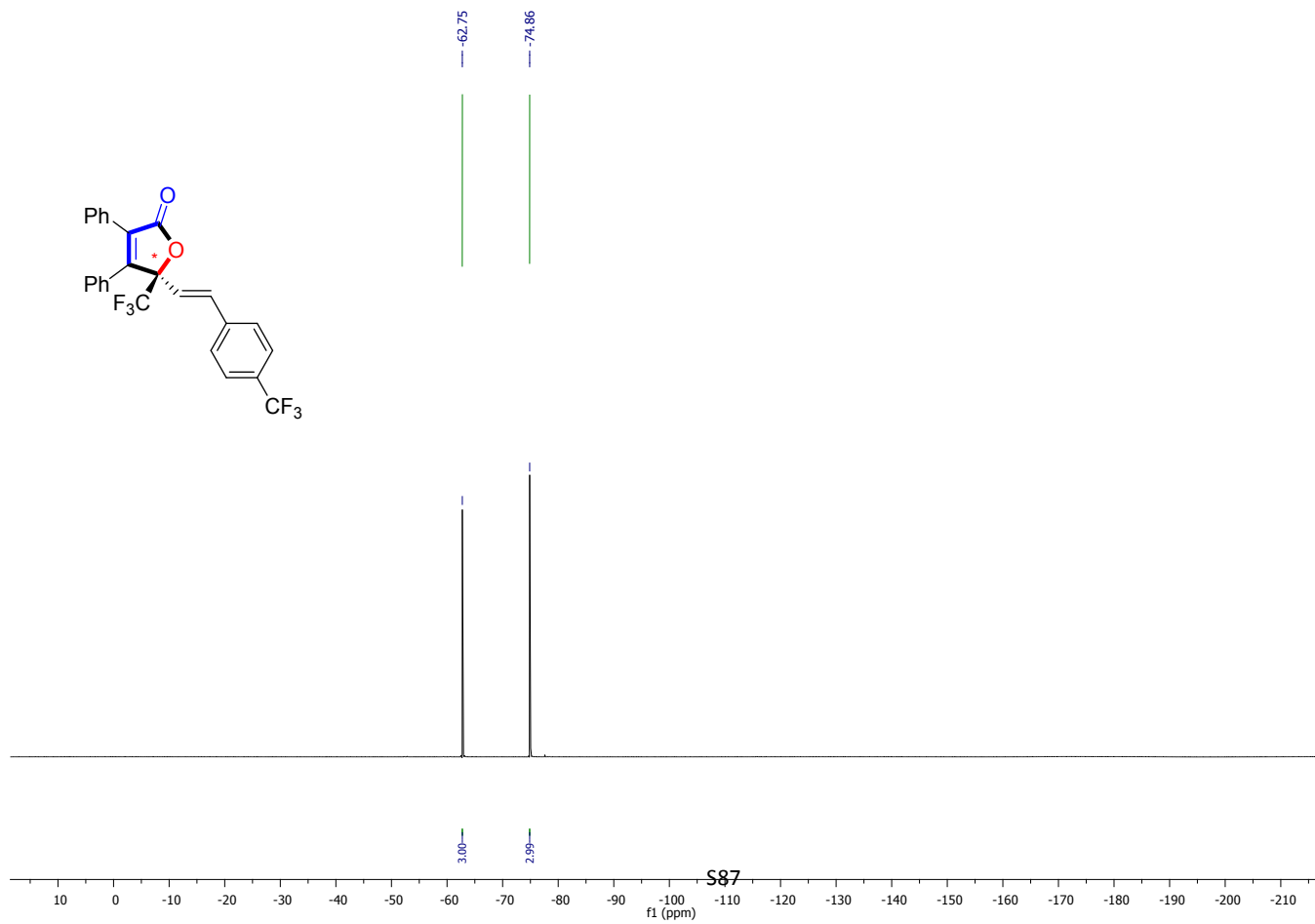
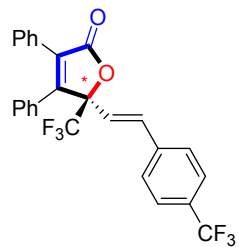


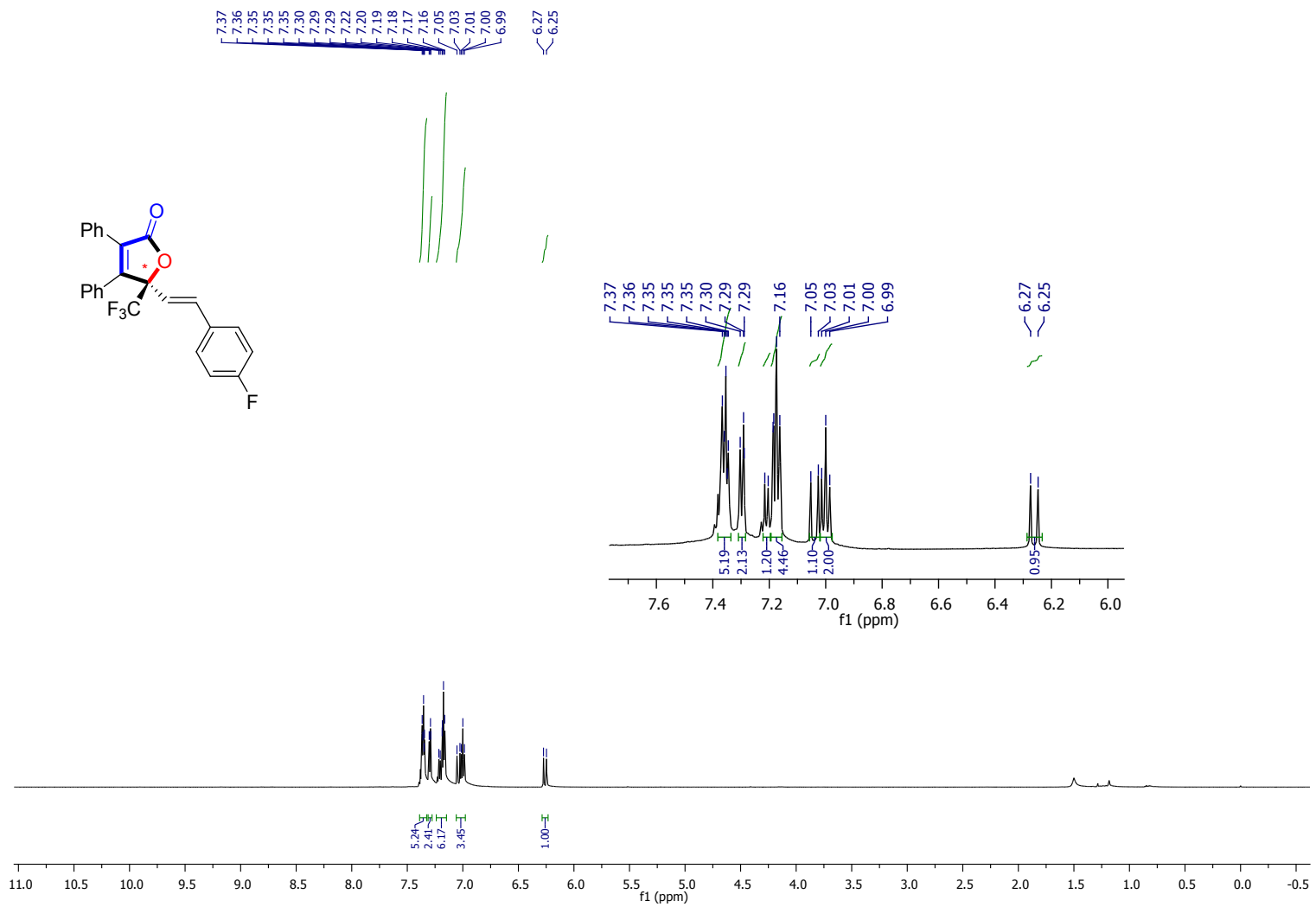
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6.41

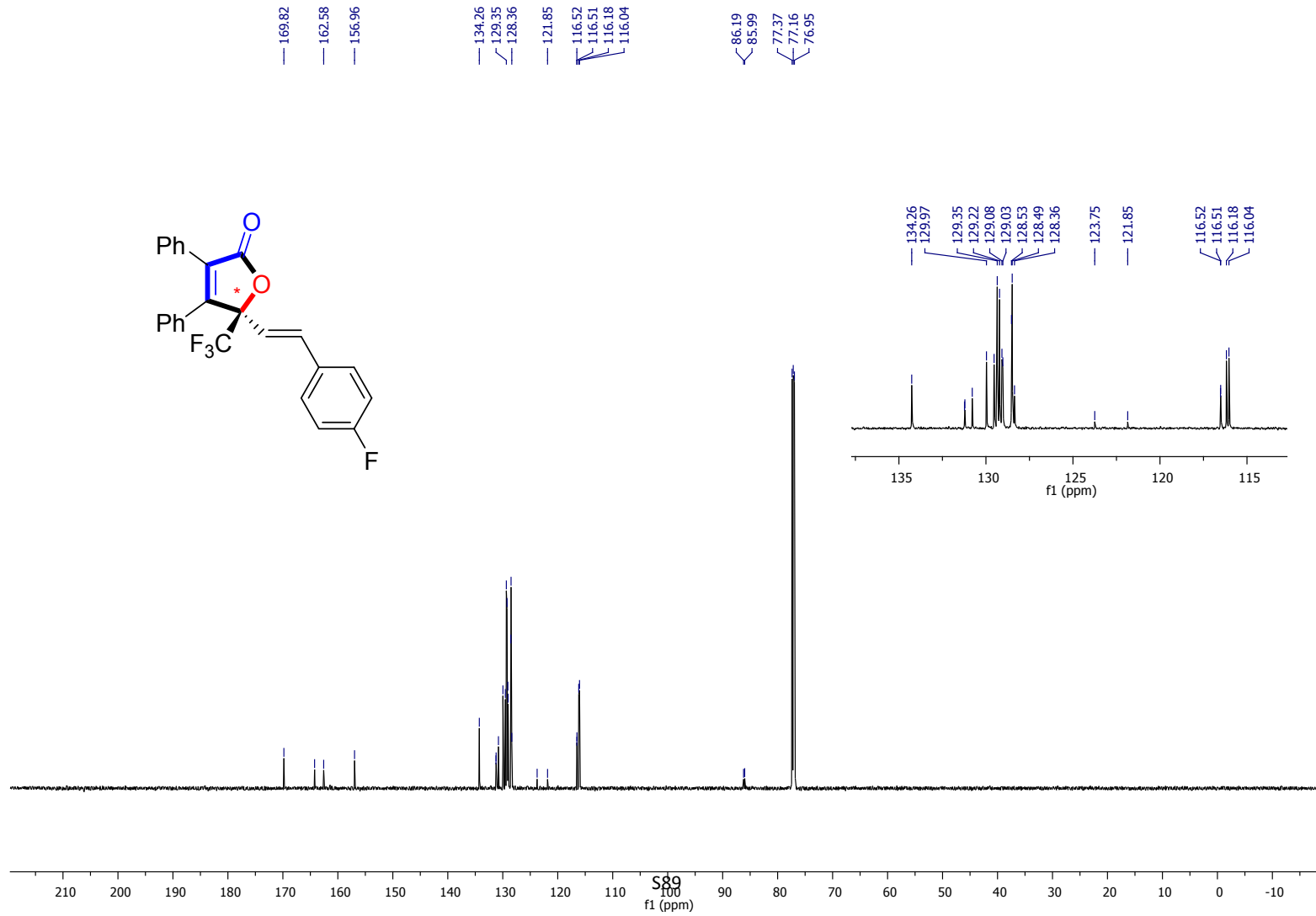
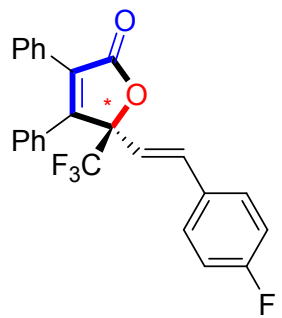


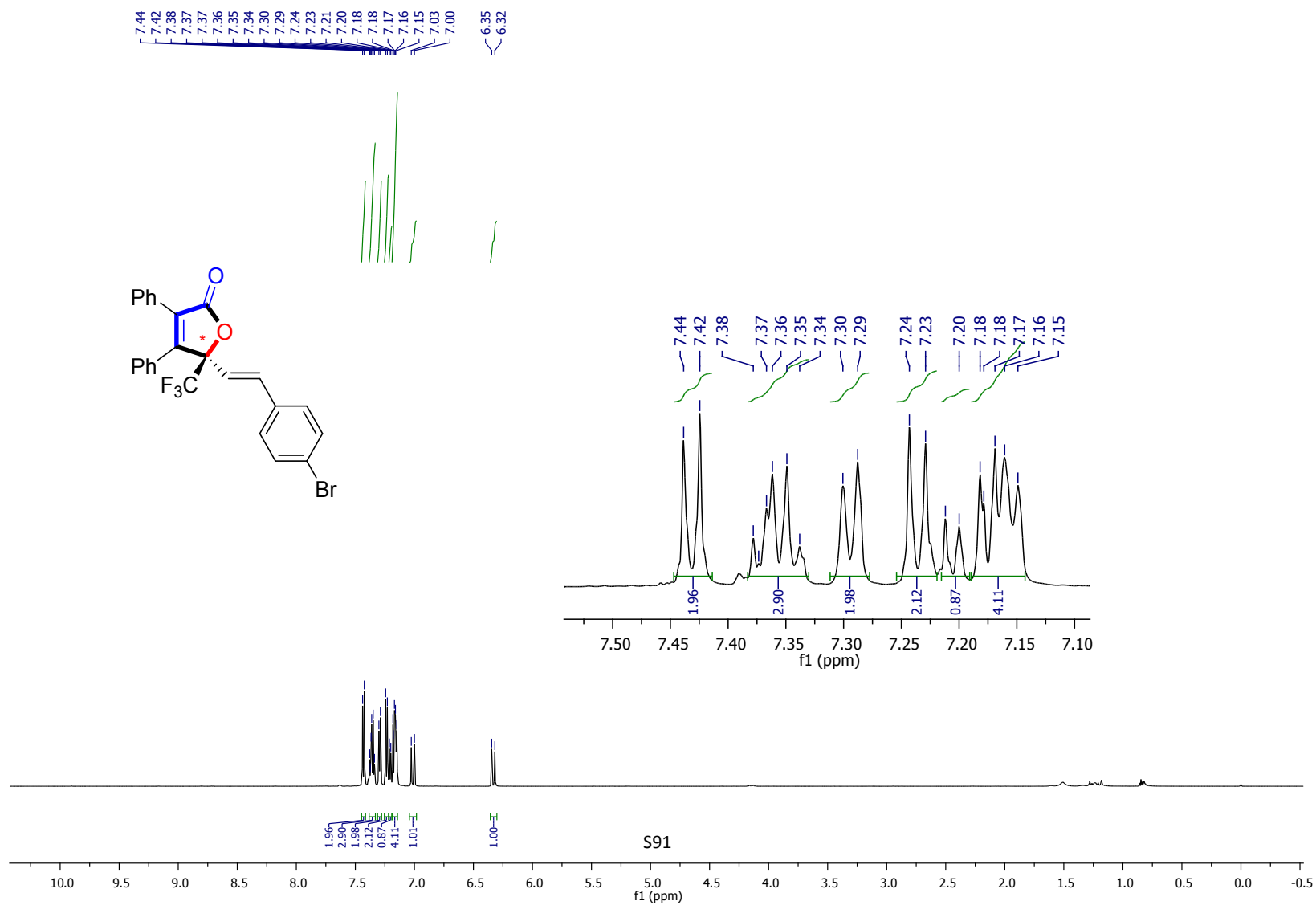


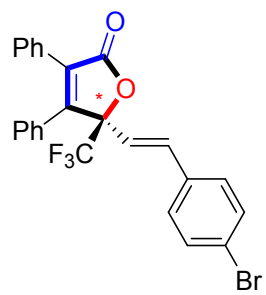
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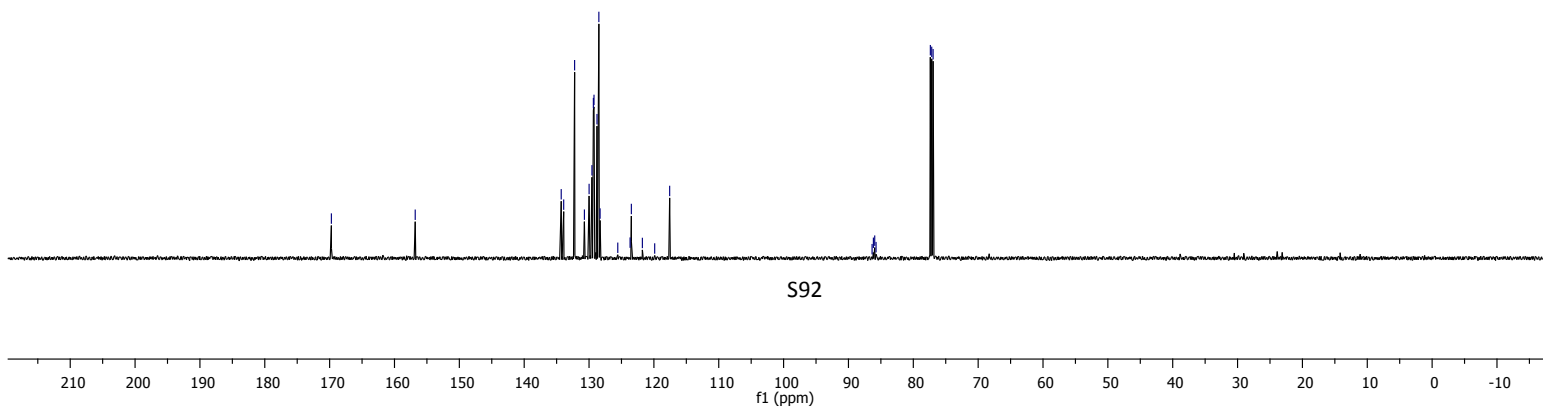
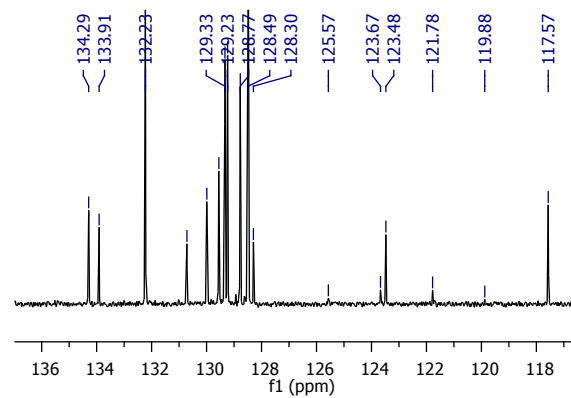


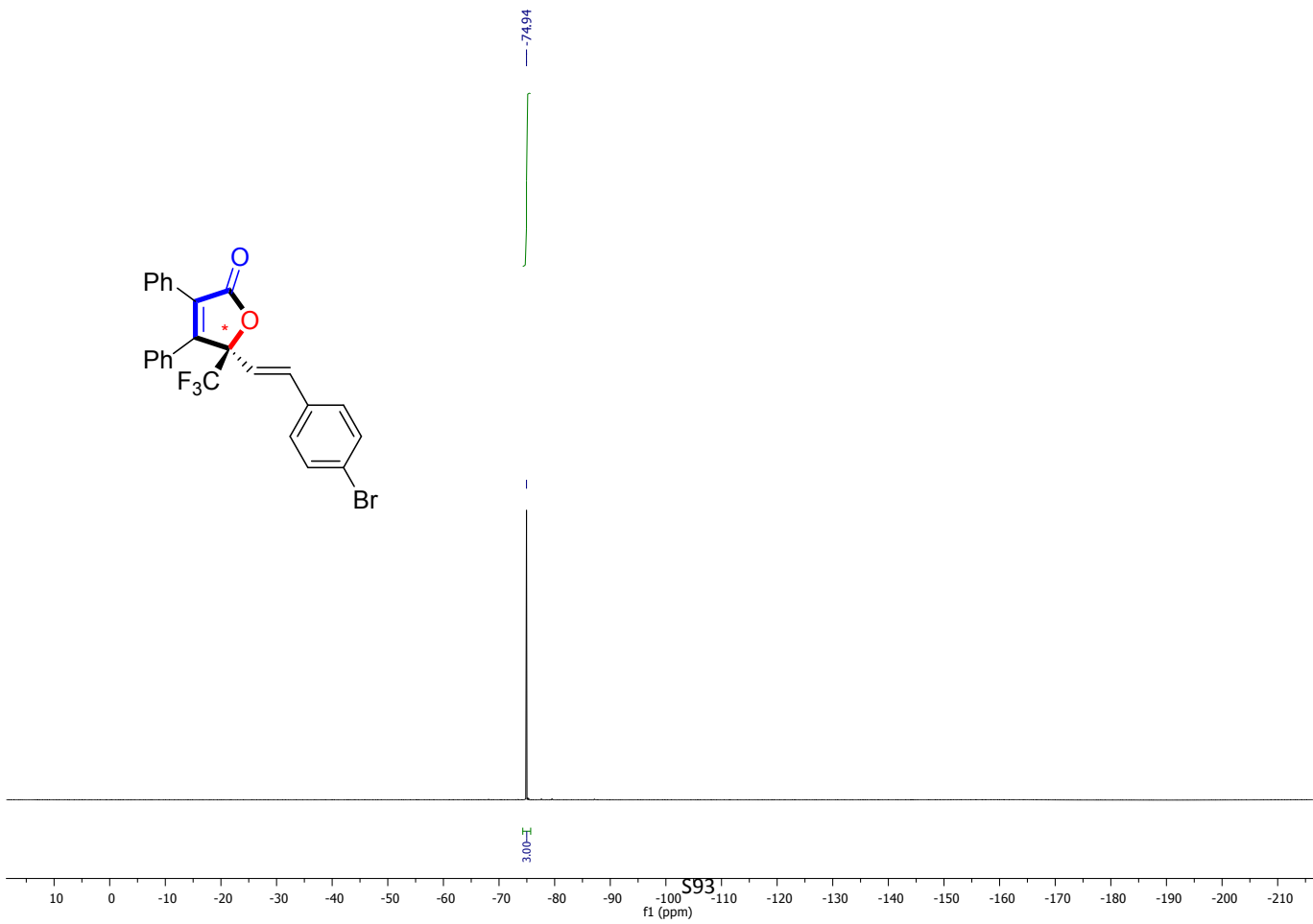
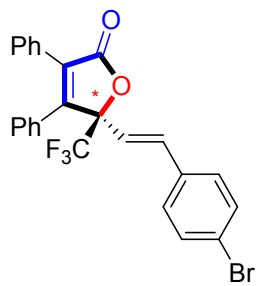
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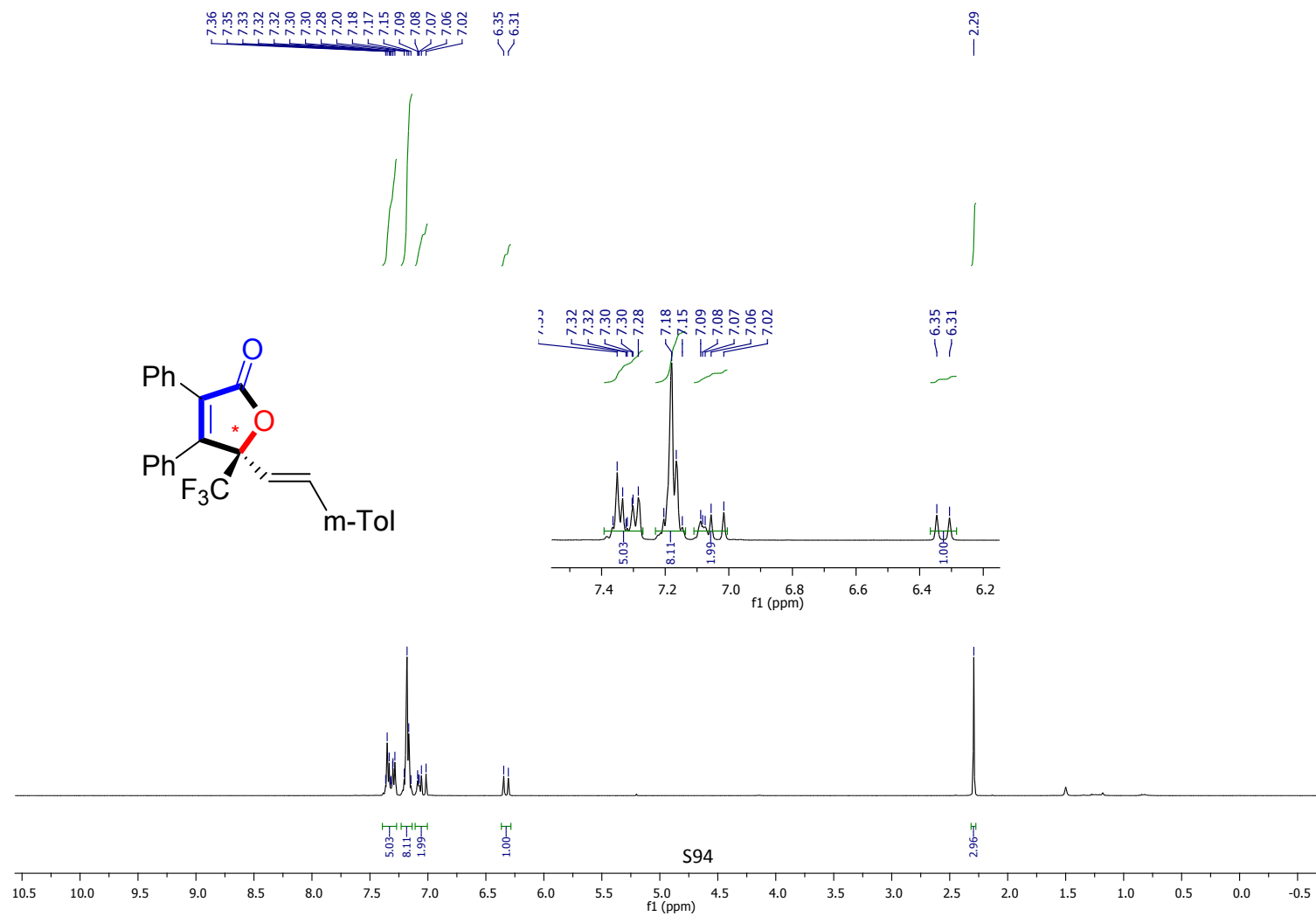
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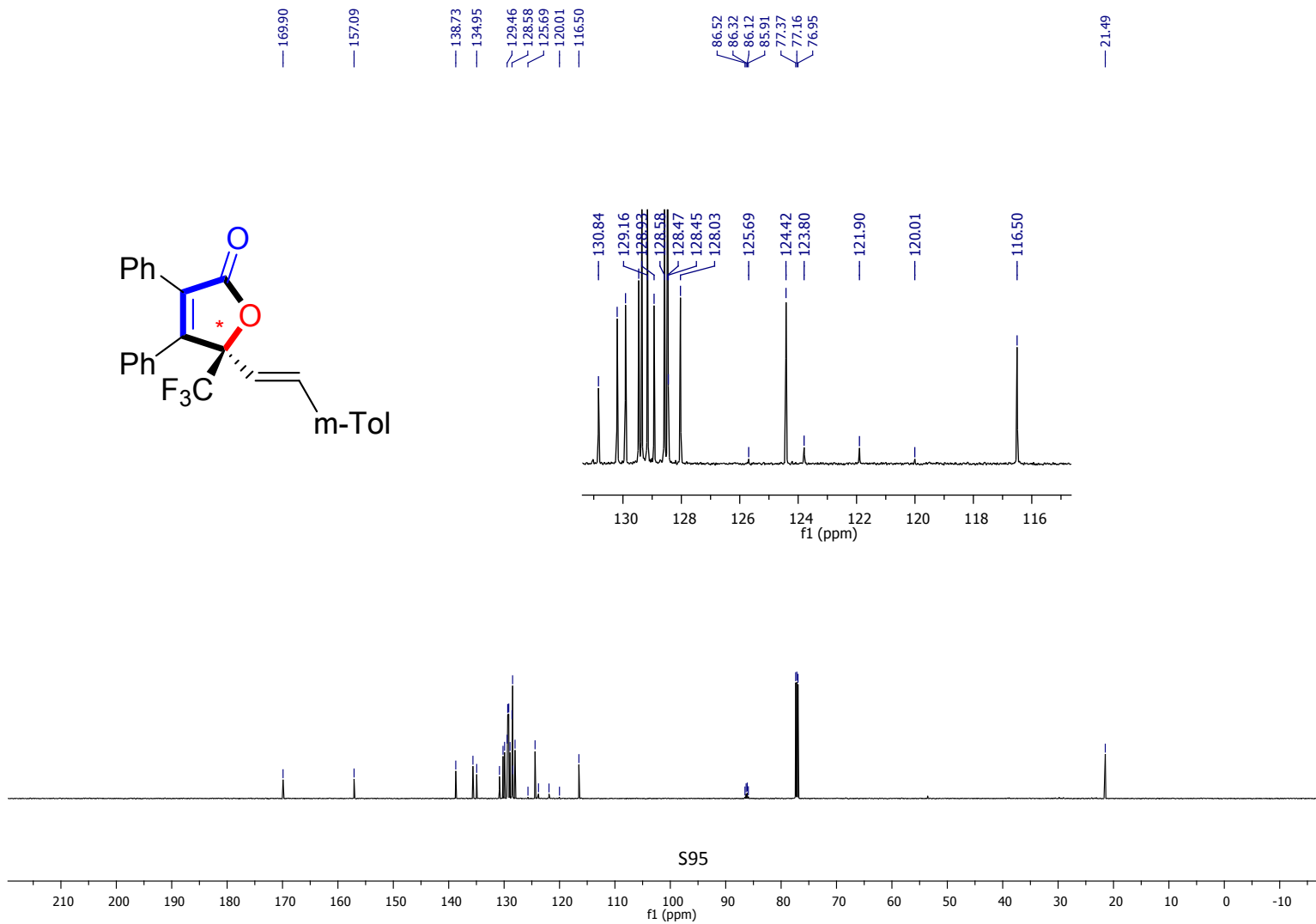
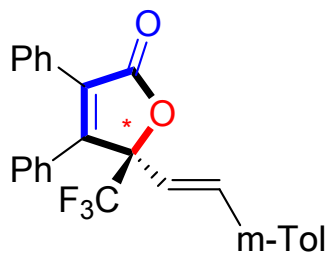
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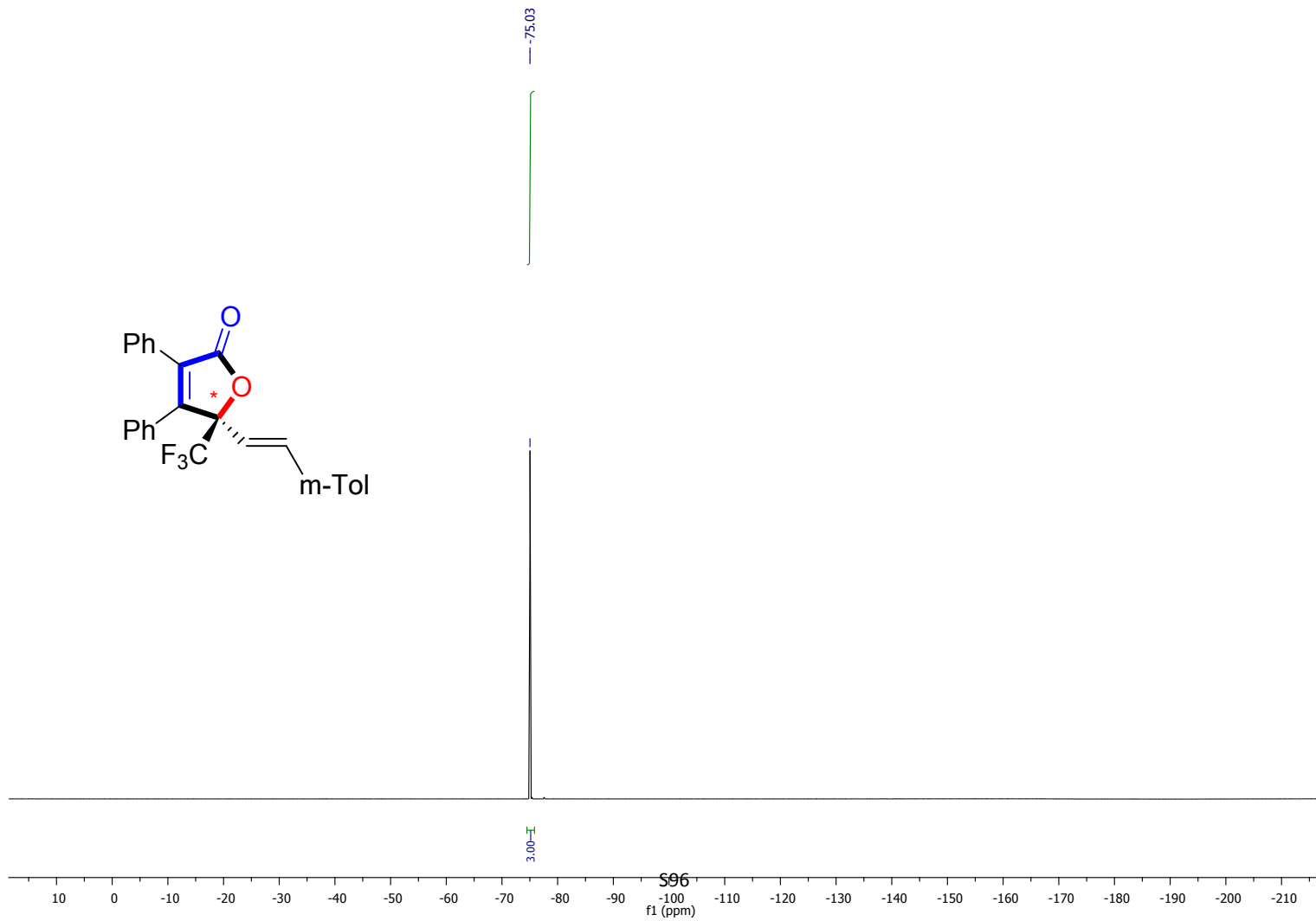
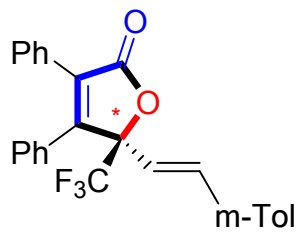


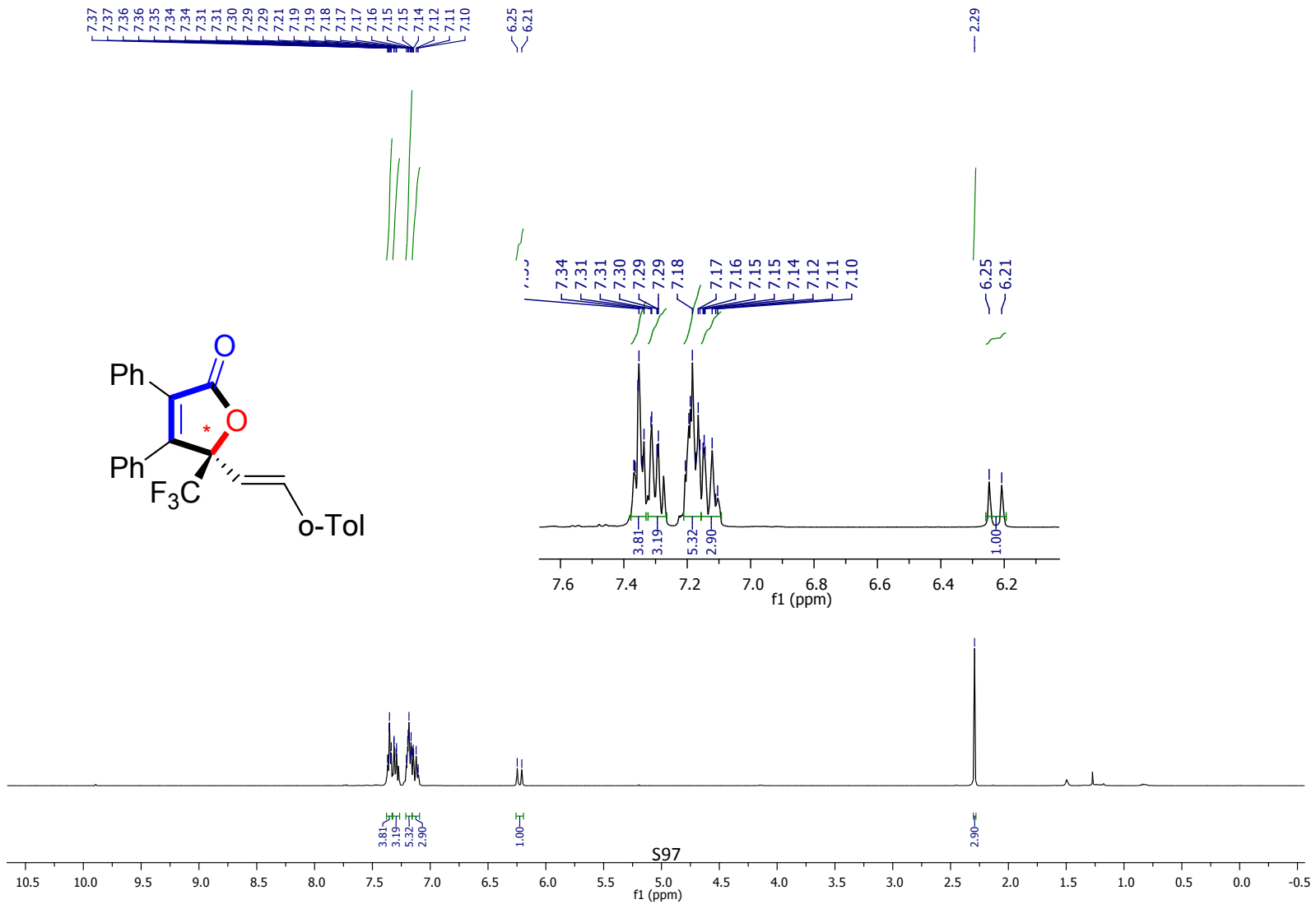
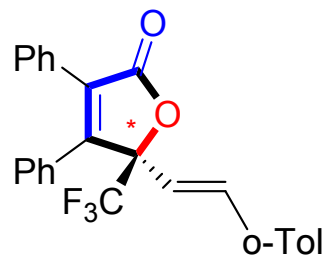


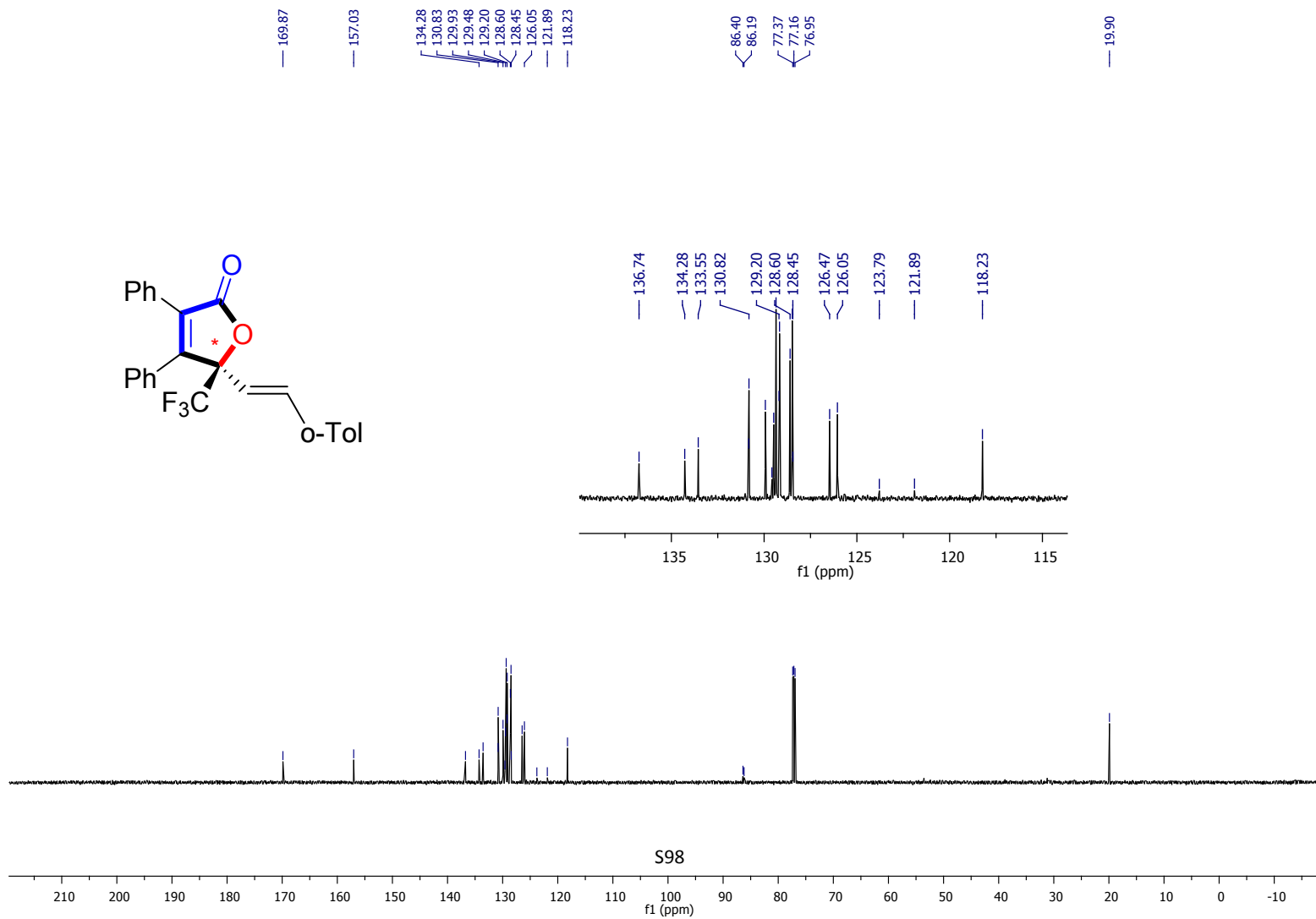
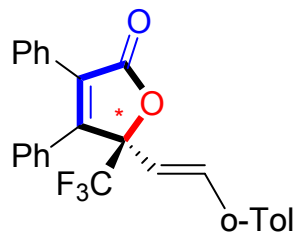




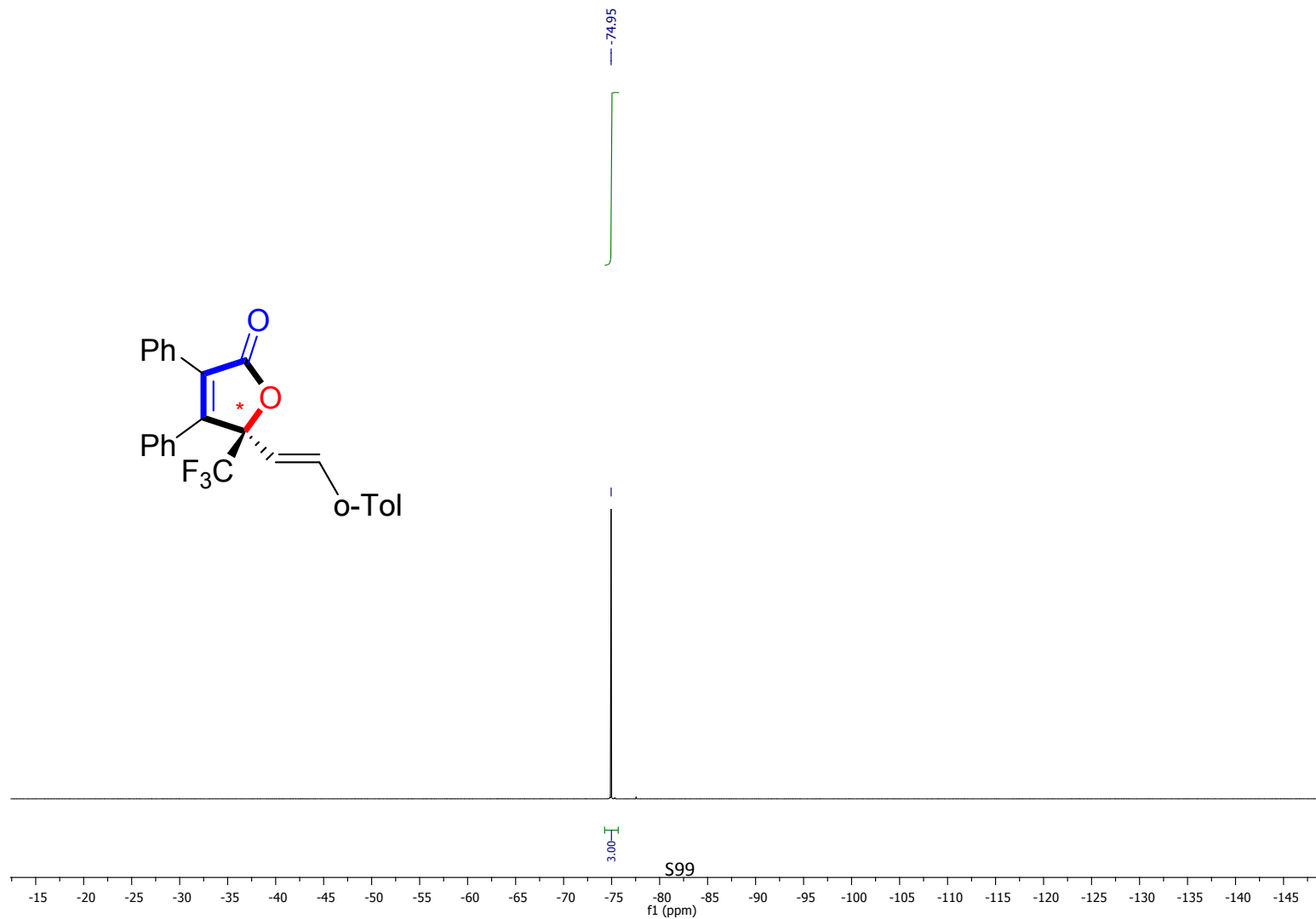
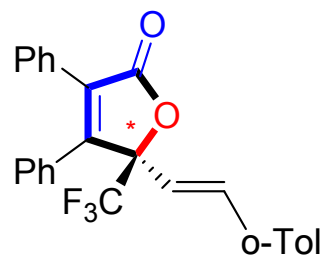
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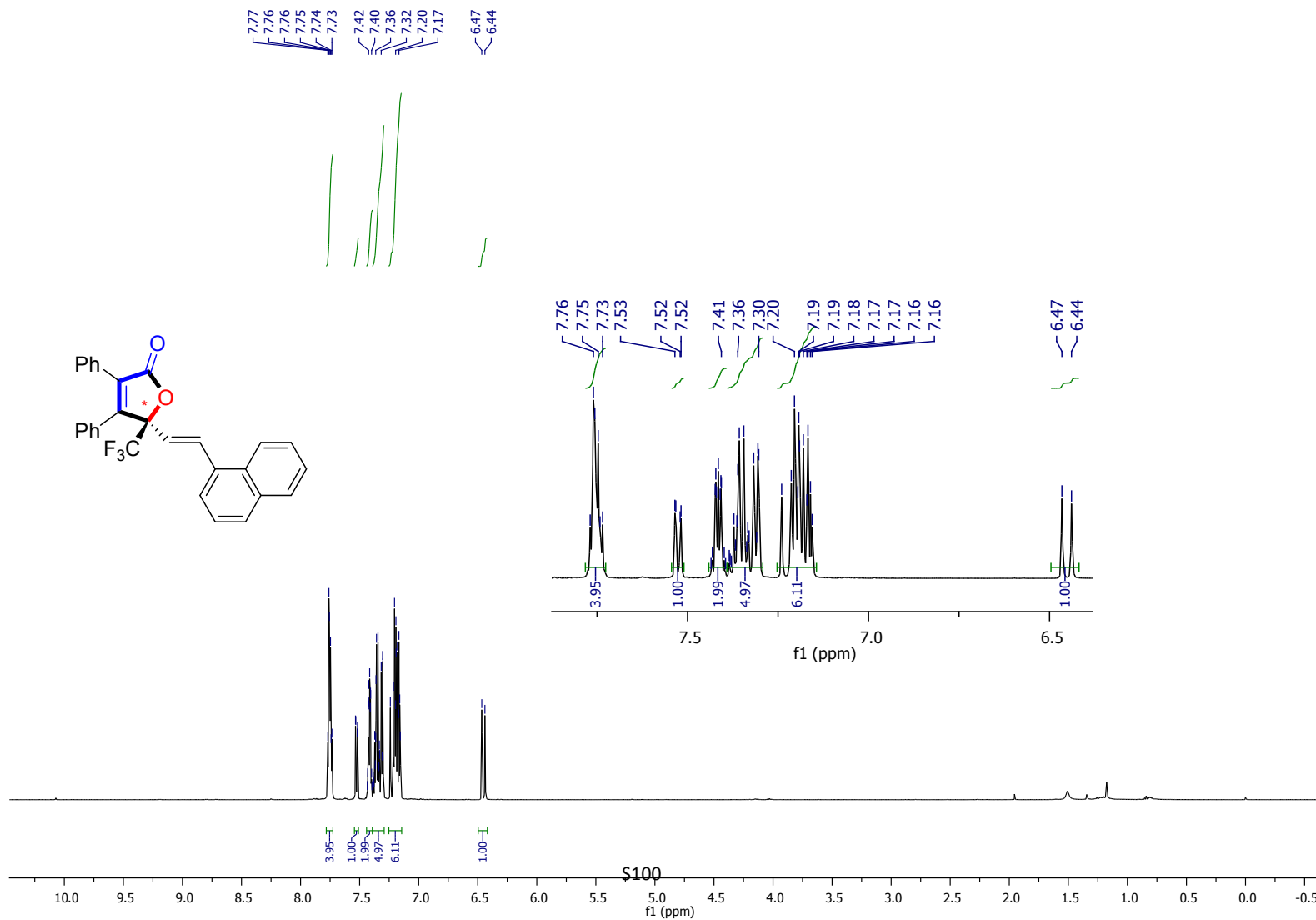


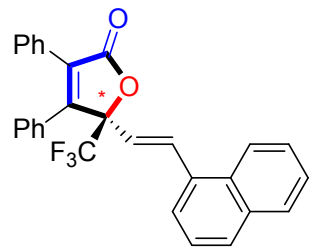




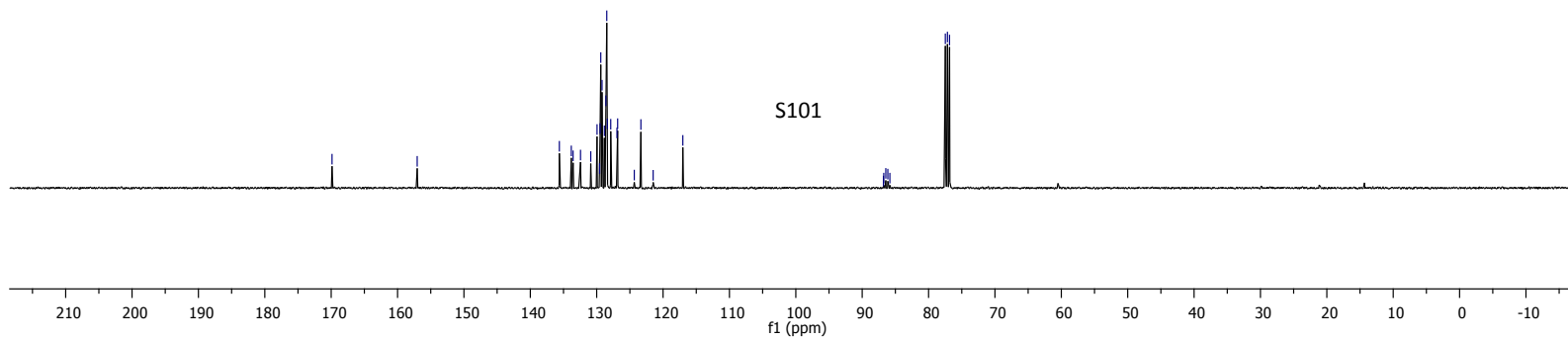
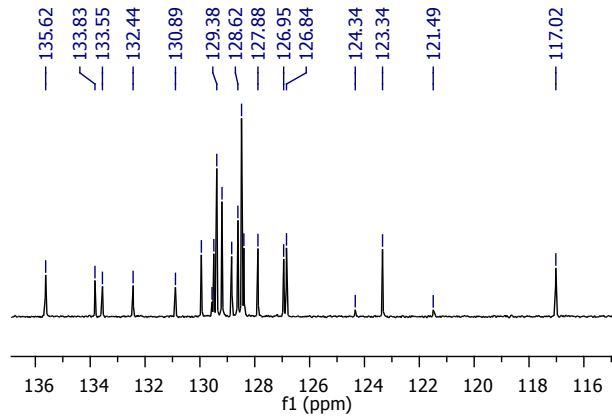
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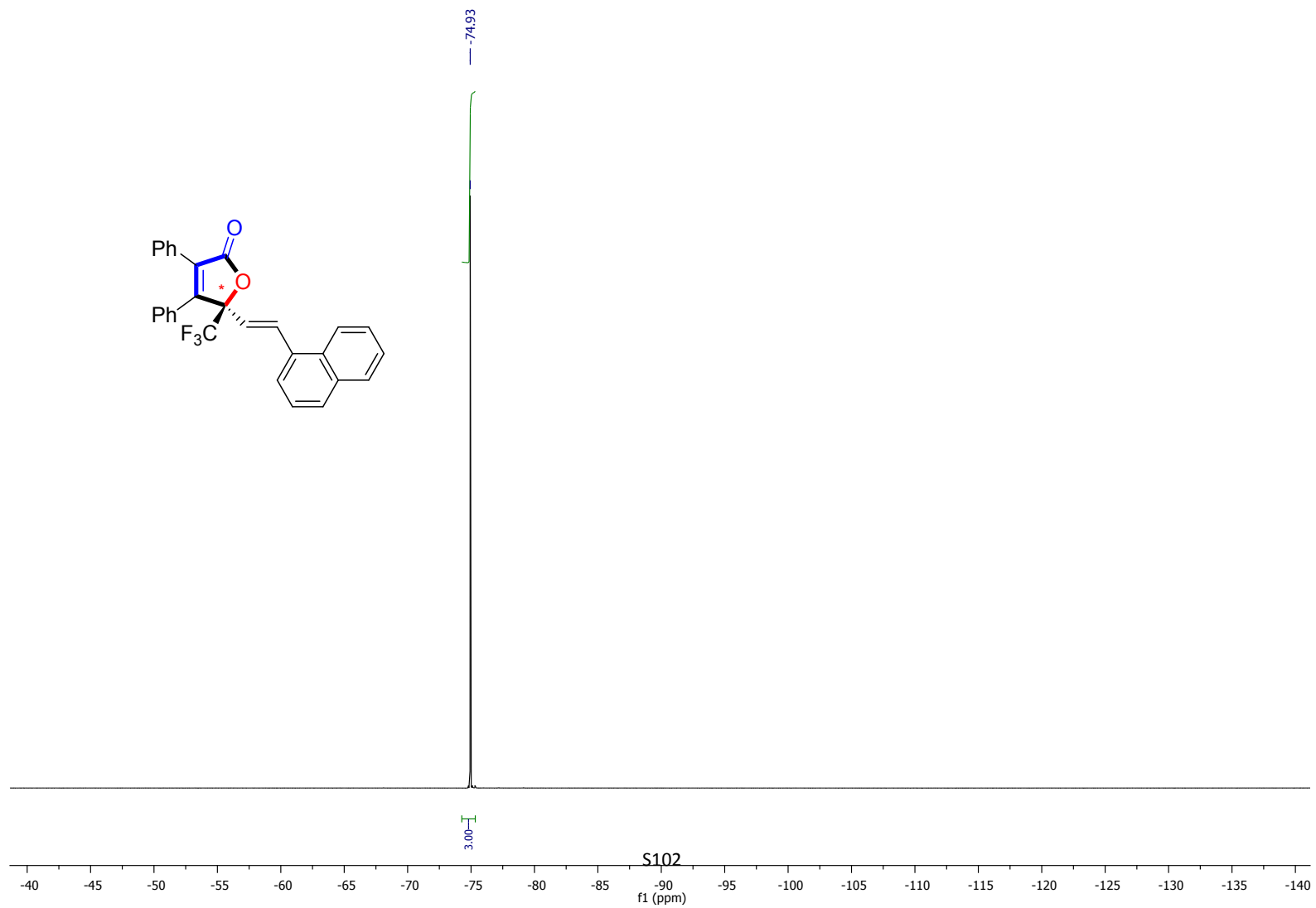
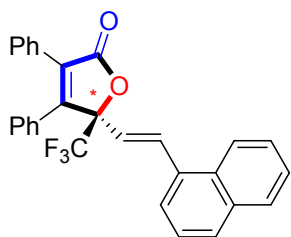


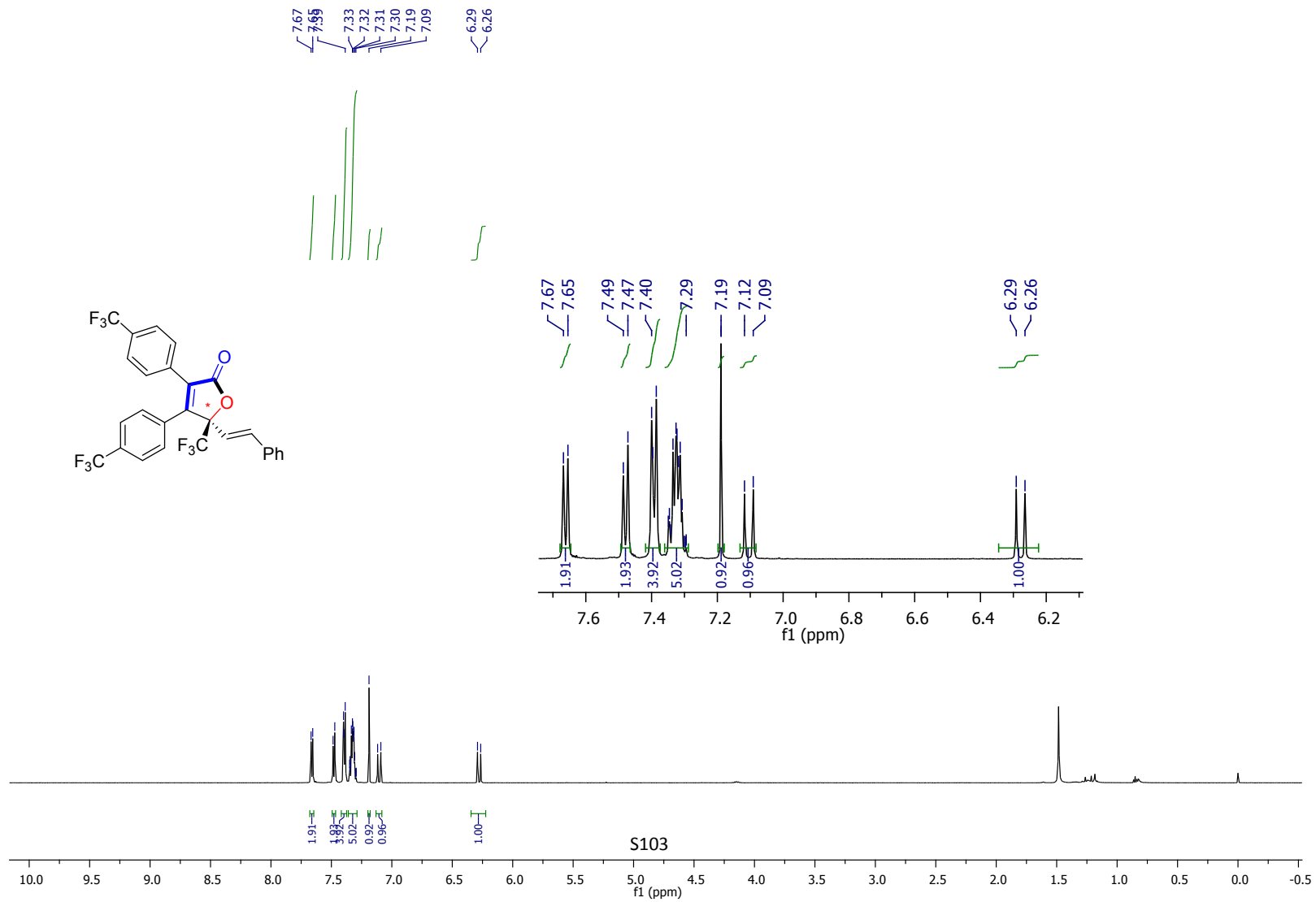


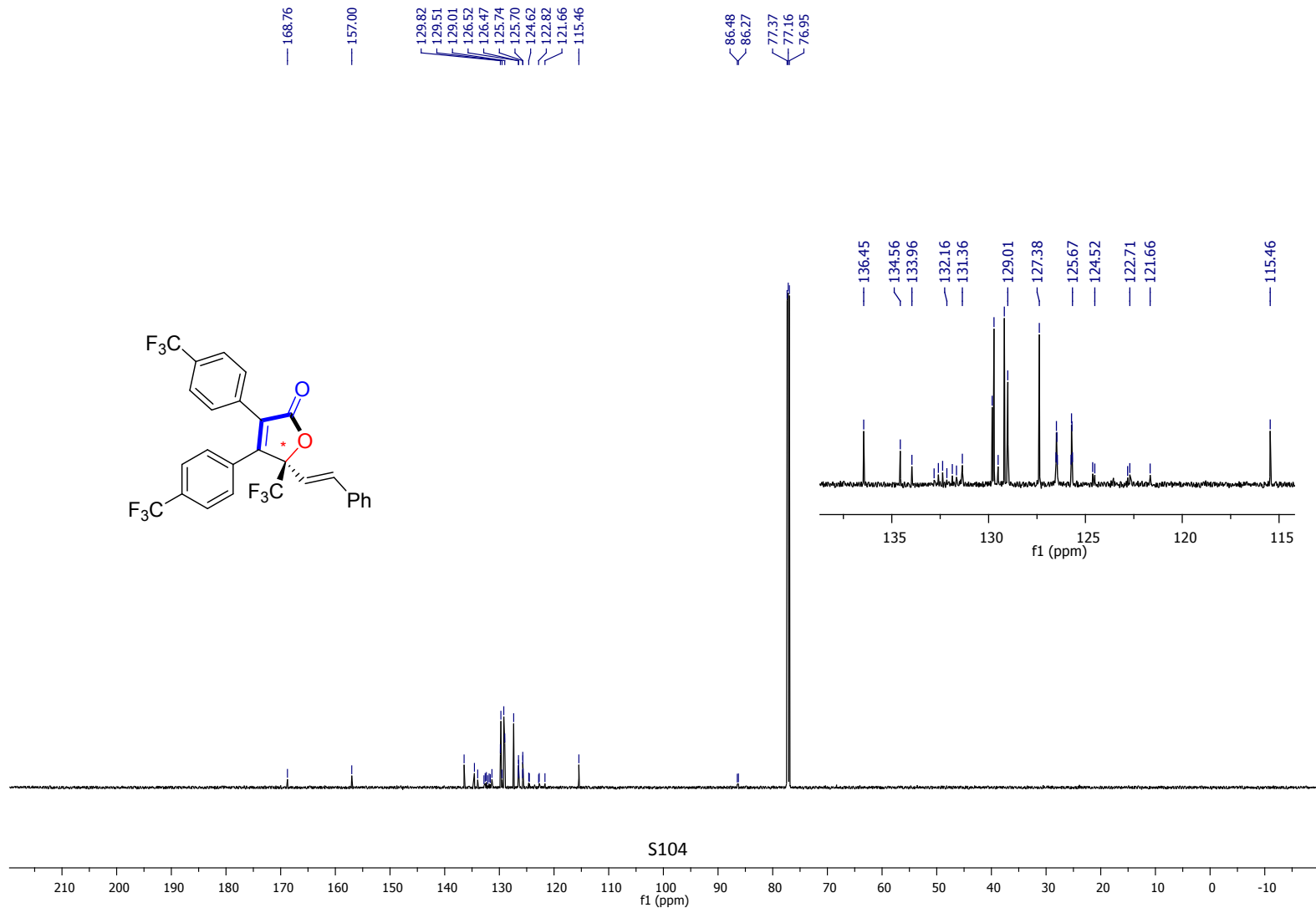


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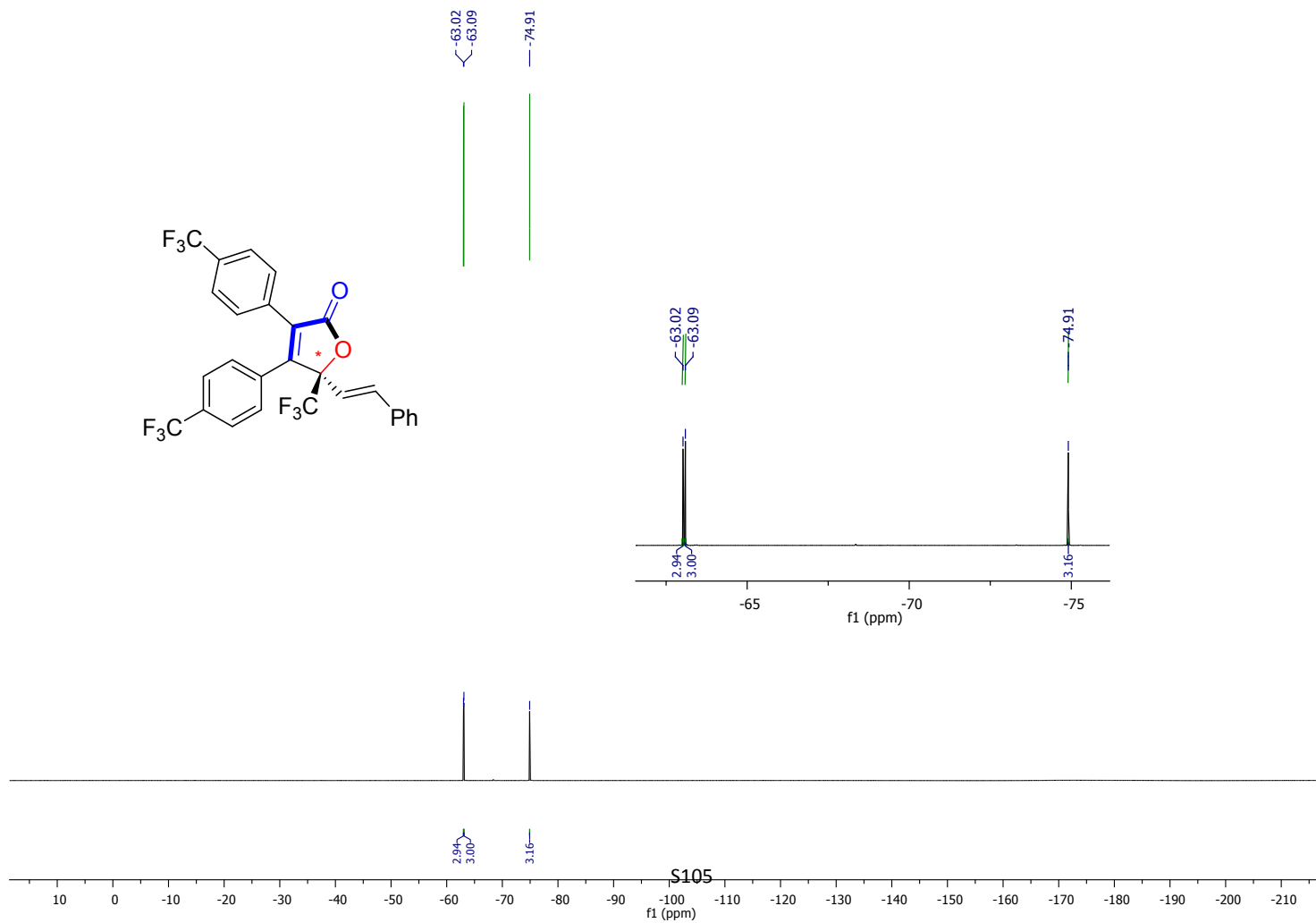
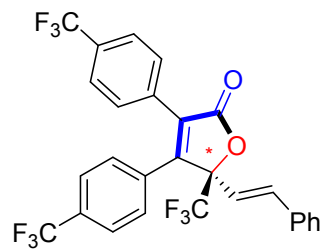




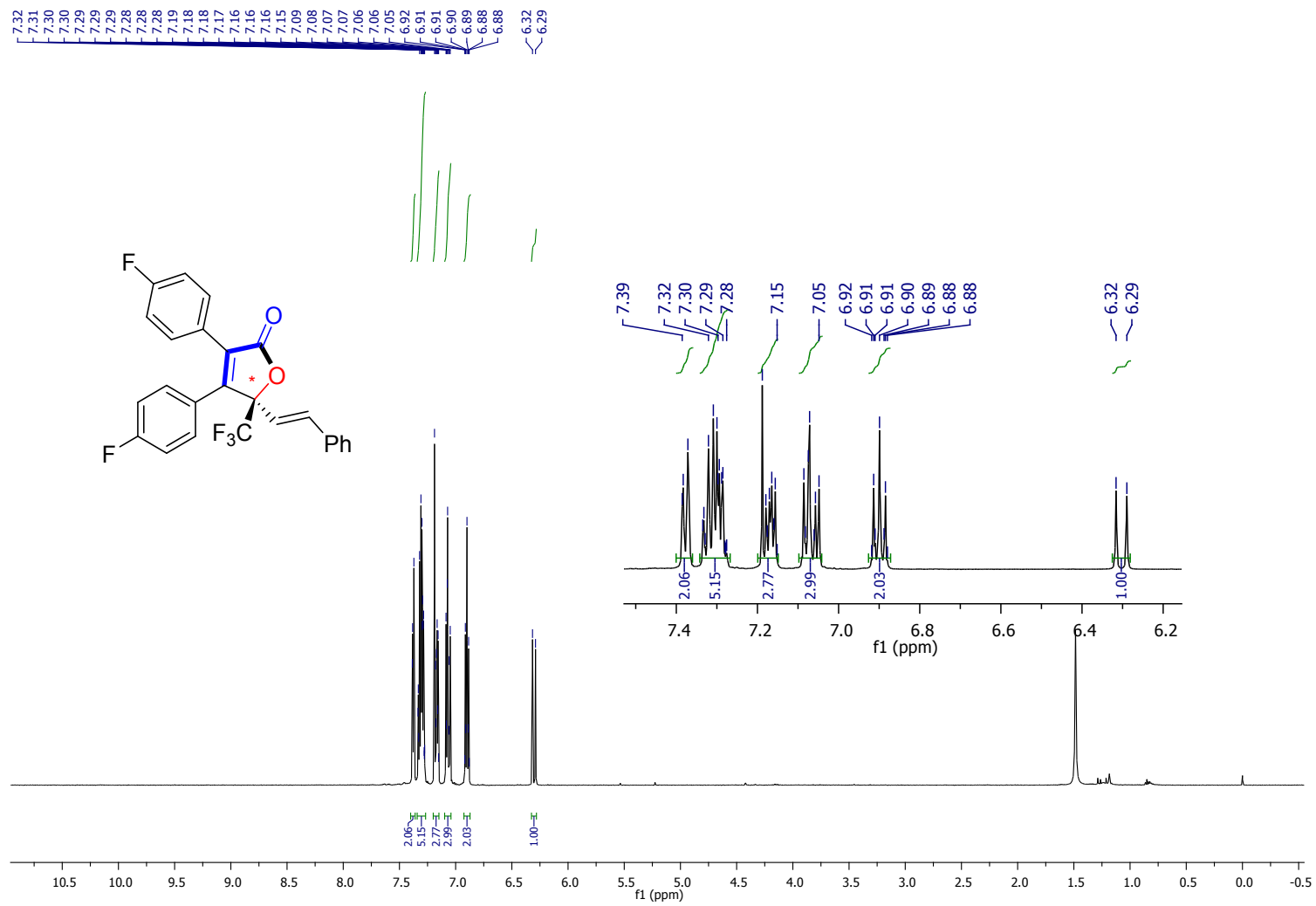


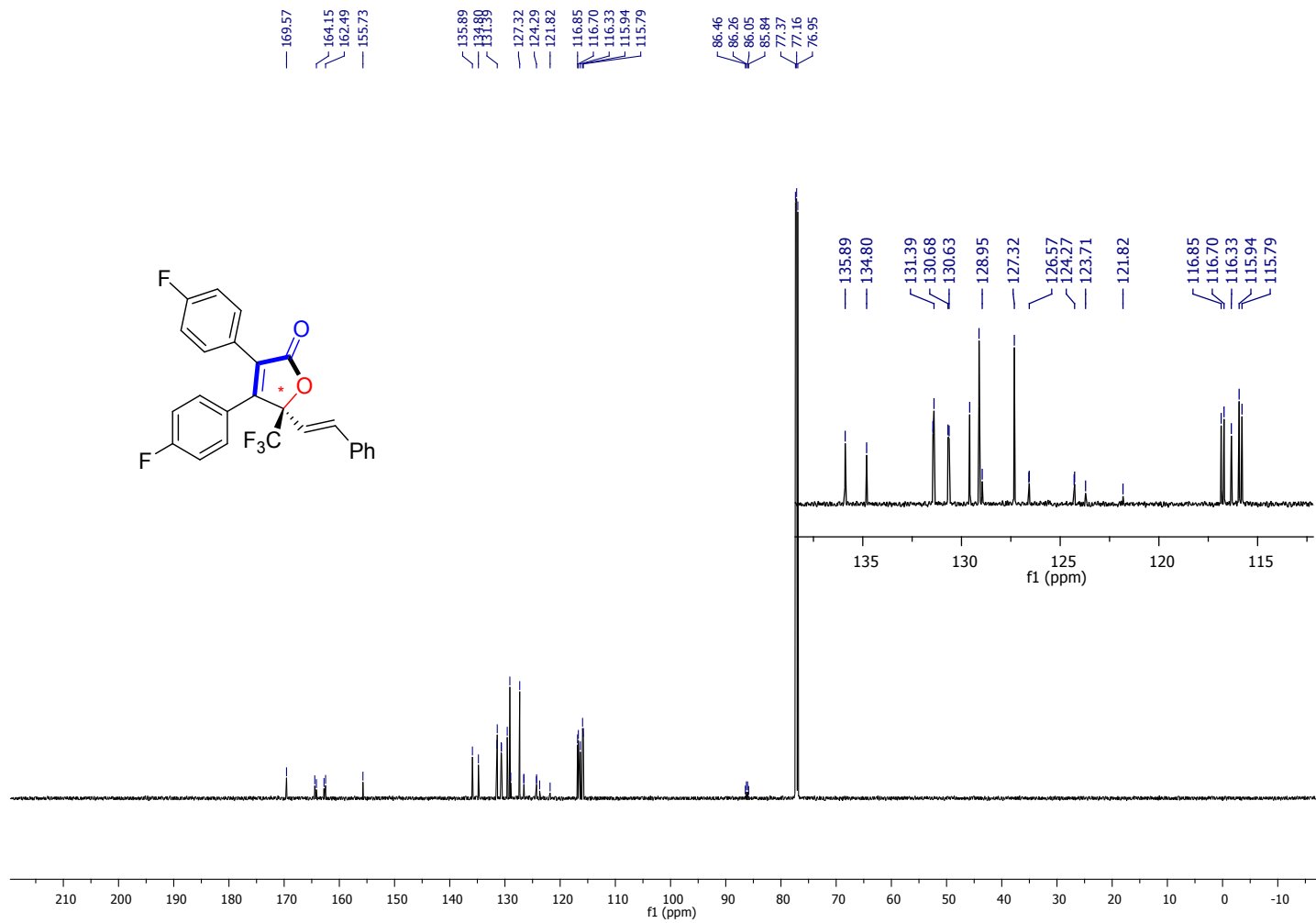


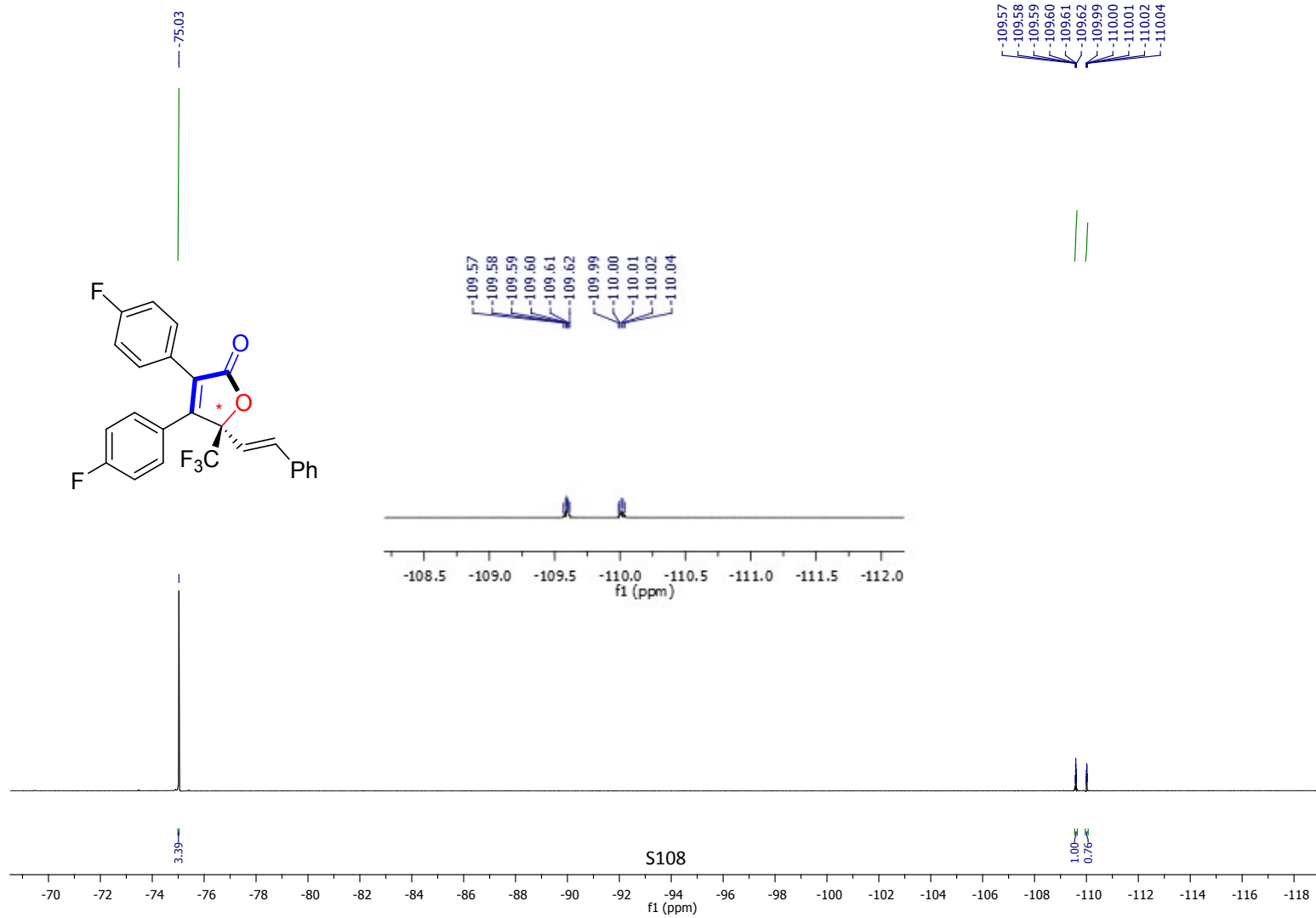
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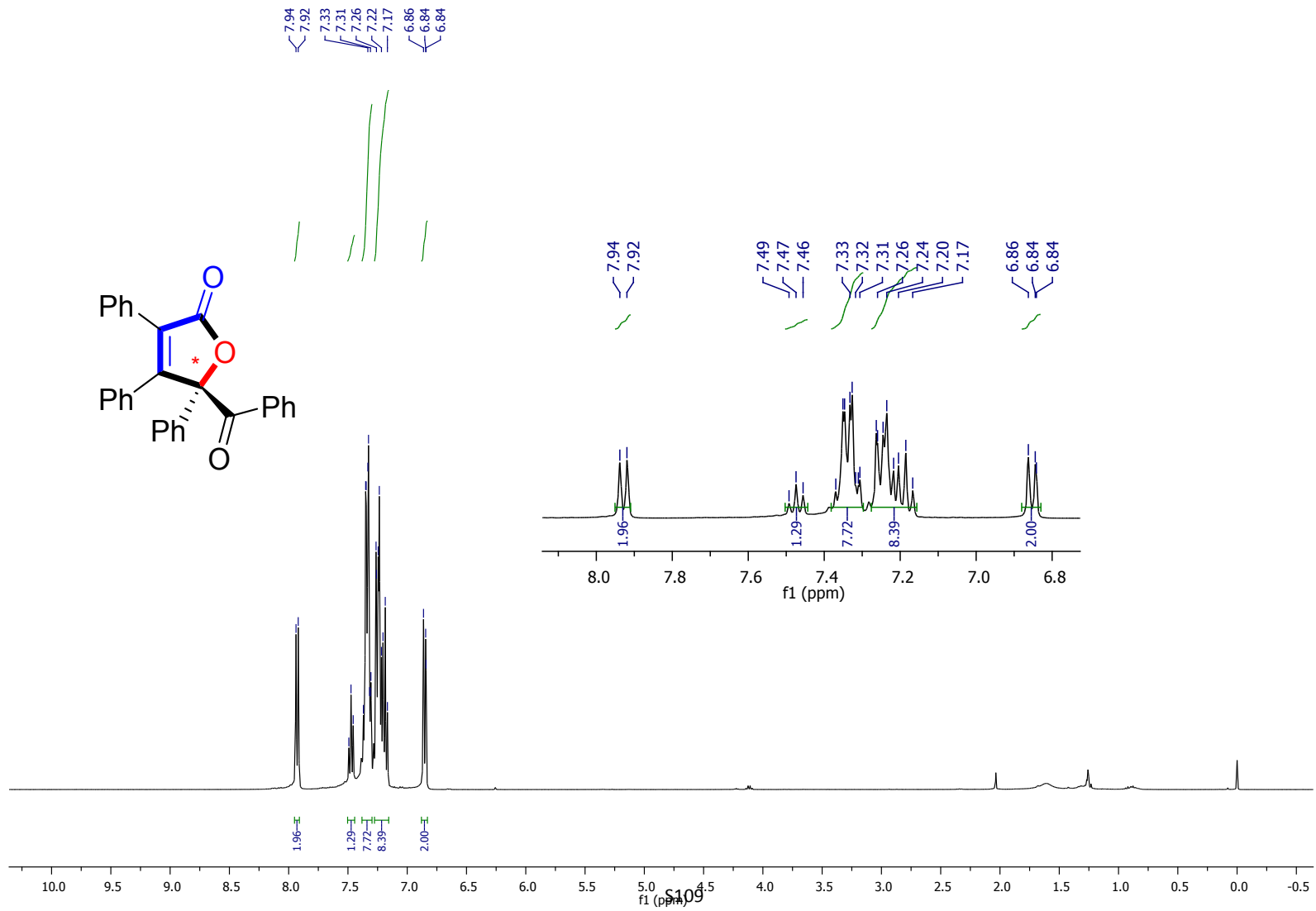


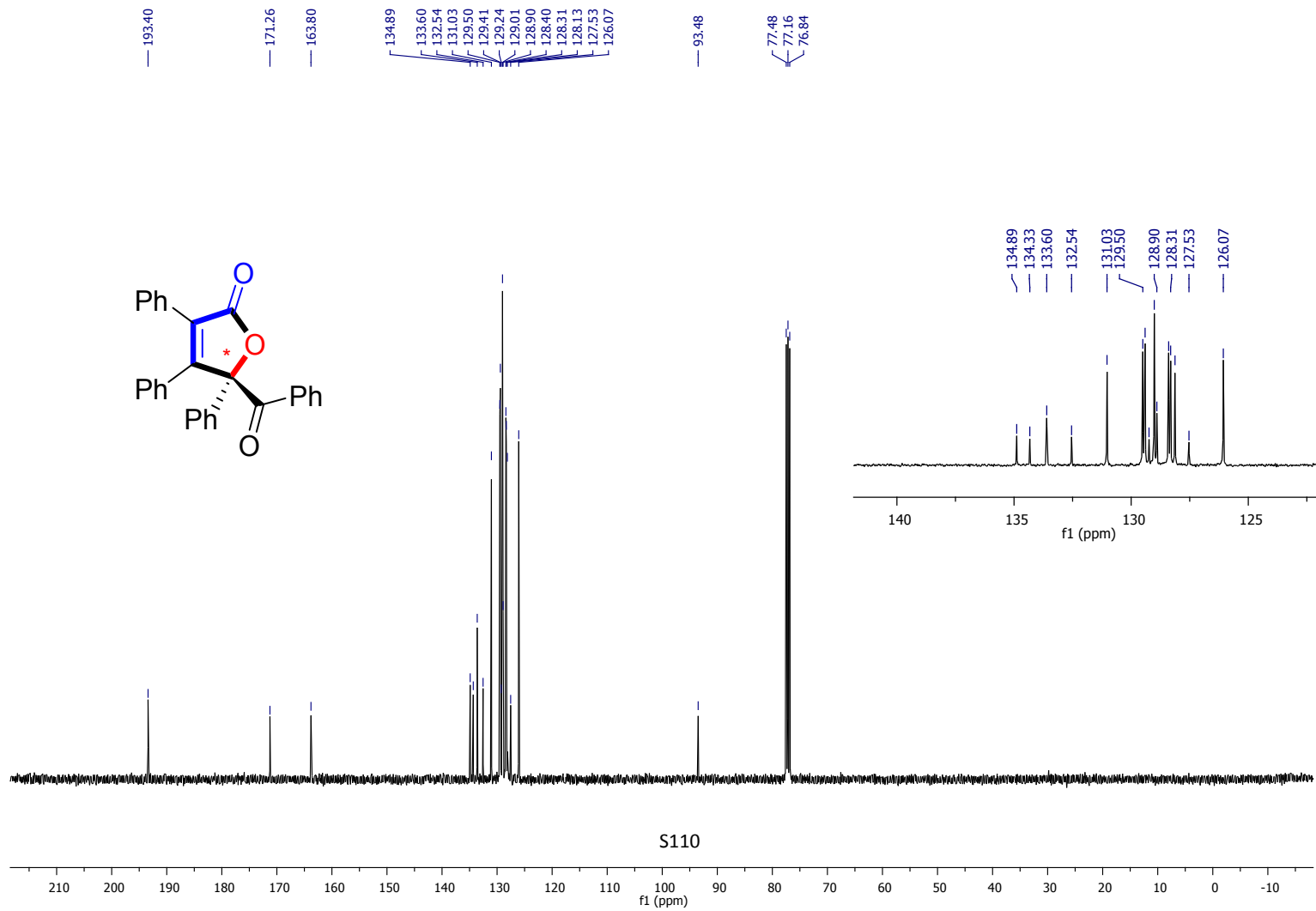
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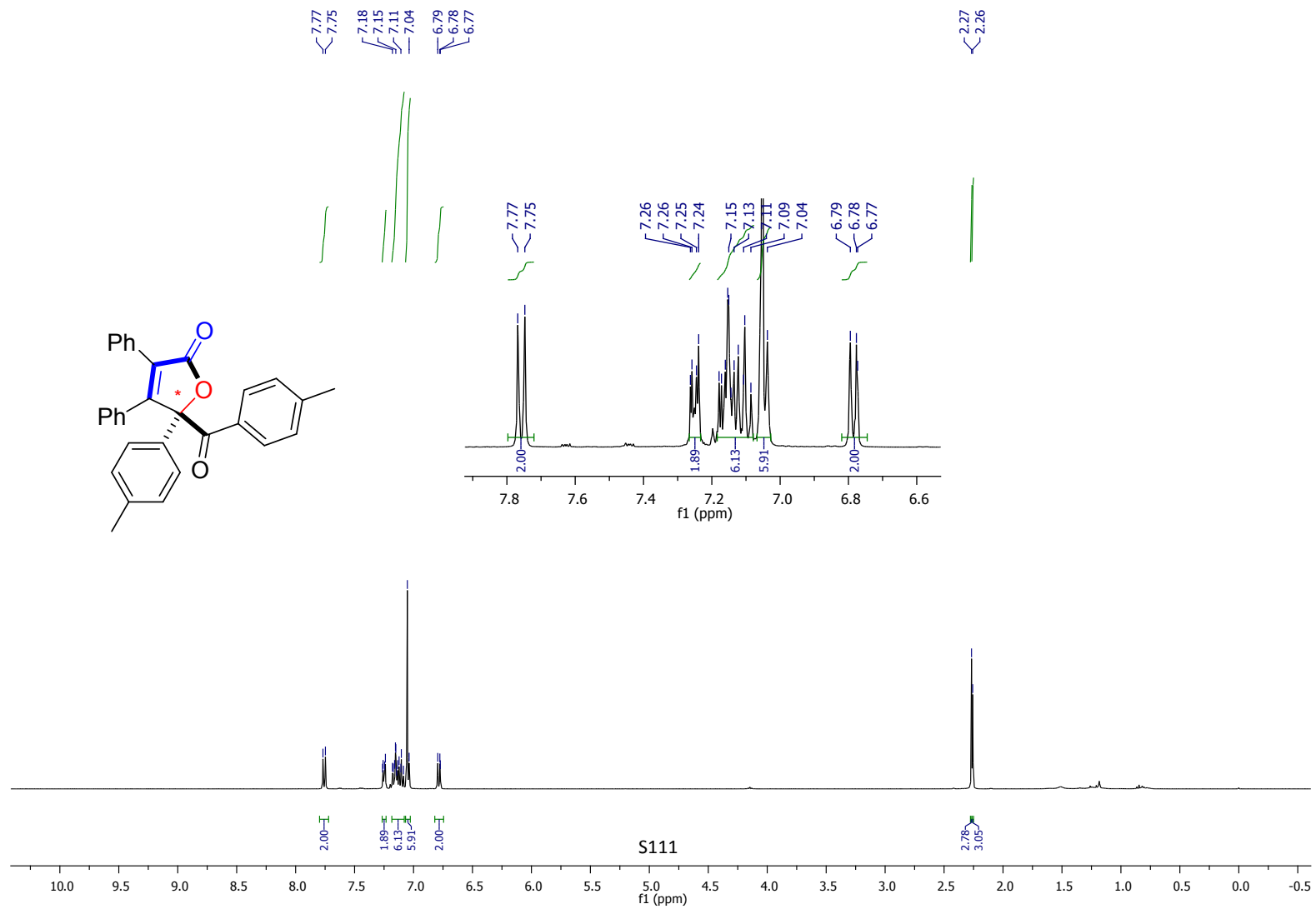
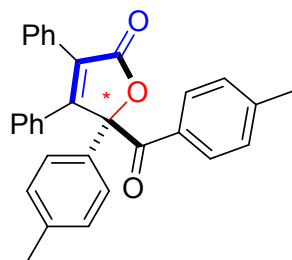




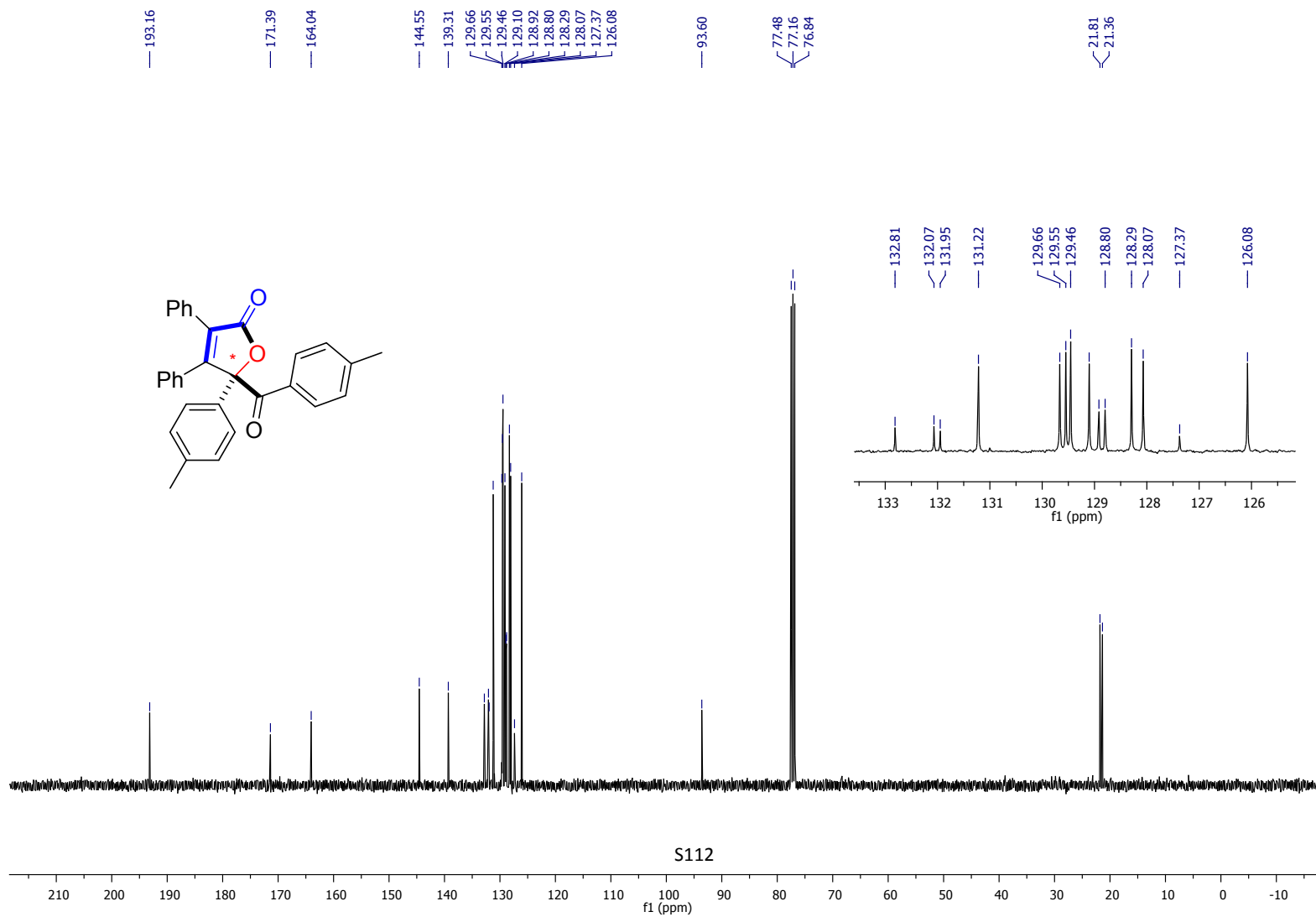


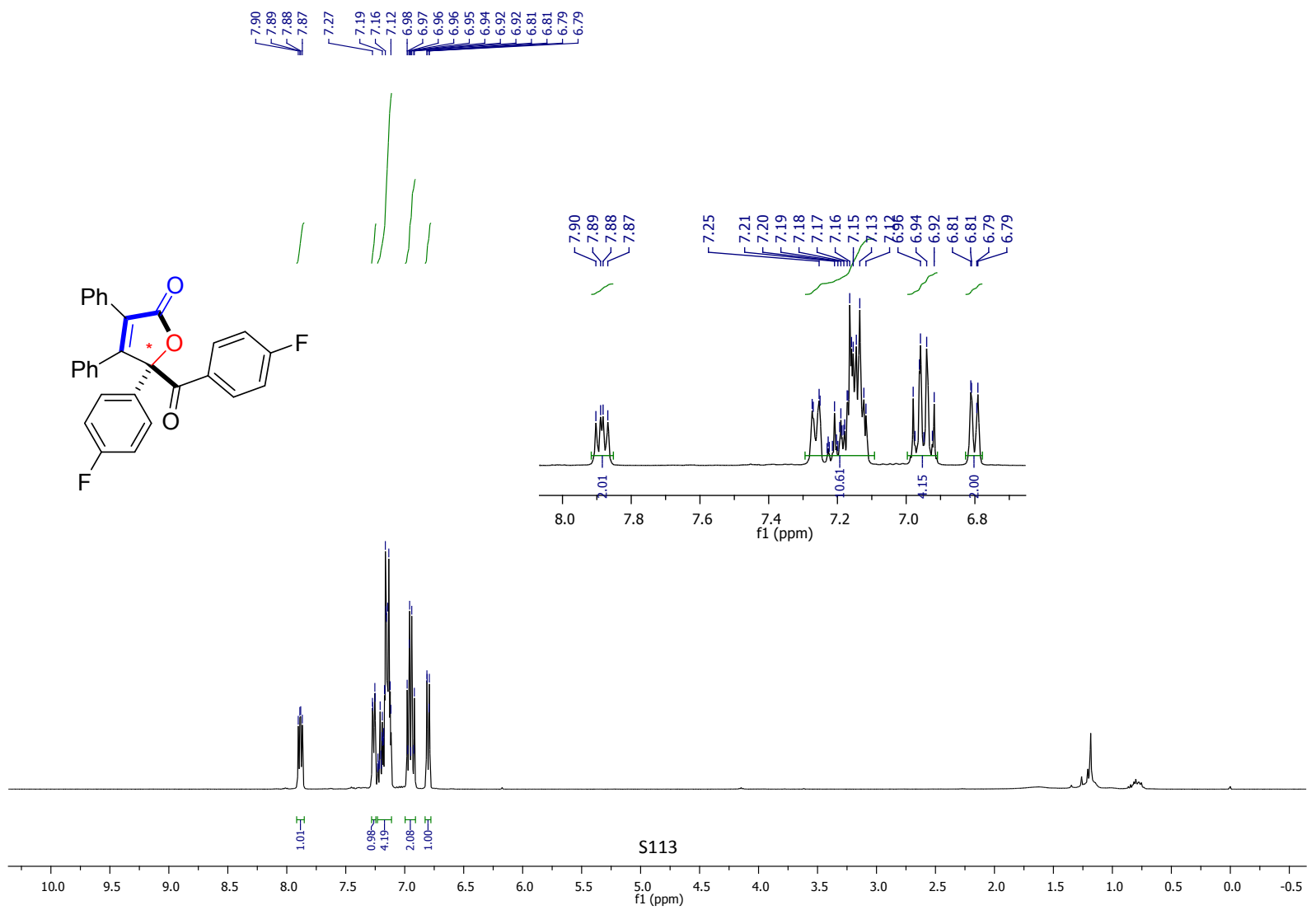


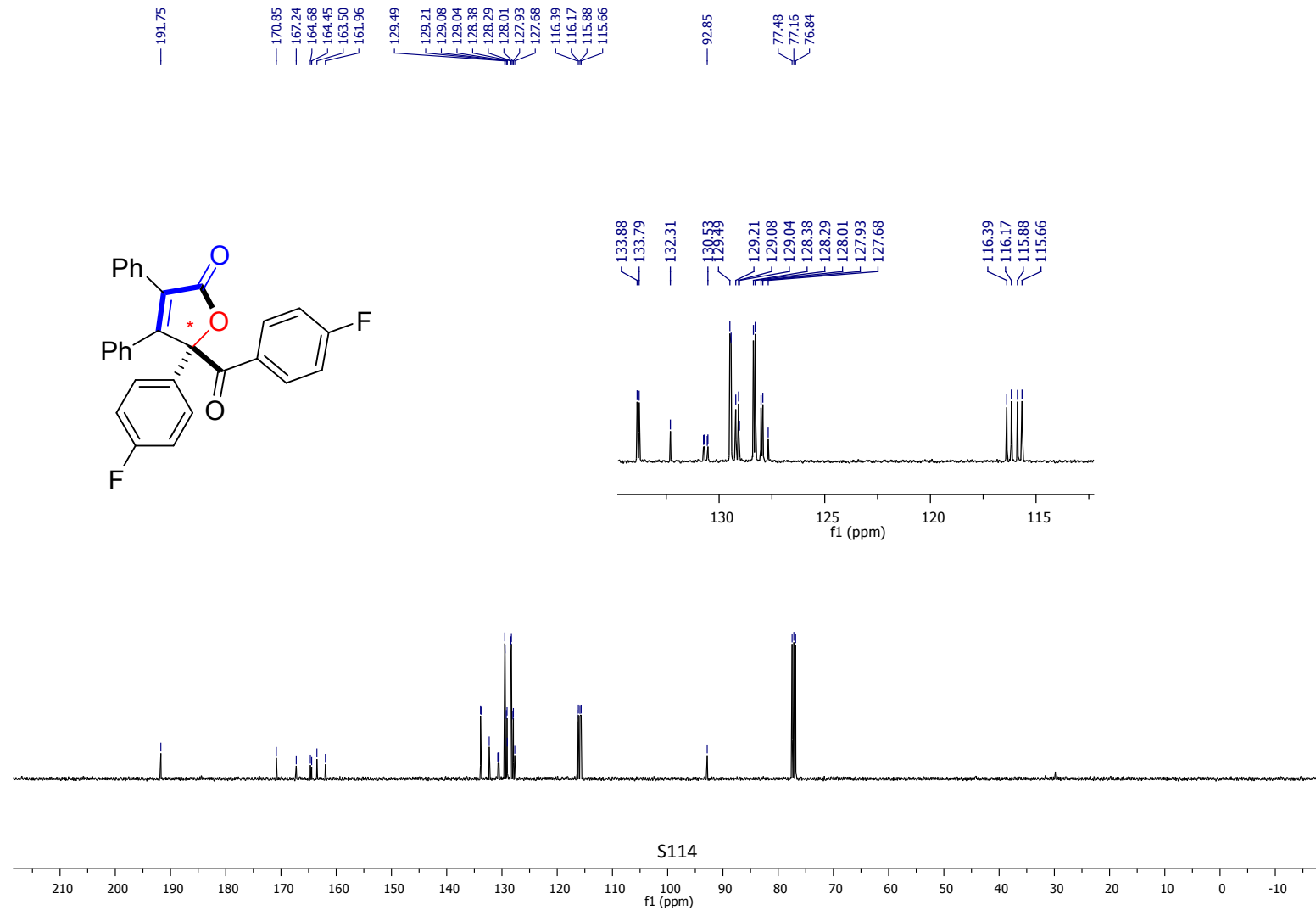
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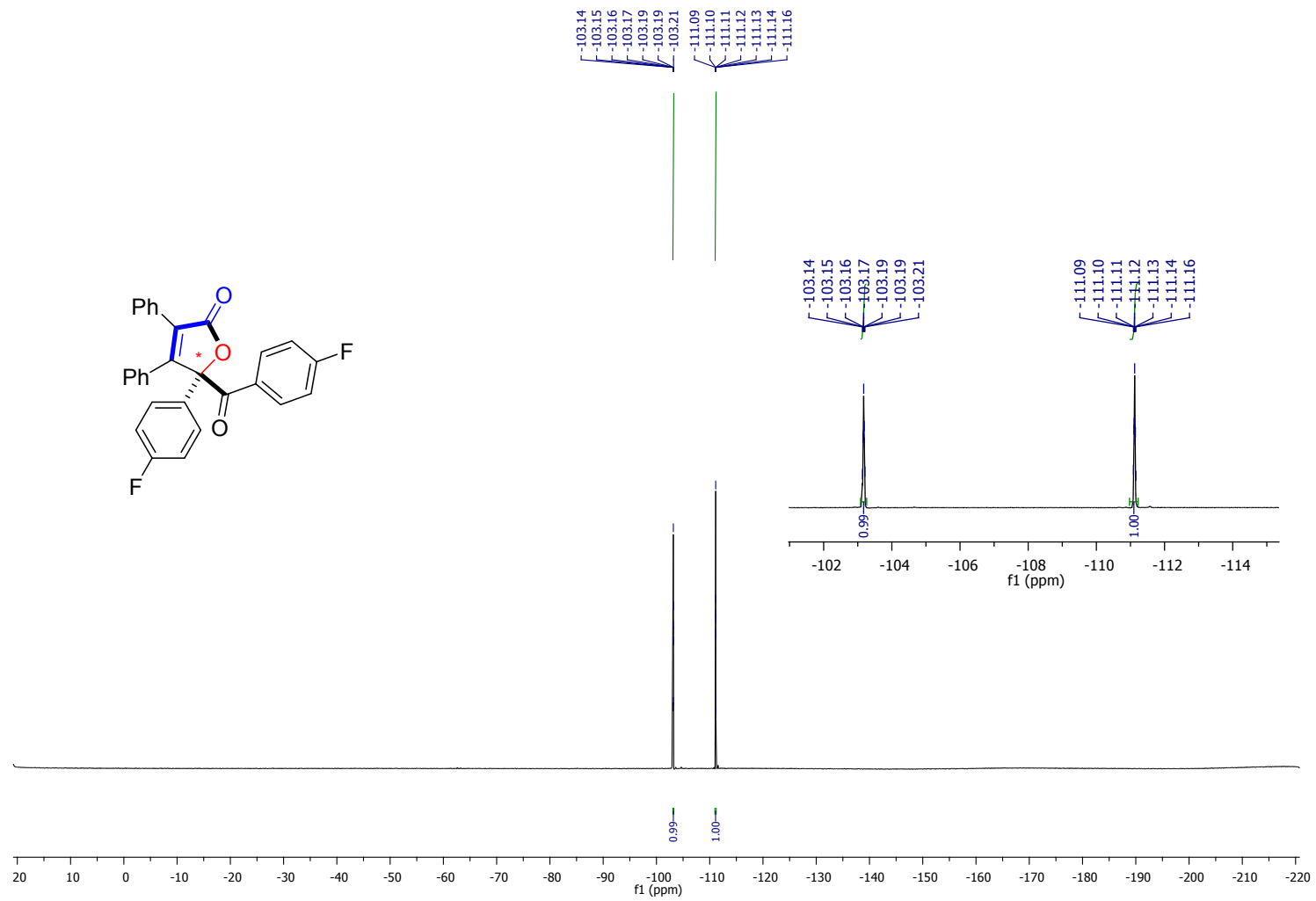


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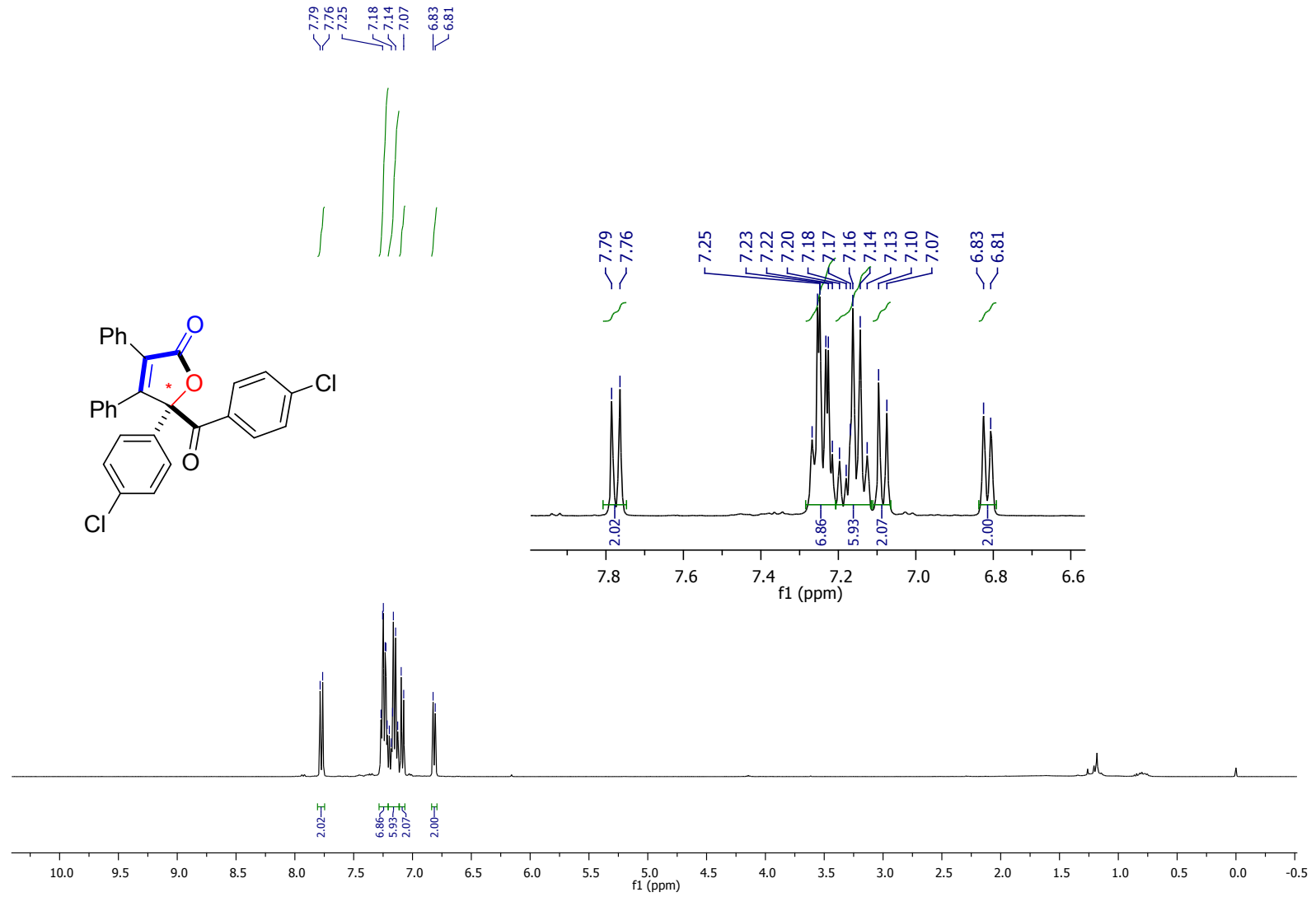


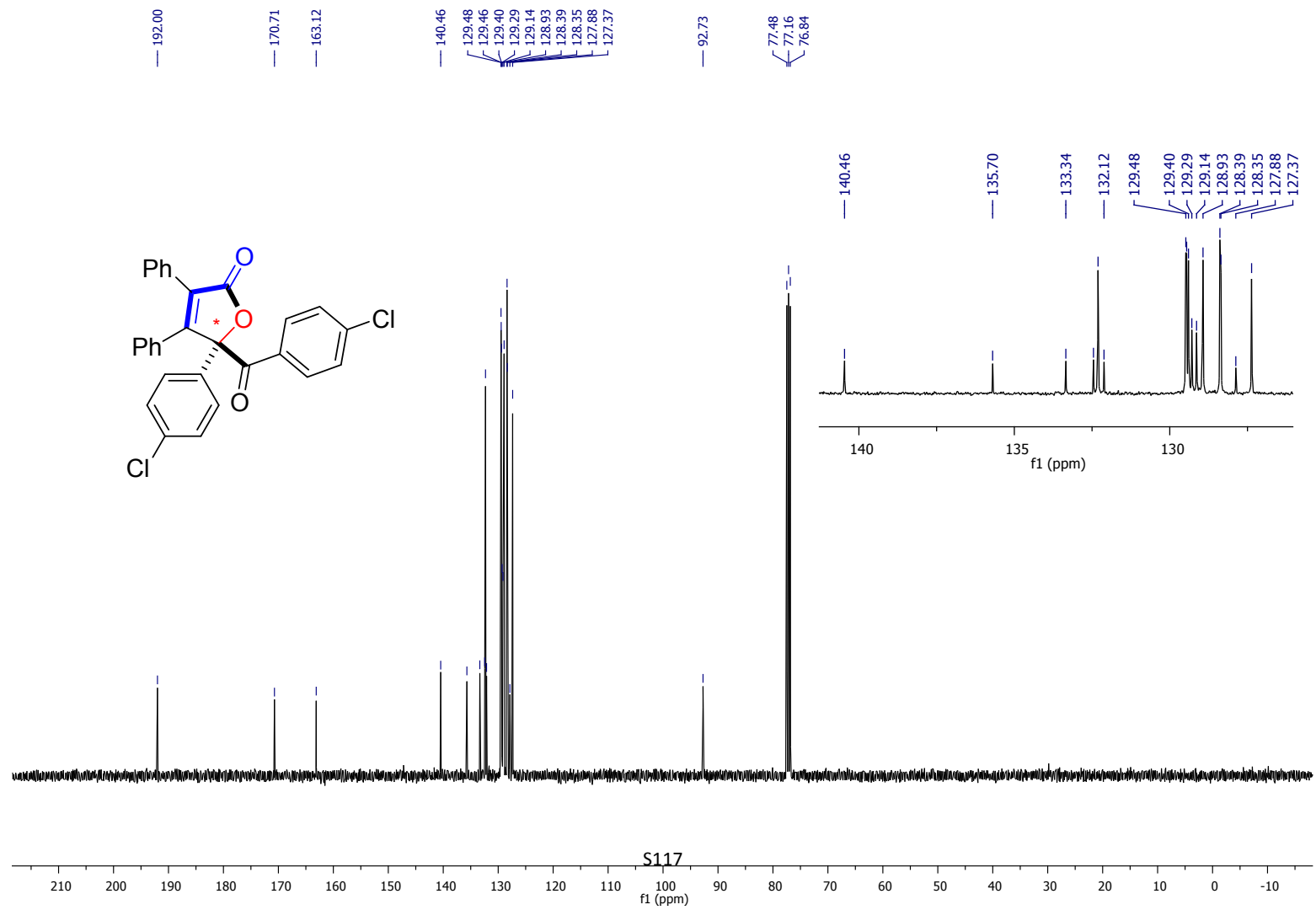




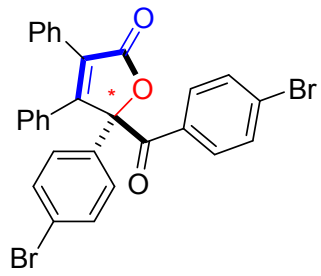


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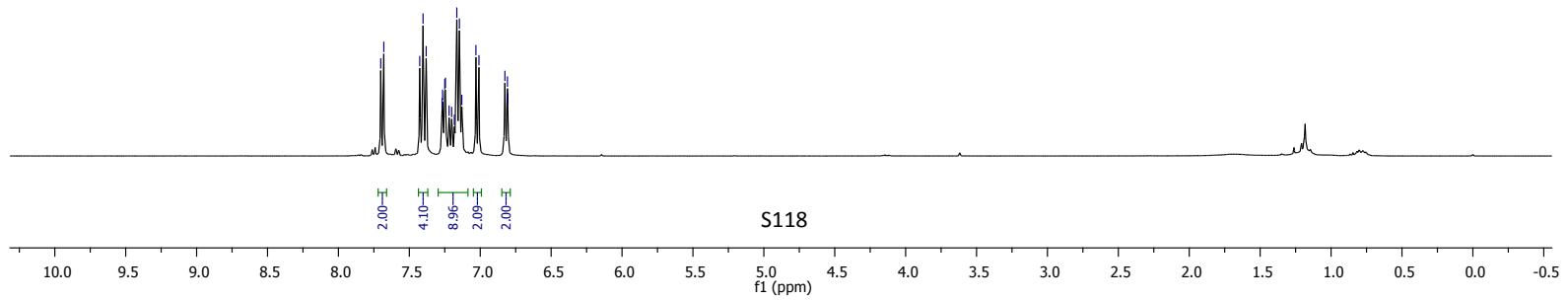
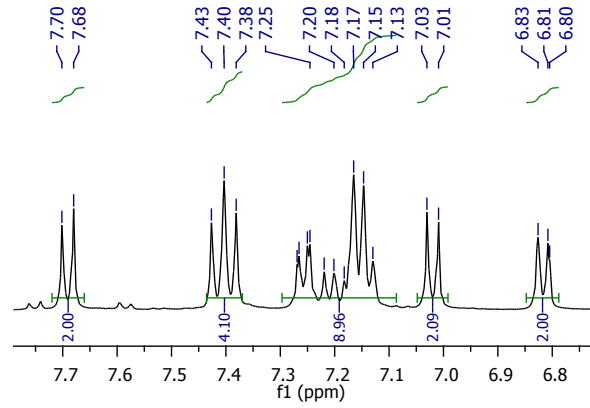




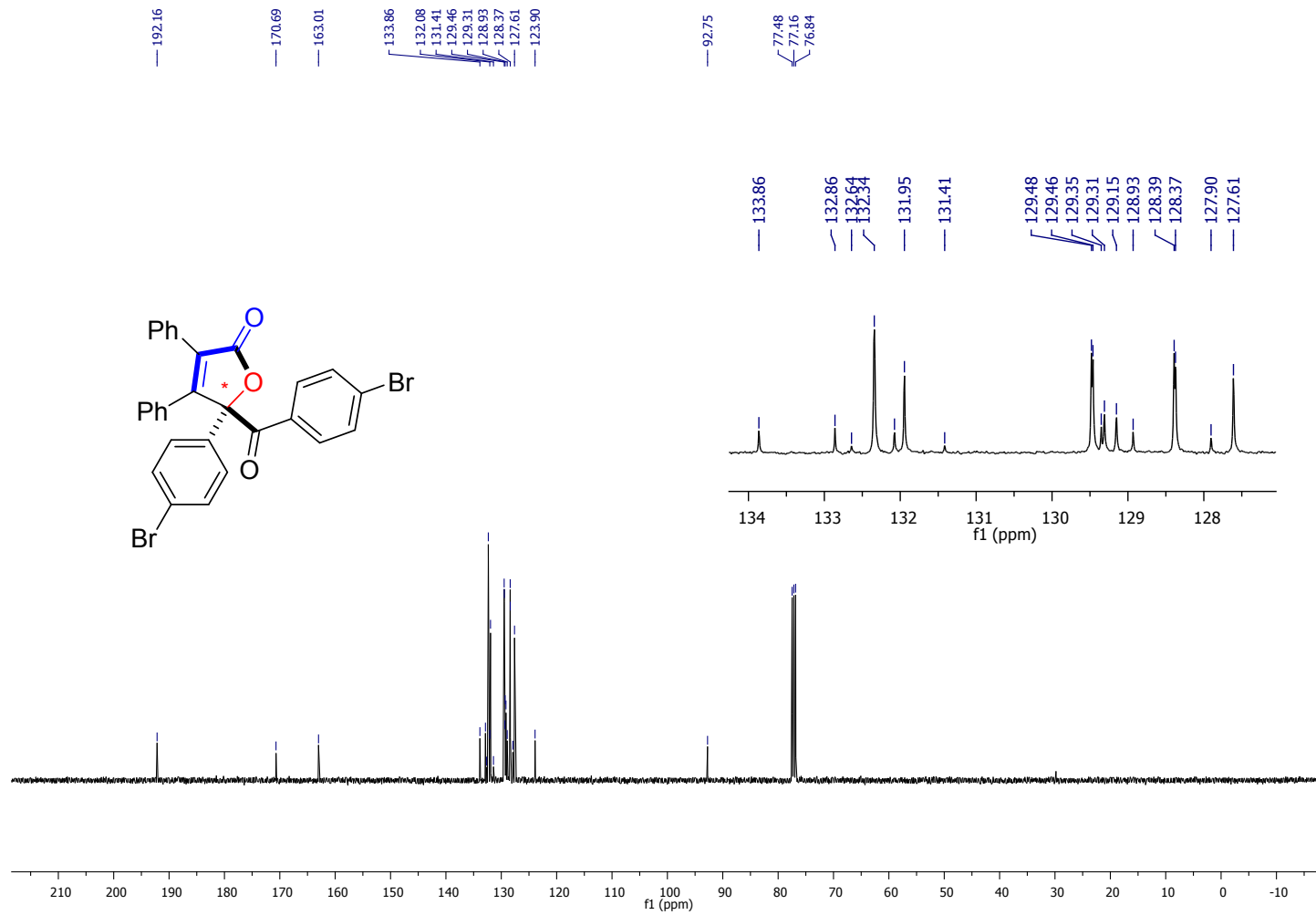
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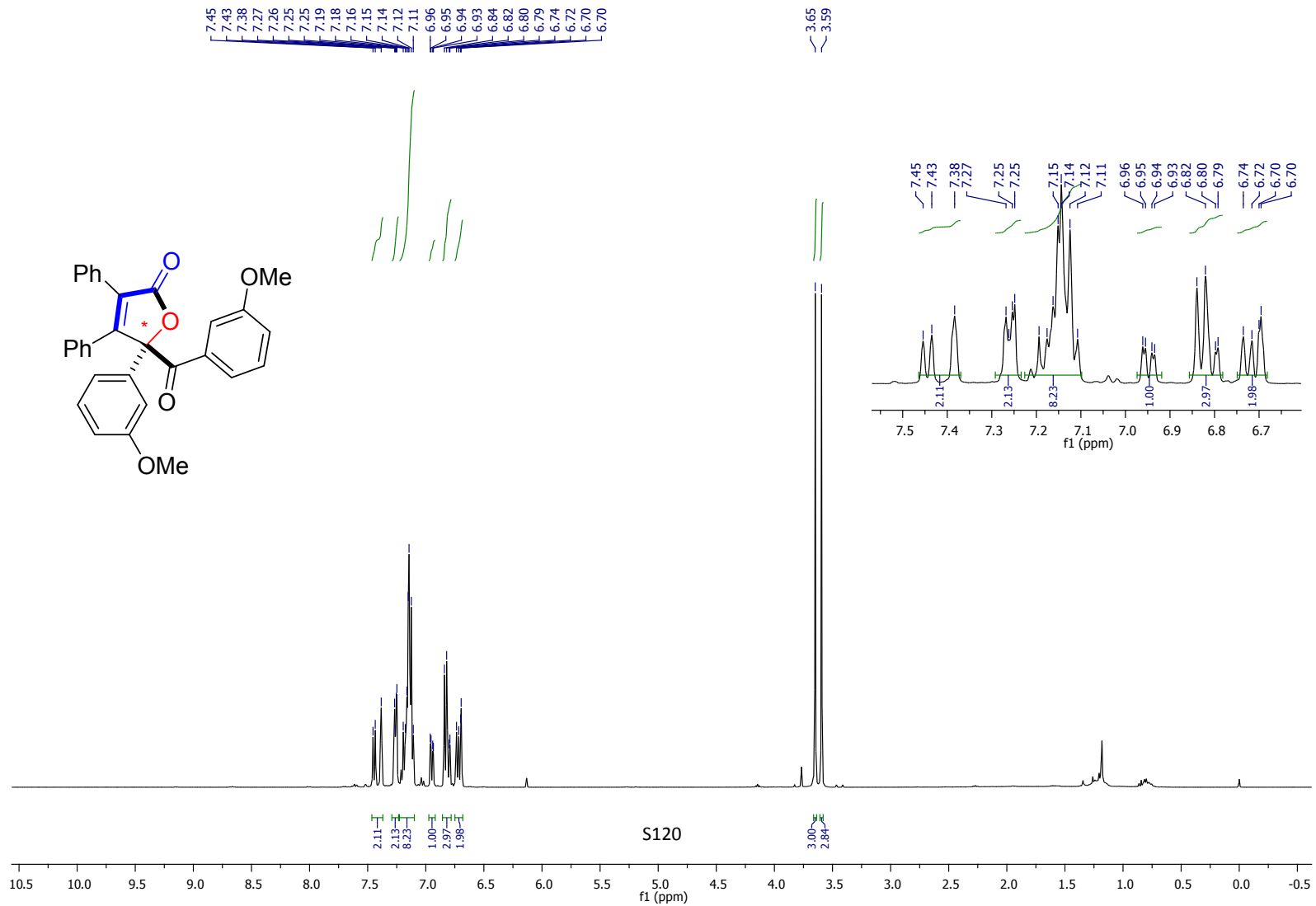
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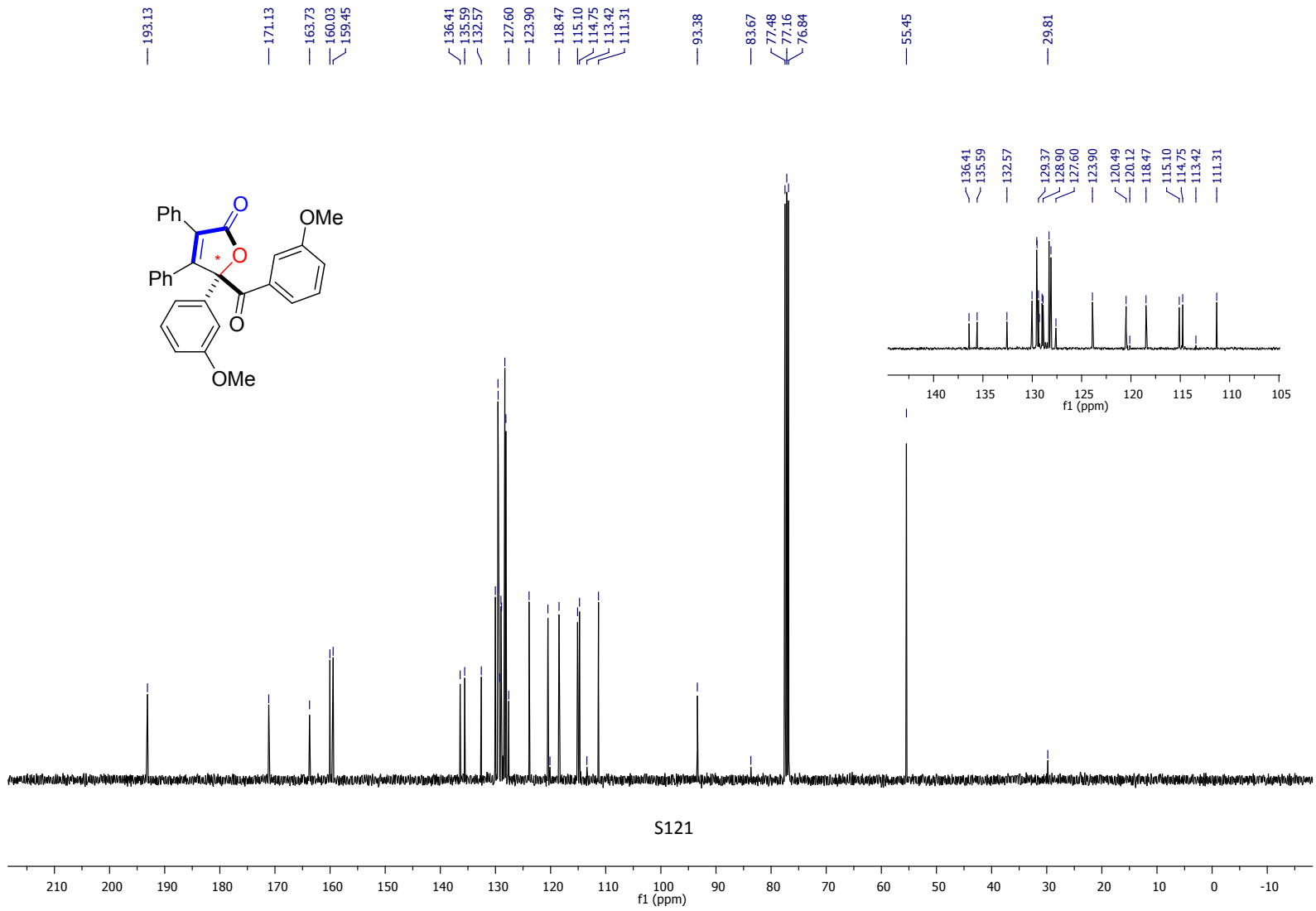


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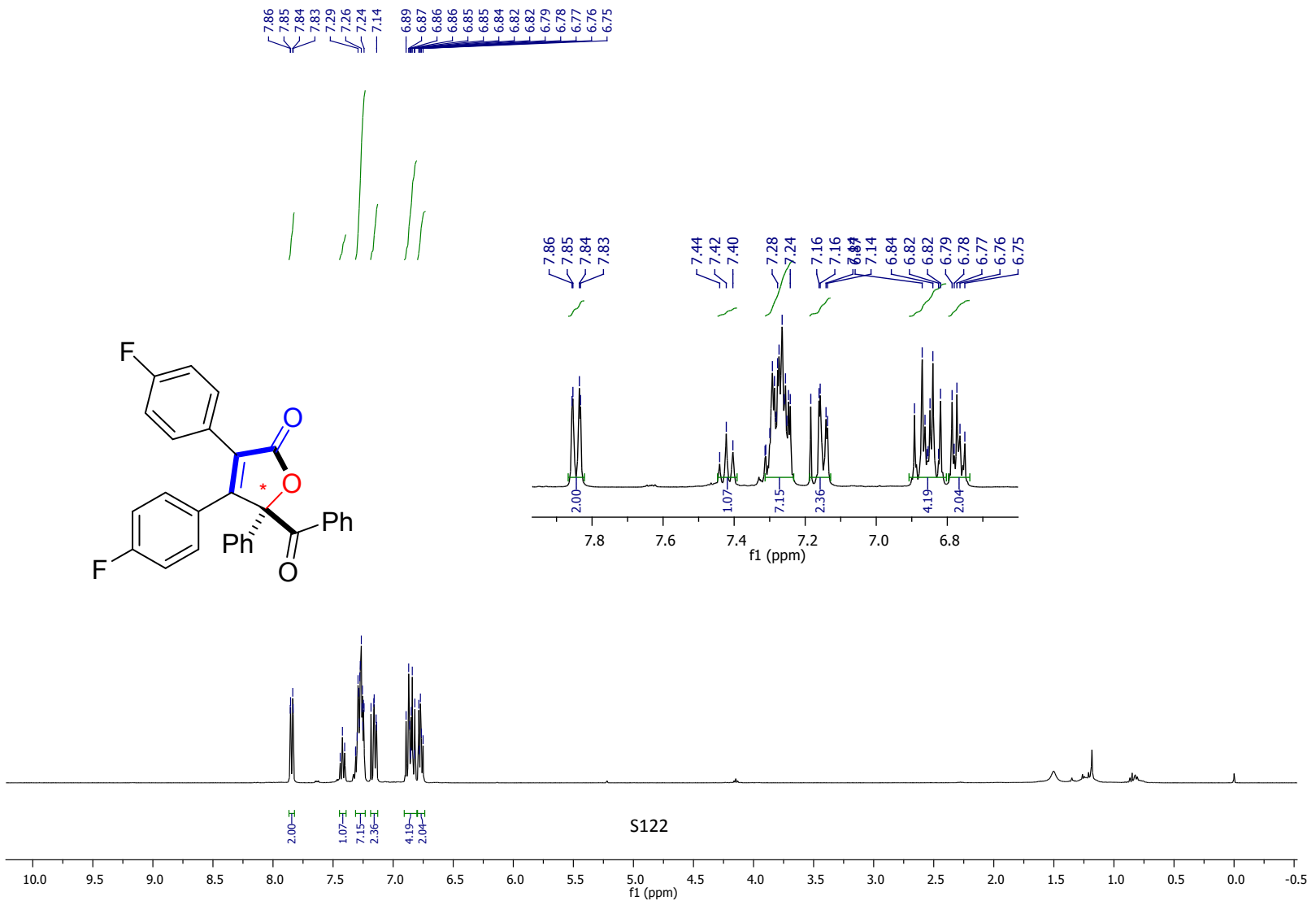


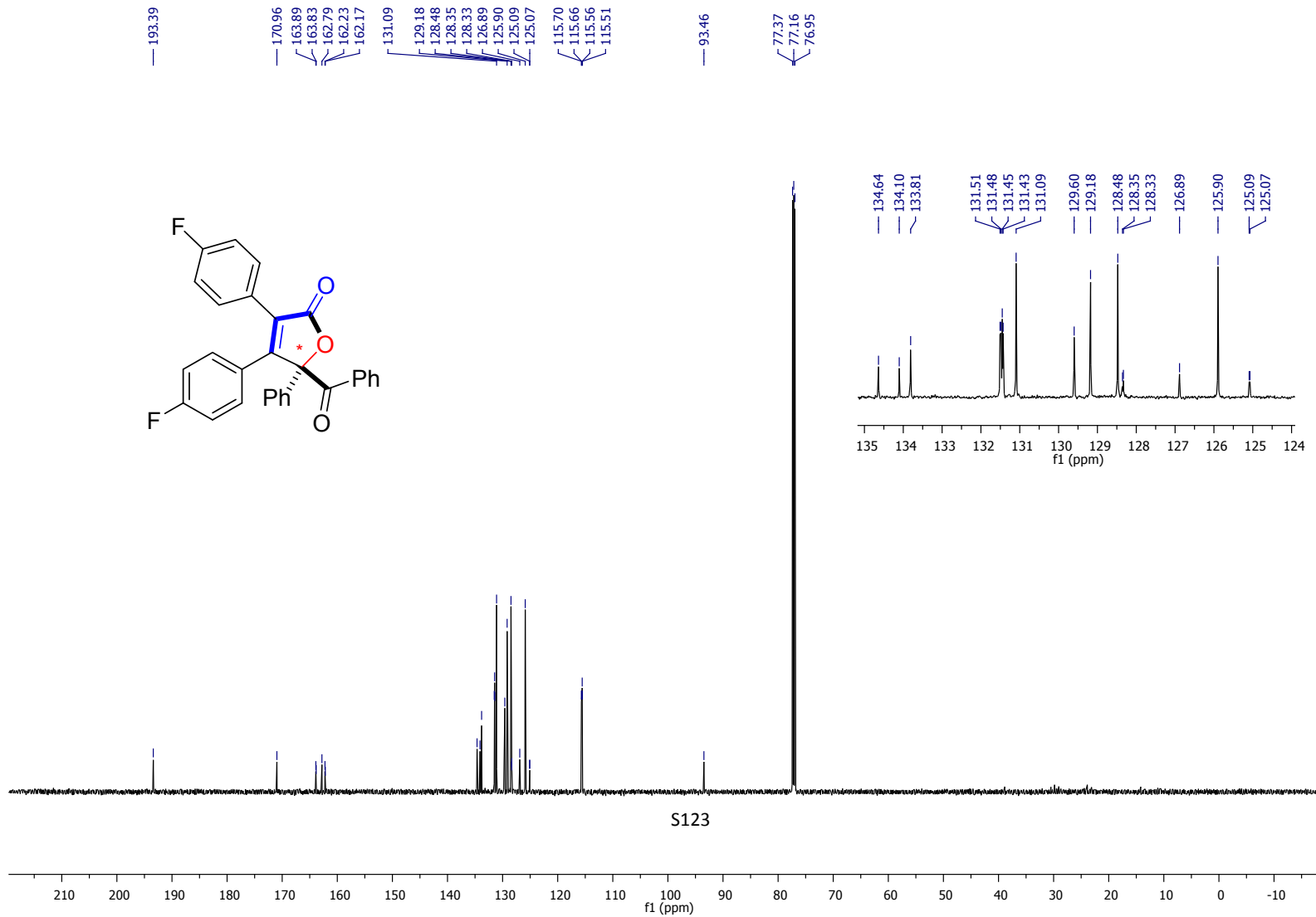
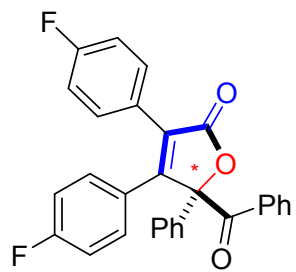
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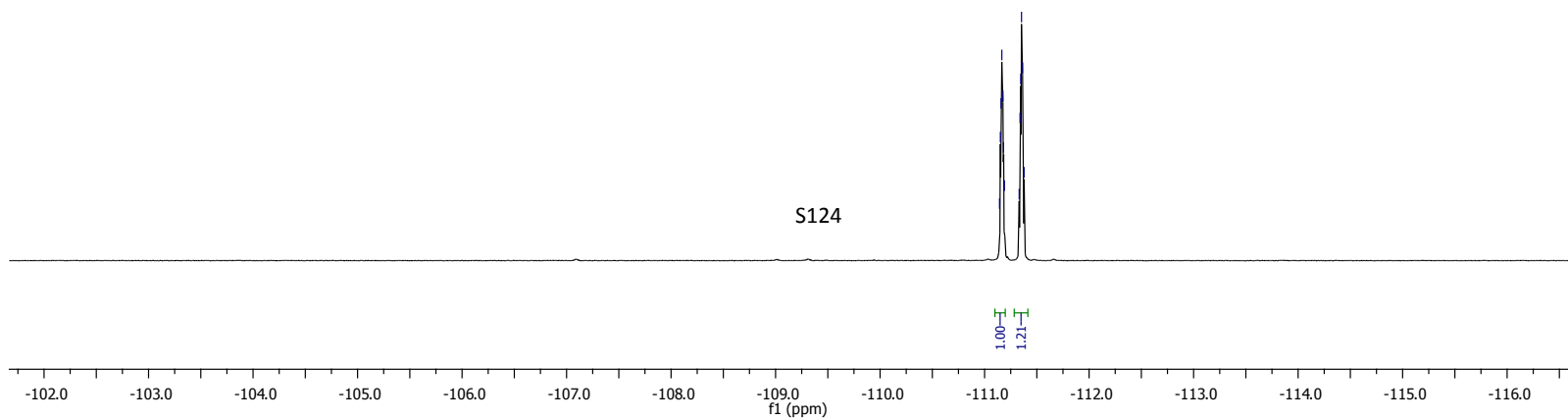
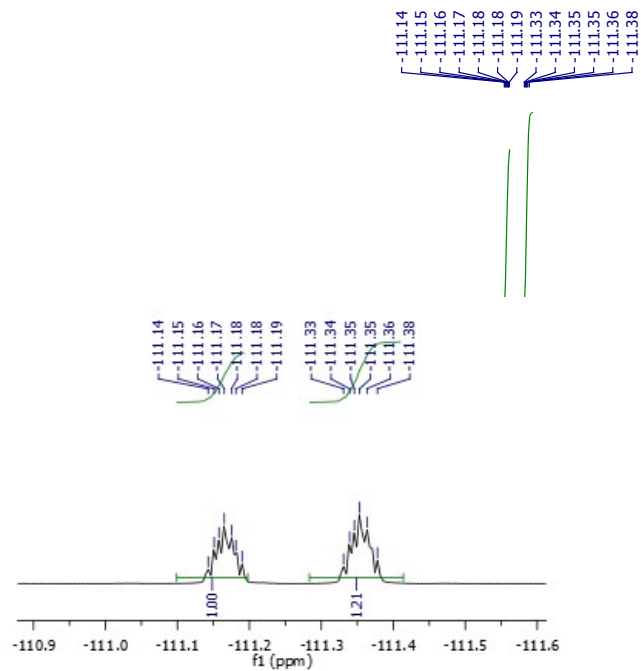
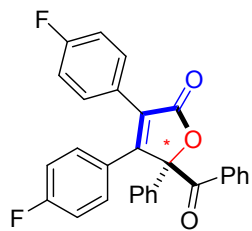


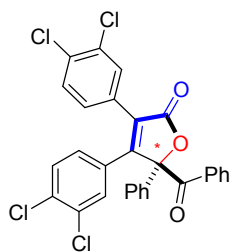
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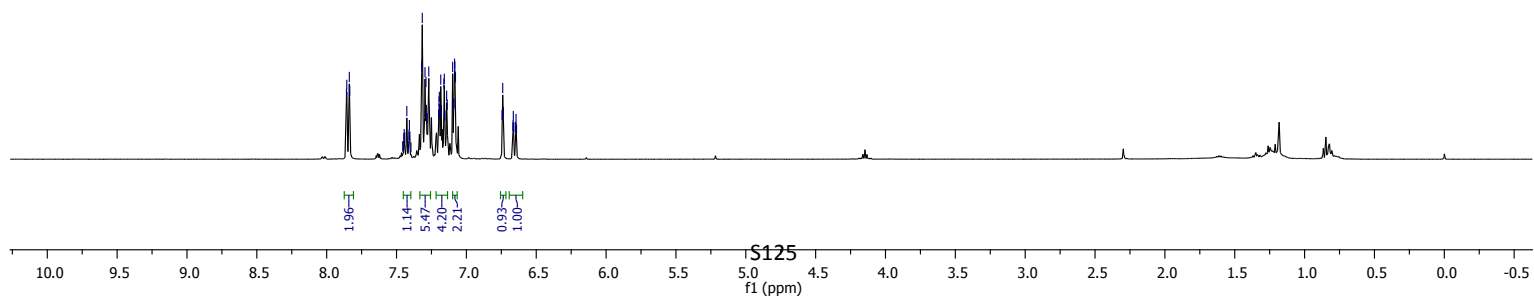
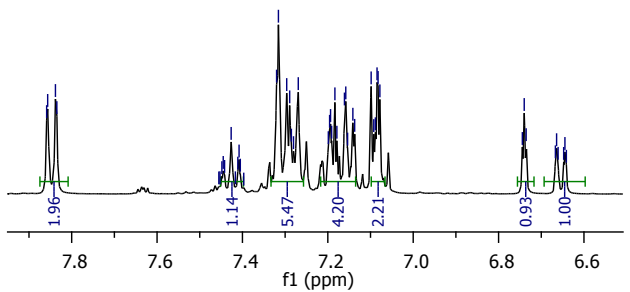
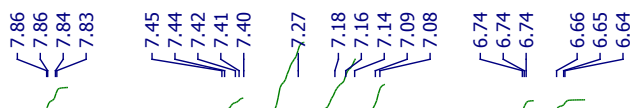
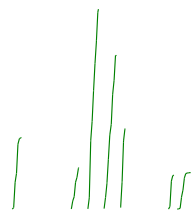


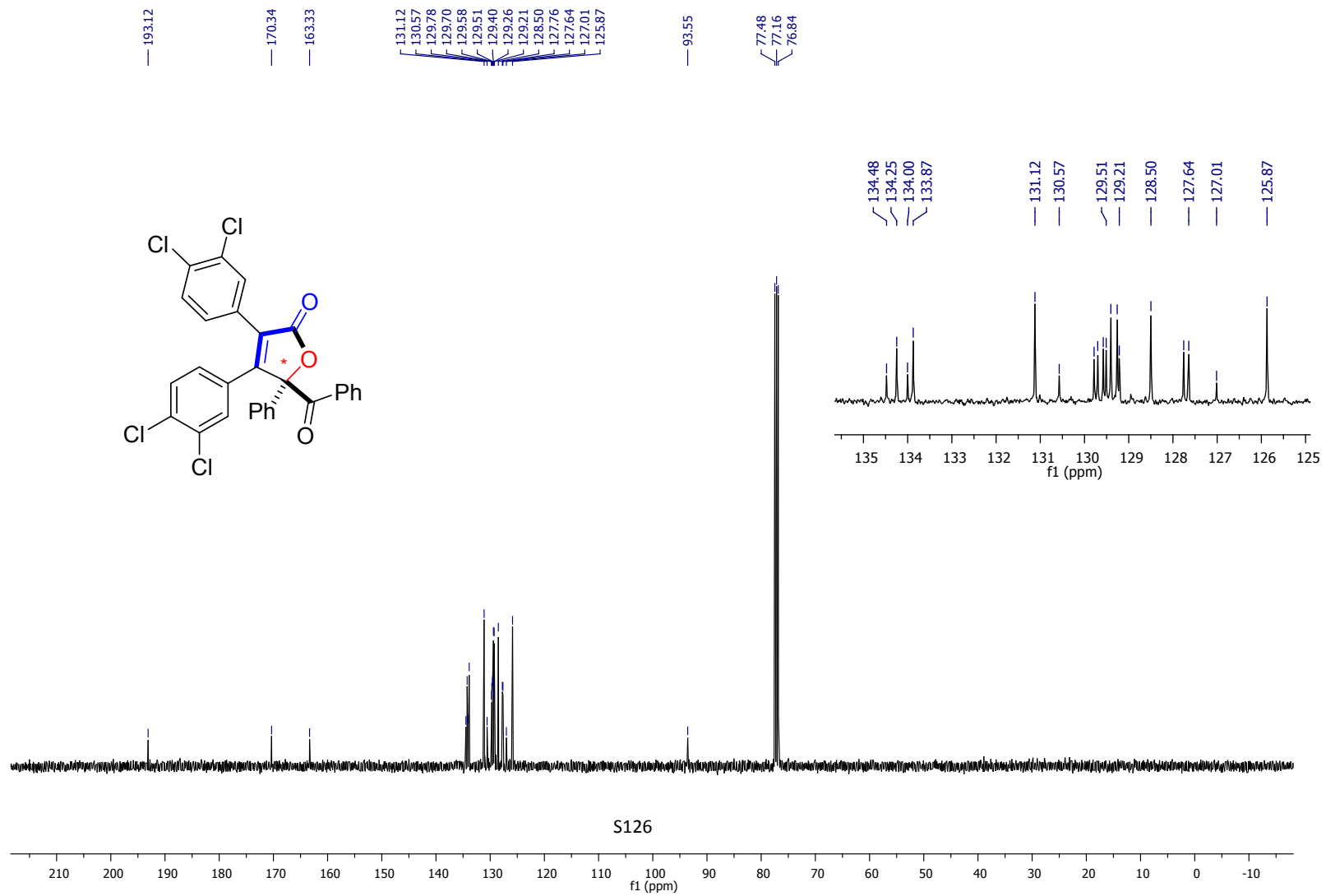
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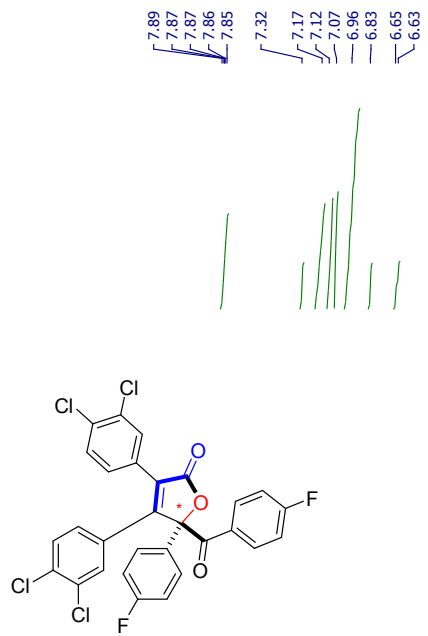




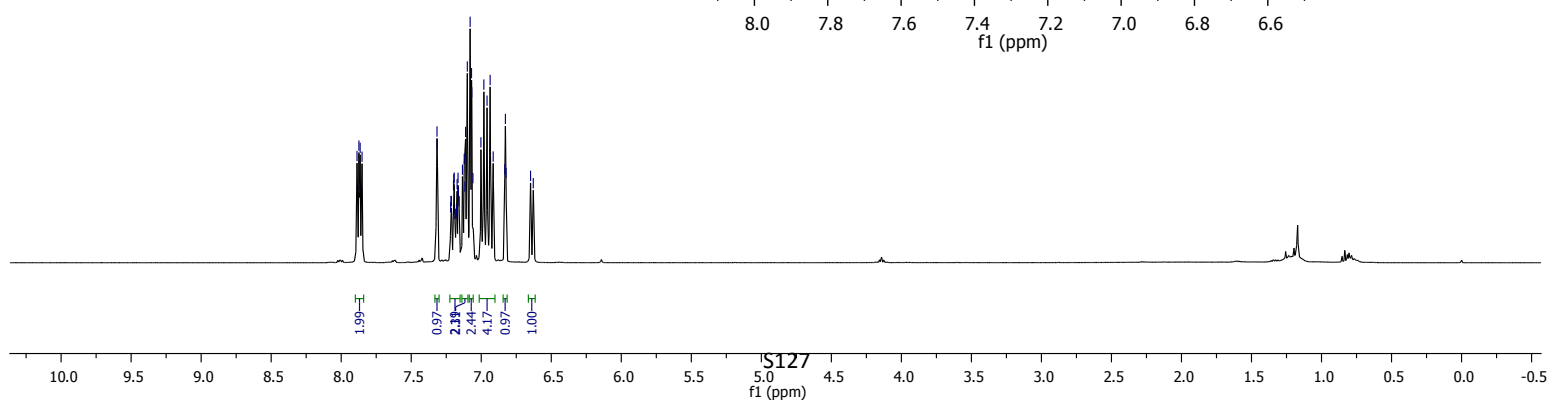
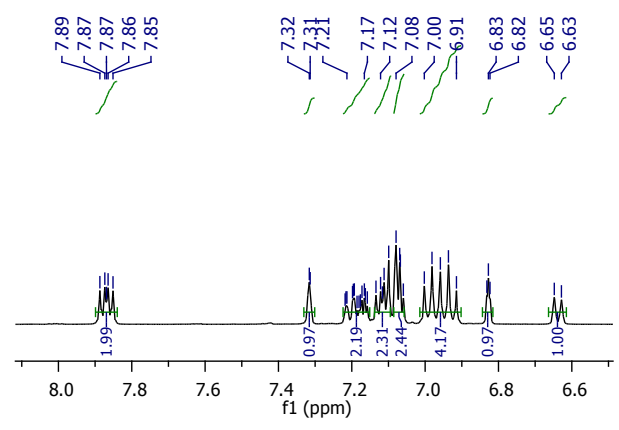
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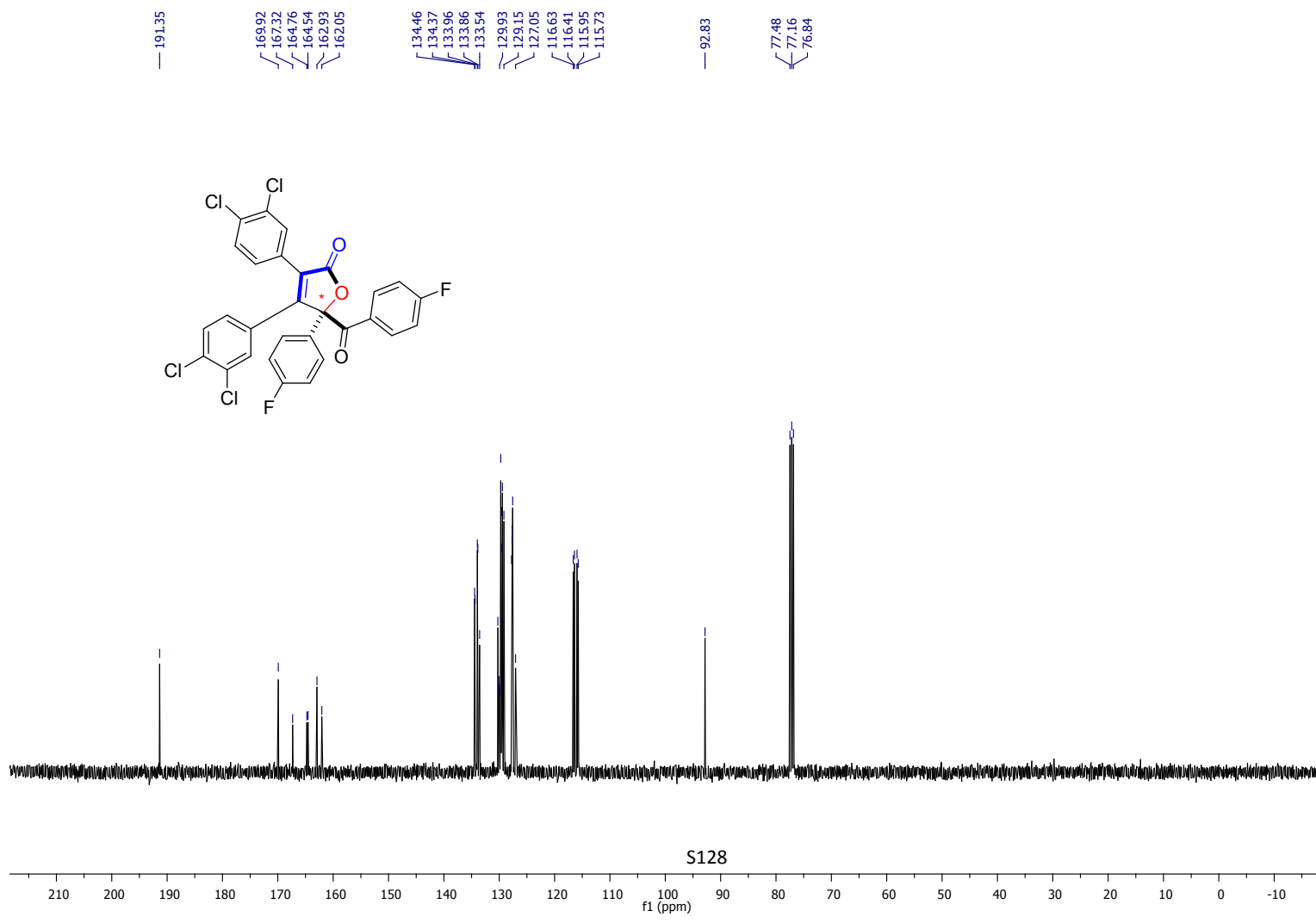
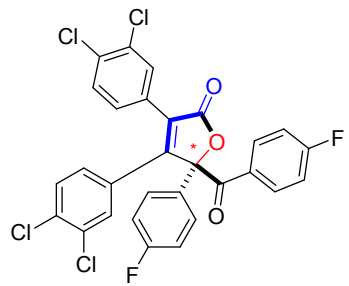




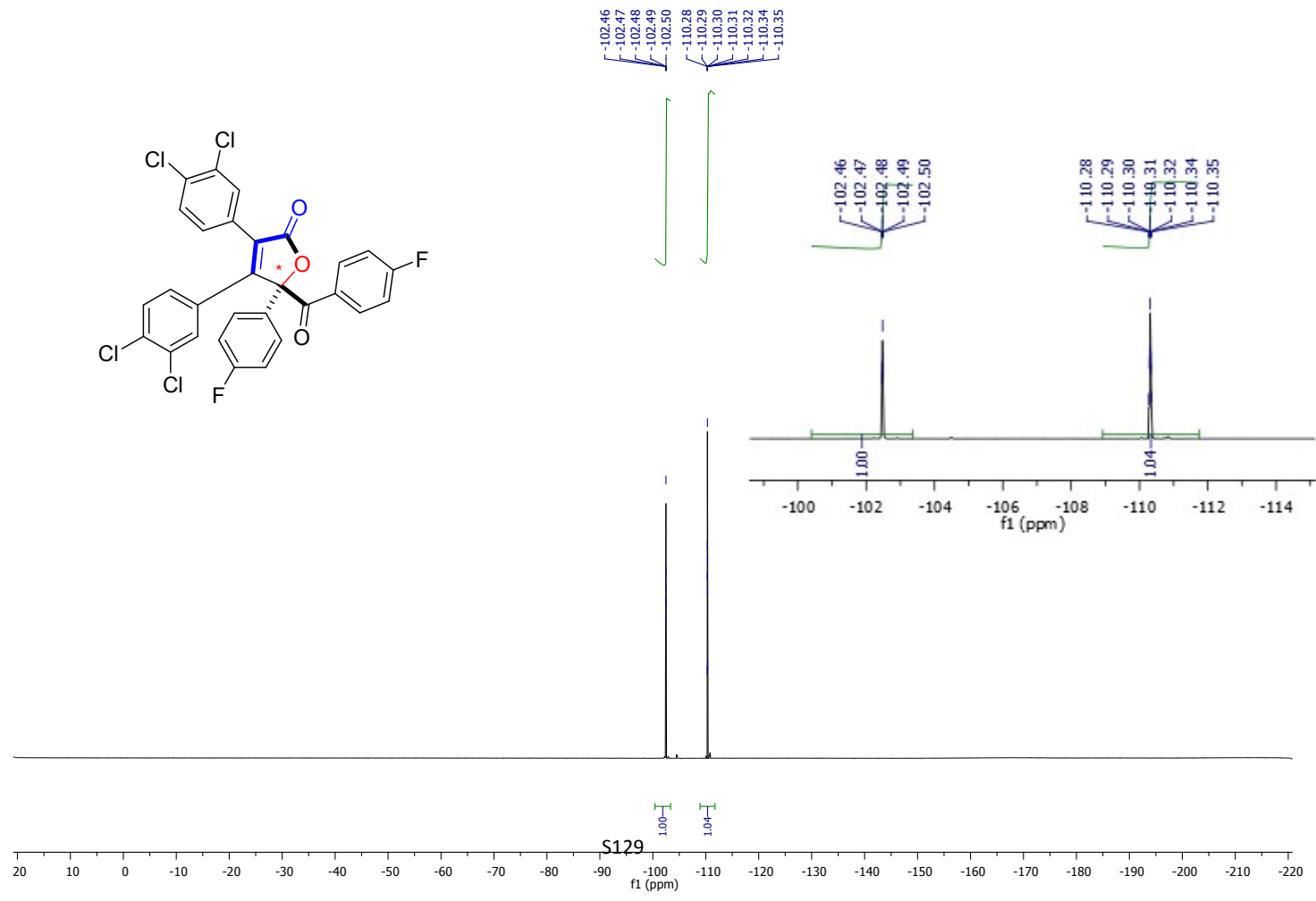


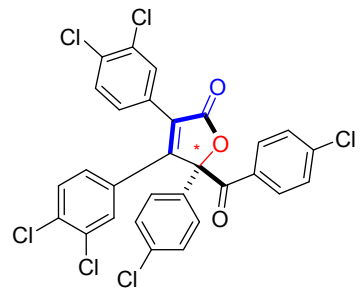
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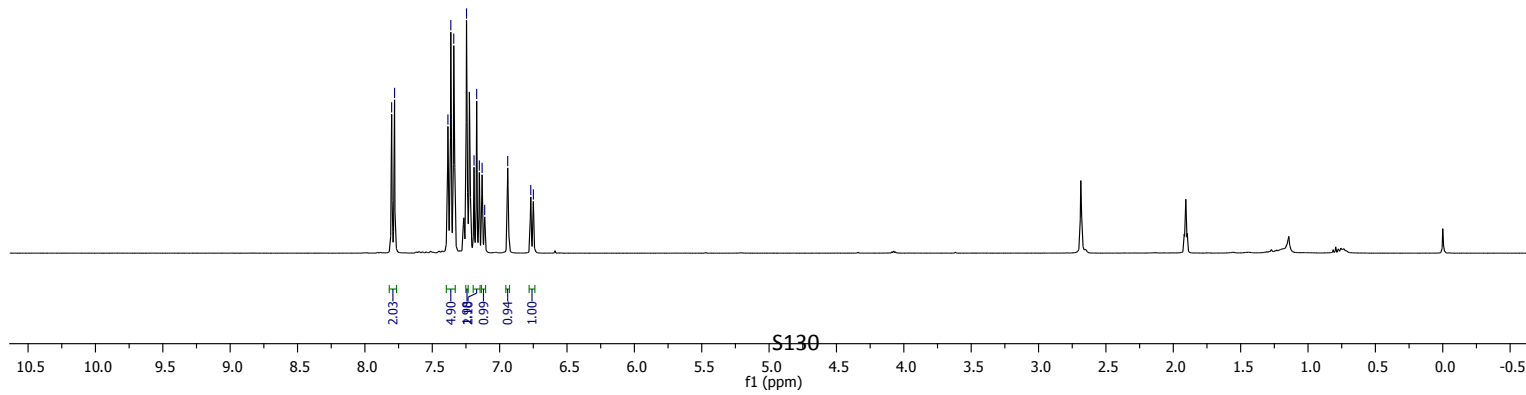
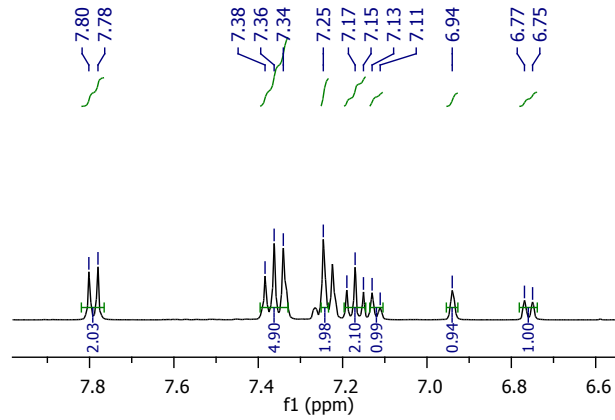


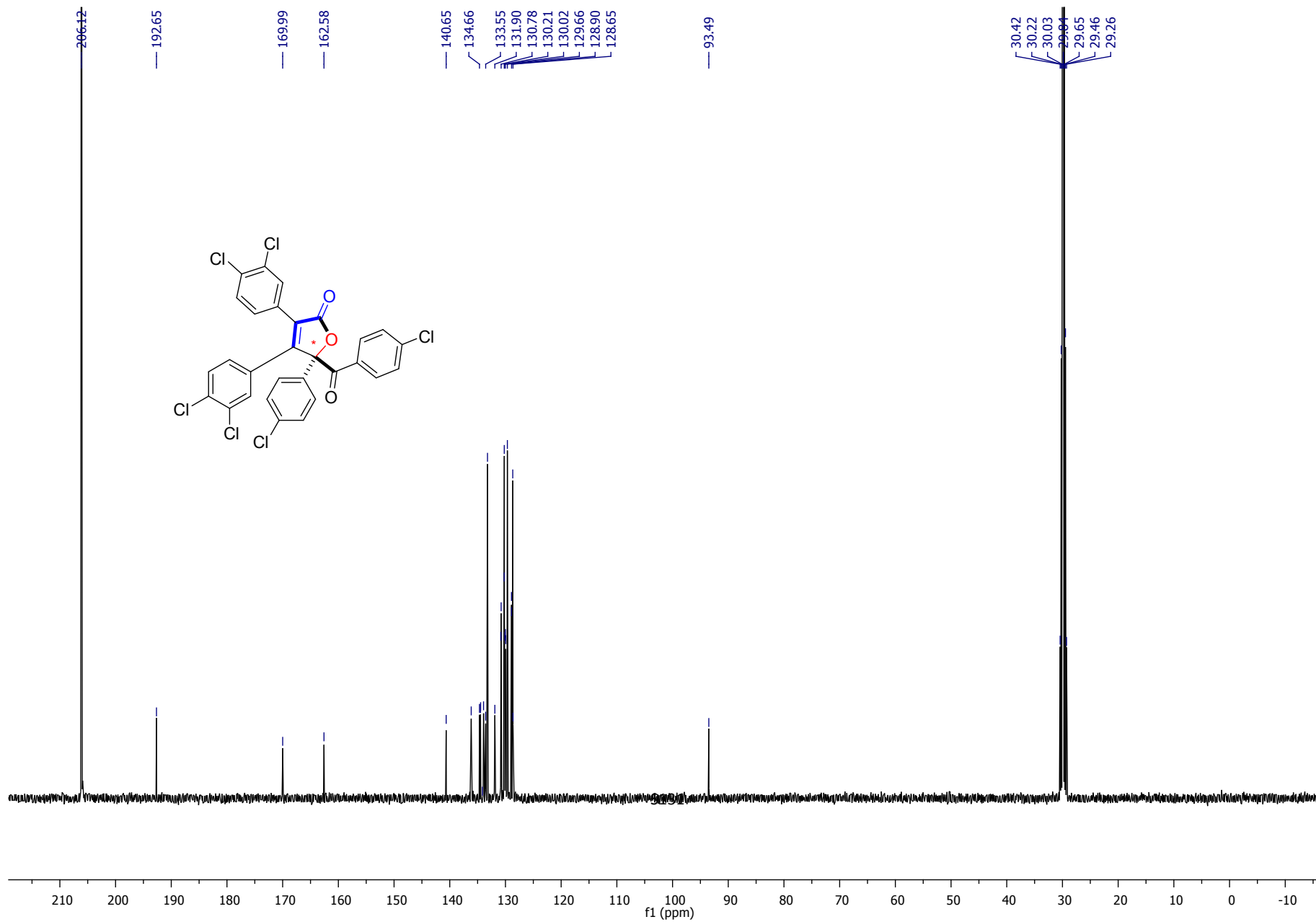
S128

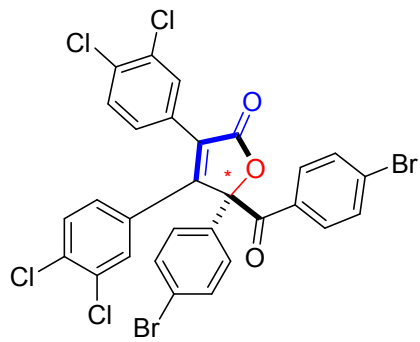




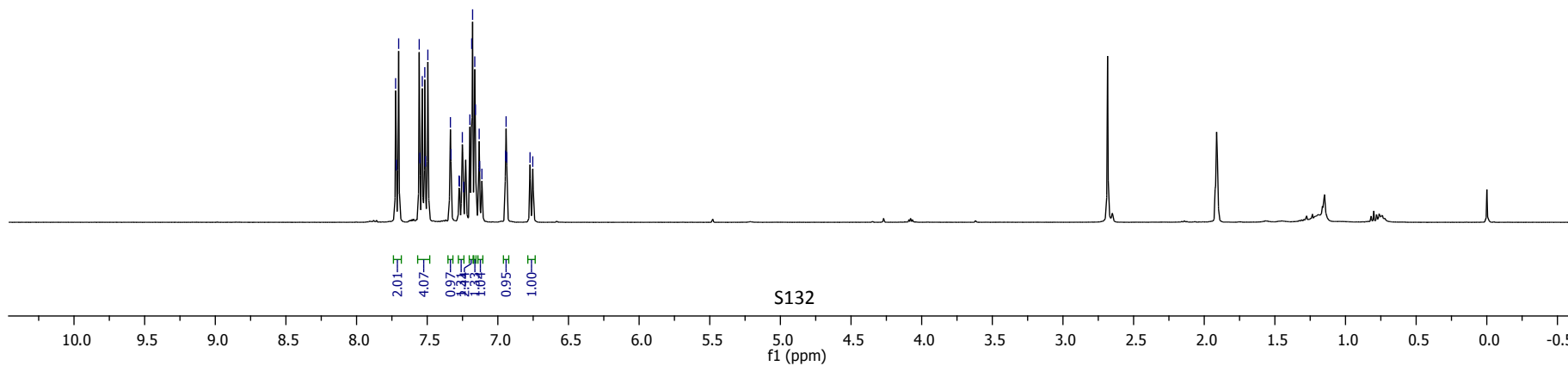
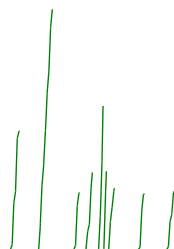
7.80
7.78
7.34
7.19
7.15
7.11
6.94
6.77
6.75

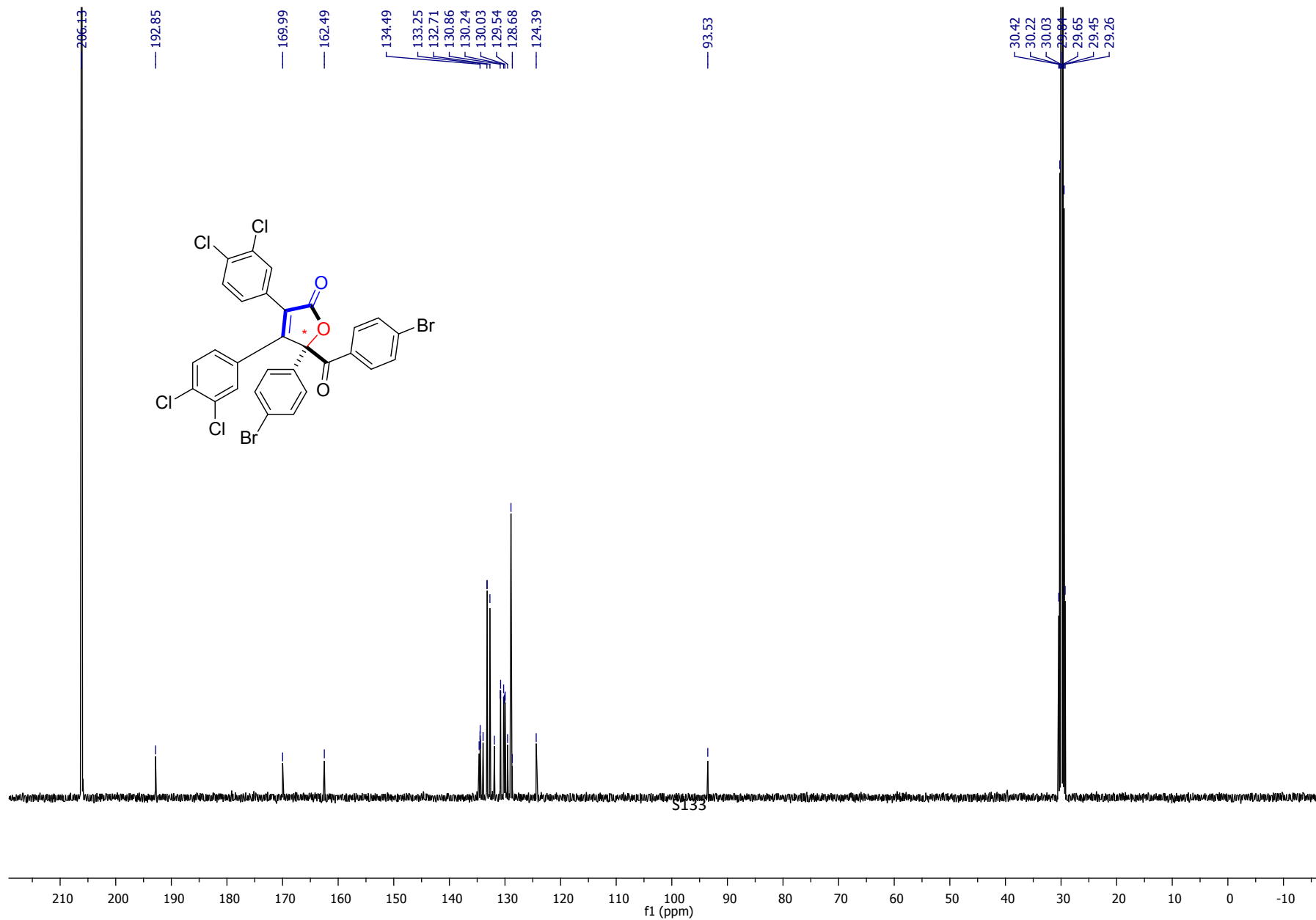




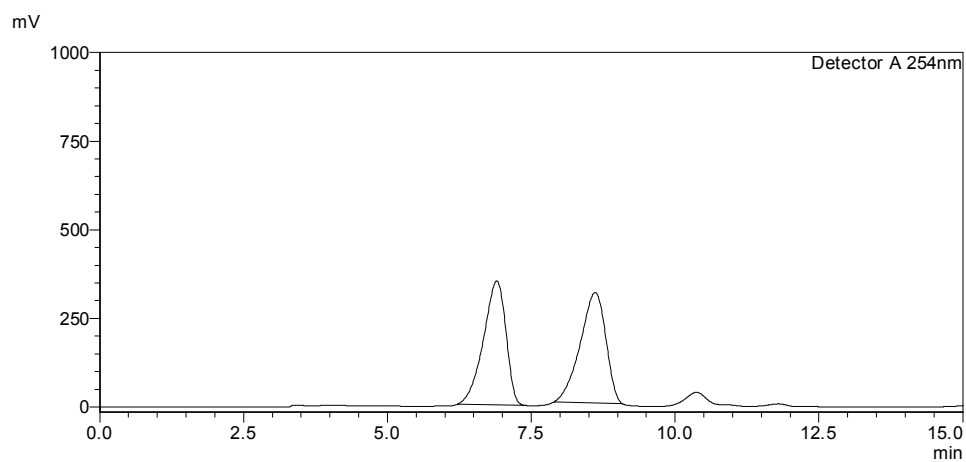
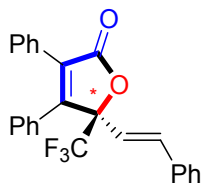


7.72
7.70
7.50
7.20
7.13
6.94
6.77
6.75

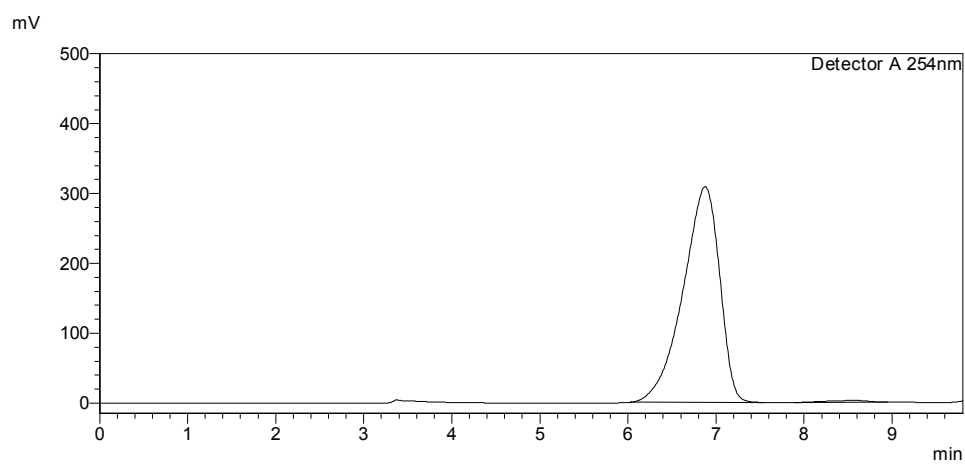




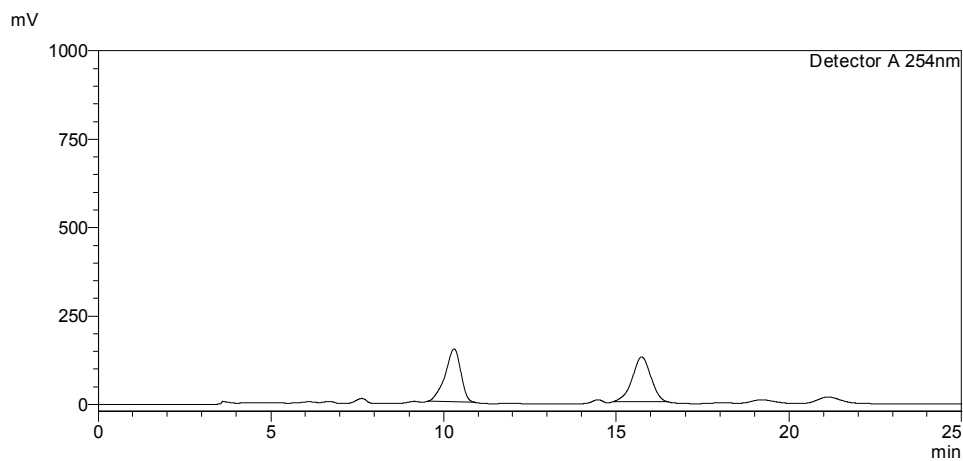
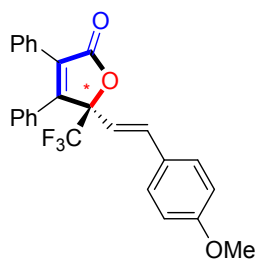
7. HPLC Spectra



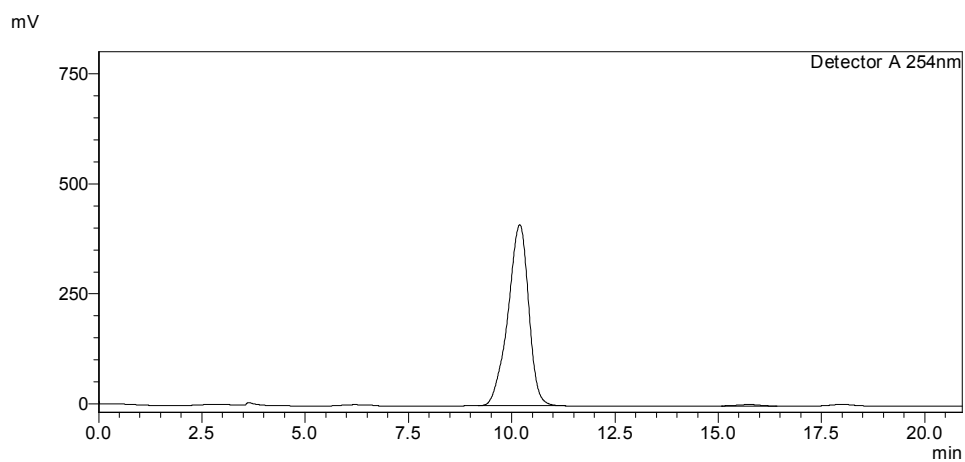
Peak#	Ret. Time	Area	Height	Conc.
1	6.900	9522529	349562	49.794
2	8.610	9601315	311032	50.206



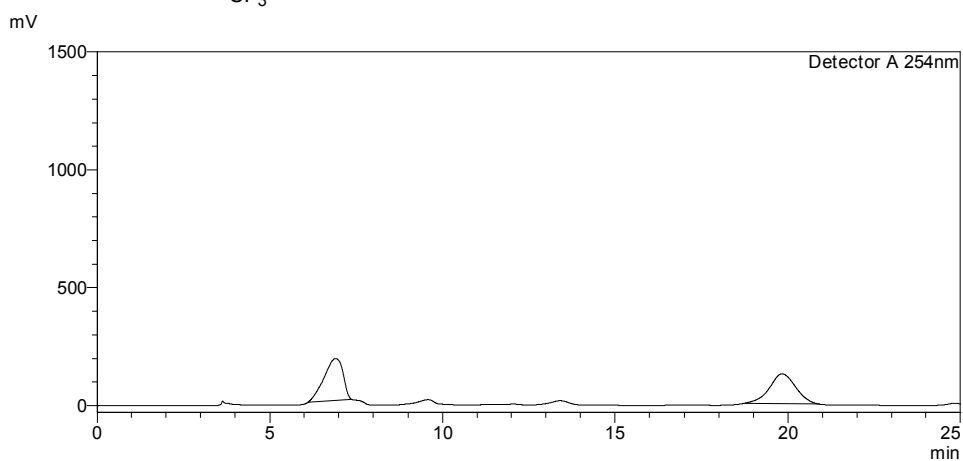
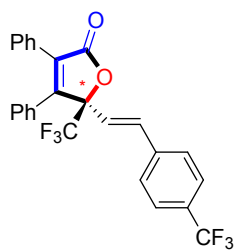
Peak#	Ret. Time	Area	Height	Conc.
1	6.876	8935670	308811	99.007
2	8.566	89627	2753	0.993



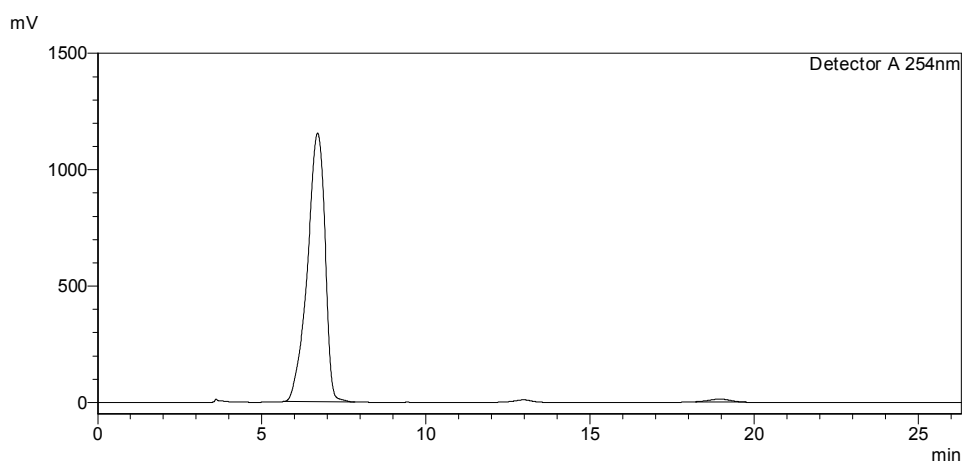
Peak#	Ret. Time	Area	Height	Conc.
1	10.307	4732520	150153	50.016
2	15.735	4729501	126467	49.984



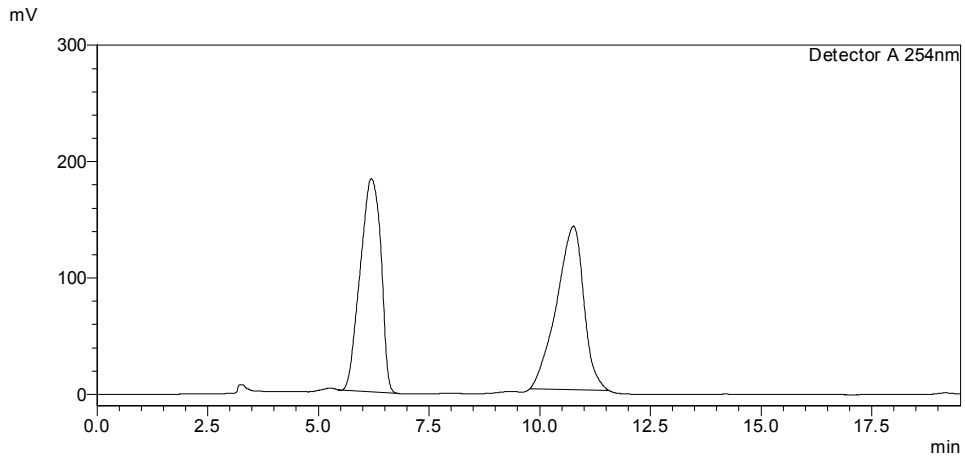
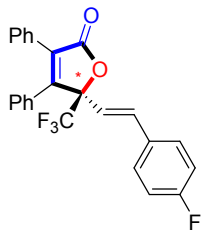
Peak#	Ret. Time	Area	Height	Conc.
1	10.193	14331406	411782	99.165
2	15.741	120707	3320	0.835



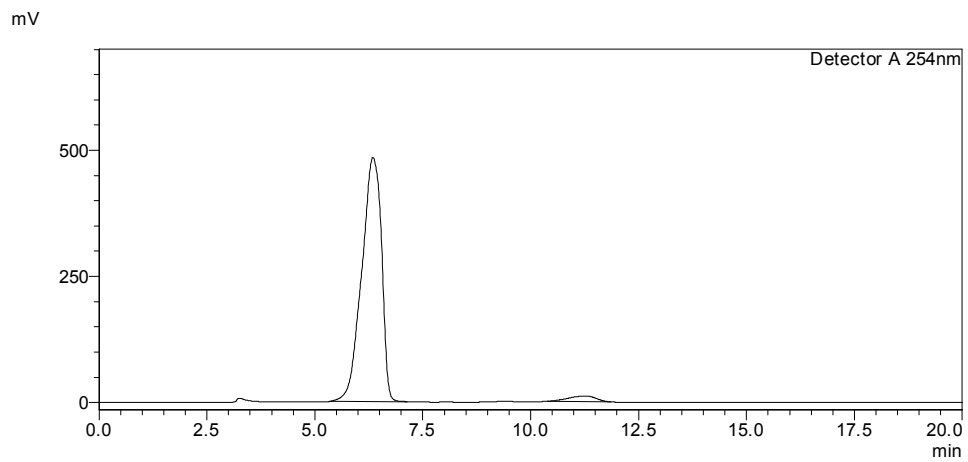
Peak#	Ret. Time	Area	Height	Conc.
1	6.911	6784433	177478	50.539
2	19.836	6639705	126240	49.461



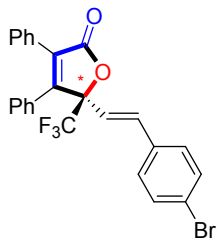
Peak#	Ret. Time	Area	Height	Conc.
1	6.698	43172402	1156514	98.769
2	18.950	538134	12302	1.231



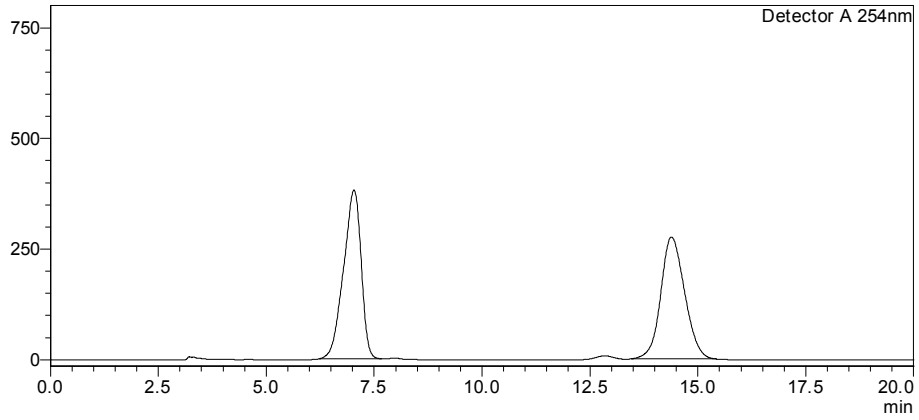
Peak#	Ret. Time	Area	Height	Conc.
1	6.196	5981045	183220	49.905
2	10.763	6003882	140425	50.095



Peak#	Ret. Time	Area	Height	Conc.
1	6.346	15423529	483548	96.937
2	11.276	487324	10753	3.063

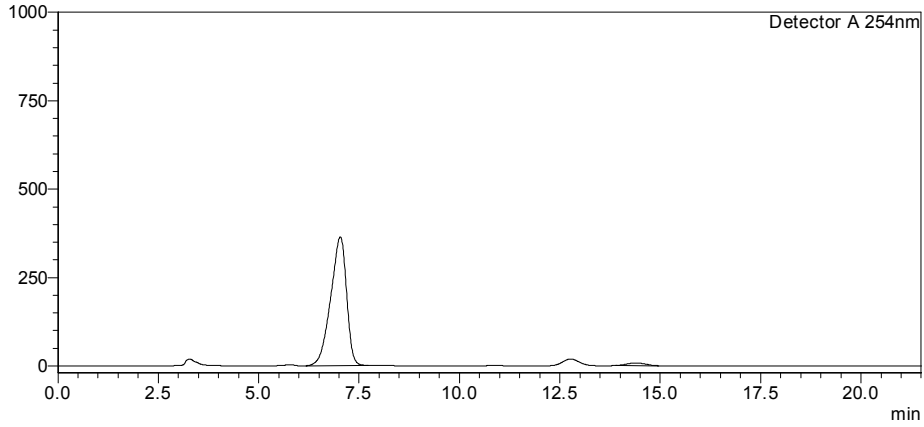


mV

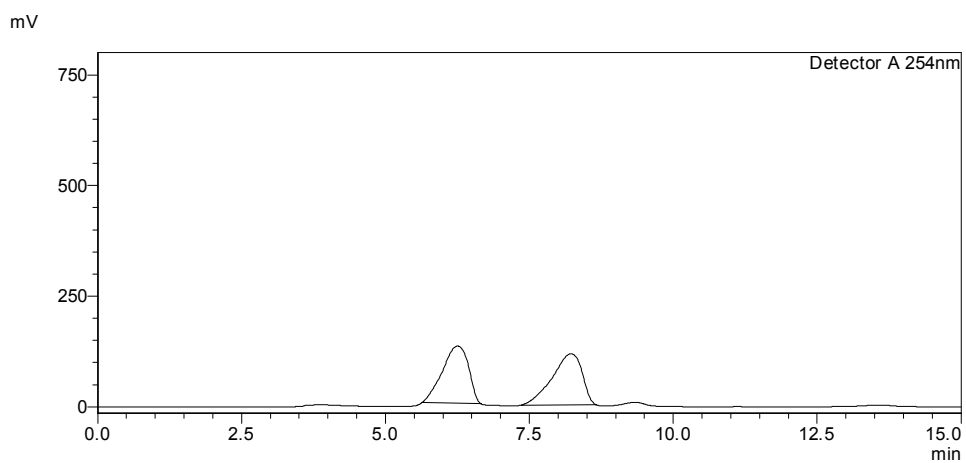
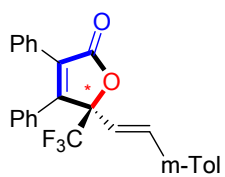


Peak#	Ret. Time	Area	Height	Conc.
1	7.032	10802978	381470	50.485
2	14.388	10595368	275466	49.515

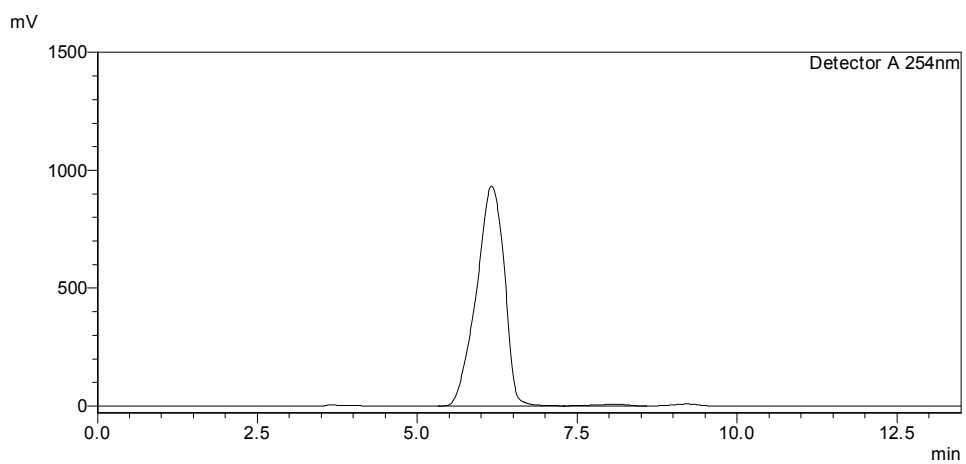
mV



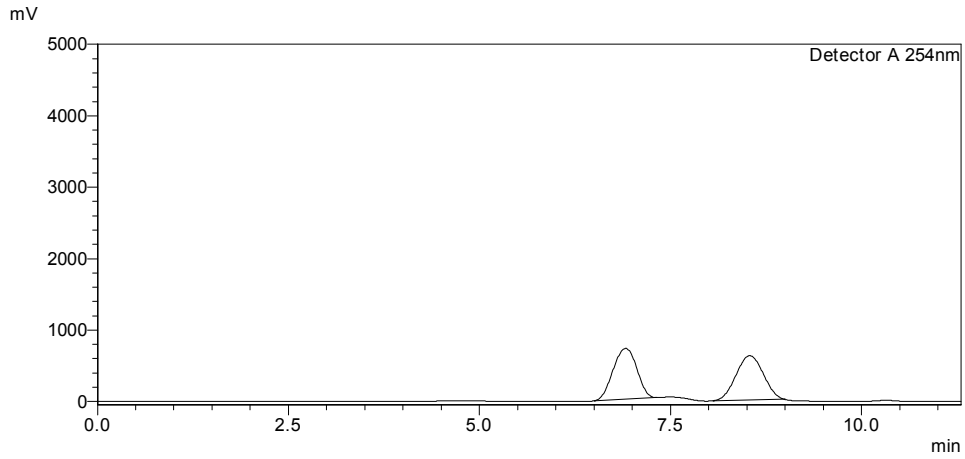
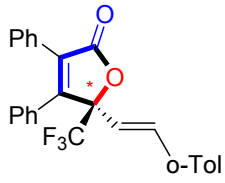
Peak#	Ret. Time	Area	Height	Conc.
1	7.032	9997595	364225	97.685
2	14.394	236955	7445	2.315



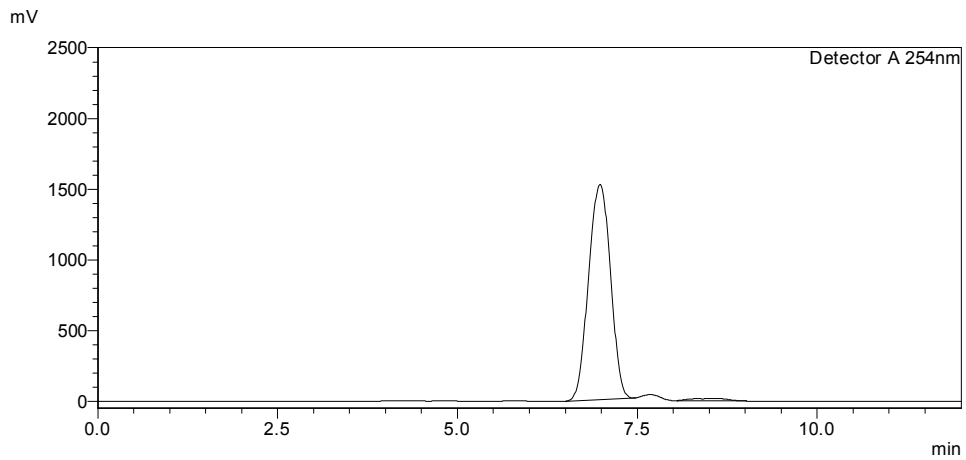
Peak#	Ret. Time	Area	Height	Conc.
1	6.254	4075777	128923	49.527
2	8.226	4153690	114946	50.473



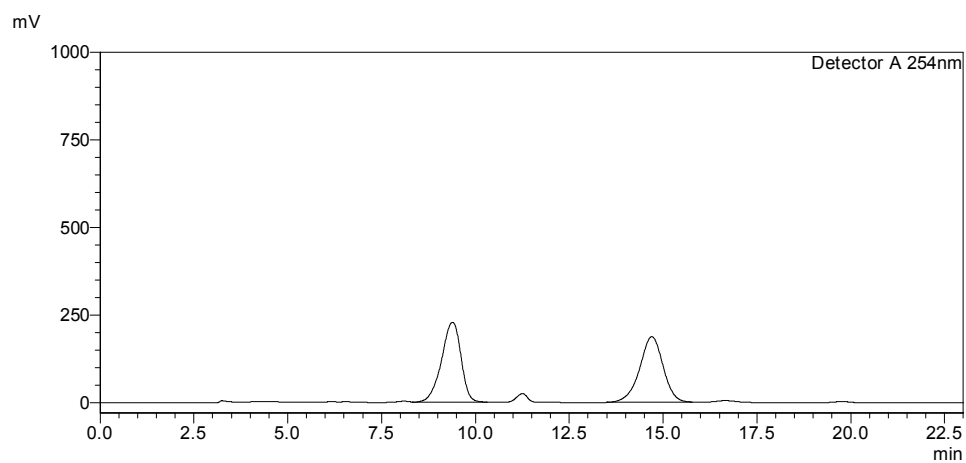
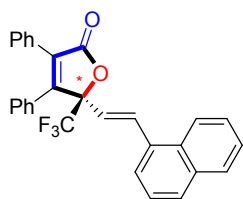
Peak#	Ret. Time	Area	Height	Conc.
1	6.162	28396599	932468	99.013
2	8.082	282992	7064	0.987



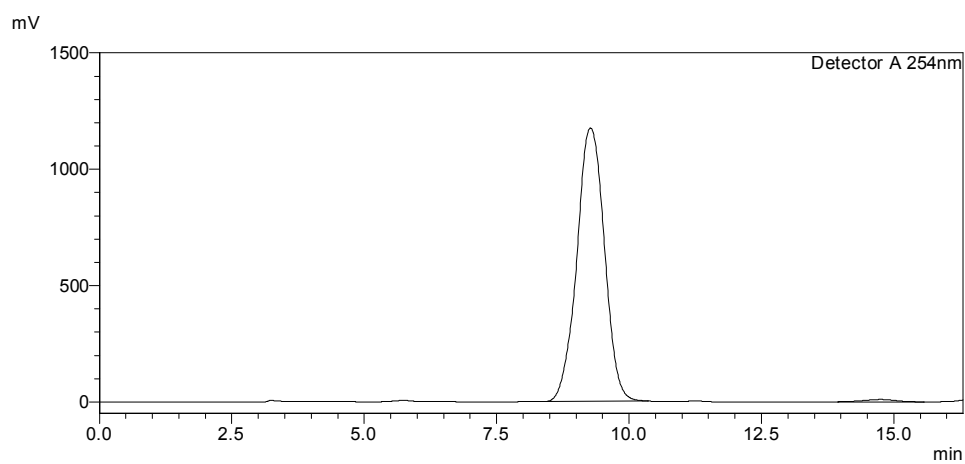
Peak#	Ret. Time	Area	Height	Conc.
1	6.914	15419302	712029	49.889
2	8.538	15487969	620756	50.111



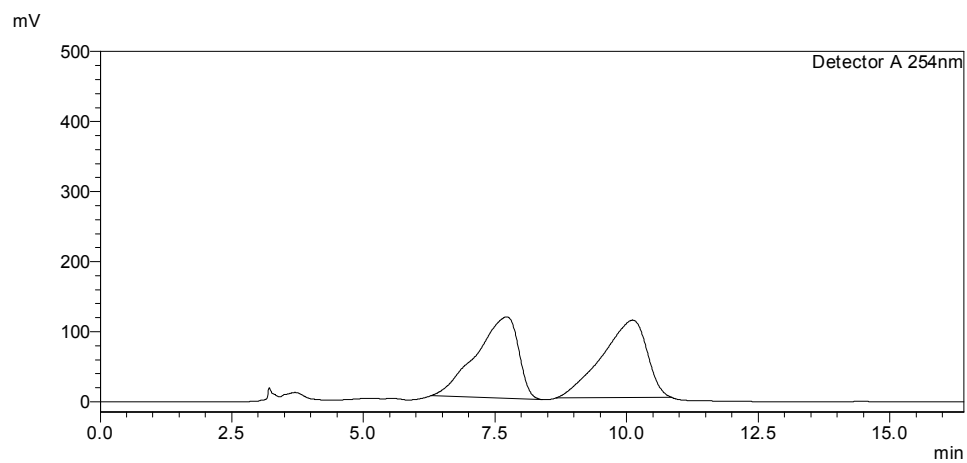
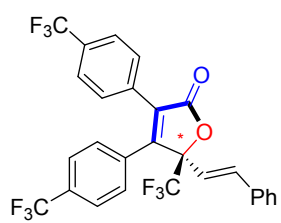
Peak#	Ret. Time	Area	Height	Conc.
1	6.981	32292923	1520847	98.239
2	8.584	578841	17528	1.761



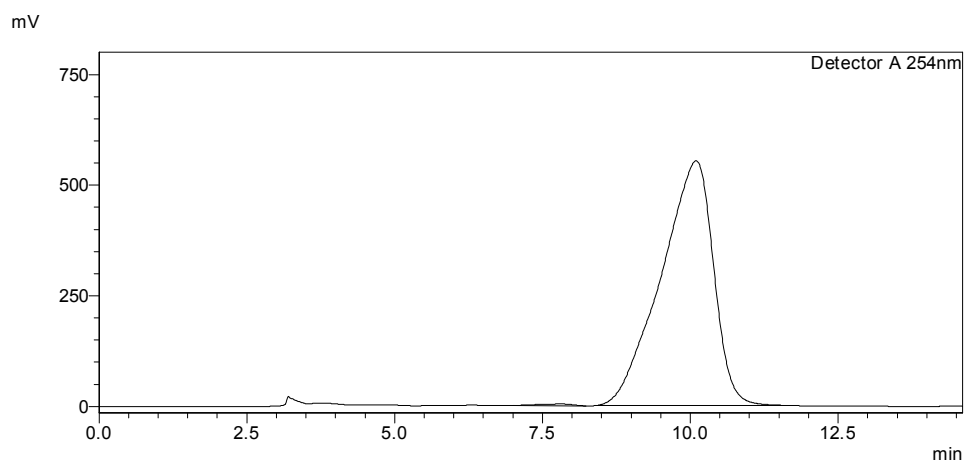
Peak#	Ret. Time	Area	Height	Conc.
1	9.390	8244066	228228	50.339
2	14.699	8133025	187241	49.661



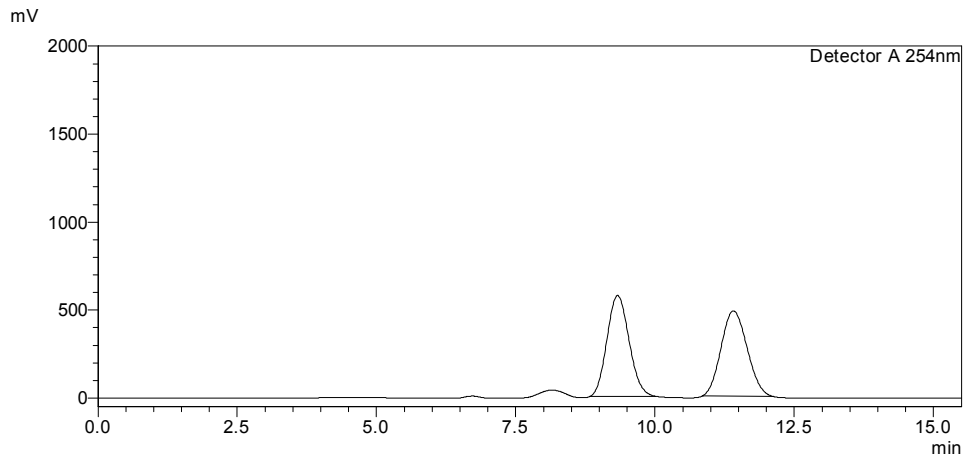
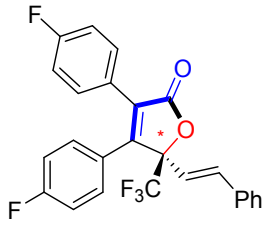
Peak#	Ret. Time	Area	Height	Conc.
1	9.272	42514800	1174134	99.044
2	14.753	410358	10066	0.956



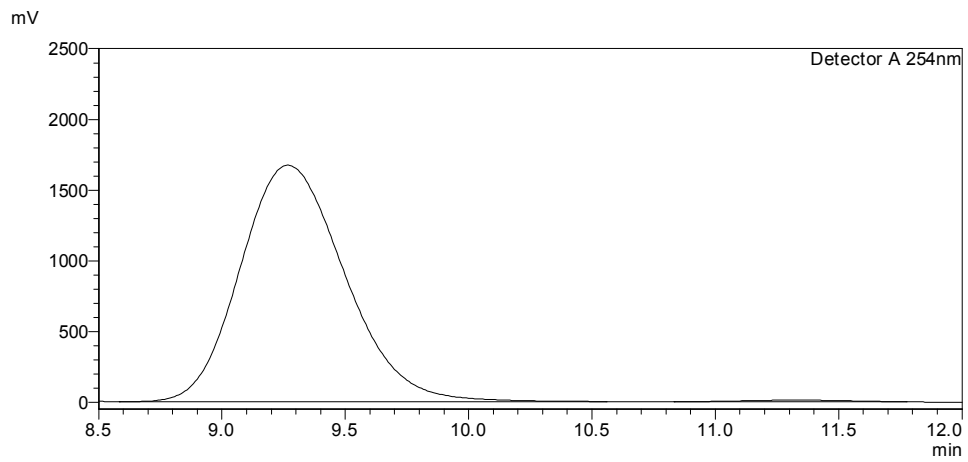
Peak#	Ret. Time	Area	Height	Conc.
1	7.720	6493127	116387	49.656
2	10.113	6583152	110540	50.344



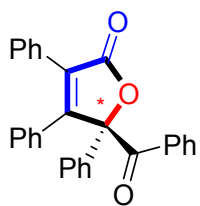
Peak#	Ret. Time	Area	Height	Conc.
1	7.816	158720	3845	0.463
2	10.097	34132817	553104	99.537



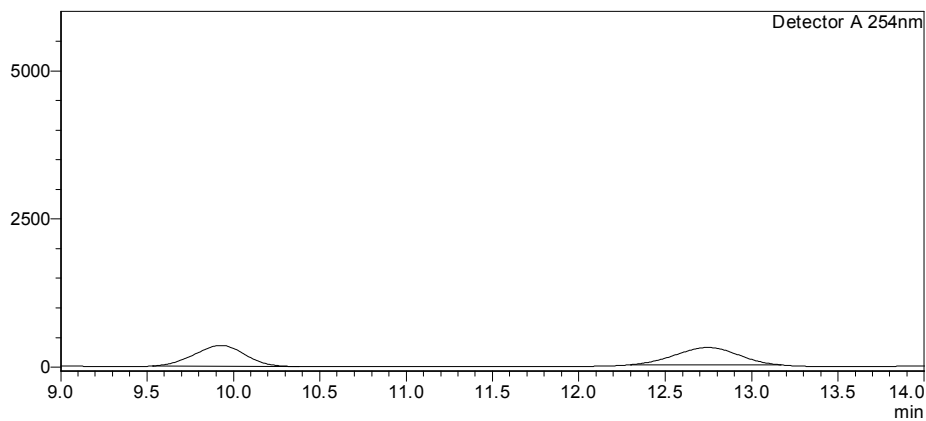
Peak#	Ret. Time	Area	Height	Conc.
1	9.328	15869993	573895	50.093
2	11.408	15811174	485662	49.907



Peak#	Ret. Time	Area	Height	Conc.
1	9.268	49221326	1671798	99.306
2	11.331	344001	11926	0.694

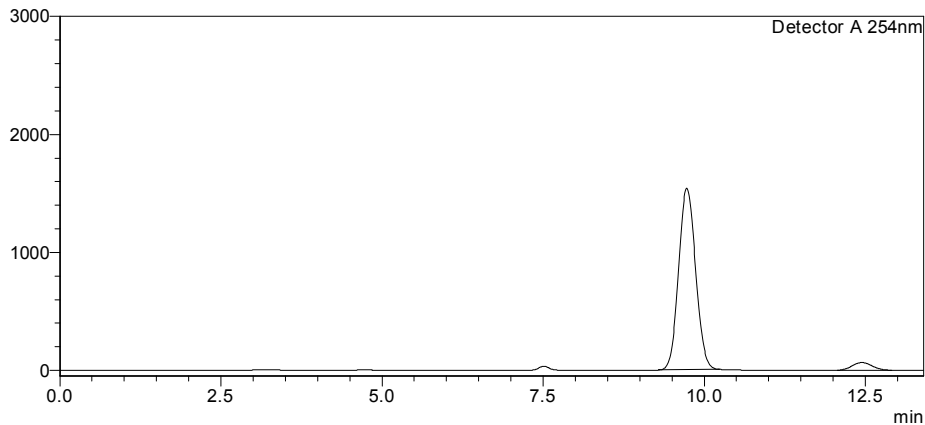


mV

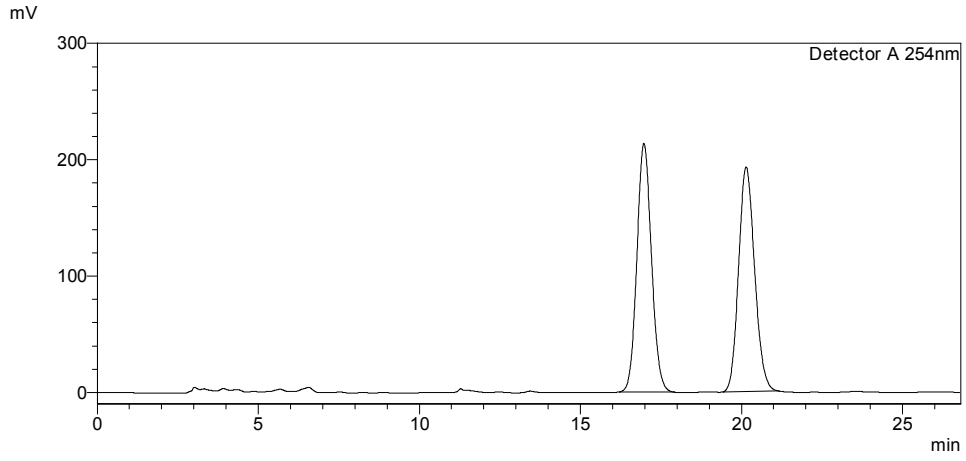
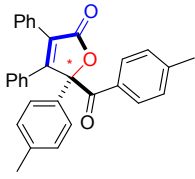


Peak#	Ret. Time	Area	Height	Conc.
1	9.929	7212760	352136	49.509
2	12.747	7355682	291955	50.491

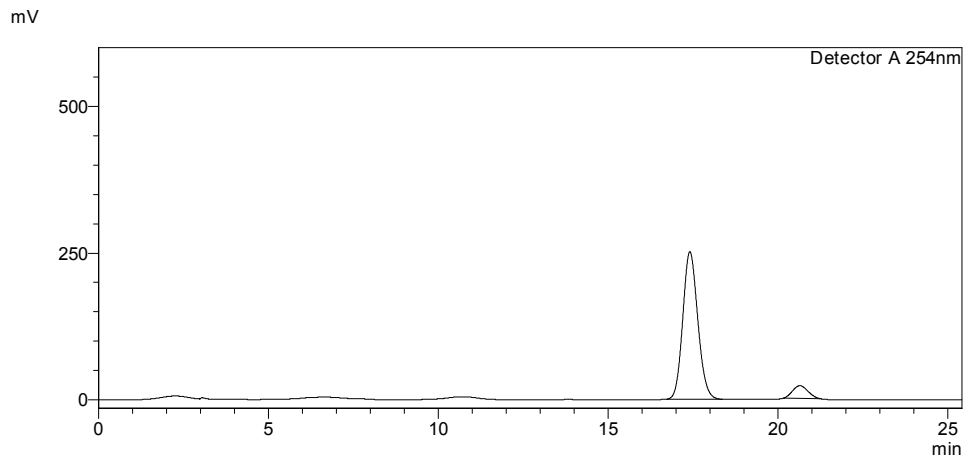
mV



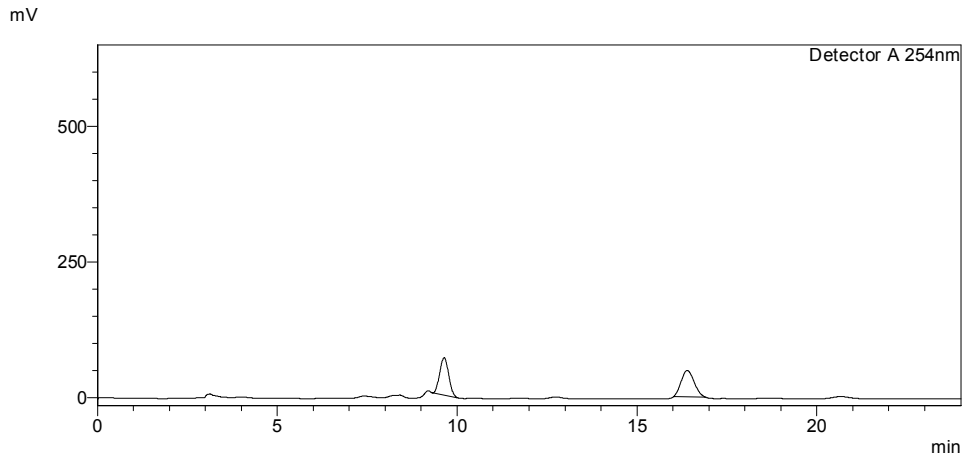
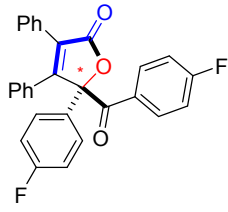
Peak#	Ret. Time	Area	Height	Conc.
1	9.729	28286914	1536880	95.262
2	12.445	1406808	65295	4.738



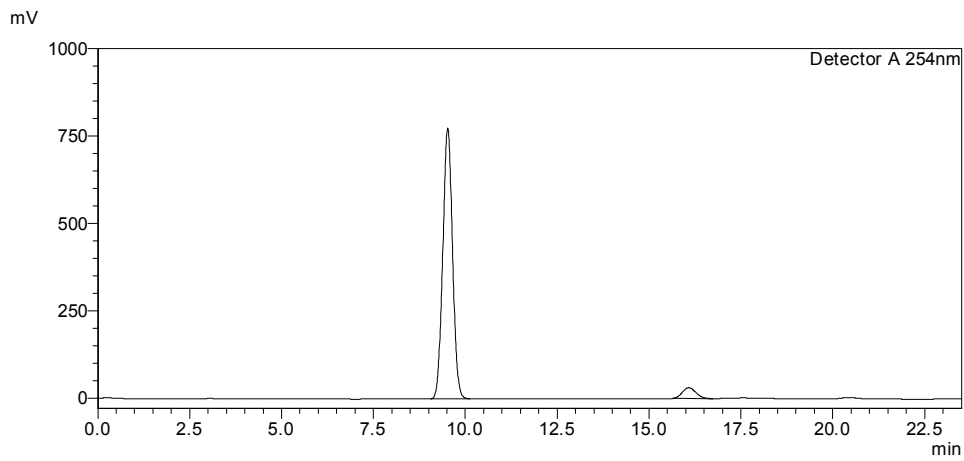
Peak#	Ret. Time	Area	Height	Conc.
1	16.971	6720650	213866	50.121
2	20.145	6688122	193089	49.879



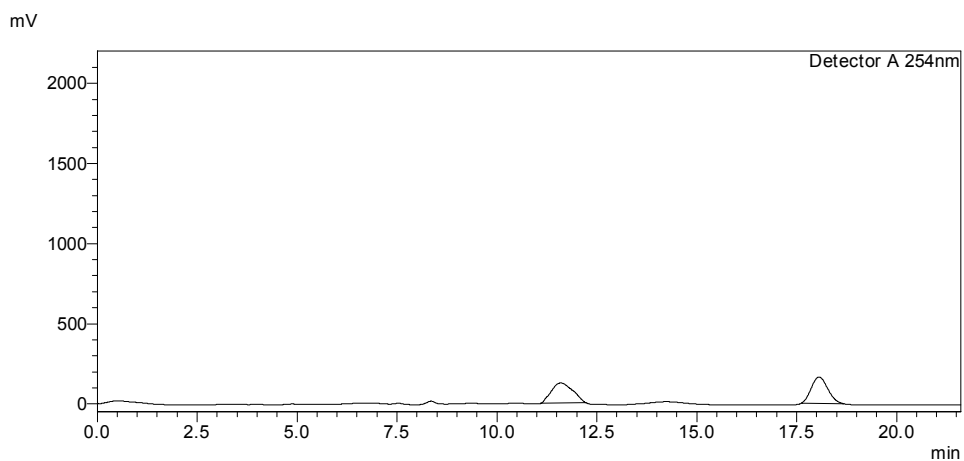
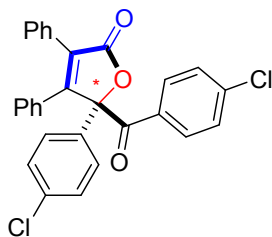
Peak#	Ret. Time	Area	Height	Conc.
1	17.402	7707763	251361	92.020
2	20.641	668455	21509	7.980



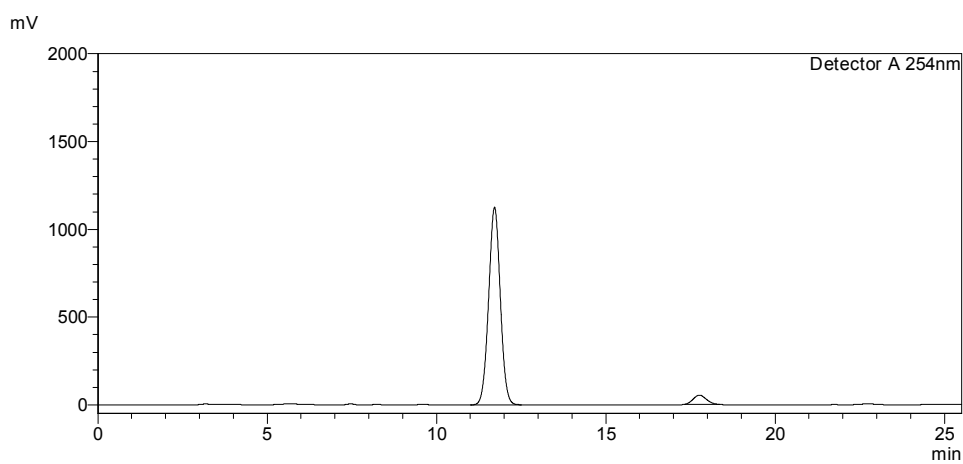
Peak#	Ret. Time	Area	Height	Conc.
1	9.639	1186960	68923	49.704
2	16.399	1201120	48207	50.296



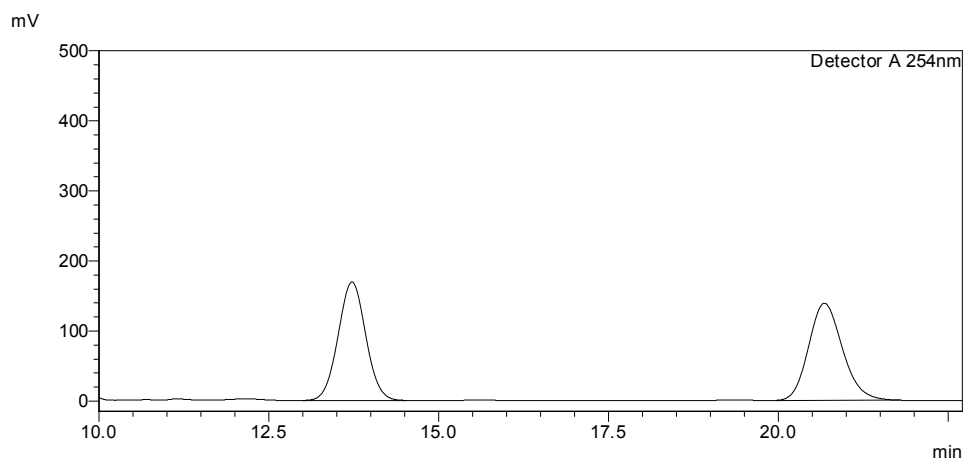
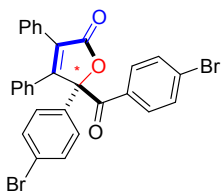
Detector A 254nm						
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark
1	9.523	14270540	775049	94.760		M
2	16.082	789135	30822	5.240		M
Total		15059675	805872			



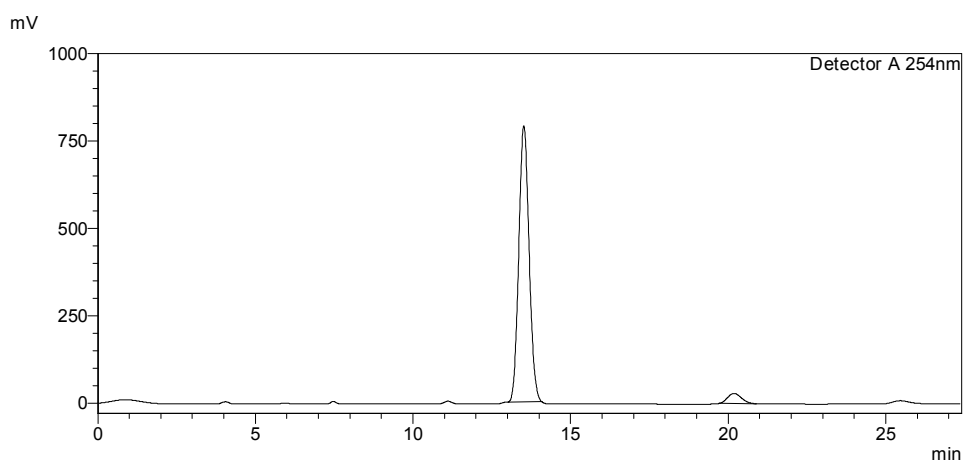
Peak#	Ret. Time	Area	Height	Conc.
1	11.596	4674351	125425	49.970
2	18.057	4680005	164363	50.030



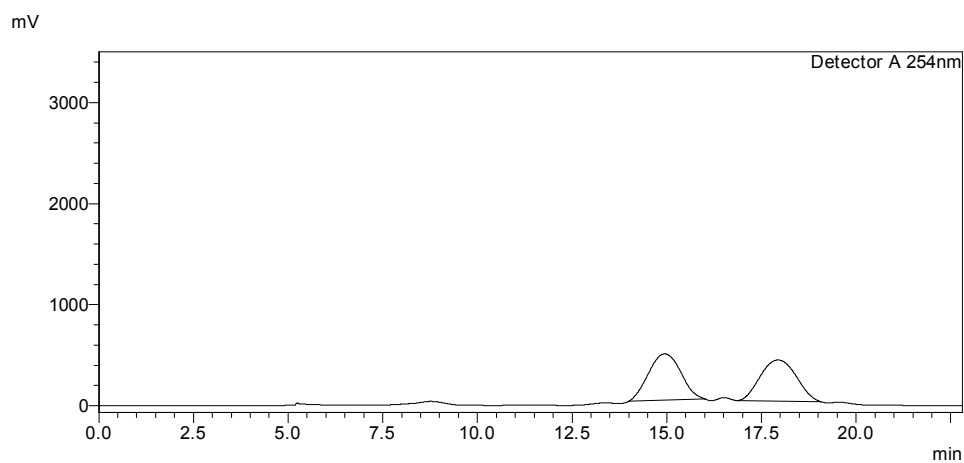
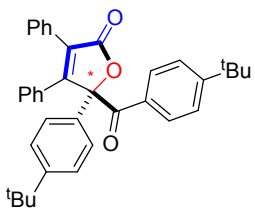
Detector A 254nm						
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark
1	11.714	26837512	1125450	94.914		M
2	17.764	1438210	52621	5.086		M
Total		28275722	1178072			



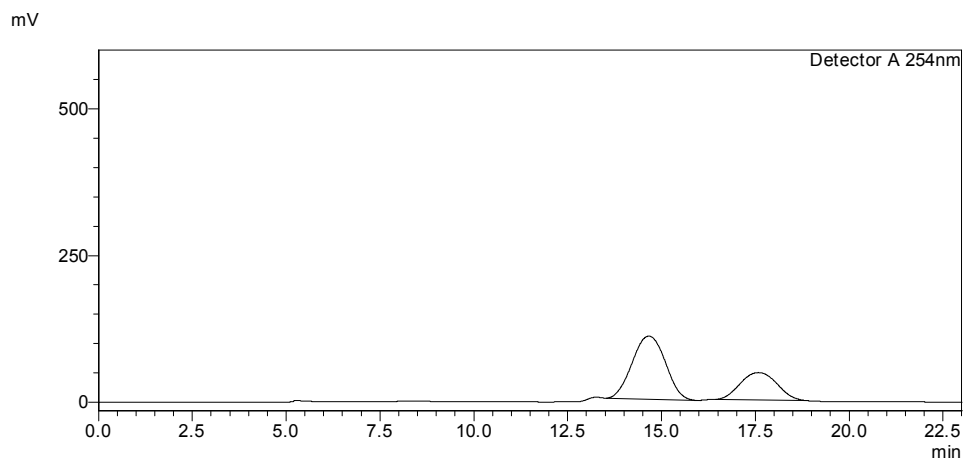
Peak#	Ret. Time	Area	Height	Conc.
1	13.723	4787077	169387	49.946
2	20.678	4797366	138584	50.054



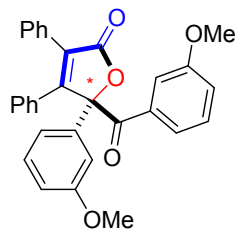
Detector A 254nm						
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark
1	13.516	17977060	790493	95.270		M
2	20.186	892525	29149	4.730		M
Total		18869584	819643			



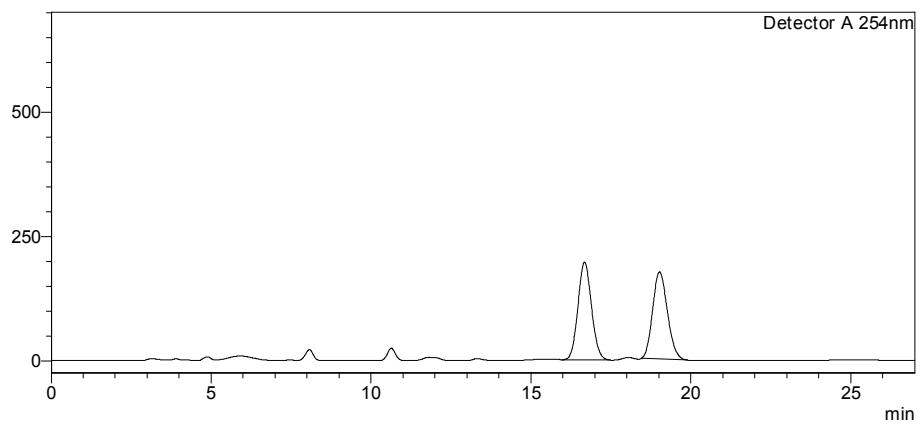
Peak#	Ret. Time	Area	Height	Conc.
1	14.947	27130130	457406	50.266
2	17.939	26842465	406457	49.734



Peak#	Ret. Time	Area	Height	Conc.
1	14.661	6589817	107361	67.355
2	17.582	3193898	46813	32.645

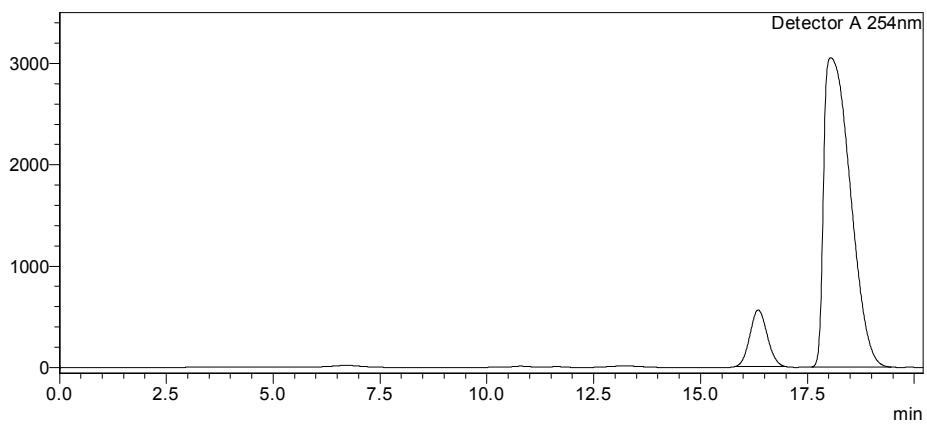


mV

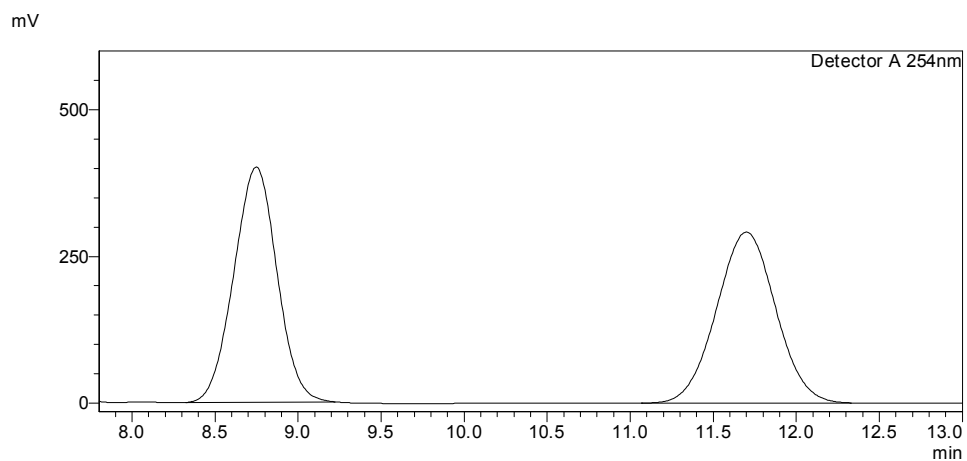
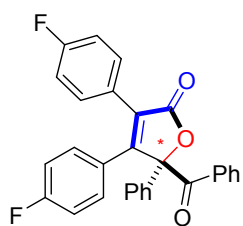


Peak#	Ret. Time	Area	Height	Conc.
1	16.676	5779667	196464	50.623
2	19.023	5637413	175319	49.377

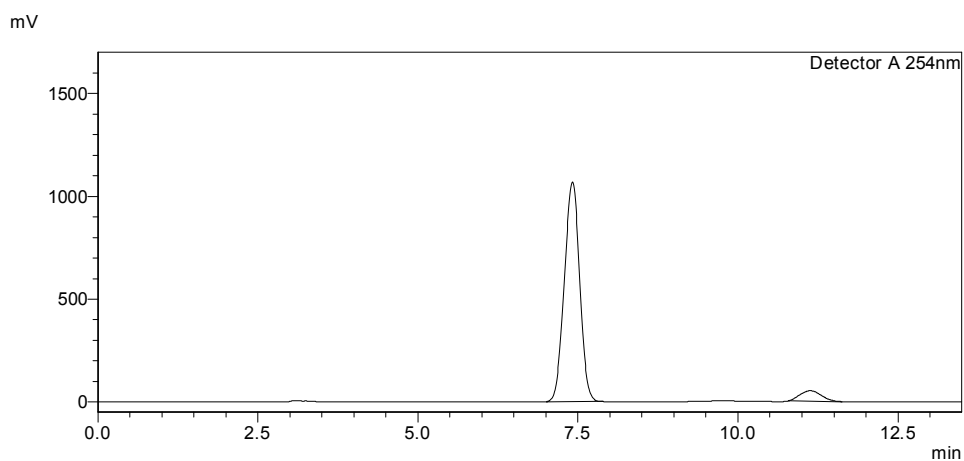
mV



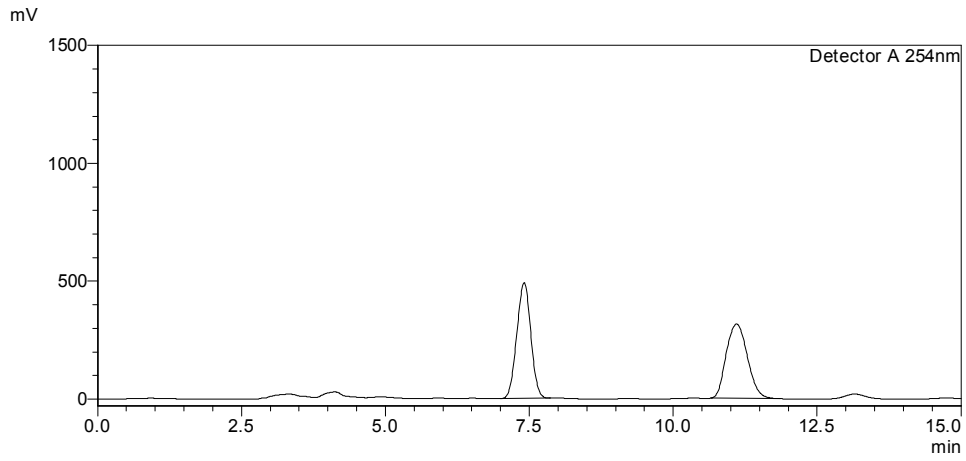
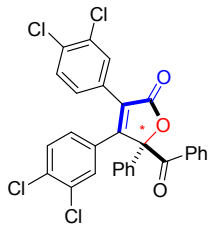
Peak#	Ret. Time	Area	Height	Conc.
1	16.348	15852791	561091	10.777
2	18.046	131245009	3052577	89.223



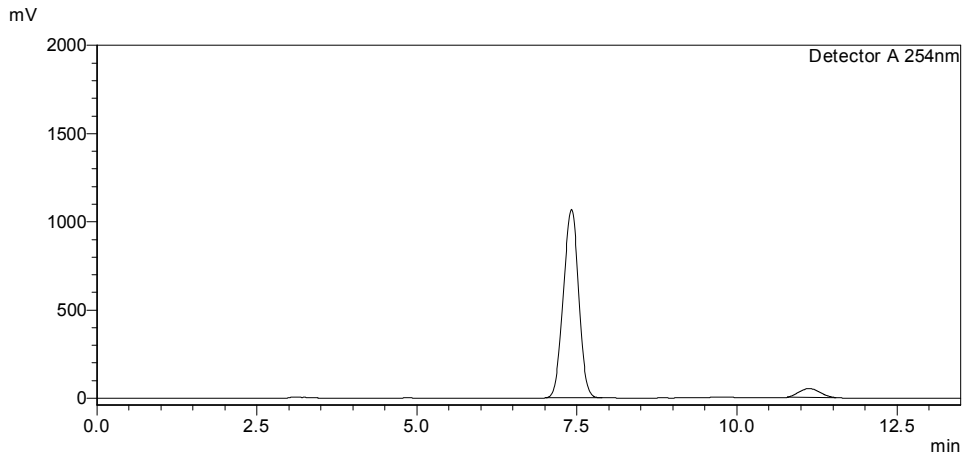
Peak#	Ret. Time	Area	Height	Conc.
1	8.747	7259272	400761	50.113
2	11.699	7226557	291514	49.887



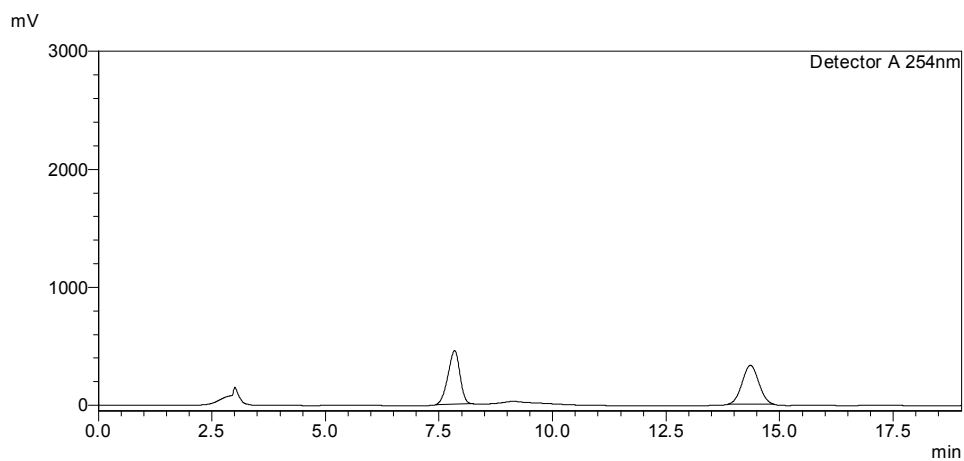
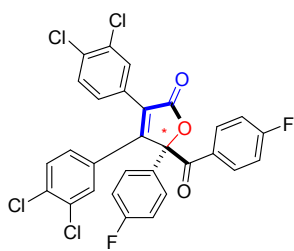
Detector A 254nm						
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark
1	7.415	17831904	1067511	93.738		M
2	11.129	1191319	50922	6.262		M
Total		19023223	1118432			



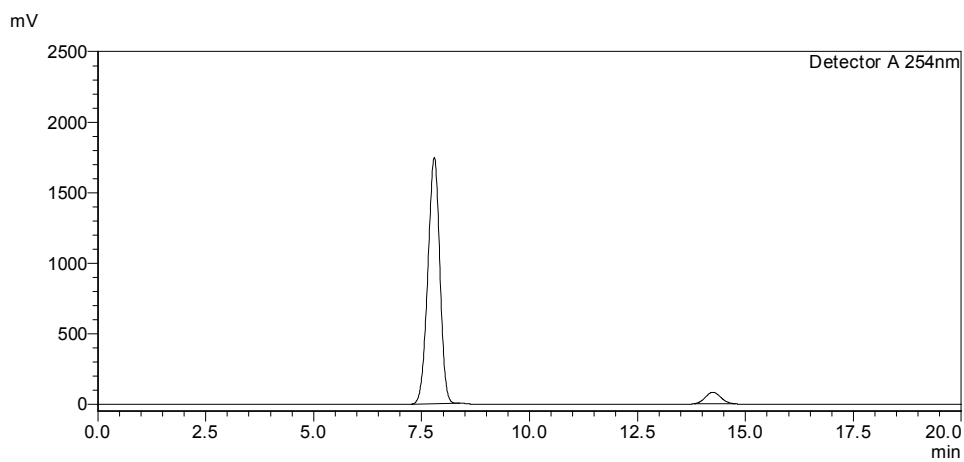
Peak#	Ret. Time	Area	Height	Conc.
1	7.412	8350398	491063	50.779
2	11.102	8094326	315217	49.221



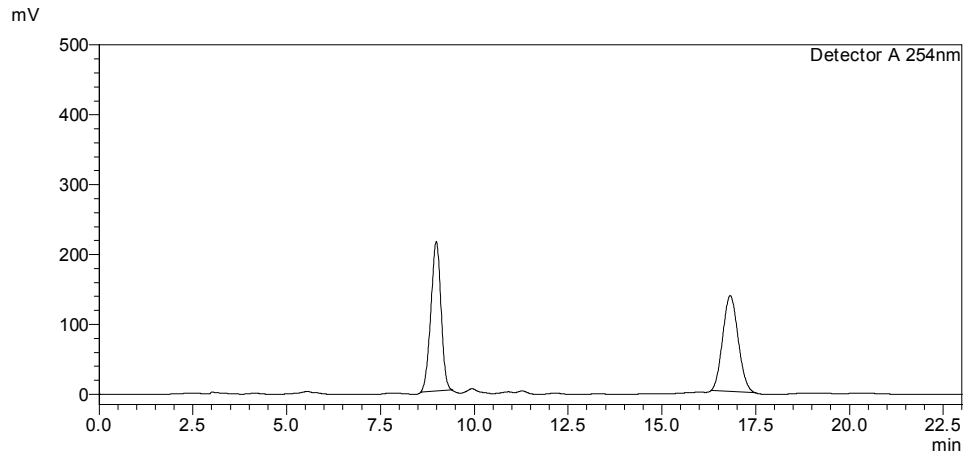
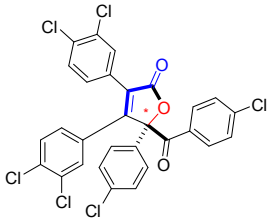
Detector A 254nm						
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark
1	7.415	17831904	1067511	93.966		M
2	11.129	1145017	50037	6.034		M
Total		18976922	1117548			



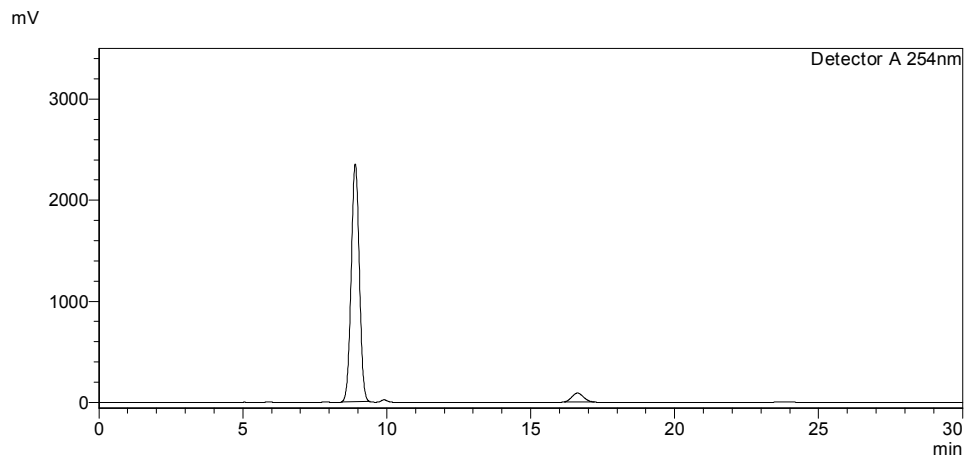
Peak#	Ret. Time	Area	Height	Conc.
1	7.841	8331288	454433	49.953
2	14.356	8347067	328835	50.047



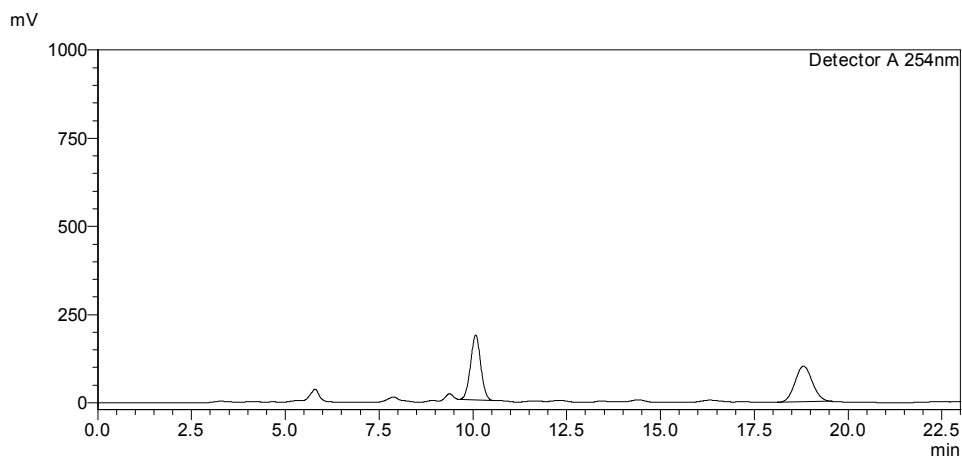
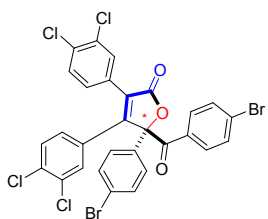
Peak#	Ret. Time	Area	Height	Conc.
1	7.794	33598601	1745100	94.337
2	14.247	2016990	81415	5.663



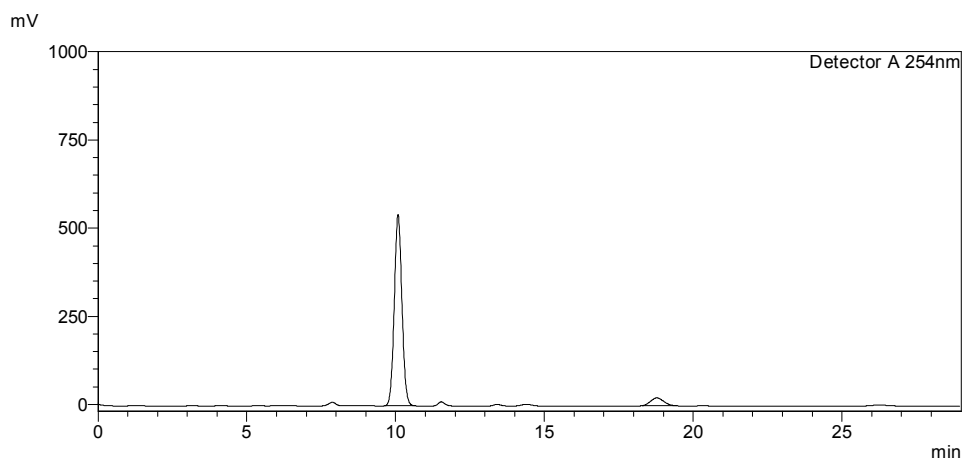
Peak#	Ret. Time	Area	Height	Conc.
1	8.987	4038164	213914	50.598
2	16.821	3942769	137214	49.402



Peak#	Ret. Time	Area	Height	Conc.
1	8.906	46308811	2355542	95.086
2	16.626	2392986	87050	4.914



Peak#	Ret. Time	Area	Height	Conc.
1	10.075	3480814	184092	51.547
2	18.812	3271901	101241	48.453



Peak#	Ret. Time	Area	Height	Conc.
1	10.083	9662481	542661	93.398
2	18.779	683055	22254	6.602