Supporting Information

Electrochemical Dual *α*,*β*-C(sp^3)–H Functionalization of Cyclic *N*-Aryl Amines

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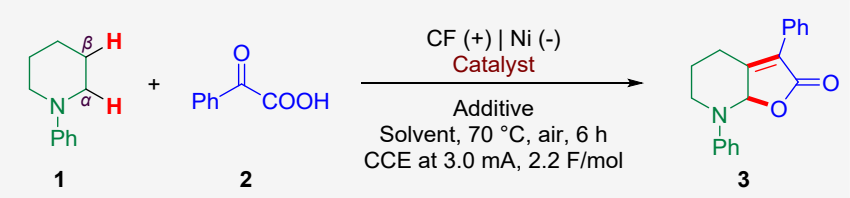
General Remarks

Catalytic reactions were carried out in undivided electrochemical cells (15 mL) using pre-dried glassware, if not noted otherwise. All the starting materials were obtained from commercial sources or synthesized according to literature methods.[1] $Fe(phen)Cl_3$ and $Fe(phen)Cl_2$ were synthesized according to literature methods.[2-3] Acetonitrile was purchased from *Energy Chemical*. Nickel electrodes (10 mm × 15 mm × 0.2 mm, 99.9%; obtained from Chuxi, Shanghai, China) and carbon felt electrodes (10 mm × 15 mm × 3 mm, Jinglong company, Beijing, China) were connected using stainless steel adapters. Electrocatalysis was conducted using an HSPY-36-03 potentiostat in constant current mode. Cyclic Voltammetry studies were performed using a Shanghai Chenhua CHI760E workstation. Yields refer to isolated compounds, estimated to be >95% purity as determined by 1H-NMR. Flash chromatography was performed using Silica gel (200-300 mesh) purchased from Qingdao Haiyang Chemical Co., China. Thin layer chromatography was used for product detection using acrylic silicone plates, with visualization effected via exposure to UV Light (λex = 254 nm). NMR spectra were recorded on Bruker AVANCE AV 400, Bruker AVANCE AV 600 and Bruker AVANCE AV 800 in the solvent indicated; using $CDCl_3$ or CD_3OD-d_4 as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature, chemical shifts (δ) are given in ppm relative to the residual solvent peak, coupling constants (J) are reported in Hertz (Hz). Multiplicities are recorded as: s = singlet, d = doublet, t = triplet, q = quadruplet, dd = doublet of doublets, m = multiplet. High-resolution mass spectrometry (HRMS) data were collected on a MicrOTOF mass spectrometer with ESI mass analyzer. Melting points were recorded on Shanghai ShenGuang WRS–2 apparatus. Visualization was achieved under a UV lamp (254 nm and 365 nm). X-ray crystallography and data were performed and collected using Rigaku XtalAB PRO MM007 DW and Olex2.

Mass spectra were acquired using an LTQ-XL mass spectrometer (Thermo-Fisher, Waltham, MA). The inlet capillary temperature of the mass spectrometer was maintained at 275 °C unless otherwise stated. The tube lens voltage on the LTQ-XL is

set to be 0 V. The mass-to-charge (*m/z*) range was adjusted to 50 – 500. All the data were analyzed by default Xcalibur package (Version 2.0.7 Thermo Fisher Scientific, US). All these experiments were carried out under atmospheric pressure.

Optimization of the Electrochemical Dual C(sp^3)–H Functionalization[a]

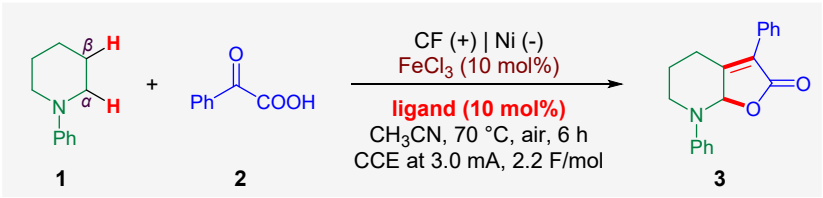


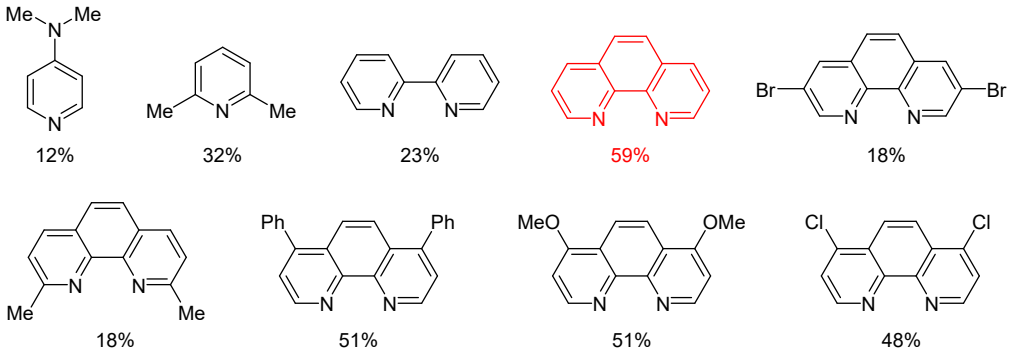
Entry	Catalyst (10 mol%)	Additive (20 mol%)	Solvent	**3** [%][b]
1	$Fe(phen)Cl_3$	--	CH_3CN	80
2	$Fe(phen)Cl_2$	--	CH_3CN	58
3	$FeCl_3$	--	CH_3CN	44
4	$FeCl_2$	--	CH_3CN	36
5	$FeCl_3$ + 1,10-phen	--	CH_3CN	59
6	Ferrocene	--	CH_3CN	N.D.[c]
7	$Fe(acac)_3$	--	CH_3CN	50
8	$Fe(OTf)_3$	--	CH_3CN	40
9	$Y(OTf)_3$	--	CH_3CN	trace
10	$Bi(OTf)_3$	--	CH_3CN	N.D.
11	$Sc(OTf)_3$	--	CH_3CN	trace
12	$Cu(OTf)_2$	--	CH_3CN	trace
13	$CuCl_2$	--	CH_3CN	33
14	$CoCl_2$	--	CH_3CN	trace
15	$InCl_3$	--	CH_3CN	trace
16	$SnCl_4$	--	CH_3CN	15
17	$MnCl_2$	--	CH_3CN	trace
18	$ZnCl_2$	--	CH_3CN	26
19	$FeCl_3 \cdot 6H_2O$	--	CH_3CN	21
20	$AlCl_3$	--	CH_3CN	N.D.
21	$BF_3 \cdot Et_3O$	--	CH_3CN	N.D.
22	$B(C_6F_5)_3$	--	CH_3CN	N.D.
23	$Fe(phen)Cl_3$	DBU	CH_3CN	34
24	$Fe(phen)Cl_3$	DABCO	CH_3CN	21
25	$Fe(phen)Cl_3$	TEMPO	CH_3CN	32
26	$Fe(phen)Cl_3$	HOAc	CH_3CN	53
27	$Fe(phen)Cl_3$		DMF	trace
28	$Fe(phen)Cl_3$		MeOH	N.D.

29	$Fe(phen)Cl_3$		DCE	22
30	$Fe(phen)Cl_3$		HFIP	N.D.
31	$Fe(phen)Cl_3$	--	CH_3CN	70[d]
32	$Fe(phen)Cl_3$	--	CH_3CN	59[e]
33	$Fe(phen)Cl_3$	--	CH_3CN	54[f]
34	$Fe(phen)Cl_3$	--	CH_3CN	56[g]
35	$Fe(phen)Cl_3$	--	CH_3CN	73[h]
36	$Fe(phen)Cl_3$	--	CH_3CN	38[i]
37	$Fe(phen)Cl_3$	--	CH_3CN	26[j]
38	$Fe(phen)Cl_3$	--	CH_3CN	66[k]
39	$Fe(phen)Cl_3$	--	CH_3CN	35[l]
40	$Fe(phen)Cl_3$	--	CH_3CN	78[m]
41	--	--	CH_3CN	trace
42	$Fe(phen)Cl_3$	--	CH_3CN	7[n]
43	$Fe(phen)Cl_3$ (1.0 equiv.)	--	CH_3CN	13[o]
44	$Fe(phen)Cl_3$ (1.0 equiv.)	--	CH_3CN	18[p]
45	$Fe(phen)Cl_3$ (1.0 equiv.)	--	CH_3CN	61[q]

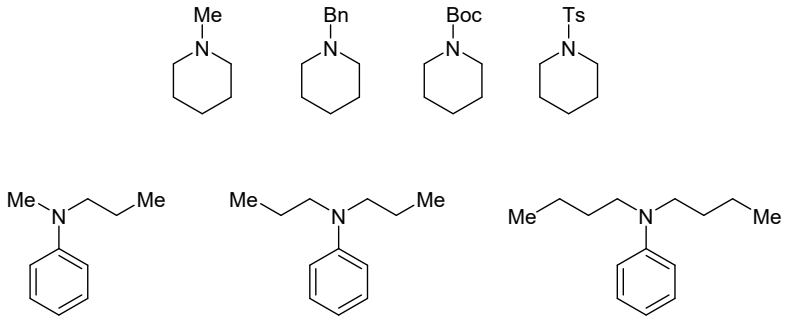
[a]Undivided cell, carbon felt anode, Ni plate cathode, constant current = 3.0 mA, **1** (0.3 mmol), **2** (0.36 mmol), catalyst (10 mol %), solvent (5.0 mL), under air, 6 h. [b]Yield of isolated product. [c]N.D. = not detected. [d]2.0 mA. [e]4.0 mA. [f]5.0 mA. [g]Graphite felt cathode. [h]Pt plate cathode. [i]Ni foam cathode. [j]Carbon felt cathode. [k]50 °C. [l]Room temperature. [m]Under Argon. [n]Without electricity. [o]Without electricity, Ar atmosphere. [p]Without electricity, air condition. [q]Without electricity, O_2 atmosphere.

Optimization of Ligands



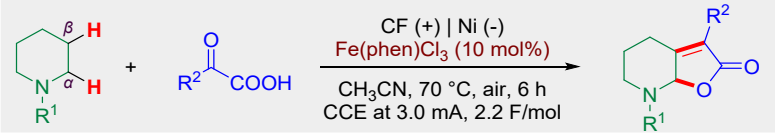


Failed substrates:



The above amines were tested, however, no desired products were afforded under the standard conditions.

General Procedure of the Electrochemical Dual C(sp^3)–H Functionalization



The electrocatalysis was carried out in an undivided cell with a carbon felt anode (10 mm × 15 mm × 3 mm) and a nickel cathode (10 mm × 15 mm × 0.2 mm). To a 15 mL pre-dried undivided electrochemical cell (15 mL) equipped with a magnetic bar was added cyclic *N*-aryl amines (0.30 mmol, 1.0 equiv.), *α*-aryl keto acids (0.36 mmol, 1.2 equiv.) and Fe(phen)Cl_3 (10.3 mg, 0.03 mmol, 10 mol%), followed by CH_3CN (5.0 mL). The electrocatalysis was performed at 70 °C with a constant current at 3.0 mA and maintained for 6 h. The carbon felt anode was washed with DCM (3 × 5 mL) in an ultrasonic bath. Evaporation of the solvent and subsequent column chromatography on silica gel afforded the corresponding products.

The consumed charge for the reaction is calculated by the following formula:

$$F/mol = \frac{i(A) \times t(s)}{x(mol) \times 10^{-3} \times 96500}$$

The efficiency of the reaction is calculated by the following formula:

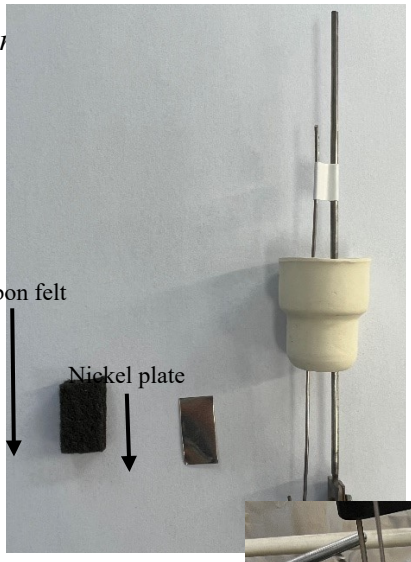
$$\eta = \frac{x(mol) \times n \times 96500}{i(A) \times t(s)} \times 100\%$$

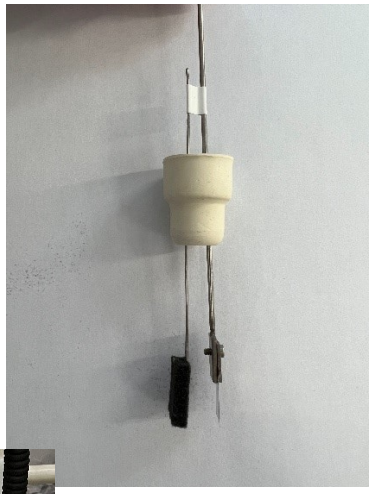
The current efficiency of each product is listed below:

3 72%	**4** 72%	**5** 77%	**6** 72%	**7** 37%	**8** 35%	**9** 23%	**10** 37%	**11** 67%
12 58%	**13** 38%	**14** 7%	**15** 15%	**16** 59%	**17** 52%	**18** 53%	**19** 60%	**20** 68%
21 67%	**22** 53%	**23** 28%	**24** 57%	**25** 64%	**26** 58%	**27** 40%	**28** 53%	**29** 70%
30 63%	**31** 56%	**32** 46%	**33** 33%	**34** 31%	**35** 35%	**36** 63%	**37** 67%	**38** 61%
39 6%	**40** 7%							

Graphical Guide

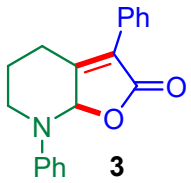
Pictu





Nickel electrodes (10 mm × 15 mm × 0.2 mm) and carbon felt electrodes (10 mm × 15 mm × 3 mm) were connected using stainless steel adapters. Electrocatalysis was conducted using an HSPY-36-03 potentiostat in constant current mode. The exact measurement of the reaction tube was 19 mm × 22 mm for the ground neck, 22 mm × 90 mm for outer diameter and length, and the volume was 10 mL. The space between of two electrodes was about 1 cm, and the rotation of the reaction was 800 rpm.

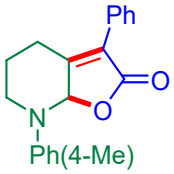
Characterization Data of Products



3

3,7-Diphenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (3)

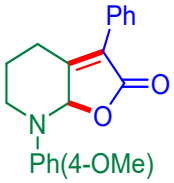
Compound **3** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **3** (69.9 mg, 80%) as a reddish solid. M.p.: 170 – 171 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.56 – 7.54 (m, 2H), 7.49 – 7.40 (m, 3H), 7.36 – 7.32 (m, 2H), 7.20 – 7.18 (m, 2H), 7.02 (t, *J* = 7.2 Hz, 1H), 5.84 (s, 1H), 3.41 (t, *J* = 5.6 Hz, 2H), 3.25 – 3.07 (m, 1H), 2.68 – 2.50 (m, 1H), 2.16 – 2.01 (m, 1H), 1.95 – 1.80 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.0, 157.4, 148.1, 129.3, 129.3, 129.1, 129.0, 128.6, 127.7, 122.0, 117.8, 90.2, 46.8, 24.3, 23.8. HR-MS (ESI) m/z calc. for $C_{19}H_{18}NO_2$ $[M+H]^+$: 292.1332, found: 292.1336. The analytical data correspond with those reported in the literature.[4]



4

3-Phenyl-7-(*p*-tolyl)-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (4)

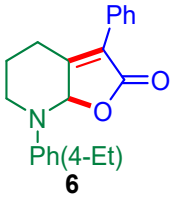
Compound **4** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **4** (74.2 mg, 81%) as a yellow solid. M.p.: 146 – 147 °C. ^{1}H NMR (400 MHz, Chloroform-*d*): δ = 7.55 – 7.53 (m, 2H), 7.48 – 7.39 (m, 3H), 7.16 – 7.10 (m, 4H), 5.73 (s, 1H), 3.36 (t, *J* = 6.0 Hz, 2H), 3.24 – 2.95 (s, 1H), 2.79 – 2.48 (s, 1H), 2.32 (s, 3H), 2.14 – 1.78 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*): δ = 171.0, 157.7, 146.0, 132.0, 129.8, 129.3, 129.1, 128.9, 128.6, 127.3, 118.6, 90.4, 48.0, 24.6, 24.2, 20.6. HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_2$ $[M+H]^+$: 306.1489, found: 306.1492. The analytical data correspond with those reported in the literature.[4]



5

7-(4-Methoxyphenyl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (5)

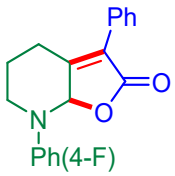
Compound **5** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 15:1) yielded **5** (40.5 mg, 86%) as a white solid. M.p.: 140 – 141 °C. ^{1}H NMR (400 MHz, Chloroform-*d*): δ = 7.54 – 7.52 (m, 2H), 7.47 – 7.38 (m, 3H), 7.20 – 7.16 (m, 2H), 6.91 – 6.87 (m, 2H), 5.55 (s, 1H), 3.79 (s, 3H), 3.52 – 2.28 (m, 4H), 2.10 – 1.82 (s, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*): δ = 171.1, 158.3, 155.9, 142.2, 129.4, 129.1, 128.9, 128.6, 126.6, 121.6, 114.5, 90.6, 55.6, 50.0, 25.1, 24.9. HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_3$ $[M+H]^+$: 322.1438, found: 322.1437. The analytical data correspond with those reported in the literature.[4]



6

7-(4-Ethylphenyl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (6)

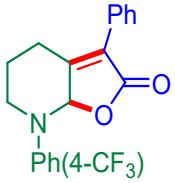
Compound **6** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **6** (27.5 mg, 80%) as a yellow solid. M.p.: 131 – 132 °C. ^{1}H NMR (400 MHz, Methanol-d_4) δ = 7.53 – 7.51 (m, 2H), 7.49 – 7.45 (m, 2H), 7.44 – 7.42 (m, 1H), 7.19 – 7.14 (m, 4H), 5.86 (s, 1H), 3.36 – 3.33 (m, 2H), 2.88 (t, J = 6.8 Hz, 2H), 2.61 (q, J = 7.6 Hz, 2H), 1.97 – 1.91 (m, 2H), 1.22 (t, J = 7.6 Hz, 3H). ^{13}C NMR (150 MHz, Methanol-d_4) δ = 171.9, 159.8, 146.6, 138.8, 129.4, 128.8, 128.5, 128.2, 128.1, 126.2, 119.3, 90.7, 49.0, 27.7, 24.5, 24.0, 14.9. HR-MS (ESI) m/z calc. for $C_{21}H_{22}NO_2$ $[M+H]^+$: 320.1645, found: 320.1641.



7

7-(4-Fluorophenyl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (7)

Compound **7** was prepared following the general procedure with constant current at 5.0 mA, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **7** (63.9 mg, 69%) as a white solid. M.p.: 163 – 164 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.55 – 7.53 (m, 2H), 7.48 – 7.39 (m, 3H), 7.19 – 7.16 (m, 2H), 7.06 – 7.01 (m, 2H), 5.63 (s, 1H), 3.38 – 3.28 (m, 2H), 3.23 – 3.10 (m, 1H), 2.65 – 2.48 (s, 1H), 2.15 – 1.99 (m, 1H), 1.96 – 1.79 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.9, 158.9 (d, $^{1}J_{C–F}$ = 240.2 Hz), 157.7, 144.6 (d, $^{4}J_{C–F}$ = 2.6 Hz), 129.2, 129.1, 129.0, 128.7, 127.1, 121.0 (d, $^{3}J_{C–F}$ = 7.9 Hz), 115.8 (d, $^{2}J_{C–F}$ = 22.1 Hz), 90.2, 49.2, 24.8, 24.5. ^{19}F NMR (375 MHz, Chloroform-*d*) δ = − 110.2. HR-MS (ESI) m/z calc. for $C_{19}H_{17}FNO_2$ $[M+H]^+$: 310.1238, found: 310.1244.

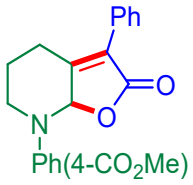


8

3-Phenyl-7-(4-(trifluoromethyl)phenyl)-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (8)

Compound **8** was prepared following the general procedure with constant current at 5.0 mA, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **8** (71.1 mg, 66%) as a light-yellow solid. M.p.: 154 – 155 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.58 – 7.55 (m, 4H), 7.50 – 7.41 (m, 3H), 7.20 – 7.18 (m, 2H), 5.95 (s, 1H), 3.61 – 3.55 (m, 1H), 3.40 – 3.33 (m, 1H), 3.23 – 3.16 (m, 1H), 2.69 – 2.61 (m, 1H), 2.19 – 2.08 (m, 1H), 1.96 – 1.87 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.6, 156.4, 150.3, 129.2, 129.1, 129.0, 128.7, 128.5, 126.6 (q, $^{4}J_{C-F}$ = 3.6 Hz), 124.5 (q, $^{1}J_{C-F}$ = 269.4 Hz), 122.8 (q, $^{2}J_{C-F}$ = 32.6 Hz), 115.8, 89.2, 44.9, 23.7, 23.0. ^{19}F NMR (375 MHz, Chloroform-*d*) δ = − 61.6. MS (ESI) m/z calc. for

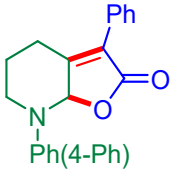
$C_{20}H_{17}F_3NO_2$ $[M+H]^+$: 360.1206, found: 360.1200.



9

Methyl 4-(2-oxo-3-phenyl-2,5,6,7a-tetrahydrofuro[2,3-*b*]pyridin-7(4*H*)-yl)benzoate (9)

Compound **9** was prepared following the general procedure with constant current at 7.0 mA, purification by column chromatography on silica gel (petroleum ether/EtOAc = 15:1) yielded **9** (63.9 mg, 61%) as a white solid. M.p.: 154 – 155 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.00 – 7.98 (m, 2H), 7.56 – 7.54 (m, 2H), 7.48 – 7.40 (m, 3H), 7.11 – 7.09 (m, 2H), 6.01 (s, 1H), 3.88 (s, 3H), 3.67 – 3.61 (m, 1H), 3.34 – 3.27 (m, 1H), 3.20 – 3.12 (m, 1H), 2.69 – 2.62 (m, 1H), 2.18 – 2.07 (m, 1H), 1.94 – 1.85 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.7, 166.9, 156.4, 151.2, 131.3, 129.2, 129.1, 129.0, 128.7, 128.6, 122.0, 114.7, 89.1, 51.8, 44.0, 23.4, 22.7. HR-MS (ESI) m/z calc. for $C_{21}H_{20}NO_4$ $[M+H]^+$: 350.1387, found: 350.1391.

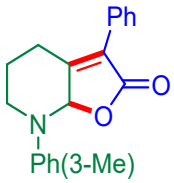


10

7-([1,1'-Biphenyl]-4-yl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (10)

Compound **10** was prepared following the general procedure with constant current at 5.0 mA, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **10** (74.9 mg, 68%) as a reddish solid. M.p.: 164 – 165 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.58 – 7.54 (m, 6H), 7.48 – 7.40 (m, 5H), 7.33 – 7.29 (t, *J* = 7.4 Hz, 1H), 7.24 – 7.22 (m, 2H), 5.86 (s, 1H), 3.45 – 3.41 (m, 2H), 3.25 – 3.08 (m, 1H), 2.69 – 2.49 (m, 1H), 2.20 – 2.02 (m, 1H), 1.97 – 1.79 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.0, 157.3, 147.4, 140.6, 134.7, 129.3, 129.1, 129.0, 128.8, 128.7, 127.9, 127.7, 126.8, 126.7, 117.9, 90.0, 46.7, 24.3, 23.7. HR-MS (ESI) m/z calc.

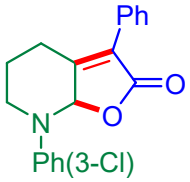
for $C_{25}H_{22}NO_2$ $[M+H]^+$: 368.1645, found: 368.1651.



11

3-Phenyl-7-(*m*-tolyl)-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (11)

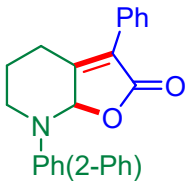
Compound **11** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **11** (68.6 mg, 75%) as a white solid. M.p.: 150 – 151 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.56 – 7.54 (m, 2H), 7.49 – 7.40 (m, 3H), 7.23 (t, *J* = 8.0 Hz, 1H), 7.01 – 6.97 (m, 2H), 6.85 (d, *J* = 7.6 Hz, 1H), 5.84 (s, 1H), 3.47 – 3.32 (m, 2H), 3.27 – 3.00 (m, 1H), 2.69 – 2.49 (m, 1H), 2.37 (s, 3H), 2.17 – 1.99 (m, 1H), 1.97 – 1.78 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.1, 157.5, 148.1, 139.2, 129.3, 129.1, 129.0, 128.6, 127.7, 122.8, 118.5, 114.7, 90.4, 46.7, 24.3, 23.7, 21.8. HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_2$ $[M+H]^+$: 306.1489 found: 306.1490.



12

7-(3-Chlorophenyl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (12)

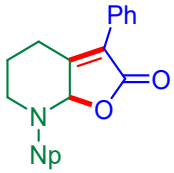
Compound **12** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **12** (63.4 mg, 65%) as a white solid. M.p.: 152 – 152 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.55 – 7.54 (m, 2H), 7.49 – 7.40 (m, 3H), 7.26 – 7.22 (m, 1H), 7.14 (t, *J* = 2.4 Hz, 1H), 7.05 (dd, *J* = 8.0, 2.4 Hz, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 5.83 (s, 1H), 3.47 – 3.32 (m, 2H), 3.21 – 3.14 (m, 1H), 2.64 – 2.56 (m, 1H), 2.15 – 2.06 (m, 1H), 1.92 – 1.83 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.8, 156.9, 149.2, 135.1, 130.3, 129.1, 129.08, 128.7, 128.0, 121.6, 117.3, 115.5, 89.6, 46.2, 24.0, 23.5. HR-MS (ESI) m/z calc. for $C_{19}H_{17}{}^{35}ClNO_2$ $[M+H]^+$: 326.0942, found: 326.0937.



13

7-([1,1'-Biphenyl]-2-yl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (13)

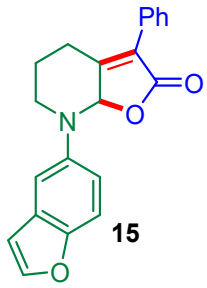
Compound **13** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **13** (47.4 mg, 43%) as a reddish solid. M.p.: 203 – 204 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.51 – 7.50 (m, 4H), 7.47 – 7.39 (m, 4H), 7.38 – 7.30 (m, 4H), 7.28 – 7.20 (m, 2H), 5.73 (s, 1H), 2.85 – 2.42 (m, 4H), 1.56 – 1.26 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.2, 159.3, 146.0, 140.2, 137.7, 131.5, 129.5, 129.3, 129.0, 128.8, 128.6, 128.2, 128.0, 126.9, 125.5, 125.0, 120.7, 88.8, 51.2, 25.3, 25.2. HR-MS (ESI) m/z calc. for $C_{25}H_{22}NO_2$ $[M+H]^+$: 368.1645, found: 368.1644. The analytical data correspond with those reported in the literature.[4]



14

7-(Naphthalen-1-yl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (14)

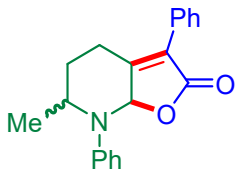
Compound **14** was prepared following the general procedure with constant current at 5.0 mA for 24 h, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **15** (54.2 mg, 53%) as a white solid. M.p.: 182 – 183 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.21 – 8.18 (m, 1H), 7.86 – 7.84 (m, 1H), 7.71 –7.69 (m, 1H), 7.59 – 7.57 (m, 2H), 7.49 – 7.40 (m, 7H), 5.86 (s, 1H), 3.57 – 3.42 (m, 1H), 3.39 – 3.24 (m, 1H), 3.06 – 2.90 (m, 1H), 2.72 – 2.52 (m, 1H), 2.06 – 2.03 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.2, 159.1, 145.3, 134.8, 130.3, 129.5, 129.0, 128.8, 128.6, 128.2, 126.1, 126.0, 125.6, 125.5, 123.3, 116.8, 89.4, 53.2, 25.9. HR-MS (ESI) m/z calc. for $C_{23}H_{20}NO_2$ $[M+H]^+$: 342.1489, found: 342.1492.



15

7-(Benzofuran-5-yl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (15)

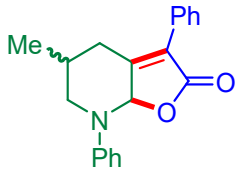
Compound **15** was prepared following the general procedure for 24 h, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **16** (64.5 mg, 65%) as a yellow solid. M.p.: 146 – 147 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.62 (d, *J* = 2.0 Hz, 1H), 7.55 – 7.54 (m, 2H), 7.49 – 7.39 (m, 5H), 7.21 (dd, *J* = 9.2, 2.4 Hz, 1H), 6.74 (d, *J* = 2.0 Hz, 1H), 5.67 (s, 1H), 3.51 – 3.29 (m, 2H), 3.29 – 2.97 (m, 1H), 2.78 – 2.38 (m, 1H), 2.16 – 1.86 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.1, 158.1, 151.7, 145.8, 144.4, 129.4, 129.1, 128.9, 128.6, 128.0, 126.8, 118.2, 112.3, 111.7, 106.8, 90.8, 50.4, 25.1, 24.8. HR-MS (ESI) m/z calc. for $C_{21}H_{18}NO_3$ $[M+H]^+$: 332.1281, found: 332.1287.



16, d.r. = 3:1

(7a*R*)-6-Methyl-3,7-diphenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (16)

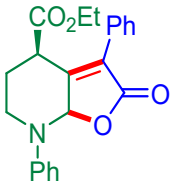
Compound **16** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **16** (60.4 mg, 66%, d.r. = 3:1) as a white solid. M.p.: 155 – 156 °C. ^{1}H NMR (800 MHz, Chloroform-*d*) δ = 7.61 – 7.51 (m, 2H), 7.47 – 7.45 (m, 2H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.36 – 7.34 (m, 2H), 7.22 – 7.21 (m, 2H), 7.14 – 7.06 (m, 1H), 6.00 (s, 0.3H), 5.81 (s, 1H), 3.81 – 3.68 (s, 1H), 3.21 – 3.04 (m, 1H), 2.84 – 2.76 (m, 0.3 H), 2.76 – 2.65 (m, 1H), 2.19 – 2.11 (m, 1H), 2.00 – 1.89 (m, 0.3 H), 1.76 – 1.66 (m, 1H), 1.15 – 0.93 (m, 4H). HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_2$ $[M+H]^+$: 306.1489, found: 306.1488.



17, d.r. = 1.67:1

(7a*R*)-5-Methyl-3,7-diphenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (17)

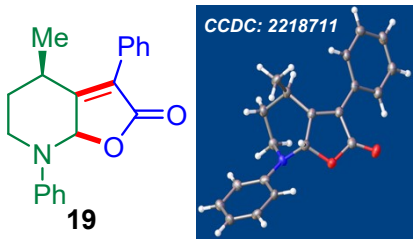
Compound **17** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **17** (53.1 mg, 58%, d.r. = 1.67:1) as a white solid. M.p.: 151 – 152 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.56 – 7.54 (m, 4H), 7.49 – 7.40 (m, 6H), 7.36 – 7.32 (m, 4H), 7.24 – 7.05 (m, 5H), 5.98 (s, 0.6H), 5.69 (s, 1H), 3.52 (d, *J* = 13.2 Hz, 2H), 3.28 – 3.14 (m, 1H), 2.94 (dd, *J* = 13.2, 9.2 Hz, 2H), 2.76 – 2.60 (m, 0.6H), 2.49 – 2.34 (m, 0.6H), 2.23 – 2.03 (m, 2H), 1.11 – 1.00 (m, 5H). HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_2$ $[M+H]^+$: 306.1489, found: 306.1486.



18

Ethyl (4*R*)-2-oxo-3,7-diphenyl-2,4,5,6,7,7a-hexahydrofuro[2,3-*b*]pyridine-4-carboxylate (18)

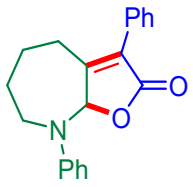
Compound **18** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 15:1) yielded **18** (64.3 mg, 59%) as a yellowish solid. M.p.: 173 – 174 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.61 – 7.58 (m, 2H), 7.51 – 7.45 (m, 3H), 7.36 – 7.32 (m, 2H), 7.17 – 7.15 (m, 2H), 7.01 (t, *J* = 7.2 Hz, 1H), 6.11 (s, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 4.14 (dd, *J* = 8.4, 4.0 Hz, 1H), 3.59 – 3.53 (m, 1H), 3.33 – 3.27 (m, 1H), 2.48 – 2.40 (m, 1H), 2.18 – 2.10 (m, 1H), 1.28 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.8, 170.5, 152.7, 147.6, 130.7, 129.6, 129.4, 129.2, 128.8, 128.6, 121.9, 117.3, 89.6, 62.2, 44.1, 40.6, 28.2, 14.2. HR-MS (ESI) m/z calc. for $C_{22}H_{22}NO_4$ $[M+H]^+$: 364.1543, found: 364.1544.



19

(4*R*)-4-Methyl-3,7-diphenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (19)

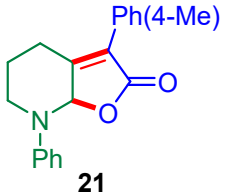
Compound **19** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **19** (61.4 mg, 67%) as a white solid. M.p.: 162 – 163 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.55 – 7.53 (m, 2H), 7.49 – 7.40 (m, 3H), 7.36 – 7.32 (m, 2H), 7.18 – 7.16 (m, 2H), 7.00 (t, *J* = 7.2 Hz, 1H), 6.04 (s, 1H), 3.60 – 3.54 (m, 1H), 3.44 – 3.36 (m, 1H), 3.31 – 3.24 (m, 1H), 2.16 – 2.08 (m, 1H), 1.81 – 1.73 (m, 1H), 1.40 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.1, 161.5, 147.7, 129.4, 129.0, 128.7, 127.8, 121.4, 116.7, 88.7, 43.7, 32.1, 28.6, 20.3. HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_2$ $[M+H]^+$: 306.1489, found: 306.1485. The analytical data correspond with those reported in the literature.[4]



20

3,8-Diphenyl-4,5,6,7,8,8a-hexahydro-2*H*-furo[2,3-*b*]azepin-2-one (20)

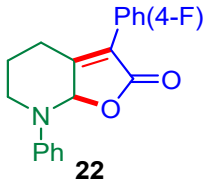
Compound **20** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **20** (69.9 mg, 76%) as a yellowish solid. M.p.: 153 – 154 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.58 – 7.55 (m, 2H), 7.48 – 7.44 (m, 2H), 7.42 – 7.38 (m, 1H), 7.33 – 7.29 (m, 2H), 7.09 – 7.07 (m, 2H), 6.94 (t, *J* = 7.2 Hz, 1H), 6.26 (s, 1H), 3.56 – 3.52 (m, 1H), 3.32 – 3.25 (m, 1H), 3.10 – 3.05 (m, 1H), 2.40 – 2.33 (m, 1H), 2.11 – 2.05 (m, 1H), 1.93 – 1.87 (m, 2H), 1.64 – 1.53 (m, 1H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ = 172.0, 159.2, 148.0, 129.7, 129.6, 129.4, 128.9, 128.8, 128.7, 120.2, 114.7, 93.9, 46.7, 29.1, 28.3, 26.7. HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_2$ $[M+H]^+$: 306.1489, found: 306.1496. The analytical data correspond with those reported in the literature.[4]



21

7-Phenyl-3-(*p*-tolyl)-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (21)

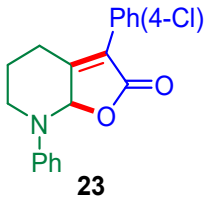
Compound **21** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **21** (68.6 mg, 75%) as a reddish solid. M.p.: 183 – 184 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.45 – 7.43 (m, 2H), 7.35 – 7.31 (m, 2H), 7.28 – 7.26 (m, 2H), 7.18 – 7.16 (m, 2H), 7.01 (t, *J* = 7.2 Hz, 1H), 5.81 (s, 1H), 3.39 (t, *J* = 6.0 Hz, 2H), 3.22 – 3.02 (m, 1H), 2.68 – 2.46 (m, 1H), 2.39 (s, 3H), 2.14 – 1.99 (m, 1H), 1.95 – 1.80 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.2, 156.7, 148.1, 139.0, 129.34, 129.31, 129.0, 127.6, 126.4, 121.9, 117.7, 90.2, 46.7, 24.2, 23.8, 21.4. HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_2$ $[M+H]^+$: 306.1489, found: 306.1487.



22

3-(4-Fluorophenyl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (22)

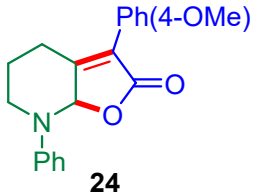
Compound **22** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded **22** (54.7 mg, 59%) as a reddish solid. M.p.: 167 – 168 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.56 – 7.53 (m, 2H), 7.36 – 7.32 (m, 2H), 7.19 – 7.14 (m, 4H), 7.03 (t, *J* = 7.2 Hz, 1H), 5.83 (s, 1H), 3.50 – 3.34 (m, 2H), 3.23 – 2.98 (m, 1H), 2.72 – 2.45 (m, 1H), 2.23 – 2.03 (m, 1H), 1.97 – 1.80 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.9, 163.0 (d, $^{1}J_{C\text{-}F}$ = 248.1 Hz), 157.2, 148.0, 131.0 (d, $^{3}J_{C\text{-}F}$ = 8.2 Hz), 129.3, 126.8, 125.3 (d, $^{4}J_{C\text{-}F}$ = 3.2 Hz), 122.1, 117.8, 115.8 (d, $^{2}J_{C\text{-}F}$ = 21.6 Hz), 90.2, 46.8, 24.3, 23.8. ^{19}F NMR (375 MHz, Chloroform-*d*) δ = − 110.1. HR-MS (ESI) m/z calc. for $C_{19}H_{17}FNO_2$ $[M+H]^+$: 310.1238, found: 310.1233.



23

3-(4-Chlorophenyl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (23)

Compound **23** was prepared following the general procedure with constant current at 5.0 mA, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded **23** (50.7 mg, 52%) as a reddish solid. M.p.: 156 – 157 °C. ^{1}H NMR (400 MHz, Methanol-d_4) δ = 7.60 – 7.55 (m, 4H), 7.35 – 7.31 (m, 2H), 7.18 – 7.16 (m, 2H), 6.97 (t, J = 7.2 Hz, 1H), 6.11 (s, 1H), 3.45 – 3.35 (m, 2H), 3.04 – 2.86 (m, 1H), 2.81 – 2.63 (m, 1H), 2.07 – 1.93 (m, 1H), 1.88 – 1.71 (m, 1H). ^{13}C NMR (100 MHz, Methanol-d_4) δ = 170.8, 160.9, 148.7, 134.0, 131.2, 129.5, 129.1, 128.6, 124.9, 121.6, 117.9, 89.8, 47.1, 24.3, 23.9, HR-MS (ESI) m/z calc. for $C_{19}H_{17}{}^{35}ClNO_2$ $[M+H]^+$: 326.0942, found: 326.0940. The analytical data correspond with those reported in the literature.[4]

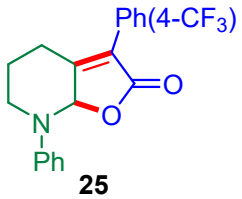


24

3-(4-Methoxyphenyl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (24)

Compound **24** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) yielded **24** (61.6 mg, 64%) as a reddish solid. M.p.: 171 – 172 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.52 – 7.50 (m, 2H), 7.36 – 7.32 (m, 2H), 7.18 – 7.16 (m, 2H), 7.03 – 6.98 (m, 3H), 5.83 (s, 1H), 3.85 (s, 3H), 3.50 – 3.34 (m, 2H), 3.24 – 3.04 (m, 1H), 2.69 – 2.49 (m, 1H), 2.16 – 1.99 (m, 1H), 1.98 – 1.78 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.3, 160.1, 155.6, 148.1, 130.5, 129.3, 127.2, 121.8, 121.7, 117.6, 114.1, 90.2, 55.4, 46.6, 24.2, 23.7. HR-MS (ESI) m/z calc. for $C_{20}H_{20}NO_3$ $[M+H]^+$: 322.1438, found: 322.1441.

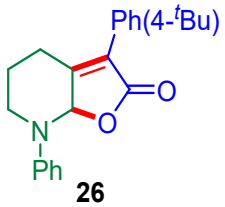
The analytical data correspond with those reported in the literature.[4]



25

7-Phenyl-3-(4-(trifluoromethyl)phenyl)-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (25)

Compound **25** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded **25** (77.5 mg, 72%) as a reddish solid. M.p.: 145 – 146 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.74 – 7.72 (m, 2H), 7.68 – 7.66 (m, 2H), 7.37 – 7.33 (m, 2H), 7.20 – 7.18 (m, 2H), 7.04 (t, *J* = 7.2 Hz, 1H), 5.86 (s, 1H), 3.42 (t, *J* = 5.6 Hz, 2H), 3.25 – 3.02 (m, 1H), 2.76 – 2.51 (m, 1H), 2.25 – 2.03 (m, 1H), 2.02 – 1.78 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.4, 159.4, 147.9, 132.9, 130.9 (d, $^{2}J_{C\text{-}F}$ = 32.5 Hz), 129.5, 129.4, 126.6, 125.6 (d, $^{4}J_{C\text{-}F}$ = 3.7 Hz), 123.9 (d, $^{1}J_{C\text{-}F}$ = 270.7 Hz), 122.3, 118.0, 90.3, 47.1, 24.4, 24.0. ^{19}F NMR (375 MHz, Chloroform-*d*) δ = − 62.7. HR-MS (ESI) m/z calc. for $C_{20}H_{17}F_3NO_2$ $[M+H]^+$: 360.1206, found: 360.1202.

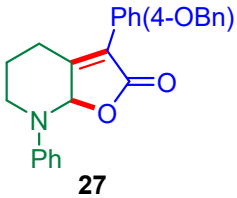


26

3-(4-(*tert*-Butyl)phenyl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (26)

Compound **26** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded **26** (67.7 mg, 65%) as a yellowish solid. M.p.: 156 – 157 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.52 – 7.48 (m, 4H), 7.36 – 7.32 (m, 2H), 7.19 – 7.17 (m, 2H), 7.02 (t, *J* = 7.2 Hz, 1H), 5.84 (s, 1H), 3.48 – 3.35 (m, 2H), 3.28 – 3.08 (m, 1H), 2.73 – 2.47 (m, 1H), 2.18 – 2.00 (m, 1H), 1.99 – 1.81 (m, 1H), 1.36 (s, 9H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.2, 156.7, 152.1, 148.1, 129.3, 128.8, 127.6, 126.4, 125.6, 121.8, 117.6, 90.2, 46.7,

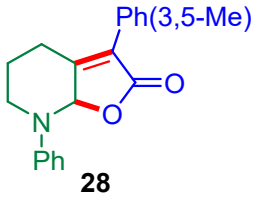
34.8, 31.3, 24.3, 23.7. HR-MS (ESI) m/z calc. for $C_{23}H_{26}NO_2$ $[M+H]^+$: 348.1958, found: 348.1963.



27

3-(4-(Benzyloxy)phenyl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (27)

Compound **27** was prepared following the general procedure with constant current at 5.0 mA, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded **27** (88.2 mg, 74%) as a yellowish solid. M.p.: 153 – 154 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.53 – 7.50 (m, 2H), 7.46 – 7.39 (m, 4H), 7.36 – 7.32 (m, 3H), 7.19 – 7.17 (m, 2H), 7.08 – 7.00 (m, 3H), 5.83 (s, 1H), 5.12 (s, 2H), 3.49 – 3.32 (m, 2H), 3.27 – 2.98 (m, 1H), 2.71 – 2.44 (m, 1H), 2.17 – 1.98 (m, 1H), 1.97 – 1.79 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ =171.3, 159.3, 155.7, 148.1, 136.7, 130.5, 129.3, 128.7, 128.1, 127.5, 127.2, 122.0, 121.8, 117.6, 115.0, 90.2, 70.1, 46.6, 24.2, 23.7. HR-MS (ESI) m/z calc. for $C_{26}H_{24}NO_3$ $[M+H]^+$: 398.1751, found: 398.1743.

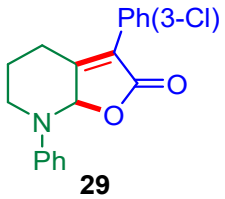


28

3-(3,5-Dimethylphenyl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (28)

Compound **28** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **28** (56.5 mg, 59%) as a white solid. M.p.: 158 – 159 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.36 – 7.32 (m, 2H), 7.19 – 7.17 (m, 2H), 7.15 (s, 2H), 7.06 (s, 1H), 7.02 (t, *J* = 7.2 Hz, 1H), 5.82 (s, 1H), 3.49 – 3.32 (m, 2H), 3.25 – 3.04 (m, 1H), 2.68 – 2.49 (m, 1H), 2.37 (s, 6H), 2.17 – 1.99 (m, 1H), 1.99 – 1.78 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.1, 157.1, 148.1, 138.2, 130.7, 129.3, 129.1, 127.9, 126.8, 121.9, 117.6, 90.2, 46.7,

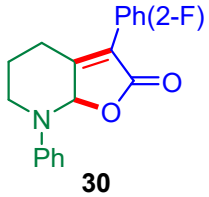
24.3, 23.8, 21.4. HR-MS (ESI) m/z calc. for $C_{21}H_{22}NO_2$ $[M+H]^+$: 320.1645, found: 320.1646.



29

3-(3-Chlorophenyl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (29)

Compound **29** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **29** (74.1 mg, 76%) as a reddish solid. M.p.: 149 – 150 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.53 (s, 1H), 7.46 – 7.42 (m, 1H), 7.40 – 7.39 (m, 2H), 7.36 – 7.32 (m, 2H), 7.19 – 7.17 (m, 2H), 7.03 (t, *J* = 7.2 Hz, 1H), 5.83 (s, 1H), 3.41 (t, *J* = 6.0 Hz, 2H), 3.26 – 3.03 (m, 1H), 2.72 – 2.48 (m, 1H), 2.22 – 2.02 (m, 1H), 1.98 – 1.78 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.5, 158.7, 148.0, 134.6, 131.0, 129.9, 129.4, 129.1, 129.05, 127.3, 126.5, 122.2, 117.9, 90.3, 46.9, 24.3, 23.9. HR-MS (ESI) m/z calc. for $C_{19}H_{17}{}^{35}ClNO_2$ $[M+H]^+$: 326.0942, found: 326.0939. The analytical data correspond with those reported in the literature.[4]

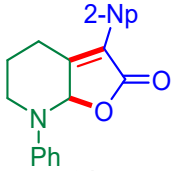


30

3-(2-Fluorophenyl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (30)

Compound **30** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **30** (34.3 mg, 70%) as a white crystalline. M.p.: 150 – 151 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.59 (t, *J* = 7.6 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.40 – 7.36 (m, 2H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.24 – 7.19 (m, 3H), 7.07 (t, *J* = 7.6 Hz, 1H), 5.89 (s, 1H), 3.46 (t, *J* = 6.0 Hz, 2H), 3.04 – 2.79 (m, 1H), 2.68 – 2.43 (m, 1H), 2.25 – 2.06 (m, 1H), 2.04 – 1.84 (m, 1H). ^{13}C

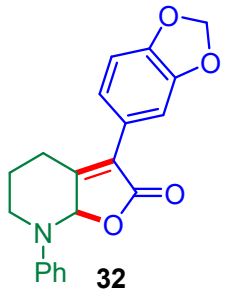
NMR (100 MHz, Chloroform-*d*) δ = 170.6, 161.0 (d, $^{1}J_{C\text{-}F}$ = 247.8 Hz), 148.1, 131.4 (d, $^{4}J_{C\text{-}F}$ = 2.8 Hz), 130.9 (d, $^{3}J_{C\text{-}F}$ = 8.1 Hz), 129.3, 124.4 (d, $^{4}J_{C\text{-}F}$ = 3.5 Hz), 122.13, 122.10, 117.9, 117.1 (d, $^{2}J_{C\text{-}F}$ = 14.8 Hz), 115.9 (d, $^{2}J_{C\text{-}F}$ = 22.0 Hz), 90.5. 47.2, 24.5 (d, $^{4}J_{C\text{-}F}$ = 4.9 Hz), 24.2. ^{19}F NMR (375 MHz, Chloroform-*d*) δ = − 113.3. HR-MS (ESI) m/z calc. for $C_{19}H_{17}FNO_2$ $[M+H]^+$: 310.1238, found: 310.1233.



31

3-(Naphthalen-2-yl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (31)

Compound **31** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **31** (64.5 mg, 63%) as a white solid. M.p.: 180 – 181 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.07 (d, *J* = 1.6 Hz, 1H), 7.94 – 7.86 (m, 3H), 7.63 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.38 – 7.34 (m, 2H), 7.21 – 7.19 (m, 2H), 7.03 (t, *J* = 7.2 Hz, 1H), 5.89 (s, 1H), 3.44 (t, *J* = 6.0 Hz, 2H), 3.32 – 3.14 (m, 1H), 2.78 – 2.56 (m, 1H), 2.21 – 2.02 (m, 1H), 2.01 – 1.81 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.0, 157.6, 148.1, 133.2, 133.1, 129.3, 128.9, 128.4, 128.3, 127.8, 127.7, 126.9, 126.7, 126.5, 126.2, 122.0, 117.8, 90.3, 46.8, 24.3, 23.9. HR-MS (ESI) m/z calc. for $C_{23}H_{20}NO_2$ $[M+H]^+$: 342.1489, found: 342.1492.

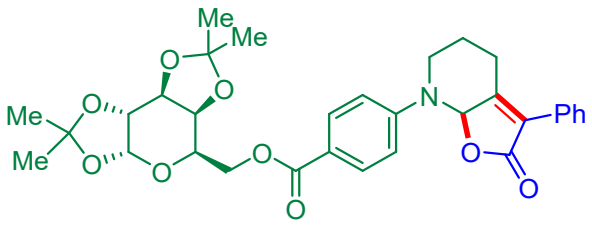


32

3-(Benzo[*d*][1,3]dioxol-5-yl)-7-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (32)

Compound **32** was prepared following the general procedure, purification by column

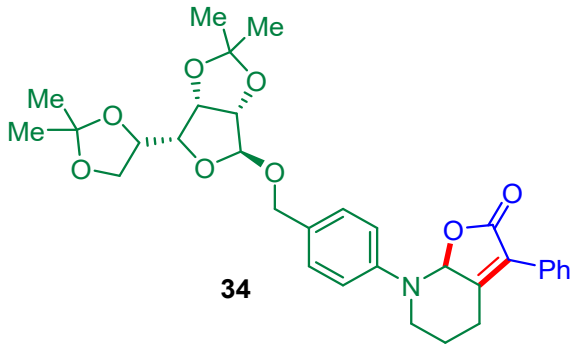
chromatography on silica gel (petroleum ether/EtOAc = 20:1) yielded **32** (51.2 mg, 51%) as a white solid, M.p.: 176 – 177 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.35 – 7.32 (m, 2H), 7.18 – 7.16 (m, 2H), 7.06 – 7.00 (m, 3H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.01 (s, 2H), 5.81 (s, 1H), 3.48 – 3.34 (m, 2H), 3.27 – 3.03 (m, 1H), 2.73 – 2.47 (m, 1H), 2.19 – 2.01 (m, 1H), 1.98 – 1.84 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.0, 156.1, 148.2, 148.1, 147.9, 129.3, 127.3, 123.3, 123.0, 121.9, 117.7, 109.4, 108.6, 101.4, 90.2, 46.7, 24.2, 23.8. HR-MS (ESI) m/z calc. for $C_{20}H_{18}NO_4$ $[M+H]^+$: 336.1230, found: 336.1233.



33

((3a*R*,5*R*,5a*S*,8a*S*,8b*R*)-2,2,7,7-Tetramethyltetrahydro-5*H*-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-5-yl)methyl 4-((*R*)-2-oxo-3-phenyl-2,5,6,7a-tetrahydrofuro[2,3-*b*]pyridin-7(4*H*)-yl)benzoate (33)

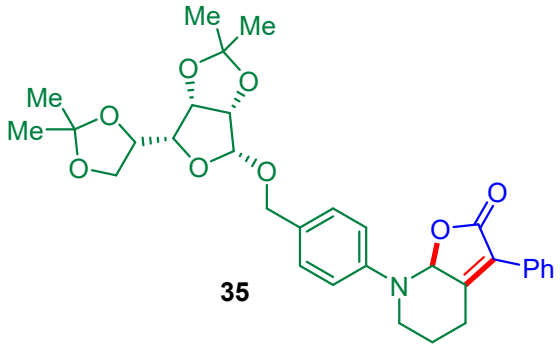
Compound **33** was prepared following the general procedure with constant current at 7.0 mA, purification by column chromatography on silica gel (petroleum ether/EtOAc = 6:1) yielded **33** (100.3 mg, 58%, *d.r.* = 1:1) as a yellow syrup. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.02 – 8.00 (m, 2H), 7.57 – 7.55 (m, 2H), 7.49 – 7.39 (m, 2H), 7.43 (t, J = 4.0 Hz, 1H), 7.12 – 7.10 (m, 2H), 6.02 (s, 1H), 5.57 (d, *J* = 4.8 Hz, 1H), 4.65 (dd, *J* = 8.0, 2.8 Hz, 1H), 4.51 (dd, *J* = 11.6, 4.8 Hz, 1H), 4.43 – 4.38 (m, 1H), 4.356 – 4.33 (m, 2H), 4.20 – 4.17 (m, 1H), 3.68 – 3.63 (m, 1H), 3.36 – 3.29 (m, 1H), 3.22 – 3.14 (m, 1H), 2.69 – 2.61 (m, 1H), 2.16 – 2.07 (m, 1H), 1.94 – 1.85 (m, 1H), 1.53 (s, 3H), 1.48 (s, 3H), 1.36 (s, 3H), 1.34 (s, 3H). HR-MS (ESI) m/z calc. for $C_{32}H_{36}NO_9$ $[M+H]^+$: 578.2385, found: 578.2393.



34

7-(4-((((3a*S*,4*S*,6*R*,6a*S*)-6-((*R*)-2,2-Dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)oxy)methyl)phenyl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (34)

Compound **34** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) yielded **34** (89.6 mg, 53%) as a yellow syrup. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.55 – 7.54 (m, 2H), 7.48 – 7.39 (m, 3H), 7.30 – 7.28 (m, 2H), 7.16 – 7.14 (m, 2H), 5.82 (s, 1H), 5.07 (s, 1H), 4.79 (dd, *J* = 6.0, 3.6 Hz, 1H), 4.65 – 4.59 (m, 2H), 4.46 – 4.39 (m, 2H), 4.14 – 4.10 (m, 1H), 4.03 – 3.96 (m, 2H), 3.45 – 3.34 (m, 2H), 3.23 – 3.08 (m, 1H), 2.68 – 2.51 (m, 1H), 2.16 – 2.04 (m, 1H), 1.94 – 1.82 (m, 1H), 1.47 (s, 6H), 1.39 (s, 3H), 1.32 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.9, 157.2, 147.9, 130.6, 129.5, 129.2, 129.1, 129.0, 128.6, 127.8, 117.6, 112.6, 109.3, 105.4, 90.1, 85.1, 80.4, 79.6, 73.2, 68.7, 67.0, 46.7, 27.0, 25.9, 25.3, 24.5, 24.2, 23.7. HR-MS (ESI) m/z calc. for $C_{32}H_{38}NO_8$ $[M+H]^+$: 564.2592, found: 564.2593.

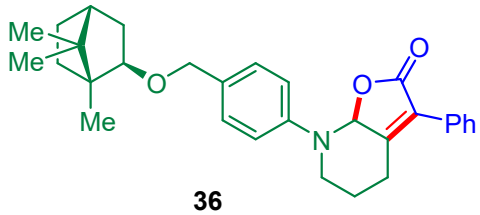


35

7-(4-((((3a*S*,4*R*,6*R*,6a*S*)-6-((*R*)-2,2-Dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)oxy)methyl)phenyl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (35)

Compound **35** was prepared following the general procedure with constant current at

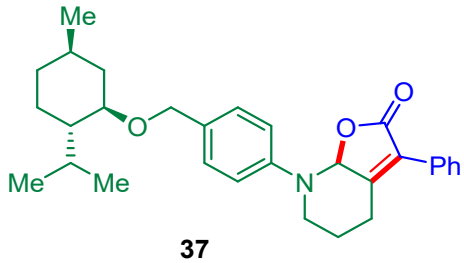
7.0 mA, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) yielded **35** (103.1 mg, 61%) as a yellow syrup. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.56 – 7.54 (m, 2H), 7.49 – 7.40 (m, 3H), 7.36 – 7.34 (m, 2H), 7.16 – 7.14 (m, 2H), 5.83 (s, 1H), 4.88 (d, *J* = 12.0 Hz, 1H), 4.73 (d, *J* = 3.6 Hz, 1H), 4.70 (dd, *J* = 6.0, 4.0 Hz, 1H), 4.63 (d, *J* = 12.0 Hz, 1H), 4.57 (dd, *J* = 6.4, 3.6 Hz, 1H), 4.50 – 4.45 (m, 1H), 4.11 (d, *J* = 5.2 Hz, 2H), 3.57 (q, *J* = 4.0 Hz, 1H), 3.41 (t, *J* = 6.0 Hz, 2H), 3.25 – 3.10 (m, 1H), 2.67 – 2.52 (m, 1H), 2.16 – 2.04 (m, 1H), 1.95 – 1.82 (m, 1H), 1.57 (s, 3H), 1.45 (s, 3H), 1.37 (d, *J* = 10.4 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.0, 157.3, 147.9, 130.5, 129.5, 129.2, 129.1, 129.0, 128.7, 127.7, 117.7, 113.7, 109.3, 100.9, 89.9, 79.8, 79.1, 73.3, 71.1, 66.9, 47.0, 27.0, 25.8, 25.3, 25.0, 24.3, 23.8. HR-MS (ESI) m/z calc. for $C_{32}H_{38}NO_8$ $[M+H]^+$: 564.2592, found: 564.2588.



36

3-Phenyl-7-(4-((((1*R*,2*R*,4*R*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)methyl)phenyl)-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (36)

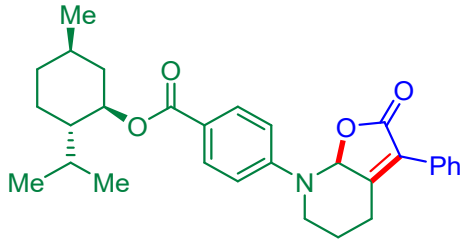
Compound **36** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded **36** (97.4 mg, 71%) as a white solid. M.p.: 133 – 134 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.56 – 7.54 (m, 2H), 7.48 – 7.39 (m, 3H), 7.30 – 7.28 (m, 2H), 7.16 – 7.14 (m, 2H), 5.80 (s, 1H), 4.50 (d, *J* = 12.0 Hz, 1H), 4.35 (d, *J* = 12.0 Hz, 1H), 3.40 (t, *J* = 5.6 Hz, 2H), 3.31 (q, *J* = 3.6 Hz, 1H), 3.24 – 3.09 (m, 1H), 2.68 – 2.48 (m, 1H), 2.17 – 2.03 (m, 1H), 1.93 – 1.80 (m, 2H), 1.71 – 1.64 (m, 2H), 1.63 – 1.57 (m, 1H), 1.52 – 1.47 (m, 1H), 1.04 (s, 3H), 0.99 (d, *J* = 8.8 Hz, 2H), 0.95 (s, 3H), 0.82 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.0, 157.5, 147.2, 133.4, 129.3, 129.1, 128.9, 128.6, 128.3, 127.6, 117.8, 90.2, 86.4, 70.2, 49.3, 47.3, 46.6, 45.1, 38.5, 34.5, 27.3, 24.4, 23.9, 20.4, 20.3, 12.0. HR-MS (ESI) m/z calc. for $C_{30}H_{36}NO_3$ $[M+H]^+$: 458.2690, found: 458.2692.



37

7-(4-((((1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)oxy)methyl)phenyl)-3-phenyl-5,6,7,7a-tetrahydrofuro[2,3-*b*]pyridin-2(4*H*)-one (37)

Compound **37** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded **37** (103.4 mg, 75%) as a white solid. M.p.: 175 – 176 °C. ^{1}H NMR (800 MHz, Chloroform-*d*) δ = 7.55 – 7.54 (m, 2H), 7.47 – 7.46 (m, 2H), 7.41 (t, *J* = 3.6 Hz, 1H), 7.32 – 7.31 (m, 2H), 7.16 – 7.15 (m, 2H), 5.80 (s, 1H), 4.61 (d, *J* = 5.6 Hz, 1H), 4.36 (d, *J* = 5.6 Hz, 1H), 3.39 (t, *J* = 2.8 Hz, 2H), 3.19 – 3.15 (m, 2H), 2.62 – 2.53 (m, 1H), 2.31 – 2.28 (m, 1H), 2.19 (d, *J* = 6.0 Hz, 1H), 2.13 – 2.06 (m, 1H), 1.92 – 1.83 (m, 1H), 1.67 – 1.62 (m, 2H), 1.40 – 1.34 (m, 1H), 1.30 – 1.27 (m, 1H), 1.00 – 0.84 (m, 9H), 0.72 (d, *J* = 3.6 Hz, 3H) . ^{13}C NMR (200 MHz, Chloroform-*d*) δ = 171.0, 157.4, 147.6, 132.8, 129.3, 129.1, 129.0, 128.6, 127.6, 117.8, 90.3, 78.6, 70.0, 48.3, 47.2, 40.4, 34.6, 31.6, 25.5, 24.3, 23.9, 23.3, 22.4, 21.1, 16.1. HR-MS (ESI) m/z calc. for $C_{30}H_{38}NO_3$ $[M+H]^+$: 460.2846, found: 460.2844.

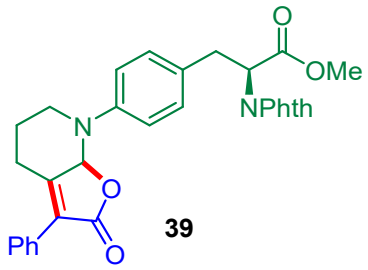


38

(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 4-(2-oxo-3-phenyl-2,5,6,7a-tetrahydrofuro[2,3-*b*]pyridin-7(4*H*)-yl)benzoate (38)

Compound **38** was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 8:1) yielded **38** (96.6 mg, 68%, *d.r.* = 1:1) as a yellowish solid. M.p.: 151 – 152 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.02 – 8.00 (m, 2H), 7.57 – 7.55 (m, 2H), 7.49 – 7.41 (m, 3H), 7.14 – 7.11 (m, 2H),

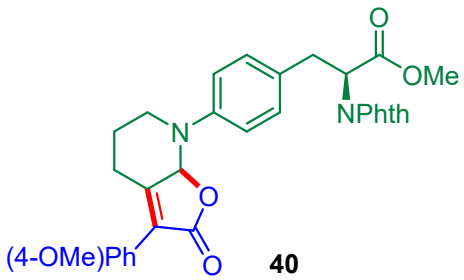
6.02 (s, 0.5H), 6.01 (s, 0.5H), 4.94 – 4.88 (m, 1H), 3.67 – 3.61 (m, 1H), 3.37 – 3.29 (m, 1H), 3.22 – 3.14 (m, 1H), 2.69 – 2.62 (m, 1H), 2.19 – 2.08 (m, 2H), 2.00 – 1.87 (m, 2H), 1.73 (d, J = 11.2 Hz, 2H), 1.61 – 1.51 (m, 2H), 1.19 – 1.05 (m, 2H), 0.97 – 0.89 (m, 7H), 0.80 (d, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.7, 166.2, 156.3, 151.2, 131.5, 129.2, 129.1, 129.0, 128.8, 128.7, 122.0, 114.7, 109.7, 108.8, 96.4, 89.18, 89.15, 71.2, 70.8, 70.6, 66.29, 66.25, 63.63, 63.57, 44.0, 26.1, 26.0, 25.0, 24.5, 23.5, 22.7. HR-MS (ESI) m/z calc. for $C_{30}H_{36}NO_4$ $[M+H]^+$: 474.6205, found: 474.6199.



39

Methyl (2*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-(4-(2-oxo-3-phenyl-2,5,6,7a-tetrahydrofuro[2,3-*b*]pyridin-7(4*H*)-yl)phenyl)propanoate (39)

Compound **39** was prepared following the general procedure with constant current at 5.0 mA for 24 h, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) yielded **39** (103.4 mg, 66%) as a yellow syrup. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.81 – 7.79 (m, 2H), 7.71 – 7.69 (m, 2H), 7.52 – 7.50 (m, 2H), 7.46 – 7.37 (m, 3H), 7.13 – 7.11 (m, 2H), 7.00 – 6.98 (m, 2H), 5.73 (s, 1H), 5.14 (dd, J = 9.6, 6.4 Hz, 1H), 3.78 (s, 3H), 3.57 – 3.49 (m, 2H), 3.35 – 3.26 (m, 2H), 3.19 – 3.02 (m, 1H), 2.63 – 2.43 (m, 1H), 2.12 – 1.96 (m, 1H), 1.90 – 1.73 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 170.9, 169.5, 167.6, 157.3, 146.8, 134.2, 131.6, 129.7, 129.2, 129.1, 129.0, 128.6, 127.7, 123.6, 90.1, 53.3, 52.9, 33.8, 24.2, 23.7. HR-MS (ESI) m/z calc. for $C_{31}H_{27}N_2O_6$ $[M+H]^+$: 523.1864, found: 523.1858.



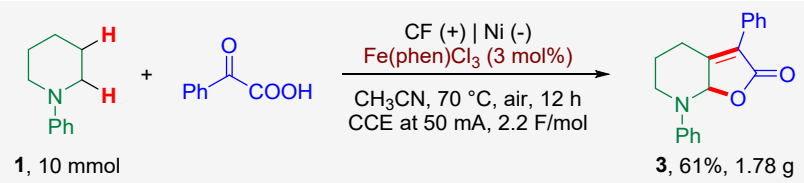
40

Methyl (2*S*)-2-(1,3-dioxoisoindolin-2-yl)-3-(4-(3-(4-methoxyphenyl)-2-oxo-

2,5,6,7a-tetrahydrofuro[2,3-*b*]pyridin-7(4*H*)-yl)phenyl)propanoate (40)

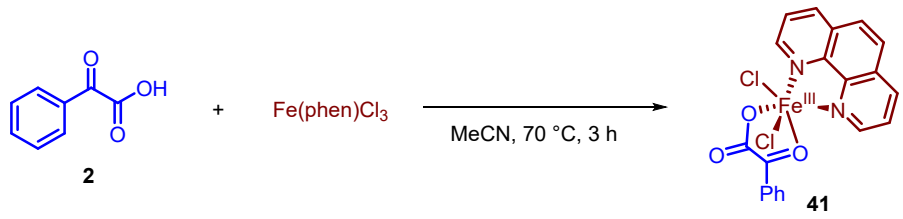
Compound **40** was prepared following the general procedure with constant current at 7.0 mA for 24 h, purification by column chromatography on silica gel (petroleum ether/EtOAc = 4:1) yielded **40** (117.7 mg, 71%) as a yellow syrup. ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.81 – 7.79 (m, 2H), 7.71 – 7.69 (m, 2H), 7.48 – 7.46 (m, 2H), 7.13 – 7.10 (m, 2H), 6.99 – 6.95 (m, 4H), 5.71 (s, 1H), 5.14 (dd, *J* = 10.0, 6.8 Hz, 1H), 3.83 (s, 3H), 3.78 (s, 3H), 3.57 – 3.48 (m, 2H), 3.36 – 3.23 (m, 1H), 3.17 – 2.99 (m, 1H), 2.65 – 2.42 (m, 1H), 2.12 – 1.93 (m, 1H), 1.91 – 1.74 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ = 171.2, 169.5, 167.6, 160.1, 155.5, 146.8, 134.2, 131.6, 130.4, 129.7, 127.2, 123.6, 121.6, 117.5, 114.1, 90.0, 55.4, 53.3, 52.9, 33.8, 29.7, 24.1, 23.7. HR-MS (ESI) m/z calc. for $C_{32}H_{29}N_2O_7$ $[M+H]^+$: 553.1969, found: 553.1973.

Gram-Scale Synthesis of 3

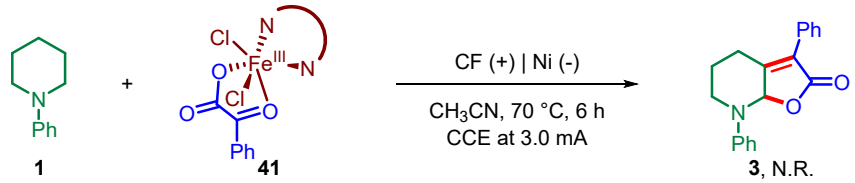


To an undivided reaction flask (diameter: 40 mm; length: 130 mm; volume: 200 mL) equipped with a teflon-coated magnetic stirring bar and teflon cap, a carbon felt anode (25 mm × 50 mm × 3 mm) and a platinum cathode (25 mm × 50 mm × 0.2 mm) were added **1** (1.62 mL, 10 mmol), **2** (1.80 g, 12 mmol, 1.2 equiv.), Fe(phen)Cl_3 (102.7 mg, 0.3 mmol, 3 mol%), followed by addition of CH_3CN (100 mL). Electrocatalysis was performed at 70 ℃ with a constant current of 50 mA and maintained for 12 h. The carbon felt anode was washed with DCM (3 × 30 mL) in an ultrasonic bath. Evaporation of the solvent and subsequent column chromatography (petroleum ether/EtOAc = 20:1) yielded **3** (1.78 g, 61%) as a reddish solid.

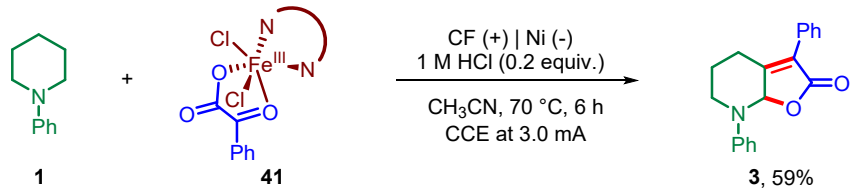
Control Experiments



(i) The Fe complex **41** was synthesized according to literature report with slight modification.[5] To a 10 mL pre-dried reaction flask was added 2-oxo-2-phenylacetic acid **2** (150.1 mg, 1.0 mmol), Fe(phen)Cl_3 (342.4 mg, 1.0 mmol) and CH_3CN (2.0 mL), then the reaction was vigorously stirred at 70 °C for 3 h. The evaporation and recrystallization using dichloromethane and hexane gave the Fe complex **41** as a deep red solid (446.8 mg, 98%).

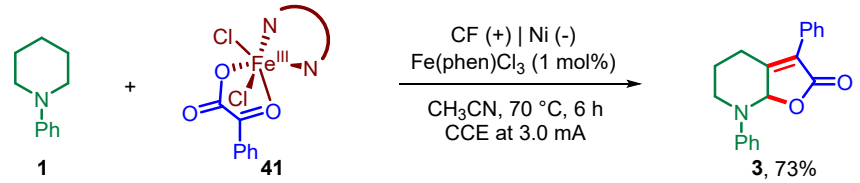


(ii) The electrocatalysis was carried out in an undivided cell with a carbon felt anode (10 mm × 20 mm × 3 mm) and a nickel plate cathode (10 mm × 15 mm × 0.2 mm). To a 15 mL pre-dried undivided electrochemical cell (15 mL) equipped with a magnetic bar was added *N*-aryl piperidine **1** (32.2 mg, 0.20 mmol, 1.0 equiv.), Fe complex **41** (0.24 mmol, 1.2 equiv.) and CH_3CN (5.0 mL). The electrocatalysis was performed at 70 °C with a constant current of 3.0 mA maintained for 6 h. The carbon felt anode was washed with DCM (3 × 5 mL) in an ultrasonic bath. And no reaction was observed.



(iii) The electrocatalysis was carried out in an undivided cell with a carbon felt anode (10 mm × 20 mm × 3 mm) and a nickel cathode (10 mm × 15 mm × 0.2 mm). To a 15 mL pre-dried undivided electrochemical cell (15 mL) equipped with a magnetic bar was added *N*-aryl piperidine **1** (32.2 mg, 0.20 mmol, 1.0 equiv.), Fe complex **41** (0.24

mmol, 1.2 equiv.), 1.0 M HCl (0.04 mL, 0.04 mmol, 0.2 equiv.) and CH_3CN (5.0 mL). The electrocatalysis was performed at 70 °C with a constant current of 3.0 mA maintained for 6 h. The carbon felt anode was washed with DCM (3 × 5 mL) in an ultrasonic bath. Evaporation of the solvent and subsequent column chromatography (petroleum ether/EtOAc = 20:1) yielded **3** (34.4 mg, 59%).



(iv) The electrocatalysis was carried out in an undivided cell with a carbon felt anode (10 mm × 20 mm × 3 mm) and a nickel cathode (10 mm × 15 mm × 0.2 mm). To a 15 mL pre-dried undivided electrochemical cell (15 mL) equipped with a magnetic bar was added *N*-aryl piperidine **1** (32.2 mg, 0.20 mmol, 1.0 equiv.), Fe complex **41** (0.24 mmol, 1.2 equiv.), $Fe(phen)Cl_3$ (0.7 mg, 1 mol%) and CH_3CN (5.0 mL). The electrocatalysis was performed at 70 °C with a constant current of 3.0 mA maintained for 6 h. The carbon felt anode was washed with DCM (3 × 5 mL) in an ultrasonic bath. Evaporation of the solvent and subsequent column chromatography (petroleum ether/EtOAc = 20:1) yielded **3** (42.5 mg, 73%).

X-ray Crystallography

*Crystal structure of compound **19** (CCDC: 2218711)*

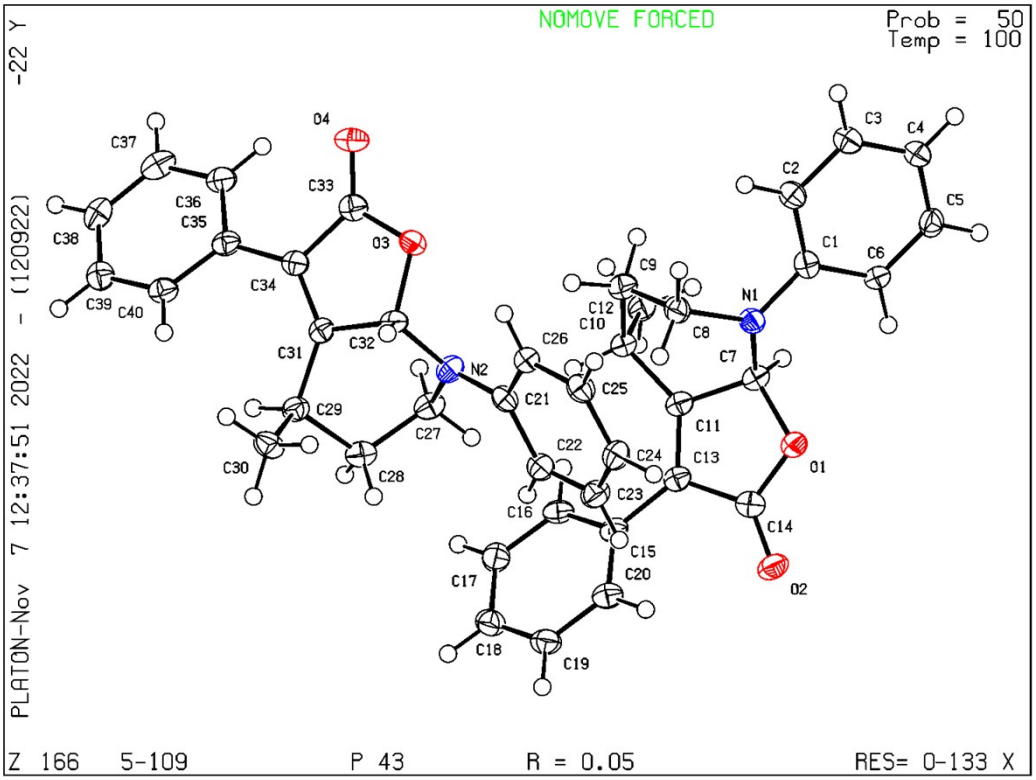


Table S-1. Crystal data and structure refinement for compound **19**.

Identification code	**19**	
Empirical formula	$C_{20}H_{19}NO_2$	
Formula weight	305.36	
Temperature	100.01(16) K	
Wavelength	1.54184 Å	
Crystal system	Tetragonal	
Space group	$P4_3$	
Unit cell dimensions	a = 9.58017(5) Å	α = 90°.
	b = 9.58017(5) Å	β = 90°.
	c = 33.7964(3) Å	γ = 90°.
Volume	3101.82(4) $Å^3$	
Z	8	
Density (calculated)	1.308 Mg/m^3	

Absorption coefficient	0.668 mm^{-1}
F(000)	1296
Crystal size	0.22 × 0.13 × 0.13 mm^3
Theta range for data collection	4.616 to 75.945°.
Index ranges	$-12 \leq h \leq 12$, $-10 \leq k \leq 10$, $-42 \leq l \leq 42$
Reflections collected	16868
Independent reflections	6166 [R(int) = 0.0327]
Completeness to theta = 67.684°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.78178
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	6166/1/417
Goodness-of-fit on F^2	1.142
Final R indices [I>2σ(I)]	$R_1 = 0.0518$, $wR_2 = 0.1242$
R indices (all data)	$R_1 = 0.0527$, $wR_2 = 0.1247$
Absolute structure parameter	0.28(9)
Extinction coefficient	n/a
Largest diff. peak and hole	0.204 and −0.308 $e.Å^{-3}$

Cyclic Voltammetry

The cyclic voltammetry was carried out with a Shanghai Chenhua CHI760E workstation. A glassy-carbon (GC) electrode (5 mm-diameter, disk-electrode) was used as the working electrode, a Pt plate was used as the counter electrode and an Ag/Ag^{+} electrode was used as the reference electrode in acetonitrile. The measurements were carried out at a scan rate of 100 mV s^{-1}, if not indicated otherwise. The operation temperature was 298 K.

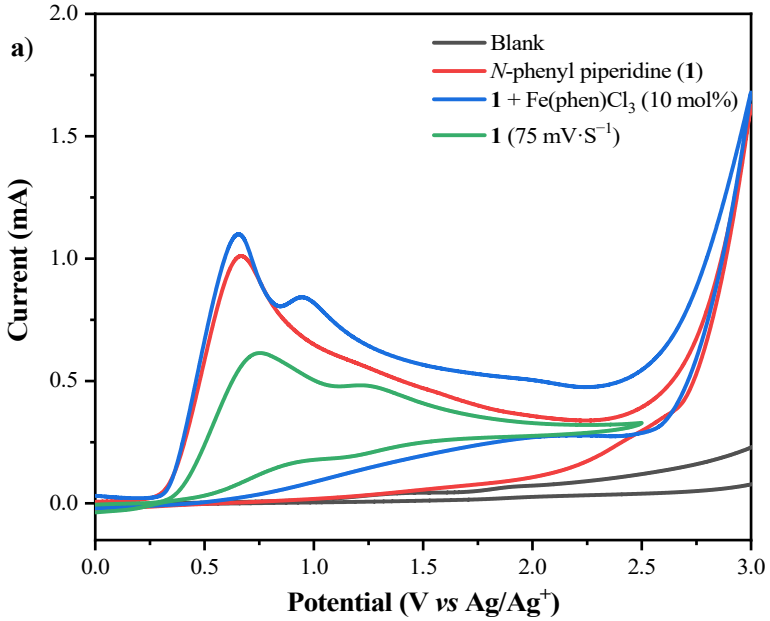


Figure S-1. Cyclic voltammograms of *N*-phenyl piperidine (**1**) and $Fe(phen)Cl_3$ at 100 mVs^{-1} in MeCN. $^{n}Bu_4NBF_4$ (0.1 M in MeCN), blank (black), **1** (10 mM, red), **1** + $Fe(phen)Cl_3$ (1 mM, blue), **1** (10 mM, 75 $mV{\cdot}s^{-1}$).

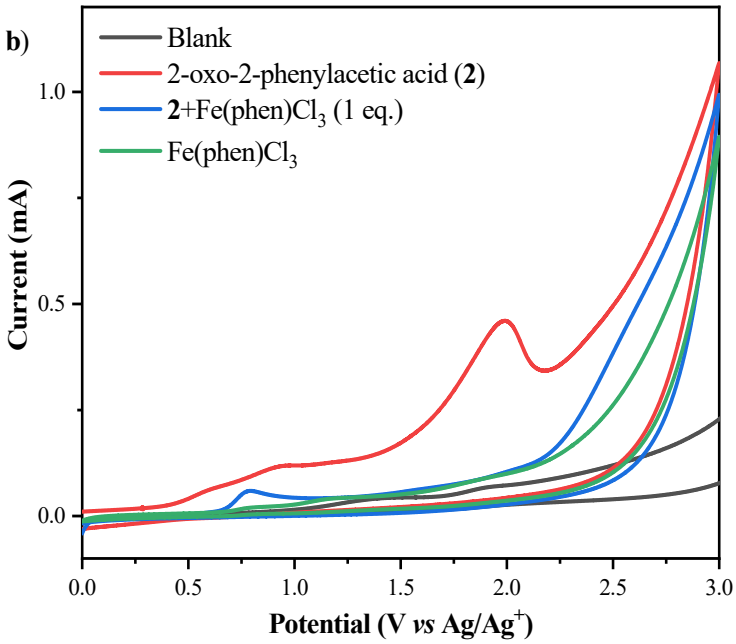
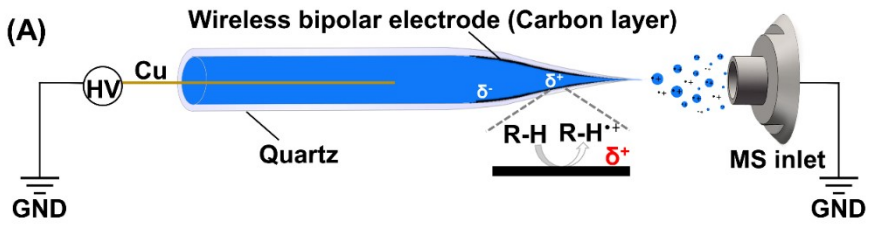


Figure S-2. Cyclic voltammograms of 2-oxo-2-phenylacetic acid (**2**) and $Fe(phen)Cl_3$ at 100 mVs^{-1} in MeCN. $^{n}Bu_4NBF_4$ (0.1 M in MeCN), blank (black), **2** (10 mM, red), **2** + $Fe(phen)Cl_3$ (blue), $Fe(phen)Cl_3$ (10 mM, red).

Bipolar Ultramicroelectrode Mass Spectrometry



A bipolar ultramicroelectrode (BUME) combined with nano-electrospray ionization mass spectrometry was used to rapidly capture short-lived reactive intermediates. The fabrication of the bipolar ultramicroelectrode has been described in **Figure S-3**. A Cu wire (0.2 mm i.d.) is inserted into the quartz capillary from its rear end and then connected to a high-voltage power supply. The BUME can directly take advantages of a high electric field, which was applied to perform electrospray ionization and to induce synergetic redox reaction at the two ends of the carbon electrode. Thus, electrospray ionization and Faradaic reaction are activated simultaneously, permitting rapid transfer of the electrochemically generated short-lived intermediates into gas phase for subsequent MS analysis.

Fabrication of bipolar ultramicroelectrode

A laser-based P-2000 pipette puller (Sutter Instrument Co., Novato, CA, USA) is used to fabricate a bare nanopipette from a quartz capillary (QF100-50-10, Sutter Instrument). The fabrication of a thin layer of carbon takes advantage of the pyrolysis of butane. Butane gas (~30 kPa) was sent into the nanopipette from its rear end and was heated by butane fire under a nitrogen atmosphere (~5 kPa through a quartz tube of O.D. 3.0 mm and I.D. 1.5 mm).

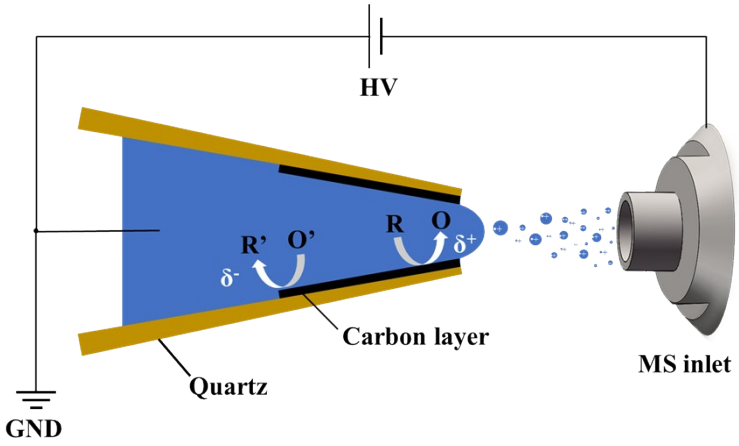


Figure S-3. Fabrication of BUME.

In this experiment, a positive high voltage of 896 V was applied to the Cu wire to induce redox reaction from a BUME nanopipette filled with 50 uM *N*-phenyl piperidine in acetonitrile. The *N*-phenyl piperidine radical cation (m/z 161.2) and the subsequently deprotonated iminium (m/z 160.2) was immediately observed (**Figure S-4**).

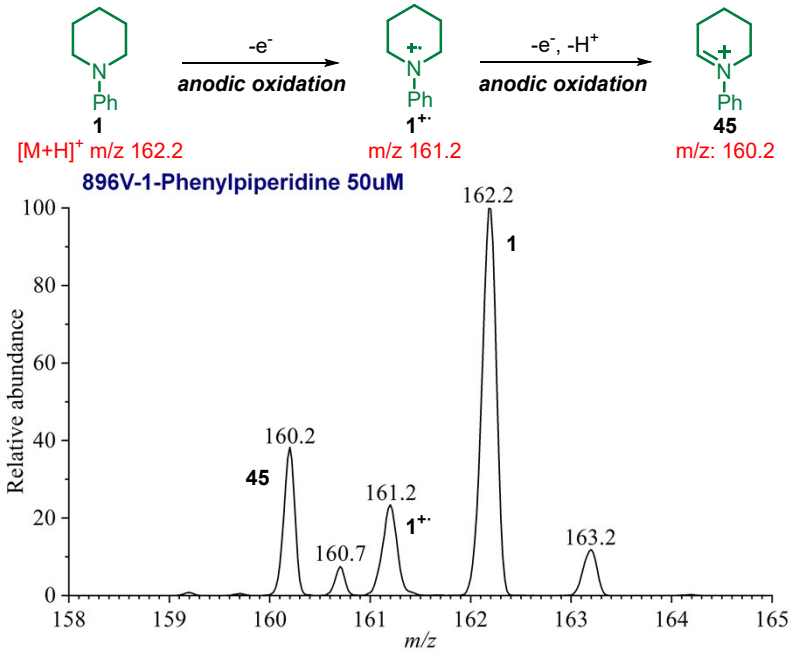


Figure S-4. Mass spectra for *N*-phenyl piperidine **1**.

DFT Calculations

General information of DFT computational studies:

Implemented in Gaussian 16, Rev. A 03[6], the unrestricted open-shell, dispersion-corrected (DFT-D3[7] with Becke-Johnson damping[8], noted as D3(BJ)) hybrid functional PBE0[9] and basis sets ma-TZVP[10] were utilized for single-point energy calculation, with the implicit solvation model SMD[11] using MeCN as the solvent and the keyword SCF = conver = 6 as an adjustment of SCF convergence criterion, while unrestricted open-shell functional PBE0[9], with D3(BJ), and basis sets def2-SVP[12] were utilized in geometric optimization and frequencies analysis, with the implicit solvation model IEFPCM[13] using MeCN as the solvent and the default settings for all convergence criteria. They are noted as SMD(MeCN) / (U)PBE0-D3(BJ) / ma-TZVP // IEFPCM(MeCN) / (U)PBE0-D3(BJ) / def2-SVP. The UltraFine integration grid was used to enhance the accuracy of our calculations. With the results of frequencies analysis, thermal corrections to Gibbs energies (TCGs) were obtained with Shermo 2.2[14] software package under T = 343.15K and p = 1atm, by applying Grimme's interpolation for entropy[15] as a treatment for low frequencies, and setting harmonic vibrational frequency scale factors for zero-point energy (ZPE), thermal energy (U), and entropy (S) to 0.9816, 0.9525, and 0.9576, individually (obtained from our fitting procedure, see the part **"**Fitting Procedure of Harmonic Vibrational Frequency Scale Factor**"** for details). All intermediates do not have an imaginary frequency, and all transition states have been optimized by the Berny algorithm[16] and verified by IRC calculations with a sole imaginary frequency. All 3D-structure figures of molecules were generated using CYLview20 software[17].

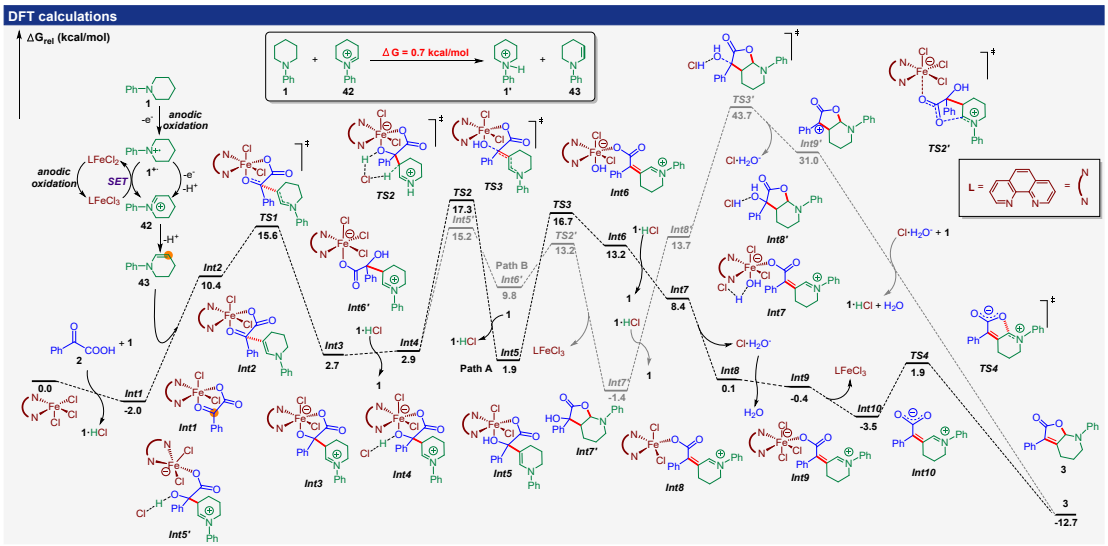
All molar Gibbs free energy changes (ΔG^{θ}) were calculated via the formula (S.1):

$$\Delta G^{o}(kcal/mol) = \left[\sum_{B}^{Products} [SPE(B) + TCG(B)] - \sum_{B}^{Reactants} [SPE(B) + TCG(B)] \right] \cdot 627.51 \quad (S.1)$$

All molar Gibbs activation energies ($\Delta G^{\ddagger}$) were calculated via the formula (S.2):

$$\Delta G^{\ddagger}(kcal/mol) = \left[[SPE(B) + TCG(B)]_{TS} - \sum_{B}^{Reactants} [SPE(B) + TCG(B)] \right] \cdot 627.51 \quad (S.2)$$

Where SPE = Single-Point Energy (Hartree), TCG = Thermal Corrections to Gibbs Free Energy (with translational, rotational and vibrational energies considered), TS = Transition State, 1 Hartree = 627.51 kcal/mol = 2625.5 kJ/mol. All SPEs and TCGs were obtained by calculation.



3D-structures of transition states:

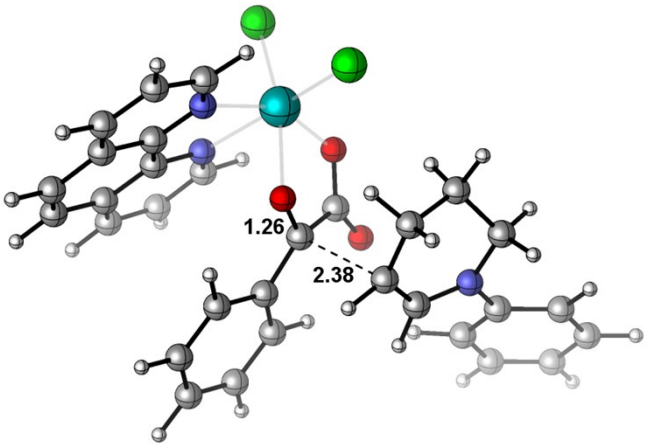


Figure S-5. 3D structure of **TS1**.

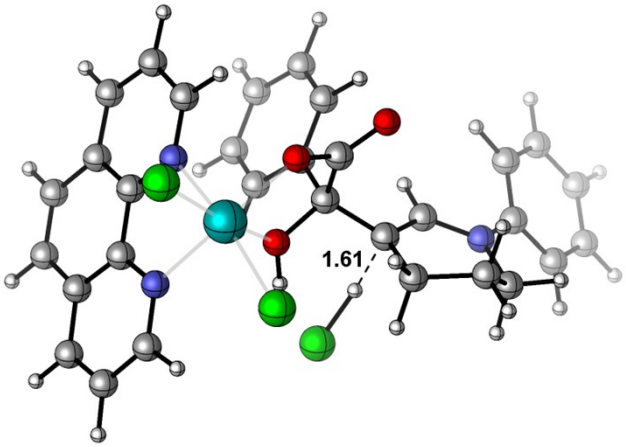


Figure S-6. 3D structure of **TS2**.

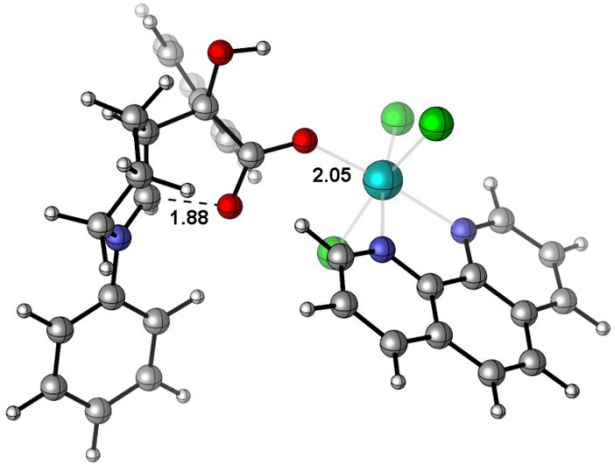


Figure S-7. 3D structure of **TS2'**.

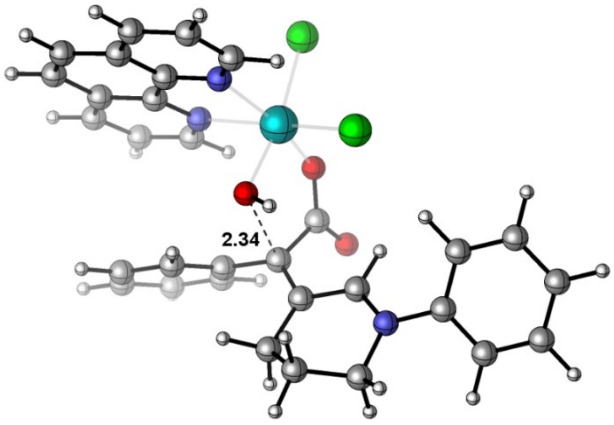


Figure S-8. 3D structure of **TS3**.

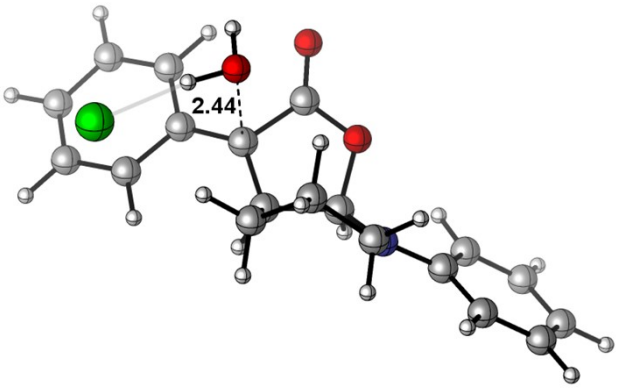


Figure S-9. 3D structure of **TS3'**.

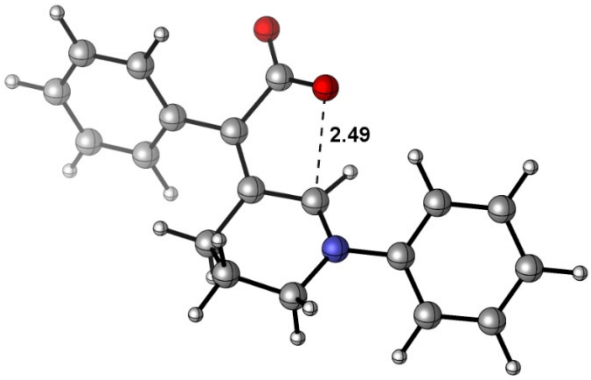


Figure S-10. 3D structure of **TS4**.

Fitting procedure of harmonic vibrational frequency scale factor:

The whole fitting procedure mainly referred to Merrick *et al*'s work[18]. According to the knowledge of statistical mechanics, in molecular vibration, for every single normal mode with a frequency v_i (wavenumber $\tilde{\nu}_i$), its contribution to the zero-point energy (ZPE), thermal energy (U, ZPE excluded) and entropy (S) can be individually evaluated by formulas (S.4), (S.5), and (S.6):

$$ZPE_{vib,m}(\tilde{\nu}_i) = \frac{1}{2} N_A h c \tilde{\nu}_i \quad (S.4)$$

$$\Delta U_{vib,m}(\tilde{\nu}_i) = N_A h c \frac{\tilde{\nu}_i}{e^{\mu_i} - 1} \quad (S.5)$$

$$\Delta S_{vib,m}(\tilde{\nu}_i) = R\left[\frac{\mu_i}{e^{\mu_i} - 1} - ln(1 - e^{-\mu_i})\right] \quad (S.6)$$

Where the temperature is set to 298.15K, N_A is Avogadro's constant, c is the speed

of light, and μ_i suffices formula (S.7):

$$\mu_i = \frac{hc\tilde{\nu}_i}{kT} \quad (S.7)$$

For a certain molecule, having obtained frequencies of all normal modes, the summation of formula (S.4), (S.5), and (S.6) equals vibrational contributions to the molecule's ZPE, thermal energy, and entropy individually.

With these theoretical bases, we prepared two test sets for experimental frequencies (with 27 molecules and 139 normal modes, see **Table S-2**) and ZPEs (with 18 experimental data, see **Table S-3**) individually. Computed wavenumbers were obtained by geometry optimization and vibration analysis for each molecule within the test set at the level of PBE0-D3(BJ)/def2-SVP, using Gaussian 16, Rev. A 03 software package with the UltraFine integration grid.

Having obtained all the experimental and computed wavenumbers ($\tilde{\nu}_i^{Exp}$ and $\tilde{\nu}_i^{Theor}$), now we can introduce the harmonic vibrational frequency scale factor λ_{ZPE}, λ_U (for thermal energy), and λ_S (for entropy). The sum of squared residuals (SSR) is chosen as the function of λ to minimize:

$$SSR(ZPE) = \sum_{i}^{All\ normal\ modes} \left[ZPE_{vib,m}(\lambda_{ZPE} \cdot \tilde{\nu}_i^{Theor}) - ZPE_i^{Exp}\right]^2 \quad (S.8)$$

$$SSR(U) = \sum_{i}^{All\ normal\ modes} \left[\Delta U_{vib,m}(\lambda_U \cdot \tilde{\nu}_i^{Theor}) - \Delta U_{vib,m}(\tilde{\nu}_i^{Exp})\right]^2 \quad (S.9)$$

$$SSR(S) = \sum_{i}^{All\ normal\ modes} \left[\Delta S_{vib,m}(\lambda_S \cdot \tilde{\nu}_i^{Theor}) - \Delta S_{vib,m}(\tilde{\nu}_i^{Exp})\right]^2 \quad (S.10)$$

Substitute every wavenumber into formula (S.8)~(S.10), use the scale factor λ as the sole independent variable to minimize the SSR function via Scipy toolkit 1.8.1 in Python 3.9, with 0.95 as an initial guess value for optimization, and we can finally obtain the fitted harmonic vibrational frequency scale factor for ZPE (λ_{ZPE}, 0.9816), thermal energy (λ_U, 0.9525), and entropy (λ_S, 0.9576)

Table S-2. All molecules and their corresponding experimental frequencies (wavenumbers) of normal modes in our test set.

Molecules	Wavenumbers of Normal Modes (cm^{-1})	Ref.
C_2H_2	612, 612, 730, 730, 1974, 3289, 3374	19
C_2H_4	825, 943, 949, 1023, 1236, 1342, 1444, 1623, 2989, 3026, 3103, 3106	19
C_2H_6	289, 822, 822, 995, 1190, 1190, 1379, 1388, 1468, 1468, 1469, 1469, 2896, 2954, 2969, 2969, 2985, 2985	19
CBr_2	196, 595, 641	20b
CH_2Cl_2	282, 717, 758, 898, 1153, 1268, 1467, 2999, 3040	19
CH_2O	1167, 1249, 1500, 1746, 2782, 2843	19
CH_3Cl	732, 1017, 1017, 1355, 1452, 1452, 2937, 3039, 3039	19
CH_3OH	250, 1033, 1060, 1165, 1345, 1455, 1477, 1477, 2844, 2960, 3000, 3681	19
CH_4	1306, 1306, 1306, 1534, 1534, 2917, 3019, 3019, 3019	19
Cl_2	554	19
CO	2143	19
CO_2	667, 667, 1333, 2349	19
F_2	894	19
H_2	4159	19
H_2O	1595, 3657, 3756	19
HCN	712, 712, 2097, 3311	19
HCOOH	625, 638, 1033, 1105, 1229, 1387, 1770, 2943, 3570	19
HF	3959	19
HNCO	610, 643, 762, 1327, 2274, 3531	19
HOBr	626, 1164, 3590	20c
N_2	2330	19
N_2O	589, 589, 1285, 2224	19
NH_3	950, 1627, 1627, 3337, 3444, 3444	19
NO_2Br	282, 290, 606, 783, 1291, 1659	20a
OH	3568	19
PH	2276	19
SH	2592	19

Table S-3. All zero-point energy (ZPE) data in our test set.

Molecules	ZPE (kJ/mol)	Ref.
C_2H_2	68.87	21
C_2H_4	131.67	22
CH_2O	69.16	22
CH_3Cl	98.11	23
CH_4	115.94	24
Cl_2	3.35	25
CO	12.93	25
F_2	5.44	25
H_2	25.98	25
H_2O	55.44	22
HCN	41.63	21
HF	24.48	25
N_2	14.06	25

N_2O	28.49	26
NH_3	89.24	26
OH	22.09	25
PH	14.02	25
SH	16.02	25

Exploration of the most stable spin-state and configuration of Fe(phen)(PhCOCOO)Cl_2 and Fe(phen)Cl_3.

Calculated and geometrically-optimized at the level of IEFPCM(MeCN)/(U)PBE0-D3(BJ)/def2-SVP, we started with the stereoisomer **Int1_1**, where the benzoylformic acid anion lies on the plane of the ligand (phen). Firstly, the impacts of different spin multiplicity (S) on single-point energy (SPE, unit: a.u.) of **Int1_1** were explored. As is shown in **Fig. S-11a**, **Int1_1** with a spin multiplicity of 6 bears the lowest SPE, while **Int1_1** with a spin multiplicity of 2 is 12.8 kcal/mol higher. The calculation for **Int1_1** with the spin multiplicity of 4 cannot proceed because of SCF convergence failure arising from improper electron distribution. Because almost all other 6-coordinated intermediates and TSs have a similar coordination sphere, the optimal stability of spin multiplicity of 6 is extrapolated to other 6-coordinated intermediates and TSs. We then explored 4 different isomers of **Int1_1**, and the calculated SPE of optimized geometries for the 4 different isomers are displayed in **Fig. S-11b**, with the most stable configuration of Fe(phen)(PhCOCOO)Cl_2 found. A similar procedure was taken to Fe(phen)Cl_3, and the calculated SPE and SPE plus thermal corrections to Gibbs free energies (TCG, not scaled) results show that Fe(phen)Cl_3 with a configuration of square-pyramid and a spin multiplicity of 6 is slightly more thermodynamically favorable than that with a configuration of bipyramid and a spin multiplicity of 6 (See **Fig. S-11c**, an SCF convergence error would occur while spin multiplicity was set to 4 in bipyramid configuration or 2 in both configurations), which indicates that both of these configurations might exist simultaneously. Likewise, we consider all other 5-coordinated intermediates and TSs should have a spin multiplicity of 6.

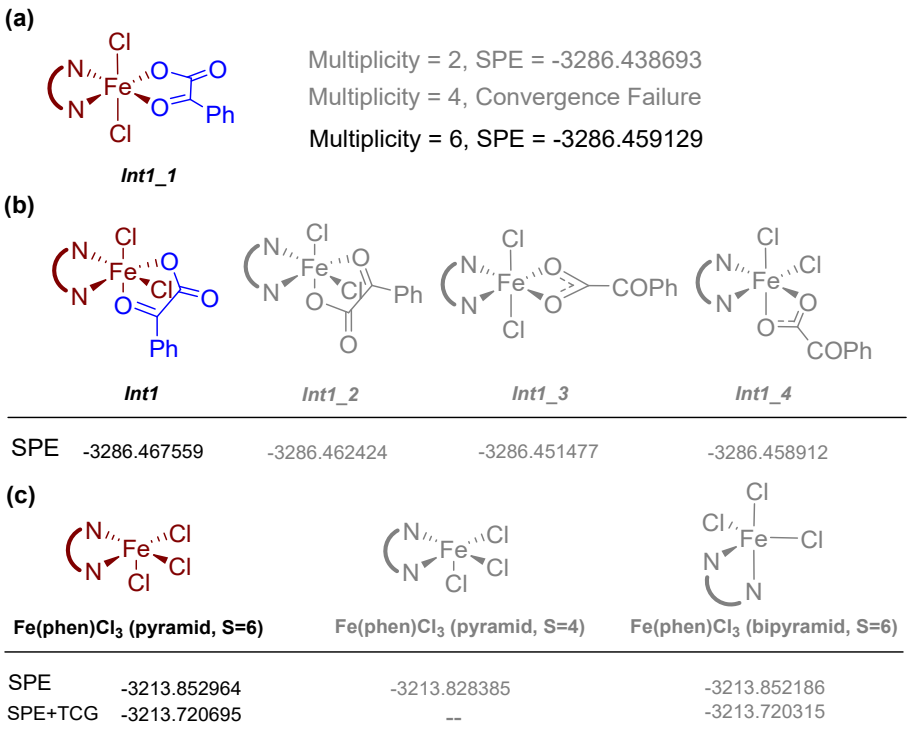


Figure S-11. Determination of optimal configuration and spin multiplicity for Fe(phen)(PhCOCOO)Cl_2 and Fe(phen)Cl_3.

Int4's deprotonation by 1.

Aside from chloride anion, in the α-H deprotonation step (from **Int4** to **Int5**), we believed that N-phenylpiperidine(**1**) might also act as a base. We have also found the TS of **Int4**'s deprotonation by 1 (**TS2"**, **Fig. S-12**), however, with a much higher energy barrier (**Fig. S-13**, 35.0 kcal/mol) , probably because of the strong steric hindrance.

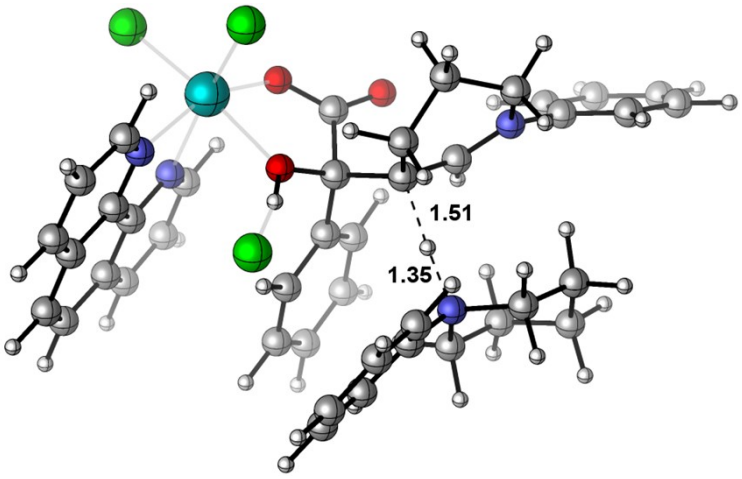


Figure S-12. 3D structure of **TS2''**.

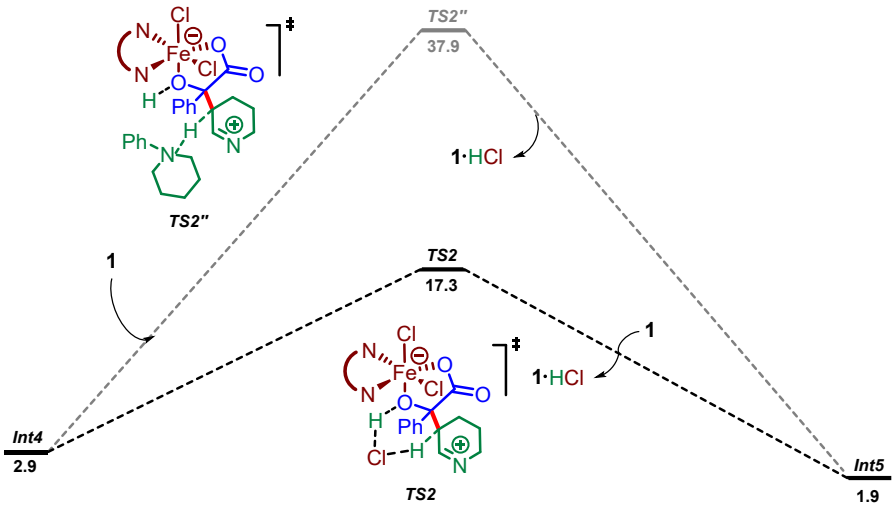


Figure S-13. Potential surfaces of **Int4**'s deprotonation, by chloride anion intramolecularly (black) and **1** (grey).

Dissociation before ring-closure vs. ring-closure before dissociation

There exist two possible pathways from **Int9** to product **3**, namely dissociation before ring-closure, and ring-closure before dissociation. The two pathways were both calculated, shown in **Fig. S-14**, which indicates that the pathway of dissociation before ring-closure is slightly favorable, in terms of energy barrier in the ring-closure-step (5.4 kcal/mol vs. 6.4 kcal/mol).

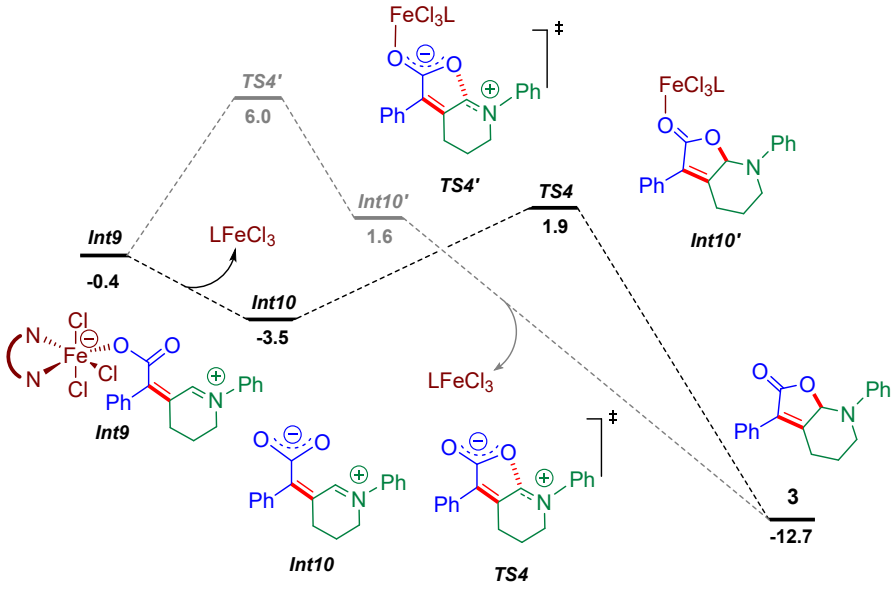


Figure S-14. Potential surfaces of **Int9**'s dissociation before ring-closure pathway (black) and ring-closure before dissociation pathway (grey).

Computed energies of stationary points

Table S-4. Thermal corrections to Gibbs free energies (TCG), single-point energies (SPE), and unscaled wavenumbers of imaginary frequencies (WIF) of transition states.

Structures	SPE[a] (Hartree)	TCG[b] (Hartree)	WIF[b] (cm^{-1})
1	-482.585240	0.194163	
1'	-483.046852	0.208833	
1·HCl	-943.294699	0.204382	
2	-533.778484	0.082814	
3	-938.787389	0.262444	
42	-481.828556	0.183956	
43	-481.367630	0.171094	
$Cl{\cdot}H_2O^-$	-536.630233	-0.006505	
H_2O	-76.3876866	0.000181	
Fe(phen)Cl_3	-3215.115469	0.121241	
Int1	-3288.217109	0.223194	
Int10	-938.769646	0.25938	
Int10'	-4153.910874	0.414552	
Int2	-3769.591847	0.421297	
Int3	-3769.611374	0.428407	
Int4	-4230.319635	0.437784	
Int5	-3769.610894	0.426781	
Int5'	-4230.299154	0.436925	
Int6	-3769.588467	0.422263	
Int6'	-4230.306442	0.435586	
Int7	-4230.307167	0.434116	
Int7'	-1015.182624	0.288252	
Int8	-3693.663609	0.414114	
Int8'	-1475.862203	0.29271	
Int9	-4153.910465	0.410807	
Int9'	-939.179435	0.2736	
TS1	-3769.588095	0.425717	102.92i
TS2'	-4230.302634	0.437143	187.18i
TS2''	-4712.876908	0.659703	1374.80i
TS2	-4230.291196	0.432269	207.12i
TS3'	-1475.814810	0.294619	102.70i

TS3	-3769.583870	0.423245	131.61i
TS4'	-4153.900989	0.411566	-76.01i
TS4	-938.762698	0.260934	47.50i

[a]Computed at the SMD[11](MeCN)/PBE0[9]-D3[7](BJ[8])/ma-TZVP[11] level.

[b]Computed at the IEFPCM[13](MeCN)/PBE0[9]-D3[7](BJ[8])/def2-SVP[12] level.

Cartesian Coordinates of Stationary Points (Unit of length: Å)

$Cl{\cdot}H_2O^-$

Charge = -1 Spin Multiplicity = 1

H	0.74302147	0.05243054	-0.09866144
H	1.91784801	-0.76085742	0.39505198
O	1.73179488	0.03033736	-0.12226727
Cl	-1.32405236	-0.08506750	0.07051873

H_2O

Charge = 0 Spin Multiplicity = 1

O	2.83041287	0.60873151	0.00000000
H	3.79270755	0.66684705	0.00000000
H	2.56397441	1.53522977	0.00000000

Int1

Charge = 0 Spin Multiplicity = 6

Fe	0.42052128	1.58996957	0.04040090
N	1.03057074	-0.07029303	1.34863562
C	1.84974676	-0.96471987	0.76454573
C	0.70084281	-0.21541358	2.61940101
C	2.37184656	-2.08105996	1.45232470
C	2.19305058	-0.74397453	-0.61010147
C	1.17049378	-1.29195067	3.39005969
H	0.04329700	0.54789121	3.04251627

C	2.00204846	-2.22690351	2.80688488
C	3.23426595	-2.98843250	0.75434880
C	3.04768314	-1.65076715	-1.27223438
N	1.67677658	0.34552372	-1.21743978
H	0.87141589	-1.37442149	4.43563954
H	2.37962847	-3.07566230	3.38157930
C	3.55735620	-2.78198431	-0.55380570
H	3.63005171	-3.85097296	1.29425242
C	3.35126103	-1.37628651	-2.62311868
C	1.97142987	0.58601307	-2.48459697
H	4.21560122	-3.47715445	-1.07879153
H	4.00926369	-2.05015579	-3.17650024
C	2.81271961	-0.25837195	-3.22676897
H	1.51677116	1.47872630	-2.92162554
H	3.02710925	-0.01842668	-4.26883398
Cl	2.04797087	2.86073175	0.92848604
O	-1.08479331	1.90388225	1.27582052
C	-2.22136266	1.32061274	1.14586799
C	-2.16784604	0.18968925	0.07645852
O	-3.23350033	1.58074328	1.76506899
C	-3.28730455	-0.70344827	-0.23327150
O	-1.09754589	0.07926388	-0.51828639
C	-4.51845268	-0.65922083	0.44517611
C	-3.09303232	-1.65039413	-1.25799797
C	-5.53065743	-1.54870417	0.09845031
H	-4.66138198	0.07741415	1.23403432
C	-4.10786470	-2.53188640	-1.59846046
H	-2.13264876	-1.67383864	-1.77577191
C	-5.32912423	-2.48151979	-0.91894315
H	-6.48582698	-1.51332491	0.62649593

H	-3.95326923	-3.26287428	-2.39482966
H	-6.12897266	-3.17618422	-1.18665998
Cl	-0.33057283	2.84931674	-1.70552933

Int10'

Charge = 0 Spin Multiplicity = 6

O	1.13253306	0.71538873	-0.76819302
C	1.84063191	-0.34129255	-0.42630178
C	3.26873437	-0.00243606	-0.38049100
O	1.30220866	-1.40602707	-0.15372064
C	4.31183363	-0.95719838	0.00697922
C	4.05372905	-1.93612272	0.98106782
C	5.58179602	-0.90535209	-0.58780820
C	5.05514240	-2.82553248	1.36171632
H	3.06448605	-2.00161480	1.43743815
C	6.57893123	-1.79733997	-0.20248713
H	5.78086847	-0.17531346	-1.37541917
C	6.31955560	-2.75735846	0.77595932
H	4.84473093	-3.57968536	2.12358105
H	7.56183706	-1.74798607	-0.67657770
H	7.10152364	-3.45864723	1.07644006
C	3.35482401	1.31849651	-0.66982582
C	1.98791865	1.83697665	-1.01418818
H	1.90578190	2.02415478	-2.10574684
N	1.57019026	2.96158611	-0.23879866
C	2.59550178	3.87677080	0.26297265
H	2.78583463	4.67226527	-0.48375039
H	2.20097104	4.37143946	1.16043527
C	0.29383126	3.48956526	-0.49720560
C	-0.66249594	2.78242255	-1.25669923

C	-0.09049852	4.73675548	0.03349236
C	-1.94763143	3.28603021	-1.42941922
H	-0.44832007	1.79993909	-1.67294323
C	-1.38298161	5.22449076	-0.14637719
H	0.61061735	5.34083644	0.60631945
C	-2.32962629	4.50496293	-0.87194860
H	-2.66461592	2.69155013	-2.00168767
H	-1.64528627	6.19073851	0.29205908
H	-3.34372380	4.88816535	-1.00304868
C	3.90360277	3.21077279	0.64317288
H	4.63442158	3.99955354	0.87335069
H	3.76937980	2.61220164	1.55815221
C	4.43883357	2.29862379	-0.46626110
H	4.62224676	2.88114152	-1.38464690
H	5.37761181	1.81426539	-0.17139798
Fe	-0.74944960	-1.95977147	0.00134487
N	-1.40656595	-0.07062136	0.99124597
C	-2.73785935	0.12480944	0.91499420
C	-0.65325280	0.84825715	1.56408879
C	-3.35623859	1.32116799	1.33808360
C	-3.54186901	-0.96243207	0.43572308
C	-1.17473433	2.06588892	2.03120817
H	0.40912835	0.62669163	1.67048450
C	-2.52288843	2.31650186	1.89236965
C	-4.77720719	1.45579430	1.21125726
C	-4.94367511	-0.81535437	0.35379541
N	-2.91555333	-2.11282633	0.10859559
H	-0.50347942	2.79919396	2.47824249
H	-2.95547642	3.26372435	2.22068805
C	-5.53974133	0.43123271	0.73526440

H	-5.23930758	2.39641818	1.51819729
C	-5.68293571	-1.93135502	-0.09375187
C	-3.62400387	-3.14997893	-0.30324137
H	-6.62335304	0.53685234	0.65147312
H	-6.76994510	-1.86060982	-0.17599325
C	-5.02284072	-3.09956527	-0.41513478
H	-3.05426683	-4.04497809	-0.56642533
H	-5.56529283	-3.98152062	-0.75784423
Cl	-0.29199510	-2.60837158	2.18666062
Cl	-0.46856170	-4.04491700	-0.90123127
Cl	-1.17621995	-0.88717186	-2.04312185

Int10

Charge = 0 Spin Multiplicity = 1

O	-2.95809989	3.44604854	0.75634973
C	-2.37370014	2.34839009	0.77522575
C	-1.81586544	1.94786955	-0.59666750
O	-2.21010242	1.55192176	1.71272687
C	-0.72085568	2.75897702	-1.14197063
C	-0.70779822	4.15941200	-1.00425792
C	0.37442276	2.13374452	-1.76705625
C	0.35727418	4.90648724	-1.49684778
H	-1.55778313	4.63222640	-0.51117213
C	1.44659799	2.88451980	-2.23866243
H	0.40270631	1.04594120	-1.84932128
C	1.43773840	4.27427750	-2.11408206
H	0.34501791	5.99438458	-1.39622332
H	2.29544753	2.38005706	-2.70590735
H	2.27513441	4.86398975	-2.49459665
C	-2.37350149	0.89855076	-1.30545963

C	-3.31347967	0.08883101	-0.61898172
H	-3.44210897	0.24678180	0.45558922
N	-4.00224485	-0.88824413	-1.16581026
C	-3.85153395	-1.21512647	-2.59175465
H	-3.13933138	-2.05089830	-2.68137085
H	-4.82767215	-1.56612032	-2.95056534
C	-4.91746070	-1.65780734	-0.38906809
C	-5.69510789	-1.03668990	0.59280624
C	-5.03866639	-3.03031767	-0.62344641
C	-6.57549570	-1.79848064	1.35564012
H	-5.63140552	0.04228722	0.74565617
C	-5.92736870	-3.78021233	0.14272840
H	-4.43032586	-3.52030948	-1.38461850
C	-6.69451596	-3.17039743	1.13471990
H	-7.18443120	-1.30870128	2.11835806
H	-6.01365526	-4.85394735	-0.03654221
H	-7.39099014	-3.76325812	1.73121546
C	-3.37503645	-0.01093818	-3.37551995
H	-3.19173953	-0.32298293	-4.41303548
H	-4.17401392	0.74771753	-3.39925002
C	-2.11601491	0.57874763	-2.75573666
H	-1.29128413	-0.14750796	-2.85036682
H	-1.80112638	1.48258068	-3.29501768

Int1_1

Charge = 0 Spin Multiplicity = 6

Fe	-0.47271618	1.20392272	0.01150523
N	1.61819441	0.65299950	0.00614169
C	2.48081156	1.69200468	-0.02396754
C	2.08477586	-0.58559412	0.02937038

C	3.88121110	1.51302869	-0.03174896
C	1.93199840	3.01850727	-0.04874964
C	3.46146332	-0.86184074	0.02384119
H	1.33342239	-1.37832920	0.05311250
C	4.35991788	0.18516360	-0.00661090
C	4.73363446	2.66571250	-0.06426316
C	2.79451552	4.13666632	-0.08071723
N	0.59092312	3.13809202	-0.04033708
H	3.79968743	-1.89867376	0.04369362
H	5.43639290	-0.00135250	-0.01152348
C	4.21250191	3.92502709	-0.08776537
H	5.81503736	2.51294631	-0.06987347
C	2.18904651	5.41161803	-0.10408702
C	0.04034030	4.33793919	-0.06252601
H	4.87018196	4.79660838	-0.11249834
H	2.81454584	6.30694254	-0.12915756
C	0.81212499	5.51138897	-0.09499726
H	-1.05215585	4.38387803	-0.05452696
H	0.31474707	6.48207836	-0.11253530
Cl	-0.68412312	1.48236945	-2.25758348
Cl	-0.64696293	1.58327241	2.26907275
O	-0.83171208	-0.75904183	0.05842864
C	-2.01660239	-1.24532937	0.07836008
C	-3.09545314	-0.12153168	0.06212903
O	-2.30987772	-2.42513130	0.10661374
C	-4.54300056	-0.35892158	0.07897267
O	-2.65302874	1.02557405	0.03328739
C	-5.11120061	-1.64550393	0.11175467
C	-5.38643921	0.76998556	0.06100561
C	-6.49541160	-1.79075326	0.12604371

H	-4.45342445	-2.51338829	0.12552641
C	-6.76486379	0.61625358	0.07542983
H	-4.93555958	1.76360853	0.03561478
C	-7.32119644	-0.66647131	0.10799198
H	-6.93387432	-2.79074630	0.15146388
H	-7.41303190	1.49523614	0.06138534
H	-8.40726835	-0.78787781	0.11936098

Int1_1 (S=2)

Charge = 0 Spin Multiplicity = 2

Fe	-0.12902797	-0.35459833	-0.00145201
N	-1.87524564	-1.21642865	-0.00077881
C	-2.90271086	-0.34282208	-0.00151303
C	-2.12385976	-2.51533549	0.00001697
C	-4.25391167	-0.73226817	-0.00131318
C	-2.54326447	1.03244374	-0.00258916
C	-3.44176342	-3.00389558	0.00024031
H	-1.25560221	-3.17787982	0.00053653
C	-4.50629817	-2.12141757	-0.00038584
C	-5.25341183	0.29890757	-0.00209295
C	-3.53265849	2.03213972	-0.00331867
N	-1.22005961	1.29178269	-0.00286495
H	-3.60665468	-4.08211988	0.00092105
H	-5.53488745	-2.48918550	-0.00018739
C	-4.90853859	1.62086640	-0.00303080
H	-6.30524656	0.00523493	-0.00192038
C	-3.07453765	3.36742698	-0.00428122
C	-0.80450962	2.54649255	-0.00373322
H	-5.68292307	2.39093734	-0.00359652
H	-3.79204937	4.19108200	-0.00487540

C	-1.71443311	3.61749015	-0.00446020
H	0.27539761	2.71098300	-0.00390225
H	-1.33128186	4.63873107	-0.00517537
Cl	-0.12363549	-0.27608674	2.25557318
Cl	-0.12344541	-0.28016148	-2.25860245
O	0.88599419	-1.95246510	0.00002472
C	2.16393966	-1.83407483	-0.00135225
C	2.58773991	-0.34400873	-0.00185032
O	2.96543169	-2.74852487	-0.00226504
C	3.96662987	0.13605778	-0.00206339
O	1.64660416	0.46100076	-0.00222457
C	5.07061778	-0.73737049	-0.00063384
C	4.18308751	1.52931571	-0.00359045
C	6.36182237	-0.21932119	-0.00069644
H	4.89315242	-1.81212345	0.00046464
C	5.47372270	2.03606617	-0.00371084
H	3.32210202	2.19979562	-0.00468930
C	6.56512007	1.16094692	-0.00224766
H	7.21726260	-0.89819568	0.00045258
H	5.63693540	3.11586742	-0.00493721
H	7.58193801	1.56142209	-0.00232286

Int1_2

Charge = 0 Spin Multiplicity = 6

Fe	-0.19994190	-0.96559021	0.54904759
N	-0.91147986	1.14290814	0.52338629
C	-2.16740034	1.27585068	0.05442239
C	-0.24569007	2.21389908	0.91541751
C	-2.80761817	2.52971712	-0.06197829
C	-2.86807326	0.07889159	-0.31828326

C	-0.79413097	3.50530809	0.83865794
H	0.76020380	2.05339354	1.31239006
C	-2.07292539	3.66457187	0.34469989
C	-4.14637009	2.58741416	-0.57126262
C	-4.18911217	0.16471146	-0.80912455
N	-2.22666987	-1.10133566	-0.17009247
H	-0.20365168	4.36071428	1.16962018
H	-2.52513686	4.65633623	0.27092313
C	-4.80876390	1.45195540	-0.93110430
H	-4.62809833	3.56326910	-0.66259291
C	-4.82950183	-1.04631994	-1.15018808
C	-2.84387625	-2.22685887	-0.49517156
H	-5.82948605	1.50304937	-1.31592655
H	-5.85187913	-1.02651083	-1.53500086
C	-4.15675912	-2.24063150	-0.99172431
H	-2.26994334	-3.14717037	-0.35809724
H	-4.62376359	-3.19326627	-1.24491367
Cl	-0.54567442	-0.89366154	2.79391099
O	0.36543039	-0.53183921	-1.34997909
C	1.56701727	-0.20777065	-1.62567208
C	2.42753116	-0.08034881	-0.33009737
O	2.03644559	-0.00113584	-2.73061927
C	3.84913718	0.25648902	-0.30009948
O	1.81368304	-0.28551116	0.72364237
C	4.59274573	0.53256465	-1.46356594
C	4.48525273	0.30079045	0.95799357
C	5.94415146	0.84617815	-1.36134875
H	4.09138956	0.49517364	-2.42984027
C	5.83281752	0.61377389	1.04964456
H	3.89952233	0.08251611	1.85273221

C	6.56353516	0.88724575	-0.11158917
H	6.52001457	1.06042359	-2.26421990
H	6.32196137	0.64566729	2.02554594
H	7.62578247	1.13372607	-0.03890307
Cl	0.29121125	-3.17944085	0.31257645

Int1_3

Charge = 0 Spin Multiplicity = 6

Fe	-0.17126800	0.15863100	0.66583100
N	-1.57297100	-1.30098900	-0.06411800
C	-2.78798200	-0.82022000	-0.39524100
C	-1.28990300	-2.57538200	-0.27698800
C	-3.79518700	-1.63120300	-0.96763500
C	-3.04374800	0.56539200	-0.13598800
C	-2.22895000	-3.46163600	-0.82791700
H	-0.29026900	-2.90865900	0.01214500
C	-3.48128900	-2.98955300	-1.17378300
C	-5.06445700	-1.04268700	-1.28610800
C	-4.29893600	1.11988900	-0.46251300
N	-2.04599000	1.28537600	0.40852900
H	-1.96042600	-4.50937500	-0.96894300
H	-4.23228700	-3.65607000	-1.60494000
C	-5.30347800	0.27825000	-1.04489400
H	-5.83428600	-1.67119600	-1.73830600
C	-4.48410700	2.49351500	-0.19034500
C	-2.23595700	2.56521900	0.66431300
H	-6.27039000	0.71953000	-1.29646000
H	-5.43681000	2.96981800	-0.43122700
C	-3.44795400	3.21415900	0.37190900
H	-1.40120400	3.11057200	1.11403700

H	-3.55265100	4.27592400	0.60164200
Cl	-0.55078300	0.12521800	2.89482100
Cl	0.14326800	1.04678000	-1.43225800
O	1.23846000	-1.36989600	0.57577100
C	2.17314100	-0.55515400	0.82492600
C	3.63916600	-0.93455500	0.82317800
O	1.89435400	0.63536400	1.08289300
C	4.52154600	-0.19655300	-0.11075300
O	4.02468000	-1.73689400	1.63827500
C	4.01914600	0.77542300	-0.98798100
C	5.88711900	-0.49705300	-0.11425000
C	4.88395300	1.42461100	-1.86702100
H	2.96392500	1.05859800	-1.02759900
C	6.75088000	0.15278300	-0.98970100
H	6.26038100	-1.25618400	0.58021700
C	6.24832700	1.11238100	-1.86994100
H	4.49319800	2.18091900	-2.54988500
H	7.81628300	-0.08753100	-0.99449100
H	6.93003200	1.62023200	-2.55733900

Int1_4

Charge = 0 Spin Multiplicity = 6

Fe	0.23014542	1.36023709	-0.13089105
N	1.09763307	0.03758046	1.40148579
C	1.98367391	-0.85233070	0.91380757
C	0.87710263	0.09388370	2.70360074
C	2.69346198	-1.75169965	1.73825612
C	2.19386000	-0.86244780	-0.50493161
C	1.53698168	-0.75612429	3.60703116
H	0.14593655	0.83131163	3.04459387

C	2.44324550	-1.67960951	3.12599491
C	3.61173512	-2.67323057	1.13596970
C	3.10197203	-1.78155793	-1.07242281
N	1.49924498	0.02755199	-1.24827977
H	1.32253381	-0.67563488	4.67352452
H	2.96902309	-2.35423612	3.80572689
C	3.80600726	-2.68858952	-0.21332817
H	4.15439861	-3.36607348	1.78255031
C	3.26082588	-1.74444420	-2.47476295
C	1.66081610	0.04552727	-2.56291521
H	4.50628178	-3.39446758	-0.66484306
H	3.95264200	-2.43783992	-2.95872830
C	2.53919171	-0.83212795	-3.21757862
H	1.06759385	0.78179781	-3.11131559
H	2.63823355	-0.77905472	-4.30249877
Cl	1.65448640	2.97237452	0.49035780
O	-1.36560494	1.57272945	1.18430714
C	-1.92594421	0.51046102	0.78104799
C	-3.25065248	0.09377851	1.41653366
O	-1.38496487	-0.21500100	-0.07512784
C	-4.41165630	-0.13885670	0.52887278
O	-3.27999698	-0.05254742	2.62053064
C	-4.36678036	0.14419516	-0.84515375
C	-5.59633849	-0.62575350	1.10231787
C	-5.49762644	-0.06223708	-1.63163259
H	-3.44996593	0.52504579	-1.30125779
C	-6.71937311	-0.83643470	0.31231019
H	-5.61162377	-0.83232976	2.17466880
C	-6.66979930	-0.55408690	-1.05615053
H	-5.46402715	0.16031344	-2.70045243

H	-7.63943458	-1.21987886	0.75933865
H	-7.55345893	-0.71810501	-1.67789549
Cl	-0.78746060	2.25850524	-1.95655611

Int2

Charge = 0 Spin Multiplicity = 6

Fe	-1.13520180	-1.44115278	0.31538892
N	-2.60812362	-0.27078716	1.46161319
C	-3.75913970	-0.03302607	0.80545207
C	-2.45578410	0.16701344	2.69854403
C	-4.82412504	0.69557029	1.37731180
C	-3.88222039	-0.56135709	-0.52189677
C	-3.45925247	0.89710496	3.35668397
H	-1.50733017	-0.06936878	3.18701546
C	-4.64050316	1.16683421	2.69516029
C	-6.01332933	0.91214379	0.60721743
C	-5.06684753	-0.33862764	-1.25570852
N	-2.84233996	-1.26724930	-1.01522240
H	-3.29088510	1.24186694	4.37757806
H	-5.43627130	1.73627987	3.18048547
C	-6.12837804	0.41697177	-0.65756761
H	-6.82879126	1.48238393	1.05678394
C	-5.13055555	-0.88873637	-2.55392784
C	-2.92043255	-1.77505510	-2.23455384
H	-7.03762006	0.58468501	-1.23849941
H	-6.02784572	-0.74186537	-3.15927267
C	-4.05767832	-1.60690569	-3.04061874
H	-2.04421544	-2.32853879	-2.58126725
H	-4.07513035	-2.04535851	-4.03902494
Cl	-1.77001686	-3.27231490	1.45293509

O	0.25379553	-0.68409603	1.50011168
C	0.77385834	0.47176119	1.30969804
C	0.08816228	1.22871128	0.13883793
O	1.68778713	0.95945036	1.94957554
C	0.37068981	2.62176459	-0.21884689
O	-0.75757930	0.58367790	-0.47943680
C	1.29923192	3.42281176	0.46921950
C	-0.33593174	3.16143337	-1.31135488
C	1.51646520	4.73523542	0.06055250
H	1.83793070	3.00161171	1.31630178
C	-0.11235393	4.46969284	-1.71255224
H	-1.05484739	2.52917250	-1.83510514
C	0.81715597	5.25834270	-1.02682717
H	2.23891550	5.35502871	0.59562245
H	-0.66069250	4.88226448	-2.56197952
H	0.99457549	6.28879897	-1.34385060
Cl	0.20787032	-2.31336946	-1.30813861
C	2.69674950	0.69872196	-1.94123021
H	2.01146346	1.54725958	-1.95699589
C	3.52250406	0.56904220	-0.88375226
H	3.47145245	1.26593143	-0.04543372
C	2.70459400	-0.26254896	-3.08773238
H	1.67001704	-0.55191834	-3.33703858
H	3.11299952	0.22319802	-3.99372302
N	4.51346681	-0.39377733	-0.79348583
C	4.79848409	-1.15131186	-2.00055860
H	5.47029795	-0.57440522	-2.66518311
H	5.32730014	-2.07156757	-1.71945541
C	3.50981578	-1.50483999	-2.73038094
H	3.75425533	-2.09373095	-3.62717435

H	2.90145771	-2.14603852	-2.07281324
C	5.29914694	-0.53566532	0.34685580
C	4.80941251	-0.16961465	1.61699048
C	6.60776741	-1.04986828	0.26197998
C	5.61090709	-0.30370591	2.74681219
H	3.78515910	0.19144614	1.73060571
C	7.39088037	-1.19208670	1.40497255
H	7.02892091	-1.32162719	-0.70662434
C	6.90592413	-0.81715974	2.65744252
H	5.20245267	-0.01751658	3.71982129
H	8.40360695	-1.59186740	1.30648675
H	7.52481256	-0.92784778	3.55045134

Int3

Charge = 0 Spin Multiplicity = 6

Fe	-1.39136989	-1.39450504	0.91670447
N	-2.24335785	0.65895042	1.09811481
C	-3.26387189	0.90486814	0.25908602
C	-1.76113009	1.63241459	1.84497055
C	-3.85259048	2.18216977	0.13324892
C	-3.75313749	-0.18983948	-0.53215569
C	-2.27349628	2.93973832	1.79000347
H	-0.93546577	1.36990055	2.51104117
C	-3.31716980	3.21574470	0.93125675
C	-4.93597079	2.36550713	-0.78671694
C	-4.82706036	0.01882308	-1.42590607
N	-3.15480141	-1.39050433	-0.38904795
H	-1.83600874	3.71659227	2.41802810
H	-3.73336311	4.22325386	0.86030692
C	-5.40499298	1.32647469	-1.53404288

H	-5.38102179	3.35874229	-0.87676677
C	-5.26840319	-1.09452247	-2.17277302
C	-3.57854258	-2.42101275	-1.09970698
H	-6.23240694	1.47314726	-2.23147546
H	-6.09697501	-0.97861173	-2.87537370
C	-4.64565855	-2.31470346	-2.00704918
H	-3.04043650	-3.36047446	-0.94397795
H	-4.96231953	-3.19376442	-2.56983032
Cl	-2.57695949	-1.80550709	2.87696259
O	0.29763377	-0.76134209	1.86040273
C	1.17806124	-0.27132533	1.08227669
C	0.69340397	0.02170777	-0.35424149
O	2.34976193	-0.02479771	1.37900385
C	0.48037961	1.53559802	-0.52699886
O	-0.45292002	-0.66054940	-0.61151947
C	1.19609941	2.51565707	0.16965130
C	-0.50884060	1.94175632	-1.43087065
C	0.92968682	3.87071599	-0.03822906
H	1.95159400	2.22196781	0.90096054
C	-0.77385089	3.29202445	-1.63863113
H	-1.08484684	1.17109727	-1.94619996
C	-0.05372570	4.26462514	-0.94224398
H	1.49252064	4.62150893	0.52198954
H	-1.55705972	3.58811651	-2.34124549
H	-0.26604304	5.32500722	-1.09842977
Cl	-0.85148039	-3.62876384	0.48293183
C	1.84052294	-0.46594825	-1.32757437
H	1.64436292	0.07430593	-2.27057591
C	3.14748288	0.04397000	-0.86908875
H	3.27717385	1.12171422	-0.74508955

C	1.81957226	-1.97266421	-1.57924719
H	0.79957175	-2.33370965	-1.39023709
H	2.05436922	-2.16528734	-2.63774195
N	4.22436222	-0.67474542	-0.76344905
C	4.21255774	-2.14146232	-0.91402130
H	4.58774404	-2.38430282	-1.92088173
H	4.93077608	-2.53732066	-0.18420461
C	2.82252186	-2.69849545	-0.70080438
H	2.83872905	-3.77281133	-0.93307856
H	2.54603403	-2.60643148	0.36098649
C	5.45468112	-0.06495892	-0.35520490
C	5.45752549	0.77776226	0.75683566
C	6.62707765	-0.33541556	-1.06149294
C	6.65305283	1.37555375	1.15046195
H	4.53158006	0.92720212	1.31559940
C	7.81528406	0.26619288	-0.65435691
H	6.61143204	-0.99566512	-1.93025459
C	7.83021799	1.12346842	0.44676451
H	6.66355588	2.03351993	2.02203168
H	8.73537719	0.06698979	-1.20777018
H	8.76559217	1.59192725	0.76043177

Int4

Charge = 0 Spin Multiplicity = 6

Fe	-1.62507282	-1.44953538	1.20459898
N	-2.31069384	0.63830850	1.22413594
C	-3.21099591	0.92641612	0.26653825
C	-1.83213800	1.60183878	1.98759084
C	-3.67054987	2.23867467	0.02847672
C	-3.69177742	-0.15948805	-0.53631823

C	-2.23029350	2.93998625	1.83211769
H	-1.10085894	1.30790117	2.74455396
C	-3.14433092	3.25922417	0.84951452
C	-4.61515200	2.46547628	-1.02434636
C	-4.62646909	0.09035513	-1.56288451
N	-3.21641751	-1.39554340	-0.27197098
H	-1.80170870	3.70667818	2.47811052
H	-3.46245729	4.29283889	0.69606370
C	-5.07361041	1.43332014	-1.78835099
H	-4.96048562	3.48557845	-1.20459276
C	-5.06695801	-1.01957901	-2.31497716
C	-3.62973704	-2.42080799	-0.99739101
H	-5.79290393	1.61341847	-2.58996120
H	-5.79286145	-0.87334180	-3.11808147
C	-4.57102421	-2.27377479	-2.02844857
H	-3.18743267	-3.39008158	-0.75427290
H	-4.88637059	-3.15128912	-2.59397571
Cl	-2.80130081	-1.77441991	3.10333994
O	0.12551019	-0.85721148	1.96143963
C	1.05677708	-0.43357072	1.19795788
C	0.63587630	-0.06322977	-0.23542337
O	2.23460554	-0.28300989	1.50952414
C	0.48932542	1.45705148	-0.36752434
O	-0.58359023	-0.69427695	-0.47516252
C	1.16358925	2.36401899	0.45918021
C	-0.36466537	1.95353002	-1.36115717
C	0.99067071	3.73848852	0.29223296
H	1.82174646	1.99993557	1.25015051
C	-0.53546951	3.32603250	-1.52317831
H	-0.89470179	1.25550943	-2.01619148

C	0.14095037	4.22479441	-0.69798766
H	1.52106746	4.43034072	0.95066179
H	-1.20995588	3.69508385	-2.29970428
H	0.00109722	5.30094278	-0.82405180
Cl	-1.04907503	-3.62330160	0.72032245
C	1.71390942	-0.62590916	-1.21006688
H	1.44452827	-0.19098271	-2.19274653
C	3.02263872	-0.04063001	-0.86601942
H	3.08562069	1.03680751	-0.69222630
C	1.71866798	-2.15652115	-1.33469368
H	0.78007790	-2.55787110	-0.92947757
H	1.72610854	-2.41489569	-2.40332617
N	4.14338566	-0.68682566	-0.86347671
C	4.20160082	-2.14245986	-1.09280979
H	4.38438899	-2.31387836	-2.16538172
H	5.06896719	-2.51599293	-0.53510975
C	2.91101092	-2.78808792	-0.63876089
H	2.95994688	-3.86310976	-0.86147588
H	2.82580702	-2.68311601	0.45397080
C	5.35767694	-0.01289278	-0.50855693
C	5.37471307	0.78381612	0.63642234
C	6.49636439	-0.18017126	-1.29616808
C	6.55161800	1.44446567	0.98185959
H	4.47955604	0.85087189	1.25856588
C	7.66608461	0.48427390	-0.93664399
H	6.46713384	-0.80798596	-2.18837820
C	7.69473223	1.29811604	0.19685051
H	6.57550887	2.06692082	1.87869525
H	8.56048312	0.36822928	-1.55215829
H	8.61613980	1.81531278	0.47278303

Cl	-1.11535502	-1.01798435	-3.22767829
H	-0.80844220	-0.83216466	-1.48811842

Int5

Charge = 0 Spin Multiplicity = 6

Fe	-0.02867148	1.22146105	2.74821284
N	-2.07087072	0.60246215	2.27129973
C	-2.59414891	-0.30396303	3.11717571
C	-2.77438027	1.00972141	1.22972585
C	-3.87945930	-0.85734157	2.93815970
C	-1.78551313	-0.71088711	4.22854577
C	-4.06231576	0.51749575	0.96478705
H	-2.30085958	1.74945302	0.58017598
C	-4.61332777	-0.41923467	1.81520037
C	-4.35898067	-1.82406366	3.88077556
C	-2.28584772	-1.65765432	5.14768273
N	-0.55651974	-0.16305971	4.34380299
H	-4.60389336	0.87544509	0.08866997
H	-5.60950039	-0.82673933	1.62939296
C	-3.59433125	-2.20663296	4.94265479
H	-5.35392365	-2.24826932	3.73136745
C	-1.44729644	-2.00920599	6.22733847
C	0.21497443	-0.50517197	5.36273521
H	-3.96718773	-2.94153174	5.65889061
H	-1.79280362	-2.73675692	6.96533664
C	-0.20032891	-1.42850805	6.33573043
H	1.20199595	-0.03707982	5.39713427
H	0.47129284	-1.67721893	7.15822314
Cl	-0.75085588	3.09595044	3.74180493
O	0.15451055	1.73381567	0.88712802

C	0.38737817	0.92566472	-0.09478242
C	0.47918067	-0.58343879	0.29144096
O	0.51336702	1.27333184	-1.25178137
C	-0.75440341	-1.30863467	-0.23719115
O	0.44668744	-0.67712498	1.73270027
C	-1.17073387	-1.14424290	-1.56366920
C	-1.46908009	-2.17789025	0.59283488
C	-2.29341772	-1.81908663	-2.03901467
H	-0.61280286	-0.46970725	-2.21424251
C	-2.59391857	-2.84965702	0.11611997
H	-1.14116426	-2.32192648	1.62230479
C	-3.01349553	-2.67054899	-1.20066566
H	-2.60889877	-1.67507756	-3.07528501
H	-3.14612865	-3.51512542	0.78427672
H	-3.89706415	-3.19372892	-1.57393532
Cl	2.22737808	1.17489480	3.32660065
C	1.77313179	-1.19146977	-0.19649678
C	2.90743498	-0.46124984	-0.07617860
H	2.86945163	0.55747172	0.31625548
C	1.81743216	-2.61062177	-0.68280122
H	1.15180927	-3.24241440	-0.07262457
H	1.41869296	-2.67434040	-1.71138889
N	4.15759902	-0.88779895	-0.44634553
C	4.24461792	-2.14301773	-1.17534714
H	4.06377660	-1.97187572	-2.25262279
H	5.26375094	-2.53745375	-1.07057948
C	3.24121717	-3.14593680	-0.62427993
H	3.32948182	-4.08740513	-1.18556862
H	3.50923396	-3.36566754	0.42242221
C	5.29465699	-0.11891382	-0.18369149

C	5.32729812	0.77250926	0.90505576
C	6.43321731	-0.22088390	-1.00200180
C	6.45779243	1.54738265	1.14623702
H	4.47597355	0.84268068	1.58575205
C	7.56342393	0.54925833	-0.73820853
H	6.43083229	-0.88864107	-1.86453852
C	7.58611400	1.44336398	0.33162781
H	6.45881393	2.23012606	1.99981012
H	8.43427363	0.45443624	-1.39181079
H	8.47316754	2.04819569	0.53130036
H	1.35898756	-0.83691476	2.02795566

Int6'

Charge = 0 Spin Multiplicity = 6

Fe	0.90274510	-1.08175578	3.93812654
N	2.27011617	-2.81909696	4.01961051
C	2.56219296	-3.23265359	5.26712190
C	2.77969327	-3.45656563	2.98287719
C	3.40003781	-4.34060959	5.52284910
C	1.99278070	-2.50123702	6.36349017
C	3.62433104	-4.56955553	3.13407030
H	2.52736609	-3.06459099	1.99569432
C	3.93380337	-5.01395693	4.40310893
C	3.66467671	-4.72004419	6.87954082
C	2.27148114	-2.89646220	7.69044536
N	1.20363733	-1.44741565	6.07450758
H	4.02335935	-5.06486383	2.24783533
H	4.58723577	-5.87662115	4.55237770
C	3.12257421	-4.02688253	7.92018907
H	4.31313582	-5.57935459	7.06295738

C	1.68351455	-2.13734509	8.72491171
C	0.66148512	-0.74660899	7.05423259
H	3.32938189	-4.32153230	8.95118623
H	1.87104173	-2.40779073	9.76664352
C	0.87913661	-1.06271582	8.40543963
H	0.03184795	0.09344206	6.74806626
H	0.41026785	-0.45579401	9.18106586
Cl	-0.78328680	-2.70505701	4.05623976
O	0.78502354	-1.12804226	1.92718439
C	1.53711876	-0.75195744	0.97960536
C	0.81381286	-0.00267263	-0.15130829
O	2.75202228	-0.92589462	0.87079121
C	0.83174603	1.49943531	0.13577147
O	-0.50128506	-0.45947619	-0.26101410
C	1.58953994	2.07323984	1.16035198
C	0.02735919	2.32389854	-0.66160415
C	1.55223507	3.45328939	1.37209285
H	2.19495837	1.45344103	1.82819814
C	-0.00391097	3.69914863	-0.45253788
H	-0.59123596	1.87573192	-1.44311986
C	0.76317887	4.26957906	0.56601774
H	2.14210797	3.88632002	2.18360476
H	-0.63438943	4.33014479	-1.08368347
H	0.73714818	5.34893618	0.73384004
Cl	-0.47162090	0.74069817	4.26324738
C	1.58889800	-0.32417558	-1.45826210
H	1.27858757	0.44013910	-2.19400122
C	3.02176217	-0.03422024	-1.21036593
H	3.28187455	0.90951161	-0.72475752
C	1.32392033	-1.72335155	-2.03451144

H	0.44065475	-2.14186270	-1.53450788
H	1.06124111	-1.62295644	-3.09794318
N	4.00694482	-0.71066071	-1.71785077
C	3.77596321	-1.98027074	-2.42946448
H	3.69620792	-1.76832340	-3.50766864
H	4.66552661	-2.60203761	-2.27098881
C	2.52331420	-2.64705612	-1.90119698
H	2.35641046	-3.57627533	-2.46382838
H	2.68834216	-2.92415454	-0.84881761
C	5.35690745	-0.32112660	-1.44345487
C	5.70933543	0.04553716	-0.14299363
C	6.29941007	-0.33276145	-2.47225373
C	7.02306969	0.42945377	0.11838701
H	4.96536307	-0.00273601	0.65524766
C	7.60933237	0.04920124	-2.19447896
H	6.01080687	-0.62256314	-3.48419028
C	7.97216381	0.43427789	-0.90314194
H	7.30653710	0.71402686	1.13391119
H	8.34998435	0.05123413	-2.99691216
H	9.00119980	0.73281200	-0.69182199
Cl	2.90650766	0.16830945	4.00089433
H	-0.73181688	-0.75386579	0.63717164

Int6

Charge = 0 Spin Multiplicity = 6

Fe	0.64293829	-0.95793274	-0.57799131
N	2.56760349	0.11149253	-0.63193197
C	3.54037675	-0.45069720	0.11080103
C	2.80214586	1.23876538	-1.27572242
C	4.81917140	0.13454692	0.24670232

C	3.25358087	-1.69889541	0.76535758
C	4.04149357	1.89672394	-1.20475776
H	1.97790431	1.63851104	-1.87026912
C	5.04818489	1.34820222	-0.43756682
C	5.80825752	-0.52094443	1.05111399
C	4.25295454	-2.32756621	1.54190333
N	2.02912597	-2.23267322	0.59756328
H	4.18526781	2.83115944	-1.74821441
H	6.02185601	1.83715142	-0.35638628
C	5.53648992	-1.70277409	1.67300845
H	6.79028468	-0.05391761	1.15161557
C	3.91764792	-3.55729227	2.14847986
C	1.73154687	-3.38359931	1.16915896
H	6.29676951	-2.19797162	2.28089545
H	4.65979739	-4.07777285	2.75823063
C	2.65709047	-4.08618526	1.96009382
H	0.71800233	-3.75730214	0.99572780
H	2.36772956	-5.03508350	2.41392980
Cl	1.46485014	-2.21132211	-2.41530757
O	-0.17360266	0.38118441	-1.85134255
C	-1.00265801	1.33957550	-1.71452987
C	-1.03635381	2.00349217	-0.35142136
O	-1.71986456	1.80601145	-2.58928875
C	0.06523671	2.95938768	-0.14107831
O	0.32516653	-0.06041661	1.05624591
C	0.29616662	3.94462036	-1.11530986
C	0.92379034	2.87024253	0.96541369
C	1.34405873	4.84911917	-0.96292904
H	-0.35975118	3.99912307	-1.98709672
C	1.97771688	3.76862341	1.10163180

H	0.79564887	2.02985407	1.64964863
C	2.18596878	4.76458131	0.14630581
H	1.50728229	5.61966147	-1.71978698
H	2.65511692	3.67878396	1.95414471
H	3.01507044	5.46716240	0.25856309
Cl	-1.27734887	-2.31629946	-0.20289409
C	-2.06214912	1.79326857	0.53310436
C	-3.07862389	0.88032577	0.14174224
H	-2.99843846	0.35271086	-0.81079798
C	-2.21365003	2.49990987	1.85342509
H	-1.23366509	2.67894353	2.30944944
H	-2.66471839	3.49239593	1.67994279
N	-4.16394376	0.63888095	0.83913091
C	-4.40215255	1.32084512	2.12061498
H	-5.00841542	2.21996200	1.92619630
H	-4.99627776	0.64078532	2.74362385
C	-3.09230001	1.68428600	2.78692370
H	-3.31270333	2.24379429	3.70631272
H	-2.56991069	0.76065893	3.08526532
C	-5.15373826	-0.27630537	0.36809011
C	-4.76245954	-1.46421698	-0.25392402
C	-6.50689873	0.02778748	0.54223823
C	-5.73839645	-2.33973823	-0.72314411
H	-3.70191920	-1.71919687	-0.34014263
C	-7.47069637	-0.85963778	0.07113169
H	-6.81235962	0.95877819	1.02156233
C	-7.09144607	-2.04198220	-0.56454816
H	-5.43209006	-3.27149975	-1.20355095
H	-8.52807873	-0.61819159	0.19815324
H	-7.85217869	-2.73487496	-0.93033980

H	-0.45934787	-0.47145792	1.44266405

Int7'

Charge = 0 Spin Multiplicity = 1

O	-1.69317570	-1.32443912	2.44630042
C	-1.17703771	-0.94857215	1.42671772
C	-1.83175148	-0.97798663	0.04921426
O	0.04901500	-0.45740815	1.34094076
C	-2.60697167	0.31969020	-0.18313117
O	-2.65802525	-2.09376170	-0.06184026
C	-2.27793675	1.52577385	0.44452424
C	-3.67293506	0.29497983	-1.08923167
C	-2.99566093	2.68869523	0.16165564
H	-1.46483011	1.57270433	1.17344476
C	-4.38738505	1.45635467	-1.37210638
H	-3.94198511	-0.65123365	-1.56230422
C	-4.04933605	2.65887881	-0.74934562
H	-2.72939711	3.62153541	0.66407018
H	-5.21710971	1.42156623	-2.08235463
H	-4.61147916	3.56944404	-0.96929625
C	-0.60236145	-1.05091662	-0.88831335
H	-0.81378274	-0.49638602	-1.81174072
C	0.44401197	-0.26501422	-0.08049093
H	0.33400322	0.81035573	-0.26642788
C	-0.15089037	-2.47331370	-1.23051894
H	-1.01872934	-3.14385629	-1.18846602
H	0.21774455	-2.48506531	-2.26810810
N	1.78365651	-0.62449288	-0.26946984
C	2.15856110	-2.02488136	-0.43981363
H	2.61425405	-2.17196228	-1.43560131

H	2.92840464	-2.28301395	0.30632214
C	0.96207001	-2.94739734	-0.31379744
H	1.27822703	-3.96554176	-0.58366861
H	0.62012353	-2.99401011	0.73291870
C	2.79247071	0.31423633	-0.03970315
C	2.54216068	1.52685195	0.63121918
C	4.10662066	0.05968635	-0.47510038
C	3.55990979	2.45792086	0.81908445
H	1.55542038	1.73803945	1.04431200
C	5.11729073	0.99592264	-0.27131980
H	4.34274168	-0.86888866	-0.99467259
C	4.85575814	2.20600158	0.36952878
H	3.33334833	3.38889658	1.34498305
H	6.12579723	0.77145211	-0.62803182
H	5.65152022	2.93713703	0.52631151
H	-3.11254803	-2.18458509	0.78938004

Int7

Charge = 0 Spin Multiplicity = 6

Fe	-0.78617962	-0.80580535	1.46382627
N	-2.42364004	0.08329204	0.34524491
C	-3.09793223	-0.76217855	-0.45569488
C	-2.78052281	1.35141194	0.41013371
C	-4.18403984	-0.34639838	-1.25328311
C	-2.68995476	-2.13646107	-0.46120574
C	-3.85412655	1.85975354	-0.33920640
H	-2.19546570	1.98528196	1.07929039
C	-4.55112580	1.01442998	-1.17648484
C	-4.85319155	-1.30947972	-2.07628763
C	-3.37667965	-3.06821484	-1.26978906

N	-1.65533964	-2.48796871	0.33128862
H	-4.11192707	2.91608657	-0.25477661
H	-5.38648381	1.38261754	-1.77648682
C	-4.46545447	-2.61658687	-2.08497322
H	-5.68776645	-0.97507531	-2.69606825
C	-2.94072806	-4.40953969	-1.21589200
C	-1.26373169	-3.75014132	0.37258698
H	-4.98372620	-3.34583365	-2.71101124
H	-3.44281614	-5.16483851	-1.82480818
C	-1.88772591	-4.74987188	-0.39151551
H	-0.41888997	-3.96920712	1.03117960
H	-1.52924379	-5.77779432	-0.32507507
Cl	-2.24238126	-1.19043788	3.16826981
O	-0.18399751	0.97415804	1.95636963
C	0.92086347	1.63160299	1.86372939
C	1.02004024	2.46976236	0.60293786
O	1.81075151	1.66146896	2.69224633
C	0.08034392	3.60137638	0.56084036
O	0.28741067	-0.56588295	-0.37826075
C	-0.01943615	4.44846580	1.67691645
C	-0.77010887	3.80496627	-0.53845151
C	-0.92159284	5.50817971	1.67577967
H	0.62743612	4.27987301	2.54148698
C	-1.68135296	4.85801240	-0.52328692
H	-0.75743353	3.08852396	-1.36856202
C	-1.75334434	5.71664447	0.57452487
H	-0.98034139	6.17072723	2.54216415
H	-2.35101469	5.00158394	-1.37479080
H	-2.46770945	6.54328184	0.57783940
Cl	1.00825487	-2.07979187	2.18002445

C	1.91102953	2.16191055	-0.38789207
C	2.69744063	0.98153924	-0.20907206
H	2.61922339	0.41721108	0.72111092
C	2.16027851	2.96756537	-1.63278749
H	1.27372434	3.54292296	-1.91515266
H	2.96049146	3.69821689	-1.41758501
N	3.55231901	0.52249725	-1.08593840
C	3.77735306	1.21046414	-2.36903883
H	4.67999787	1.83300825	-2.26268917
H	3.98976891	0.43445052	-3.11534470
C	2.57856709	2.04362807	-2.76376674
H	2.84214252	2.61798875	-3.66285671
H	1.72486655	1.39227772	-3.01500875
C	3.70202662	-1.71005793	-0.09697216
C	5.59263830	-0.80143329	-1.31727429
C	4.43251071	-2.86554766	0.16187558
H	2.67695565	-1.63191963	0.27069656
C	6.30990357	-1.96590299	-1.05521753
H	6.06003130	0.00632987	-1.88089838
C	5.73590778	-2.99951487	-0.31544744
H	3.96492094	-3.66885575	0.73532391
H	7.33117471	-2.05946868	-1.43020409
H	6.30379850	-3.91044073	-0.11491215
H	0.49796507	-1.41261395	-0.79272297
H	-0.11933867	-0.00036879	-1.13072930
Cl	-0.83031704	0.90062471	-2.60732305
C	4.28922072	-0.67487312	-0.82873474

Int8'

Charge = 0 Spin Multiplicity = 1

O	-1.70451601	-1.22215751	2.64257346
C	-1.19901225	-0.88920183	1.60398423
C	-1.89959435	-0.87969767	0.24791769
O	0.05078360	-0.48166577	1.46228403
C	-2.55430614	0.47612890	-0.00291967
O	-2.84039127	-1.91939930	0.20412832
C	-2.27643116	1.60355508	0.77573066
C	-3.45377594	0.59211212	-1.07045875
C	-2.88312464	2.82769799	0.49028153
H	-1.58455909	1.54336050	1.61964253
C	-4.06007944	1.81278960	-1.35211907
H	-3.68385652	-0.28108882	-1.68481661
C	-3.77556518	2.93582722	-0.57309292
H	-2.65635236	3.69856936	1.10937548
H	-4.76050091	1.88765010	-2.18719687
H	-4.25201004	3.89346182	-0.79512602
C	-0.71114182	-1.10835587	-0.70921547
H	-0.91496261	-0.62635818	-1.67429925
C	0.37710813	-0.30427859	0.01586552
H	0.24472694	0.76783515	-0.17750666
C	-0.32658912	-2.58036749	-0.92568976
H	-1.17507265	-3.22909578	-0.67497208
H	-0.12837056	-2.72992201	-1.99771967
N	1.70251506	-0.65802894	-0.24323107
C	2.06470580	-2.05383964	-0.46115943
H	2.37132907	-2.20992243	-1.51180938
H	2.93666334	-2.29519384	0.16771491
C	0.90937575	-2.97959502	-0.13751433
H	1.20250384	-4.00881272	-0.39045370
H	0.70971573	-2.96568639	0.94571845

C	2.71482835	0.29504303	-0.10809815
C	2.50375552	1.50602535	0.57837888
C	3.98750995	0.05765703	-0.65895956
C	3.51999315	2.45254774	0.67423531
H	1.55210955	1.70271487	1.07379191
C	4.99832568	1.00902969	-0.54531055
H	4.18834175	-0.86807905	-1.19847122
C	4.77533384	2.21692409	0.11404028
H	3.32671982	3.38255125	1.21487103
H	5.97477810	0.79919488	-0.98932772
H	5.57080977	2.96015187	0.19894042
H	-3.42069923	-2.54862369	-1.24196636
H	-3.32178885	-1.93083664	1.04662569
Cl	-3.70424805	-2.96703881	-2.46452359

Int8

Charge = 1 Spin Multiplicity = 6

Fe	-0.39962972	-1.26809335	0.72971514
N	-2.22765680	-0.16133765	1.14436192
C	-3.20047274	-0.31266421	0.22647811
C	-2.43811896	0.60410298	2.20331625
C	-4.44903455	0.33419474	0.32423973
C	-2.91885368	-1.17161970	-0.88236481
C	-3.65445848	1.27688906	2.39792107
H	-1.61222428	0.69606662	2.91230271
C	-4.65723170	1.14883534	1.45730599
C	-5.41469226	0.13724091	-0.71569264
C	-3.89042883	-1.35995657	-1.88572722
N	-1.70666460	-1.76757257	-0.91558239
H	-3.78588592	1.89801028	3.28446616

H	-5.60836222	1.67182049	1.57887239
C	-5.14512220	-0.67483115	-1.77737415
H	-6.37447890	0.65182028	-0.63954612
C	-3.55179385	-2.22292134	-2.94997079
C	-1.40696351	-2.57393717	-1.92310319
H	-5.88594586	-0.82137751	-2.56575364
H	-4.27147755	-2.40073780	-3.75212948
C	-2.31305287	-2.83165406	-2.96330457
H	-0.40890650	-3.01723077	-1.90977137
H	-2.02113514	-3.50467207	-3.77009673
Cl	-0.76228327	-2.89513020	2.16489058
O	0.44346630	0.18880887	1.68661116
C	0.69593668	1.42541788	1.41266234
C	0.86552311	1.73640022	-0.05948925
O	0.76757577	2.32274321	2.22721282
C	-0.39559607	2.08684818	-0.72938736
C	-1.31083722	2.96288576	-0.12029710
C	-0.76451035	1.43357428	-1.91895516
C	-2.54843569	3.20244644	-0.70784092
H	-1.03830941	3.45494288	0.81534654
C	-2.01150115	1.66394700	-2.49150827
H	-0.09070750	0.69694279	-2.36085939
C	-2.90307560	2.55370772	-1.89234876
H	-3.24806727	3.89179050	-0.23061424
H	-2.29308040	1.13298993	-3.40337841
H	-3.88273937	2.73113385	-2.34122688
Cl	1.43821553	-1.77489833	-0.53491408
C	2.08079536	1.60776772	-0.67216040
C	3.11108718	0.96382572	0.08076119
H	2.92995137	0.66962057	1.11699077

C	2.42548587	2.04158049	-2.06946609
H	1.53385834	2.11658296	-2.70023588
H	2.85394081	3.05774329	-2.01413537
N	4.28607897	0.65194165	-0.39584126
C	4.66983467	0.99008191	-1.77765417
H	5.22271293	1.94227263	-1.75450653
H	5.35806038	0.20719384	-2.11927003
C	3.44795618	1.08760420	-2.66712910
H	3.76926819	1.42774457	-3.66089062
H	3.00366529	0.08627557	-2.78556135
C	4.76009611	-1.16954978	1.15749290
C	6.56344826	0.27521007	0.39858096
C	5.66713992	-1.87783628	1.94138156
H	3.71271293	-1.47592985	1.10063635
C	7.45857378	-0.44441765	1.18498072
H	6.91100856	1.12370448	-0.19257935
C	7.01393428	-1.51684705	1.95902809
H	5.31703323	-2.72850549	2.52962493
H	8.51224351	-0.15831865	1.19589725
H	7.72231055	-2.07802417	2.57197720
C	5.21480835	-0.08705449	0.40066627

Int9'

Charge = 1 Spin Multiplicity = 1

O	-0.95745679	0.88976343	3.00426501
C	-0.59810086	0.58439821	1.90061534
C	-1.45777456	0.23344940	0.70269485
O	0.66754531	0.47809073	1.52944223
C	-2.81797477	0.49348756	0.58199195
C	-3.54571294	1.12144382	1.64642568

C	-3.51648362	0.11556506	-0.61229055
C	-4.89972027	1.34012035	1.51679290
H	-3.01133183	1.40628888	2.55198472
C	-4.86803753	0.34012330	-0.72104089
H	-2.97644741	-0.35101324	-1.43674272
C	-5.55768351	0.95200467	0.34102075
H	-5.45942436	1.81509582	2.32350976
H	-5.40445160	0.05207090	-1.62590399
H	-6.63114185	1.13258461	0.24462595
C	-0.58136836	-0.42623392	-0.27473307
H	-0.82928685	-0.14238997	-1.30561697
C	0.81509217	0.10344131	0.10461420
H	1.00226580	1.04723787	-0.42184067
C	-0.67875134	-1.98288956	-0.14498095
H	-1.68013260	-2.26690655	0.20597886
H	-0.56577563	-2.38814606	-1.16130967
N	1.89201271	-0.75554307	-0.08608464
C	1.77462569	-2.18310705	0.19871494
H	1.94254488	-2.76056296	-0.72640081
H	2.56466015	-2.47269665	0.90996769
C	0.40862783	-2.53308867	0.75292203
H	0.32085800	-3.62796724	0.80318028
H	0.30120525	-2.16616886	1.78577181
C	3.16025987	-0.22446809	-0.35873297
C	3.46042370	1.12787242	-0.11341258
C	4.17259355	-1.05071619	-0.87722957
C	4.71874082	1.63873184	-0.41901637
H	2.72556650	1.78470459	0.35371871
C	5.43006057	-0.52875936	-1.16780970
H	3.97801737	-2.10493593	-1.07322167

C	5.71346646	0.81906285	-0.95063997
H	4.92544046	2.69252491	-0.21723059
H	6.19677394	-1.19112809	-1.57700291
H	6.70115471	1.22324732	-1.18153238

Int9

Charge = 0 Spin Multiplicity = 6

Fe	-0.63379630	-0.69672931	1.24715509
N	-2.45211175	0.18266939	0.40009138
C	-3.24194621	-0.68835324	-0.25532505
C	-2.80974863	1.44785854	0.50460947
C	-4.45476599	-0.29927523	-0.86367658
C	-2.81717339	-2.05823953	-0.31548607
C	-3.99990396	1.93160717	-0.06580606
H	-2.12911782	2.09841394	1.05881076
C	-4.82022576	1.06050660	-0.75311709
C	-5.24029077	-1.28489384	-1.54660772
C	-3.61223225	-3.00887762	-0.99219686
N	-1.65865393	-2.38468445	0.29078448
H	-4.25347752	2.98718887	0.03960849
H	-5.75026581	1.40784599	-1.20899267
C	-4.83524075	-2.58513538	-1.60887333
H	-6.17496037	-0.97206443	-2.01682963
C	-3.14145331	-4.33952446	-1.01600972
C	-1.23222632	-3.63347983	0.26061026
H	-5.44027464	-3.33007194	-2.12988405
H	-3.72288602	-5.10903686	-1.52911200
C	-1.95201008	-4.65040259	-0.38900172
H	-0.28445926	-3.82953505	0.76980340
H	-1.56175937	-5.66900314	-0.38893052

Cl	-1.99146647	-1.14367659	3.09444173
O	-0.07357988	1.07024309	1.87436161
C	1.03219897	1.72316507	1.82626479
C	1.21330857	2.52921209	0.55477188
O	1.87710348	1.78061785	2.70129081
C	0.18960586	3.56481080	0.34760997
C	-0.13071223	4.46308674	1.37651654
C	-0.56034636	3.58505506	-0.83915296
C	-1.15491357	5.39024148	1.20450304
H	0.43432808	4.43572094	2.31149337
C	-1.59176545	4.50554269	-1.00117984
H	-0.36312706	2.83569507	-1.60865136
C	-1.88600494	5.41485468	0.01564325
H	-1.38879028	6.09370679	2.00661010
H	-2.17939981	4.50234144	-1.92193440
H	-2.69535888	6.13705657	-0.11356536
Cl	1.19257178	-1.93152510	1.96858536
C	2.21217993	2.25042759	-0.33310993
C	2.93903197	1.03218899	-0.13759809
H	2.72965900	0.39849560	0.72820263
C	2.57034719	3.08066675	-1.53526280
H	1.72127144	3.68786706	-1.86665500
H	3.36250373	3.79046849	-1.23768258
N	3.85190519	0.58831012	-0.96133388
C	4.23424458	1.33944301	-2.16864678
H	5.11107517	1.96038960	-1.92569362
H	4.54051248	0.60221087	-2.92099568
C	3.07964505	2.18883584	-2.65496366
H	3.42072965	2.78592184	-3.51163757
H	2.26983817	1.53000855	-3.00763734

C	4.45765570	-0.68965393	-0.75203478
C	3.65276376	-1.77471689	-0.40457999
C	5.83771273	-0.83399930	-0.91444702
C	4.24793893	-3.01494951	-0.18624929
H	2.57064426	-1.64988260	-0.31555105
C	6.41597712	-2.08214815	-0.70190405
H	6.45923547	0.02177923	-1.18303948
C	5.62509734	-3.17244041	-0.33424590
H	3.62060424	-3.86337483	0.09545384
H	7.49551383	-2.20008833	-0.81653126
H	6.08613971	-4.14827752	-0.16665629
Cl	0.25297757	-0.37869908	-0.97949947

Fe(phen)Cl_3

Charge = 0 Spin Multiplicity = 6

Fe	-1.59224477	-0.08022418	-0.14549318
N	0.20808060	-1.33816992	0.02265042
C	1.37305818	-0.66274121	0.04123513
C	0.22222078	-2.65899115	-0.03475357
C	2.62940258	-1.30495736	0.02050872
C	1.29891459	0.76696537	0.08322807
C	1.42100912	-3.38951320	-0.07015821
H	-0.75336133	-3.15101270	-0.04315183
C	2.62476636	-2.71516735	-0.03865183
C	3.81993386	-0.50831138	0.05857941
C	2.48650994	1.52800062	0.12004936
N	0.06922439	1.32667792	0.08278456
H	1.38312311	-4.47840804	-0.11847457
H	3.57203325	-3.25859580	-0.06008033
C	3.75064384	0.85206353	0.10936604

H	4.78709711	-1.01495933	0.04616593
C	2.34750317	2.93178273	0.16360168
C	-0.03827037	2.64622002	0.11977530
H	4.66170438	1.45308660	0.13963067
H	3.23839932	3.56294788	0.19561732
C	1.08485644	3.48747076	0.16355740
H	-1.05620636	3.04306222	0.11632935
H	0.94119246	4.56803774	0.19603203
Cl	-2.78058443	-1.74115997	0.82104353
Cl	-3.08226772	1.59245070	0.24801480
Cl	-1.60517092	-0.32094100	-2.35664268

Fe(phen)Cl_3 (S=4)

Charge = 0 Spin Multiplicity = 4

Fe	1.34323038	-0.02924770	-0.09473967
N	-0.22727439	-1.31121117	-0.18610164
C	-1.41968337	-0.67327287	-0.13520809
C	-0.19168451	-2.63344942	-0.16550018
C	-2.64939328	-1.35707452	-0.07511757
C	-1.38986445	0.75136947	-0.14048545
C	-1.36649635	-3.39966101	-0.10159810
H	0.80151240	-3.08648649	-0.21279843
C	-2.59322557	-2.76783773	-0.05957858
C	-3.86116905	-0.59213841	-0.03033800
C	-2.59054688	1.48538639	-0.08860285
N	-0.17087476	1.33746284	-0.19238774
H	-1.29071199	-4.48744183	-0.08889636
H	-3.51846435	-3.34626004	-0.01269161
C	-3.83296472	0.77171101	-0.03729229
H	-4.81250337	-1.12612478	0.01186714

C	-2.47626767	2.89281664	-0.08746901
C	-0.08203020	2.65749591	-0.18465303
H	-4.76144440	1.34493652	-0.00112203
H	-3.37691152	3.50936924	-0.04805185
C	-1.22441796	3.47267329	-0.13336565
H	0.92965111	3.06879475	-0.22565910
H	-1.10367474	4.55647730	-0.13173378
Cl	2.73249489	-1.60738157	-0.84381159
Cl	2.86402522	1.52520176	-0.58235284
Cl	1.38591454	-0.10875259	2.17599030

Fe(phen)Cl_3 (S=6, bipyramid)

Fe	-1.52649200	-0.02258400	-0.01184800
N	0.27349000	-1.29271200	-0.04723800
C	1.44826200	-0.64036600	-0.03462900
C	0.25690600	-2.61361600	-0.03099700
C	2.69250800	-1.30576500	-0.01846600
C	1.39518900	0.79090700	-0.03993600
C	1.44046500	-3.36839100	-0.00325100
H	-0.72675800	-3.08906100	-0.04626400
C	2.65821200	-2.71646000	-0.00020800
C	3.89590100	-0.52728600	-0.02251600
C	2.59487500	1.53283200	-0.04651800
N	0.17300200	1.36903600	-0.03775900
H	1.38240900	-4.45736100	0.01226000
H	3.59380500	-3.27995200	0.01618900
C	3.84781700	0.83500700	-0.03946800
H	4.85528500	-1.04858800	-0.01353700
C	2.47858900	2.93923100	-0.05945600
C	0.08778700	2.69148800	-0.04675300

H	4.76852500	1.42188000	-0.04571900
H	3.37937700	3.55696800	-0.06901400
C	1.22465700	3.51472000	-0.05983300
H	-0.92330900	3.10509000	-0.04537300
H	1.09811700	4.59784600	-0.07002800
Cl	-2.01030100	-0.87841600	1.99642300
Cl	-2.98058100	1.72109700	-0.11002800
Cl	-2.36153800	-1.28666300	-1.67600200

2

Charge = 0 Spin Multiplicity = 1

O	-1.14434602	1.67754465	1.55156074
C	-2.25516031	1.45675323	0.87001012
C	-2.09184719	0.26779573	-0.09021809
O	-3.25014151	2.13179317	0.93979844
C	-3.26164730	-0.59574705	-0.36597714
O	-1.01423157	0.11511036	-0.62235973
C	-4.45650078	-0.53302858	0.36776152
C	-3.12793120	-1.54555347	-1.39162305
C	-5.49876426	-1.40762100	0.07182672
H	-4.57376276	0.20058252	1.16515129
C	-4.17306821	-2.41005229	-1.68839147
H	-2.18799920	-1.58490636	-1.94566391
C	-5.36094552	-2.34152110	-0.95509464
H	-6.42642316	-1.35849934	0.64601450
H	-4.06595152	-3.14248161	-2.49147612
H	-6.18381281	-3.02227729	-1.18607548
H	-1.28130457	2.46452479	2.10579183

42

Charge = 1 Spin Multiplicity = 1

C	-2.72598838	1.23037014	-0.48360564
H	-2.95099633	2.01417388	0.26639769
C	-1.26039370	1.09761454	-0.47035653
H	-0.64385438	1.93761831	-0.80712425
C	-3.47333106	-0.06368823	-0.20479935
H	-4.49930783	0.16120652	0.11551502
H	-3.54881137	-0.65235188	-1.13283575
N	-0.62489976	0.04696485	-0.07518232
C	-1.32051834	-1.16819702	0.40343842
H	-1.30759076	-1.89505266	-0.42307356
H	-0.70691491	-1.57455842	1.21738675
C	-2.73335698	-0.86503791	0.85341768
H	-3.23728056	-1.81981552	1.05804082
H	-2.70315527	-0.30633291	1.80309526
C	0.81263356	0.02231618	-0.06101045
C	1.50655847	1.06262572	0.55551629
C	1.48261250	-1.04836772	-0.65287978
C	2.89926474	1.03742862	0.56001483
H	0.96385790	1.87291244	1.04672410
C	2.87458994	-1.06038139	-0.63954764
H	0.92936392	-1.85445120	-1.13684786
C	3.58324094	-0.02057998	-0.03673691
H	3.44927638	1.84662066	1.04431804
H	3.40773488	-1.88874577	-1.11015844
H	4.67499103	-0.03843158	-0.02808396
H	-3.00270100	1.69297014	-1.44543546

43

Charge = 0 Spin Multiplicity = 1

C	-2.65891811	1.23468645	-0.37214010
H	-3.12719144	2.18008625	-0.65524224
C	-1.31471076	1.16940852	-0.36670861
H	-0.71390163	2.04207345	-0.62852467
C	-3.51510881	0.06069202	-0.00959429
H	-4.34536353	0.37636470	0.64435834
H	-3.99643977	-0.35851625	-0.91311641
N	-0.59342389	0.01414334	-0.10235668
C	-1.34860495	-1.22486400	-0.02524145
H	-1.52351549	-1.63266950	-1.03939314
H	-0.75372499	-1.96483016	0.52637261
C	-2.67746693	-1.00465453	0.68639891
H	-3.21659171	-1.96194668	0.74290746
H	-2.46739745	-0.69059009	1.72231950
C	0.79587371	0.01402166	-0.04208735
C	1.51141567	1.17796362	0.30559352
C	1.53307099	-1.15281875	-0.32531556
C	2.90190836	1.17117889	0.35126208
H	0.97490644	2.08993899	0.57128290
C	2.92418689	-1.14857921	-0.26089846
H	1.01877798	-2.06783592	-0.62105690
C	3.62470301	0.01032688	0.07205628
H	3.42652549	2.08918598	0.62891486
H	3.46674520	-2.06959828	-0.48979456
H	4.71576671	0.00889962	0.11686594

1'

Charge = 1 Spin Multiplicity = 1

C	-2.69738110	-0.22746035	1.24453352
H	-2.82606669	-1.32223208	1.29879878

C	-1.22120167	0.11189639	1.25271821
H	-0.68373220	-0.35662952	2.08714182
C	-3.39539863	0.32634066	0.00943791
H	-4.45083418	0.01854631	-0.00020089
H	-3.38481482	1.42909233	0.04235739
N	-0.55477284	-0.36685792	-0.01090985
C	-1.22092310	0.19023390	-1.24198585
H	-1.05835196	1.27654018	-1.21858673
H	-0.68117454	-0.22290506	-2.10358094
C	-2.69611219	-0.15253388	-1.25582144
H	-3.13361313	0.30840357	-2.15353712
H	-2.82178077	-1.24261507	-1.37409706
C	0.89670207	-0.15624399	-0.00467824
C	1.72546289	-1.27231510	-0.03720247
C	1.41092435	1.13658683	0.03273371
C	3.10697793	-1.08845321	-0.03195865
H	1.30106188	-2.27928441	-0.06601743
C	2.79327919	1.30651689	0.03717767
H	0.75628899	2.00944404	0.05814161
C	3.64026738	0.19861306	0.00501312
H	3.76513613	-1.95893257	-0.05696256
H	3.20814504	2.31579631	0.06602192
H	4.72287679	0.34048729	0.00885636
H	-3.13437696	0.18101742	2.16755247
H	-1.05528317	1.19681878	1.29832700
H	-0.69265470	-1.38416478	-0.04356527

1·HCl

Charge = 0 Spin Multiplicity = 1

C	2.68083988	-0.20378674	-1.24220601

H	2.77440332	-1.30155428	-1.26854332
C	1.20522321	0.14746967	-1.24343427
H	0.67154395	-0.32546259	-2.07871014
C	3.38197633	0.34515896	-0.00631837
H	4.43790669	0.03591557	0.00107276
H	3.37390441	1.44915163	-0.03165360
N	0.54819552	-0.33532804	0.00848743
C	1.20454285	0.20440425	1.23733806
H	1.04831740	1.29384817	1.25021443
H	0.67034595	-0.22968724	2.09311752
C	2.68013989	-0.14653064	1.25306043
H	3.12526622	0.29101196	2.15909114
H	2.77367764	-1.24193461	1.32975968
C	-0.89567819	-0.12740748	0.00339183
C	-1.72567389	-1.24536518	0.02920012
C	-1.42143797	1.16332515	-0.02661577
C	-3.10812121	-1.06387787	0.02477279
H	-1.27224902	-2.24013876	0.05230157
C	-2.80432846	1.33153335	-0.03074038
H	-0.76862811	2.03823676	-0.04676871
C	-3.64844535	0.22074486	-0.00511273
H	-3.76491433	-1.93629137	0.04491507
H	-3.22292415	2.33984827	-0.05420419
H	-4.73189817	0.35897719	-0.00849013
H	3.12646744	0.19177205	-2.16709498
H	1.04903382	1.23516913	-1.30642791
H	0.72406211	-1.41441797	0.03329932
Cl	1.13767716	-3.23418110	0.07525763

1

Charge = 0 Spin Multiplicity = 1

C	-2.69425797	1.24599518	-0.27698482
H	-2.63567618	1.69425514	0.72979592
C	-1.28487366	1.00233982	-0.79004182
H	-0.71938363	1.94094755	-0.78234630
C	-3.47723457	-0.05704309	-0.21371290
H	-4.48094707	0.10649751	0.20928529
H	-3.62397929	-0.44454002	-1.23815044
N	-0.58364728	0.00149605	0.00150010
C	-1.28536900	-1.26347099	0.09068954
H	-1.31142330	-1.77710397	-0.89582489
H	-0.73974474	-1.92311462	0.77916782
C	-2.70545173	-1.07769390	0.60860126
H	-3.21403081	-2.05460288	0.60867200
H	-2.65499255	-0.73974079	1.65798810
C	0.80823564	0.00000483	-0.00591495
C	1.53258991	1.21079663	0.07007516
C	1.55650007	-1.19444214	-0.05651261
C	2.92181494	1.21916273	0.10152105
H	0.99948973	2.16064463	0.13343498
C	2.95027921	-1.17375163	-0.01392765
H	1.05185570	-2.15625152	-0.14460218
C	3.65029570	0.02771083	0.06261571
H	3.44350128	2.17763712	0.16936050
H	3.49321795	-2.12195203	-0.05591748
H	4.74193998	0.03898922	0.09095810
H	-3.19320162	1.97844314	-0.93096242
H	-1.33481796	0.67131733	-1.85071148

3

Charge = 0 Spin Multiplicity = 1

O	-2.82089014	0.24752173	0.62916931
C	-2.09753995	1.39294092	0.57163162
C	-1.47708985	1.48936790	-0.77233746
O	-2.03418178	2.14534989	1.50613660
C	-0.62156783	2.60910547	-1.17800237
C	-0.89838238	3.91531803	-0.74363549
C	0.49249999	2.39382205	-2.00477139
C	-0.09309324	4.97794736	-1.14556693
H	-1.75170023	4.09273600	-0.08771302
C	1.29571394	3.45898026	-2.40440984
H	0.74437049	1.37820691	-2.31755775
C	1.00354895	4.75507109	-1.97894869
H	-0.32458539	5.98990550	-0.80474278
H	2.16086848	3.27362455	-3.04533394
H	1.63478100	5.59046115	-2.29099863
C	-1.88034162	0.41491407	-1.47972388
C	-2.72515753	-0.45777496	-0.59081163
H	-2.19705935	-1.41084944	-0.36566609
N	-4.02444187	-0.70803675	-1.18122333
C	-3.89667954	-1.20710757	-2.54722474
H	-3.36887925	-2.18403823	-2.58163460
H	-4.91161492	-1.37957725	-2.93168759
C	-4.95470738	-1.39075341	-0.35361249
C	-5.51850169	-0.72421609	0.74679923
C	-5.36473503	-2.70506050	-0.62243683
C	-6.44518049	-1.36409620	1.56370821
H	-5.22673423	0.30651772	0.94549514
C	-6.30801115	-3.33419627	0.19077679
H	-4.94604811	-3.25174435	-1.46808749

C	-6.84884022	-2.67260281	1.29054130
H	-6.87127945	-0.82582031	2.41409856
H	-6.61512166	-4.35743072	-0.03976995
H	-7.58560136	-3.16825887	1.92679730
C	-3.16684729	-0.21939690	-3.43903448
H	-3.11531230	-0.62207559	-4.46123347
H	-3.73743404	0.72193448	-3.47938977
C	-1.75683479	0.06150197	-2.91269371
H	-1.13898685	-0.84855693	-3.01565098
H	-1.26153902	0.86124679	-3.47918509

TS1

Charge = 0 Spin Multiplicity = 6

Fe	-1.28315748	-1.71658742	0.77383324
N	-2.05450096	0.28459847	1.41456086
C	-3.03459444	0.76278904	0.62767282
C	-1.52945139	1.05665367	2.34790102
C	-3.51812762	2.08473776	0.73398906
C	-3.58979382	-0.12930104	-0.34937450
C	-1.94204088	2.38696335	2.53410788
H	-0.74718304	0.61115390	2.96758872
C	-2.92878328	2.90475565	1.71988781
C	-4.55743304	2.52087996	-0.15037575
C	-4.62805440	0.32083316	-1.19291121
N	-3.08538926	-1.37982169	-0.42091617
H	-1.47249549	2.99181436	3.31065154
H	-3.26269523	3.93875370	1.83166133
C	-5.09197806	1.67233902	-1.07345937
H	-4.91613767	3.54874506	-0.06649944
C	-5.15051800	-0.60571539	-2.12065071

C	-3.58616086	-2.23264604	-1.29878656
H	-5.88811825	2.00828058	-1.74100261
H	-5.95656430	-0.30121037	-2.79215782
C	-4.63413036	-1.88402952	-2.16661795
H	-3.12444888	-3.22288227	-1.32348052
H	-5.01575433	-2.62486466	-2.87017941
Cl	-2.20620531	-2.54898512	2.67051926
O	0.47690816	-1.13971157	1.46988733
C	1.08838050	-0.13879940	0.93119948
C	0.36433145	0.34305228	-0.34600733
O	2.08958148	0.39159755	1.37646809
C	0.28582917	1.78337069	-0.68938187
O	-0.54942926	-0.41991165	-0.75053291
C	1.10378778	2.76246291	-0.10351676
C	-0.72543377	2.18125412	-1.57980935
C	0.91030853	4.10724997	-0.40804153
H	1.87041257	2.45682835	0.60753946
C	-0.91215127	3.52485611	-1.88250185
H	-1.36818393	1.41539745	-2.01761293
C	-0.09395153	4.49315455	-1.29674195
H	1.54685689	4.86222480	0.05909334
H	-1.70606563	3.82092335	-2.57209010
H	-0.24296647	5.55021986	-1.52946604
Cl	-0.78073266	-3.67707248	-0.29898832
C	2.00751593	-0.27351493	-1.94841039
H	1.47807719	0.44844251	-2.57008557
C	3.14185167	0.16735190	-1.31520428
H	3.34667247	1.23712328	-1.24073044
C	1.74379933	-1.73000670	-2.13220551
H	0.66600954	-1.93247318	-2.01897167

H	2.01084377	-2.02928532	-3.16226140
N	4.06697982	-0.64469818	-0.76011318
C	3.97245870	-2.08367515	-1.00812673
H	4.52092848	-2.32747367	-1.93550499
H	4.47590652	-2.60202087	-0.18150516
C	2.52766254	-2.54032657	-1.10901092
H	2.51440080	-3.61019350	-1.36146520
H	2.04156239	-2.44965018	-0.12589447
C	5.18562199	-0.12633569	-0.08092988
C	5.09806125	1.08267704	0.62604477
C	6.41027475	-0.81037519	-0.11245037
C	6.21987782	1.60372825	1.26264737
H	4.13401696	1.58184895	0.71625354
C	7.52303733	-0.28413648	0.54009775
H	6.50693749	-1.74620035	-0.66374302
C	7.43976619	0.92681564	1.22548858
H	6.13065531	2.54296006	1.81391008
H	8.46963972	-0.82841026	0.50033588
H	8.31533941	1.33574755	1.73421293

TS2'

Charge = 0 Spin Multiplicity = 6

Fe	1.71416474	1.07419790	0.23905705
N	1.98538138	-1.05416942	0.78488928
C	3.15943839	-1.57374620	0.37789443
C	1.13660085	-1.80787398	1.45719262
C	3.52610003	-2.91342701	0.63492051
C	4.05810857	-0.71476111	-0.33980212
C	1.40905747	-3.15223884	1.76113419
H	0.19842866	-1.34130921	1.76066405

C	2.60312941	-3.70694074	1.34926739
C	4.79308409	-3.39506446	0.16912045
C	5.30113618	-1.21523133	-0.78587337
N	3.67180666	0.55790225	-0.56132957
H	0.67392492	-3.73641684	2.31626144
H	2.84375634	-4.74953015	1.56918517
C	5.64540752	-2.57963725	-0.51322062
H	5.06244502	-4.43335734	0.37386792
C	6.14132438	-0.32256970	-1.48527855
C	4.46975491	1.38121710	-1.21816643
H	6.60923722	-2.95334272	-0.86498862
H	7.11223956	-0.66748009	-1.84833922
C	5.72448325	0.97494376	-1.70066834
H	4.09329076	2.39748119	-1.36289130
H	6.34988886	1.68942130	-2.23738200
Cl	2.75264120	1.46743662	2.28542556
O	-0.12117055	1.23169964	1.14972339
C	-1.26430487	0.80654824	0.88640825
C	-2.46308707	1.72281787	1.14352367
O	-1.55137155	-0.32349068	0.42583759
C	-2.67893219	2.63133740	-0.06596834
O	-2.26551755	2.47443400	2.30221847
C	-2.00820288	2.45854652	-1.27957898
C	-3.58781023	3.68846903	0.07042682
C	-2.25568035	3.32595071	-2.34596017
H	-1.26390254	1.66659798	-1.41028310
C	-3.83418411	4.54914751	-0.99450933
H	-4.09325782	3.83957726	1.02724063
C	-3.16883908	4.36805287	-2.20955888
H	-1.71788718	3.18444704	-3.28649506

H	-4.54639243	5.36929851	-0.87598616
H	-3.35936854	5.04532021	-3.04549561
Cl	1.77024450	3.24053298	-0.52510360
C	-3.64624370	0.73817401	1.31846548
H	-4.57004886	1.26318909	1.02820399
C	-3.42766576	-0.31363296	0.26772077
H	-3.40228302	0.03736210	-0.76733282
C	-3.80337141	0.16185474	2.73522650
H	-3.20082618	0.76049561	3.43017643
H	-4.85230165	0.28046760	3.04490114
N	-3.86275487	-1.55801701	0.41451608
C	-4.15190194	-2.10484544	1.74697005
H	-5.24066818	-2.08847953	1.92142483
H	-3.82963123	-3.15486421	1.74942656
C	-3.42894549	-1.30942278	2.81396671
H	-3.69475752	-1.71762379	3.79952747
H	-2.34339086	-1.44581419	2.69057842
C	-3.85381767	-2.44402960	-0.69799879
C	-2.85293920	-2.34431373	-1.67120937
C	-4.84435312	-3.42498587	-0.80690065
C	-2.86765596	-3.21048734	-2.76275750
H	-2.04513852	-1.61829171	-1.55843513
C	-4.84097226	-4.29106634	-1.89751612
H	-5.62645546	-3.50325033	-0.04993738
C	-3.85825962	-4.18434682	-2.88187314
H	-2.08240829	-3.12997430	-3.51790420
H	-5.62102109	-5.05121118	-1.98044850
H	-3.86074593	-4.86448273	-3.73634966
Cl	0.81422201	0.17594990	-1.75657721
H	-1.34636318	2.78120797	2.27218051

TS2''

Charge = 0 Spin Multiplicity = 6

Fe	-2.19345197	-2.20761440	-0.63785587
N	-2.85932391	-1.38549044	1.30071748
C	-3.75081130	-0.38505104	1.19020090
C	-2.41206894	-1.73788336	2.49119306
C	-4.23486654	0.32808097	2.30802587
C	-4.21105059	-0.05630389	-0.12730493
C	-2.83359323	-1.09142417	3.66469614
H	-1.69132916	-2.55843256	2.51712783
C	-3.74036673	-0.05516012	3.57301869
C	-5.18339854	1.38224721	2.10231318
C	-5.16034720	0.97201676	-0.29933854
N	-3.71198353	-0.76540622	-1.16028490
H	-2.43194024	-1.40914819	4.62740213
H	-4.07945064	0.47244777	4.46742288
C	-5.62965965	1.68780414	0.85047909
H	-5.54762118	1.93391749	2.97151647
C	-5.59609803	1.22941493	-1.61640360
C	-4.11749498	-0.49700093	-2.38882671
H	-6.35817076	2.48772443	0.70224758
H	-6.33548100	2.01318851	-1.79689149
C	-5.07883318	0.48970891	-2.65827621
H	-3.65704290	-1.08674710	-3.18525488
H	-5.39086522	0.66595761	-3.68834327
Cl	-3.61754249	-3.94392237	-0.29499176
O	-0.61069046	-2.90501857	0.28909996
C	0.47105166	-2.22729260	0.39530065
C	0.32584437	-0.68323841	0.15301602

O	1.55400841	-2.70845357	0.69435032
C	0.20506320	0.00993862	1.51300573
O	-0.87583822	-0.55314848	-0.55077298
C	0.93652989	-0.39437008	2.63561604
C	-0.68415246	1.08624415	1.63831877
C	0.80140293	0.27873252	3.85114014
H	1.59999810	-1.25891633	2.57261838
C	-0.82713958	1.74607585	2.85608449
H	-1.26169086	1.41734308	0.77123132
C	-0.07975054	1.35142776	3.96691661
H	1.38346782	-0.04996238	4.71525563
H	-1.52970046	2.57944321	2.93525148
H	-0.19195241	1.87193945	4.92072748
Cl	-1.57627293	-2.62633544	-2.82074051
C	1.54820458	-0.18791976	-0.68423793
H	1.93439827	1.22569513	-0.33052245
C	2.75413841	-0.73599136	-0.20234193
H	2.92150684	-0.79212224	0.87136526
C	1.36890330	-0.23781268	-2.20185361
H	0.31499213	-0.41639154	-2.44424604
H	1.62217053	0.73734831	-2.64715036
N	3.78897994	-1.11309297	-0.94361503
C	3.68468370	-1.15312949	-2.40511583
H	4.10876024	-0.22649240	-2.82803158
H	4.30342630	-1.99019350	-2.75512663
C	2.23870755	-1.31849751	-2.82375038
H	2.18428432	-1.28590931	-3.92148442
H	1.87785768	-2.31134536	-2.50917283
C	4.98296972	-1.58391875	-0.32936106
C	4.90946737	-2.35579764	0.83495691

C	6.22478493	-1.28160135	-0.89625304
C	6.08231330	-2.79110072	1.44643121
H	3.93220211	-2.63951848	1.23083545
C	7.39049969	-1.73151367	-0.28011448
H	6.28635129	-0.68405408	-1.80721086
C	7.32534522	-2.47879861	0.89545465
H	6.02030811	-3.39657347	2.35347315
H	8.35863226	-1.48680206	-0.72264878
H	8.24226294	-2.82657859	1.37603213
Cl	-1.76649182	1.80161911	-1.79593519
H	-1.11208204	0.36927500	-0.98940638
C	4.82242182	2.06417610	-0.16541558
H	4.77031227	0.98412989	-0.35091592
C	3.62339212	2.75956340	-0.77982730
H	3.53030676	2.46186998	-1.82976047
C	4.93841479	2.31502720	1.32624734
H	5.77822252	1.74399365	1.74988701
H	5.14469469	3.38288364	1.51542861
N	2.31635906	2.49611236	-0.10077495
C	2.45362795	2.66031348	1.37237267
H	2.56514455	3.73923046	1.57404536
H	1.51949049	2.32521945	1.83418486
C	3.62863866	1.92313563	1.98391005
H	3.62716442	2.15769616	3.05902500
H	3.47975483	0.83563335	1.91674850
C	1.29290481	3.37819902	-0.65277065
C	1.23598683	3.59758680	-2.03385071
C	0.38133309	4.04526469	0.17032570
C	0.31153611	4.48541393	-2.57181311
H	1.91204834	3.07980706	-2.71299512

C	-0.54809192	4.92709291	-0.37809109
H	0.37495047	3.89307886	1.24670206
C	-0.58196082	5.16394507	-1.74739097
H	0.29061869	4.63920125	-3.65301037
H	-1.24954080	5.43596463	0.28724185
H	-1.30693840	5.86188925	-2.17184634
H	5.71129688	2.42248473	-0.70646925
H	3.77477033	3.85214329	-0.76158279

TS2

Charge = 0 Spin Multiplicity = 6

Fe	2.20630531	-1.40422568	-0.96891306
N	2.54485053	0.77145583	-1.08177407
C	3.08033439	1.31191029	0.02721149
C	2.20477848	1.55063740	-2.09147339
C	3.29493598	2.69901540	0.16981585
C	3.42472398	0.41904681	1.09460657
C	2.37723916	2.94388944	-2.04693518
H	1.77541044	1.05607732	-2.96592294
C	2.91791406	3.51889286	-0.91543970
C	3.85931247	3.19524671	1.38962294
C	3.98812762	0.93341793	2.28211844
N	3.18449852	-0.89825877	0.91486771
H	2.07264371	3.55026512	-2.90043689
H	3.05453258	4.60044795	-0.84802068
C	4.19349990	2.34700310	2.40327216
H	4.01757086	4.27081040	1.49161653
C	4.31583323	0.00434939	3.29279560
C	3.49817067	-1.75378582	1.87478125
H	4.62544750	2.73126298	3.32954862

H	4.75532585	0.35736531	4.22850560
C	4.07550937	-1.33839709	3.08534687
H	3.26841110	-2.80345343	1.67471419
H	4.31764306	-2.08180141	3.84563417
Cl	4.03611531	-1.70595340	-2.24602846
O	0.79468970	-1.15718428	-2.30274599
C	-0.40633494	-0.76983561	-2.04093907
C	-0.64291495	-0.27242657	-0.58139500
O	-1.32697276	-0.75790725	-2.83549042
C	-0.71746678	1.25347044	-0.55595682
O	0.50019846	-0.70329191	0.15388136
C	-1.32394741	1.98191976	-1.58727380
C	-0.18684393	1.94653603	0.53718603
C	-1.38910495	3.37305710	-1.52649861
H	-1.74307458	1.44894752	-2.44205025
C	-0.25183485	3.33731395	0.59509380
H	0.28497159	1.39737356	1.35261514
C	-0.85127544	4.05689952	-0.43718511
H	-1.86152822	3.92520454	-2.34239215
H	0.17696626	3.86004098	1.45338635
H	-0.89752086	5.14750880	-0.39356679
Cl	1.76408448	-3.55394188	-0.29639540
C	-1.87885237	-0.96523742	-0.03800350
H	-1.65339636	-0.71299247	1.53148184
C	-3.08006583	-0.29324849	0.00284881
H	-3.09116916	0.79346440	-0.09447799
C	-1.87453823	-2.48161948	-0.05362997
H	-1.12308508	-2.84976579	-0.76821213
H	-1.55673669	-2.87374195	0.92767573
N	-4.27197134	-0.86984730	0.23655726

C	-4.32982505	-2.31807810	0.42145325
H	-4.20088498	-2.56055167	1.49066752
H	-5.32946913	-2.65799171	0.12025407
C	-3.25768689	-3.00187868	-0.40892254
H	-3.32484001	-4.08707226	-0.24775473
H	-3.45650259	-2.81176205	-1.47614313
C	-5.44819404	-0.09682797	0.35990369
C	-5.61232658	1.08184315	-0.38144442
C	-6.47047261	-0.51140780	1.22331255
C	-6.76976329	1.84147379	-0.23786077
H	-4.84609643	1.39774324	-1.09187706
C	-7.63075987	0.24969558	1.34798276
H	-6.35583724	-1.41980292	1.81608333
C	-7.78632477	1.43128726	0.62504481
H	-6.88297725	2.75609048	-0.82452230
H	-8.41686466	-0.08488628	2.02890391
H	-8.69641864	2.02595749	0.72782830
Cl	-1.03721118	-0.79414456	2.82787185
H	0.28676841	-0.90005087	1.08670695

TS3

Charge = 0 Spin Multiplicity = 6

Fe	0.64821305	-1.12303468	-0.85604043
N	2.51744750	0.04753113	-0.86593369
C	3.44202438	-0.38009159	0.01332480
C	2.73559162	1.14336460	-1.56728591
C	4.65133346	0.31558820	0.23608866
C	3.17769221	-1.60057083	0.72601042
C	3.90683828	1.90433409	-1.41876419
H	1.95449533	1.43148048	-2.27398098

C	4.86149263	1.49463069	-0.51096509
C	5.59293467	-0.20333898	1.18449707
C	4.13219788	-2.09616992	1.64211826
N	2.01685377	-2.23782393	0.47758277
H	4.03974358	2.80845277	-2.01350983
H	5.78006189	2.06804836	-0.36630182
C	5.34446475	-1.36169355	1.85817029
H	6.52082574	0.34764481	1.35203206
C	3.82561470	-3.30820847	2.29743386
C	1.74591239	-3.37095603	1.09807004
H	6.06973444	-1.75393866	2.57429815
H	4.53499904	-3.72796359	3.01438583
C	2.63405238	-3.94745955	2.02205250
H	0.78223769	-3.83010355	0.85933829
H	2.36903808	-4.88606811	2.51064669
Cl	1.52164509	-2.34546021	-2.63927670
O	-0.22554446	0.23710149	-2.03828490
C	-0.94077789	1.23380749	-1.69594706
C	-0.87165322	1.75660212	-0.26086104
O	-1.65417699	1.88994933	-2.44415563
C	0.23894627	2.71571825	-0.03887794
O	0.24570404	-0.06690362	0.69638123
C	0.43402173	3.74010531	-0.97875055
C	1.09902308	2.63142701	1.06578933
C	1.45809686	4.66935165	-0.80568678
H	-0.23014620	3.80531209	-1.84285142
C	2.12634033	3.55561709	1.22592290
H	0.98163130	1.78986092	1.74745439
C	2.30800665	4.57982823	0.29517136
H	1.59385162	5.46427336	-1.54264186

H	2.80163985	3.46612950	2.08017802
H	3.11832901	5.30130923	0.42342051
Cl	-1.22254749	-2.50891795	-0.42650566
C	-1.98864640	1.70264574	0.56072970
C	-3.02562242	0.83537220	0.17731298
H	-2.91521665	0.21563195	-0.71511950
C	-2.13437792	2.48873947	1.83647043
H	-1.16557110	2.57972549	2.34336494
H	-2.45569824	3.51725242	1.59599075
N	-4.16563840	0.69408756	0.83141209
C	-4.43683299	1.51406705	2.01830899
H	-4.94106133	2.44119698	1.70036328
H	-5.13260671	0.95302065	2.65454328
C	-3.14767554	1.82347870	2.75417841
H	-3.38025798	2.46721450	3.61370398
H	-2.73172211	0.88384868	3.15339760
C	-5.14609609	-0.24287053	0.40075109
C	-4.74999291	-1.48639403	-0.10166529
C	-6.50237733	0.08581752	0.48990559
C	-5.71779016	-2.38793178	-0.53688693
H	-3.69162462	-1.76226445	-0.12968868
C	-7.45925492	-0.82919605	0.05827754
H	-6.81344543	1.05836318	0.87400372
C	-7.07244751	-2.06516655	-0.45971084
H	-5.40412564	-3.35949757	-0.92516726
H	-8.51746092	-0.56654470	0.12145124
H	-7.82725618	-2.77880247	-0.79678910
H	-0.52507454	-0.46935598	1.11906004

TS3'

Charge = 0 Spin Multiplicity = 1

O	-0.86369096	1.69838834	2.22063472
C	-0.40536989	1.12016424	1.26990062
C	-1.14300957	0.48759469	0.11517105
O	0.89179701	0.92503783	1.09051981
C	-2.43841456	0.81898809	-0.28169592
O	-1.78896354	-1.05518235	1.89070084
C	-3.22599129	1.77569684	0.43688938
C	-3.01124801	0.18822854	-1.43130704
C	-4.46183990	2.14214302	-0.03446979
H	-2.81517379	2.22090467	1.34224331
C	-4.24746914	0.60997455	-1.91795628
H	-2.42531704	-0.53068006	-2.00176147
C	-4.96170058	1.57731100	-1.22891510
H	-5.05323084	2.88697341	0.50084645
H	-4.65321757	0.16234790	-2.82610153
H	-5.93076601	1.90766425	-1.61103905
C	-0.15345673	-0.28549874	-0.68536223
H	-0.29463053	-0.03439221	-1.74557465
C	1.19168815	0.31181792	-0.21911834
H	1.45395948	1.15883074	-0.86559147
C	-0.21312724	-1.82457750	-0.54558614
H	-1.25601730	-2.13810039	-0.39584491
H	0.12445599	-2.25475078	-1.50150514
N	2.28677753	-0.55113811	-0.14213069
C	2.13481960	-1.94786063	0.25277162
H	2.48345568	-2.59897930	-0.56810424
H	2.78442453	-2.14957119	1.12097037
C	0.69569321	-2.29189460	0.57150879
H	0.61756531	-3.38252396	0.69225827

H	0.37641590	-1.84375853	1.52320410
C	3.57817641	-0.02578252	-0.25927568
C	3.82480435	1.35816939	-0.17430716
C	4.67711481	-0.88215890	-0.45740908
C	5.11427528	1.86009688	-0.32694139
H	3.01520076	2.05327628	0.05005529
C	5.96308308	-0.36636918	-0.59800216
H	4.53184616	-1.96018287	-0.51927212
C	6.19567955	1.00689127	-0.54322699
H	5.27276611	2.93906523	-0.25506604
H	6.79478961	-1.05715043	-0.75811123
H	7.20600888	1.40585880	-0.65454573
H	-2.50943054	-1.44823687	1.32687375
H	-2.23072269	-0.36301725	2.39974702
Cl	-3.80372869	-2.07439350	-0.05459185

TS4'

Charge = 0 Spin Multiplicity = 6

Fe	-1.10925644	-0.97068253	1.11234714
N	-2.63463975	0.36704968	0.22990916
C	-3.64271711	-0.26366867	-0.39993293
C	-2.62232879	1.68454407	0.28853267
C	-4.69661437	0.43249296	-1.03186436
C	-3.63011433	-1.69841923	-0.40325089
C	-3.62575854	2.46704916	-0.30873674
H	-1.78904237	2.13800132	0.82789106
C	-4.66025087	1.84264354	-0.97441874
C	-5.73437736	-0.31129814	-1.68308053
C	-4.66943569	-2.40574942	-1.04710563
N	-2.61216536	-2.31927483	0.22617820

H	-3.56736476	3.55383555	-0.23748236
H	-5.45328778	2.42310615	-1.45140700
C	-5.72065437	-1.67417184	-1.69098848
H	-6.54124220	0.23876460	-2.17202144
C	-4.60673865	-3.81510934	-1.01163918
C	-2.57032863	-3.63959348	0.25067790
H	-6.51566866	-2.23487871	-2.18709059
H	-5.38929621	-4.40264057	-1.49726351
C	-3.55701991	-4.43038446	-0.36137648
H	-1.71763959	-4.07884961	0.77564237
H	-3.47890185	-5.51733604	-0.31401825
Cl	-2.43201469	-0.79840945	3.01481685
O	0.02005099	0.63443746	1.61602562
C	1.15638332	0.82694972	1.08665484
C	1.39202156	2.04396858	0.24423826
O	2.13009141	0.04965031	1.17530960
C	0.51957708	3.21818323	0.31388791
C	0.07131002	3.69488600	1.55700897
C	0.08793371	3.86249924	-0.85563966
C	-0.77800311	4.79493555	1.62558152
H	0.38609971	3.19043528	2.47240235
C	-0.76677758	4.96010259	-0.78463493
H	0.39807706	3.47608100	-1.82870420
C	-1.20009657	5.42964132	0.45529092
H	-1.11819247	5.15739646	2.59817412
H	-1.10468396	5.44445141	-1.70350700
H	-1.87361690	6.28802910	0.51093567
Cl	0.17862857	-2.73196113	1.83955792
C	2.47699430	1.89459045	-0.54897463
C	3.10773728	0.56780198	-0.50763588

H	2.56831073	-0.30109627	-0.89960728
C	3.18104837	2.93662824	-1.36668352
H	2.89401091	2.83604647	-2.42571603
H	2.83225980	3.92719786	-1.04275037
N	4.42005944	0.52018192	-0.43940144
C	5.10906112	1.78579215	-0.15902402
H	4.82978332	2.12744068	0.84987437
H	6.18915722	1.60438149	-0.17360125
C	4.71264718	2.80137995	-1.22518389
H	5.15770125	3.77157531	-0.96347367
H	5.15919294	2.48914308	-2.18026435
C	5.14259698	-0.69581149	-0.60500238
C	4.80662861	-1.57200556	-1.63985175
C	6.17854064	-1.00820821	0.27797218
C	5.50476604	-2.76845307	-1.78084580
H	4.01372906	-1.31214277	-2.34407933
C	6.87687002	-2.20341115	0.12173843
H	6.42746560	-0.32988586	1.09613554
C	6.54146258	-3.08697565	-0.90359757
H	5.24259838	-3.44971185	-2.59314213
H	7.68367269	-2.44779281	0.81600889
H	7.09021217	-4.02377991	-1.02118079
Cl	-0.16783642	-0.88329074	-1.09425255

TS4

Charge = 0 Spin Multiplicity = 1

O	0.04048890	2.22549845	0.43829695
C	-1.13286623	1.99864655	0.04949708
C	-1.51707615	0.50446223	-0.09369831
O	-2.01481149	2.82539872	-0.22095816

C	-2.94113768	0.16060360	-0.15187012
C	-3.87178757	0.80716799	0.68145157
C	-3.41018381	-0.81528672	-1.04887894
C	-5.21932533	0.46479930	0.63736552
H	-3.52444430	1.57999749	1.36706277
C	-4.76223236	-1.14102766	-1.10756681
H	-2.70646323	-1.30159211	-1.72810356
C	-5.66966432	-0.50723514	-0.25809806
H	-5.92736168	0.96525976	1.30215921
H	-5.10948977	-1.89164995	-1.82132401
H	-6.73050452	-0.76613411	-0.29814394
C	-0.54042266	-0.45378534	-0.11201750
C	0.82693835	-0.02977029	-0.25118758
H	1.05326530	0.90475314	-0.75619397
N	1.85616788	-0.75457597	0.11096049
C	1.70865306	-2.09021817	0.71013493
H	2.00196909	-2.82445808	-0.05648646
H	2.43035937	-2.16483424	1.53476998
C	3.17681404	-0.23476582	-0.05218992
C	3.39372933	1.13417742	0.13846525
C	4.23667724	-1.08609968	-0.37228406
C	4.67625264	1.65083786	-0.01994278
H	2.56105152	1.78158469	0.42600884
C	5.51544773	-0.55487883	-0.52384677
H	4.07261104	-2.15362605	-0.52122970
C	5.73924508	0.81065793	-0.35208978
H	4.84600920	2.71880171	0.13243279
H	6.34268545	-1.21878708	-0.78346526
H	6.74489962	1.21963132	-0.47010495
C	0.29478304	-2.35064375	1.18243648

H	0.20239758	-3.42194795	1.41115319
H	0.10807206	-1.80182345	2.11913327
C	-0.73005697	-1.92565158	0.13562905
H	-0.58582115	-2.50680051	-0.79136799
H	-1.74919329	-2.12693664	0.48814727

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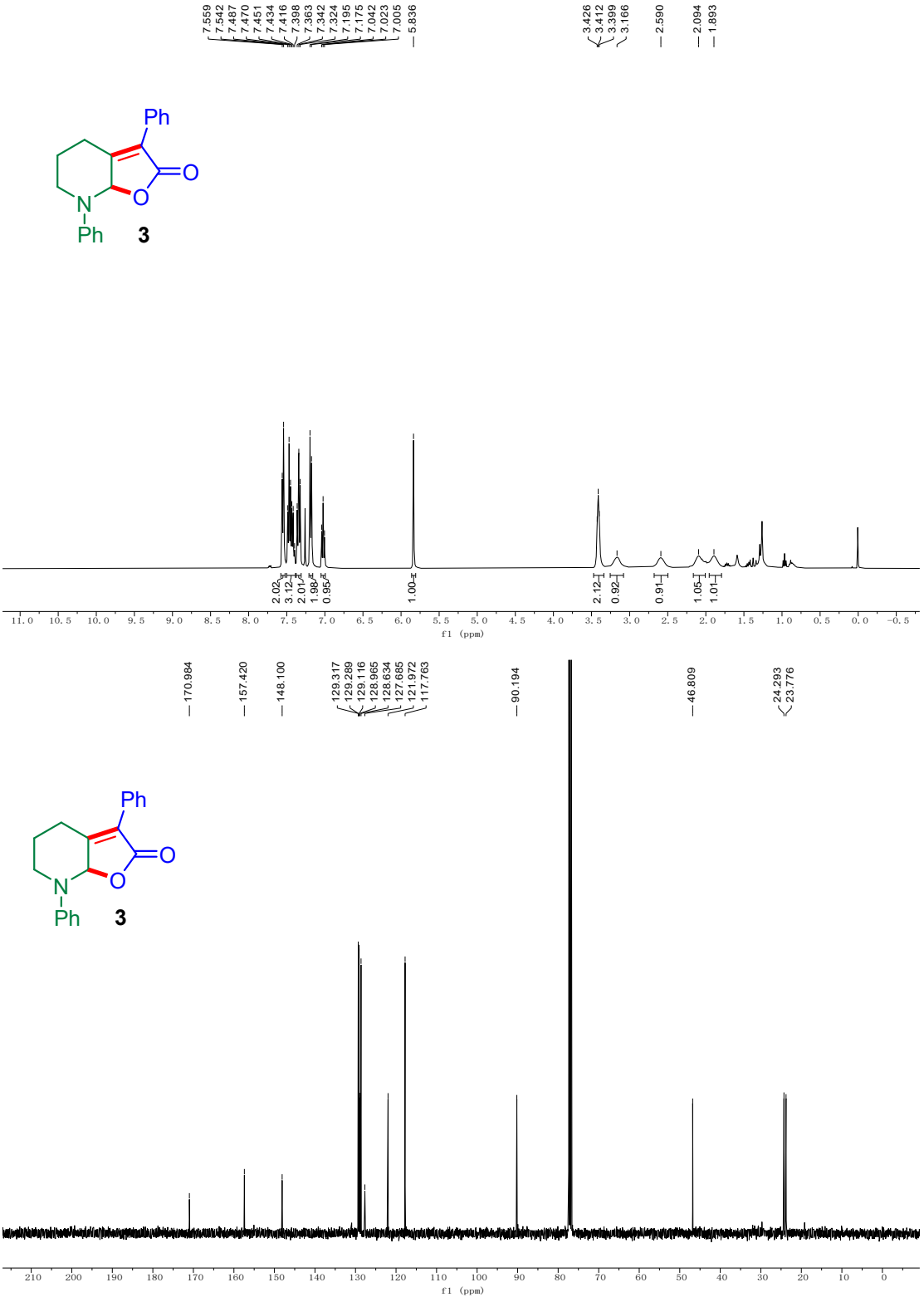
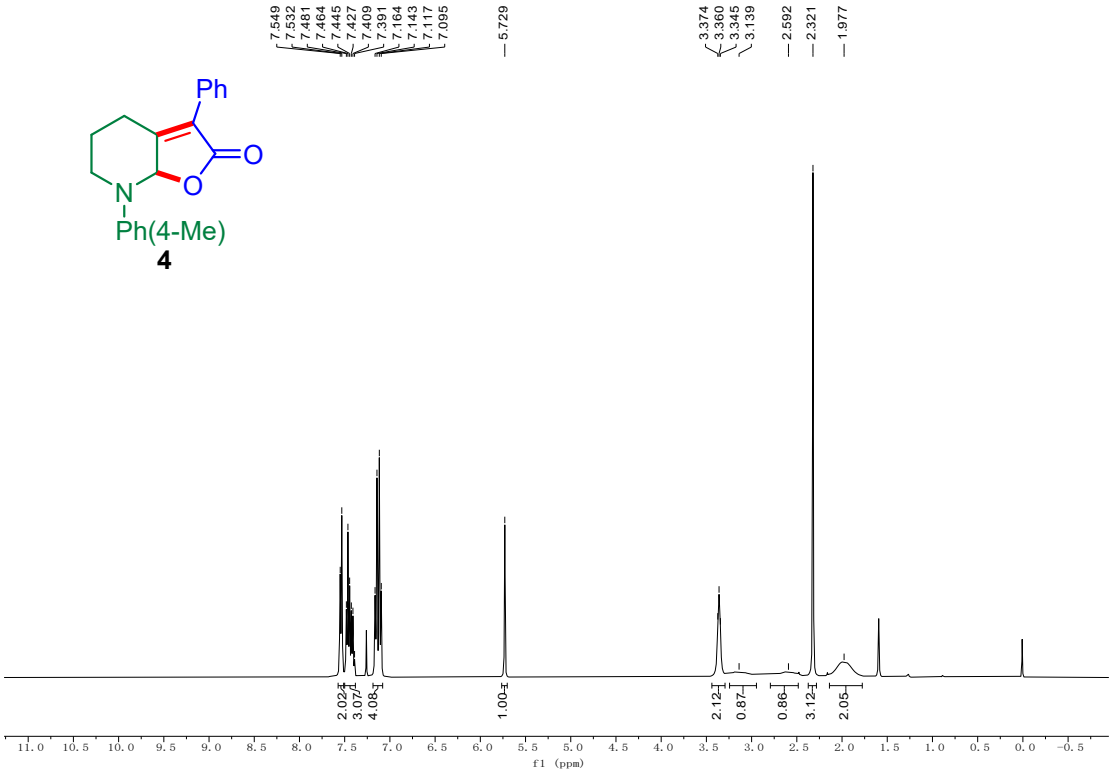
NMR Spectrum

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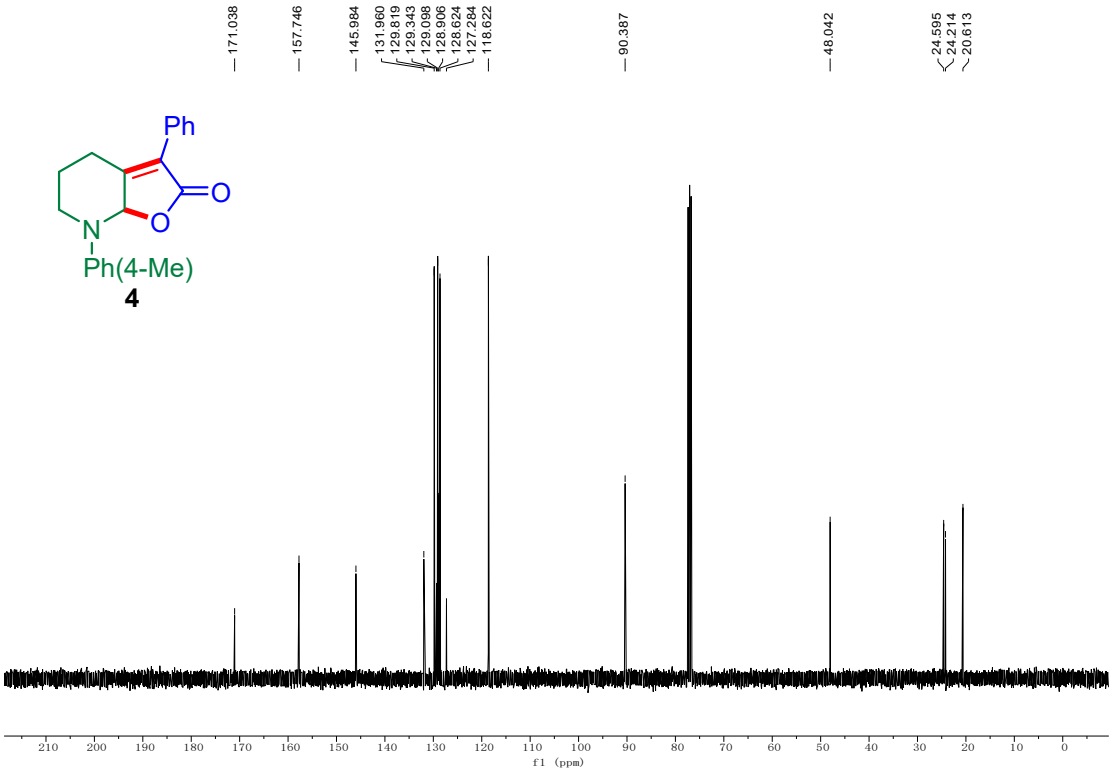
7.532
7.481
7.464
7.445
7.427
7.409
7.391
7.164
7.143
7.117
7.095
5.729
3.374
3.360
3.345
3.139
2.592
2.321
1.977
Ph
O
O
N
Ph(4-Me)
4
2.02
3.07
4.08
1.00
2.12
0.87
0.86
3.12
2.05
f1 (ppm)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157.746
145.984
131.960
129.819
129.343
129.098
128.906
128.624
127.284
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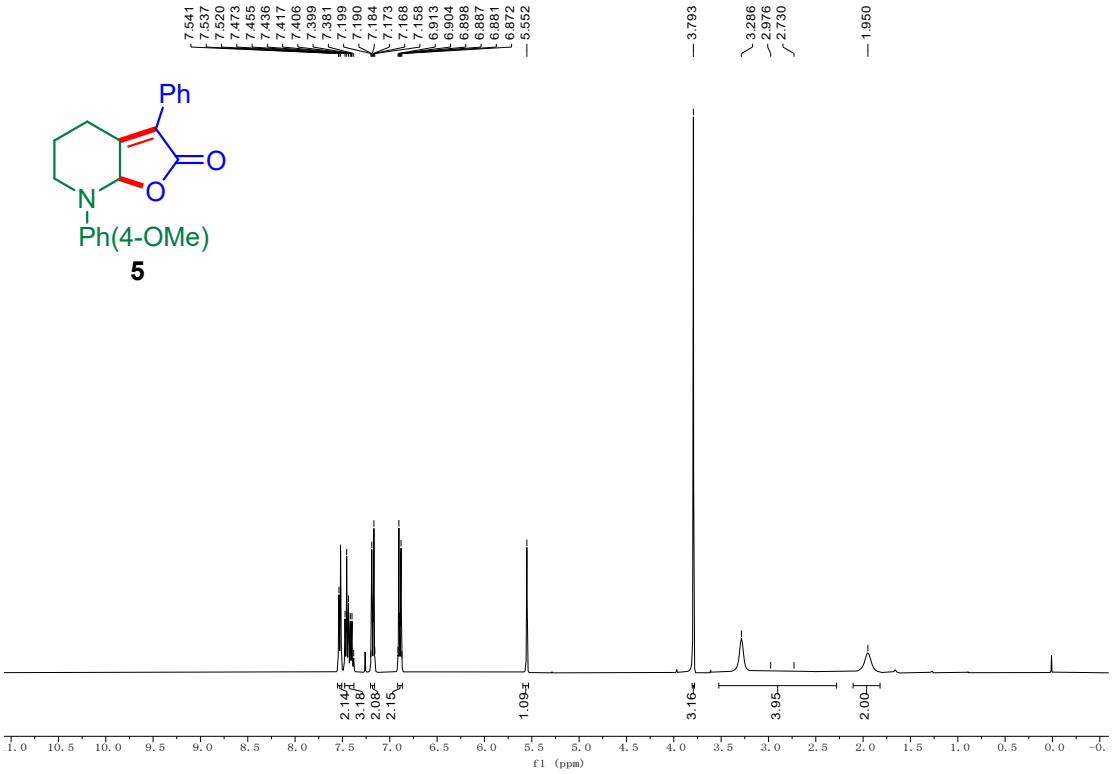
90.387
48.042
24.595
24.214
20.613
Ph
O
O
N
Ph(4-Me)
4
f1 (ppm)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7.537
7.520
7.473
7.455
7.436
7.417
7.406
7.399
7.381
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7.190
7.184
7.173
7.168
7.158
6.913
6.904
6.898
6.887
6.881
6.872
5.552
3.793
3.286
2.976
2.730
1.950
Ph
O
N
O
Ph(4-OMe)
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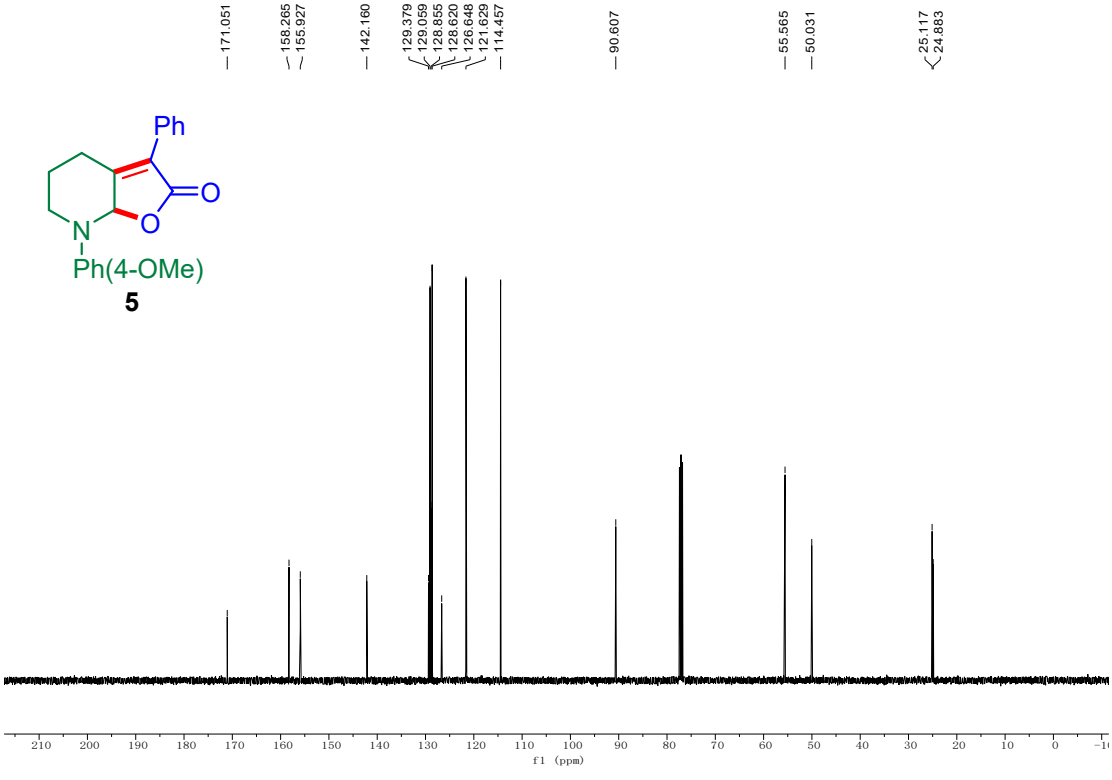
2.14
3.18
2.08
2.15
1.09
3.16
3.95
2.00
f1 (ppm)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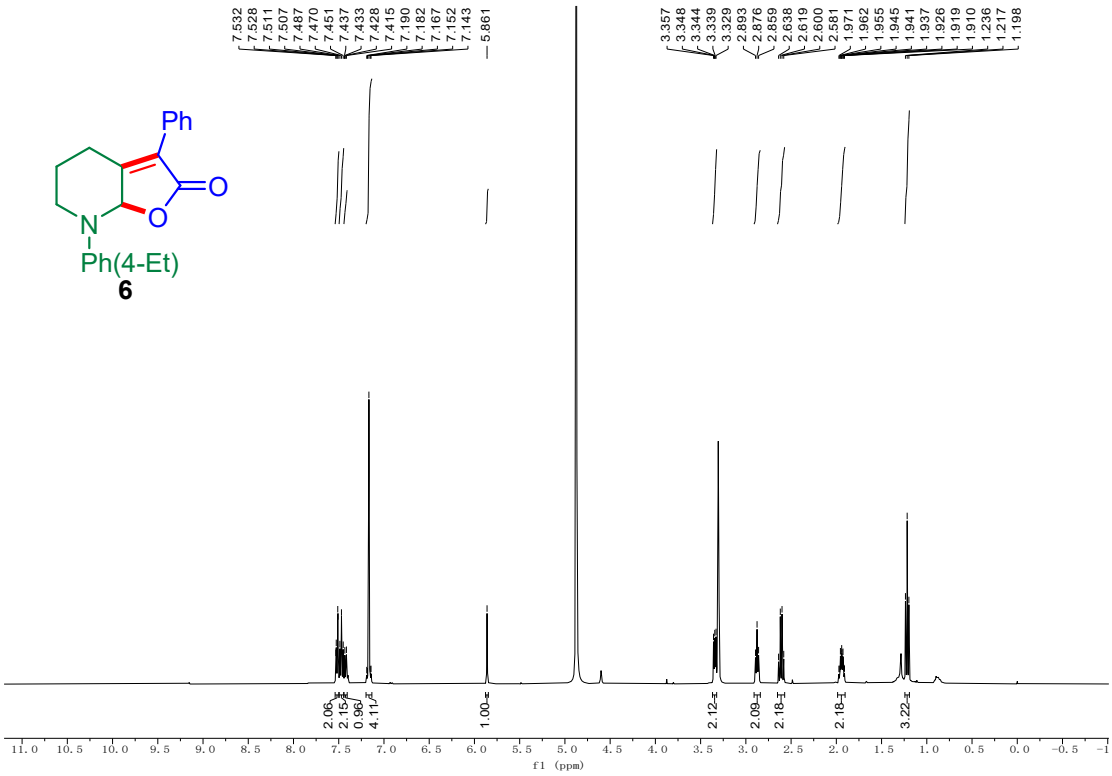
158.265
155.927
142.160
129.379
129.059
128.855
128.620
126.648
121.629
114.457
90.607
55.565
50.031
25.117
24.883
Ph
O
N
O
Ph(4-OMe)
5
f1 (ppm)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7.511
7.507
7.487
7.470
7.451
7.437
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7.428
7.415
7.190
7.182
7.167
7.152
7.143
5.861
3.357
3.348
3.344
3.339
3.329
2.893
2.876
2.859
2.638
2.619
2.600
2.581
1.971
1.962
1.955
1.945
1.941
1.937
1.926
1.919
1.910
1.236
1.217
1.198
Ph
O
N
O
Ph(4-Et)
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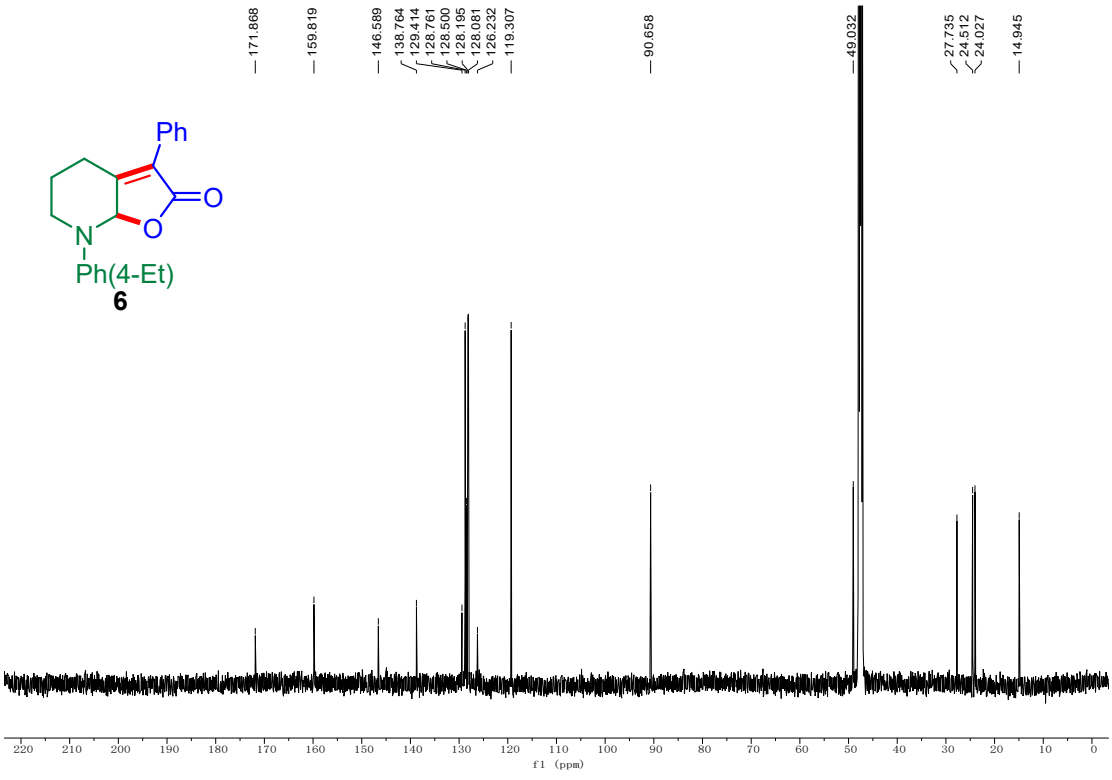
2.15
0.96
4.11
1.00
2.12
2.09
2.18
2.18
3.22
f1 (ppm)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146.589
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129.414
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128.195
128.081
126.232
119.307
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49.032
27.735
24.512
24.027
14.945
Ph
O
N
O
Ph(4-Et)
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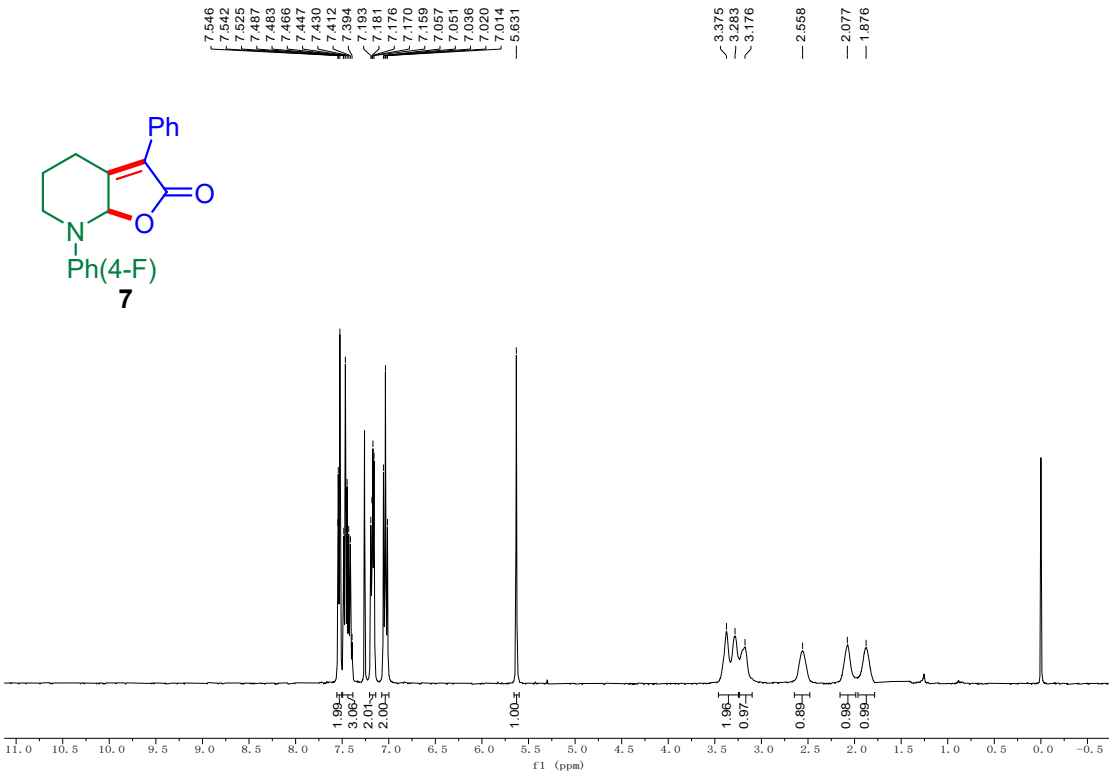
f1 (ppm)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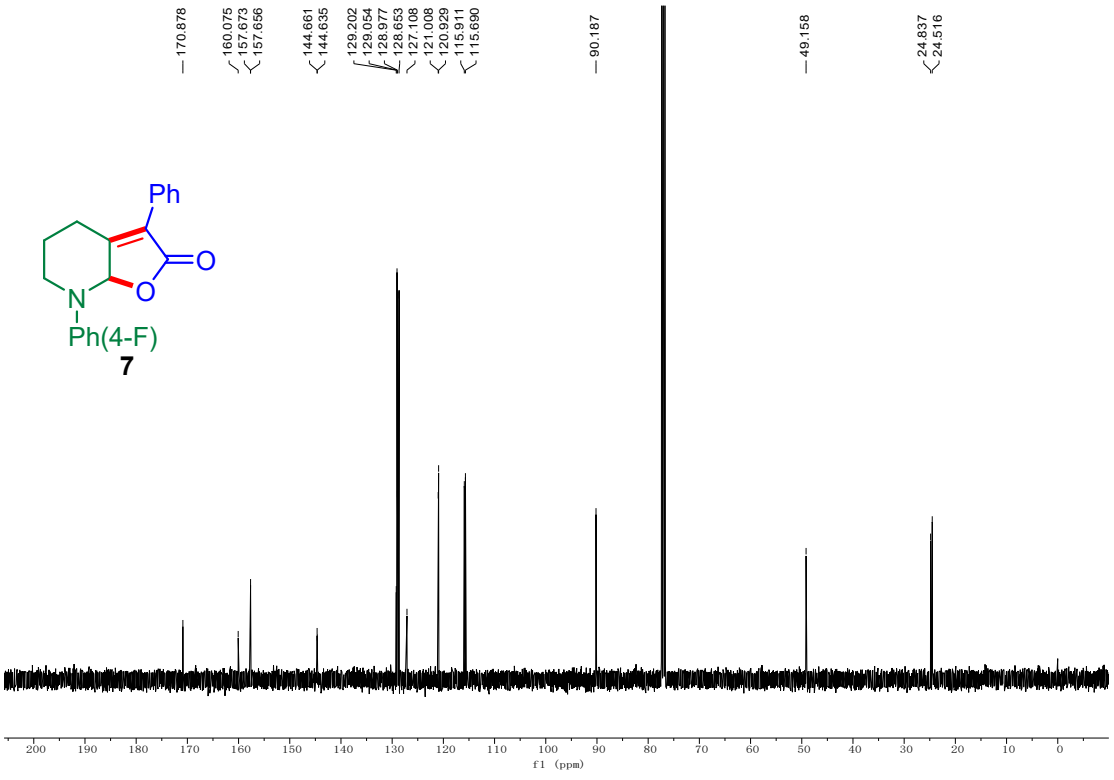
7.487
7.483
7.466
7.447
7.430
7.412
7.394
7.193
7.181
7.176
7.170
7.159
7.057
7.051
7.036
7.020
7.014
5.631
3.375
3.283
3.176
2.558
2.077
1.876
Ph
O
N
O
Ph(4-F)
7
1.99
3.06
2.01
2.00
1.00
1.96
0.97
0.89
0.98
0.99
f1 (ppm)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144.635
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129.054
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128.653
127.108
121.008
120.929
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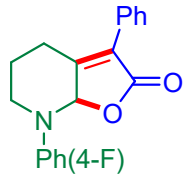
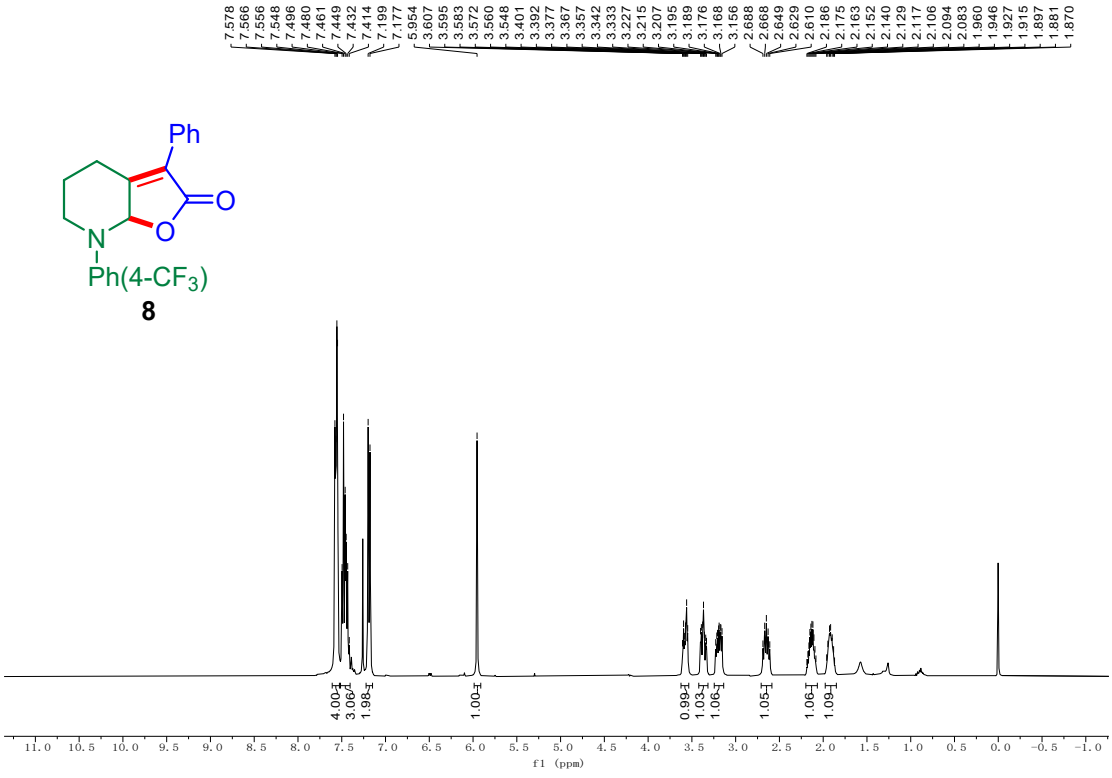
115.690
90.187
49.158
24.837
24.516
Ph
O
N
O
Ph(4-F)
7
f1 (ppm)



7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7.414
7.199
7.177
5.954
3.607
3.595
3.583
3.572
3.560
3.548
3.401
3.392
3.377
3.367
3.357
3.342
3.333
3.227
3.215
3.207
3.195
3.189
3.176
3.168
3.156
2.688
2.668
2.649
2.629
2.610
2.186
2.175
2.163
2.152
2.140
2.129
2.117
2.106
2.094
2.083
1.960
1.946
1.927
1.915
1.897
1.881
1.870
Ph
O
N
O
Ph(4-CF3)
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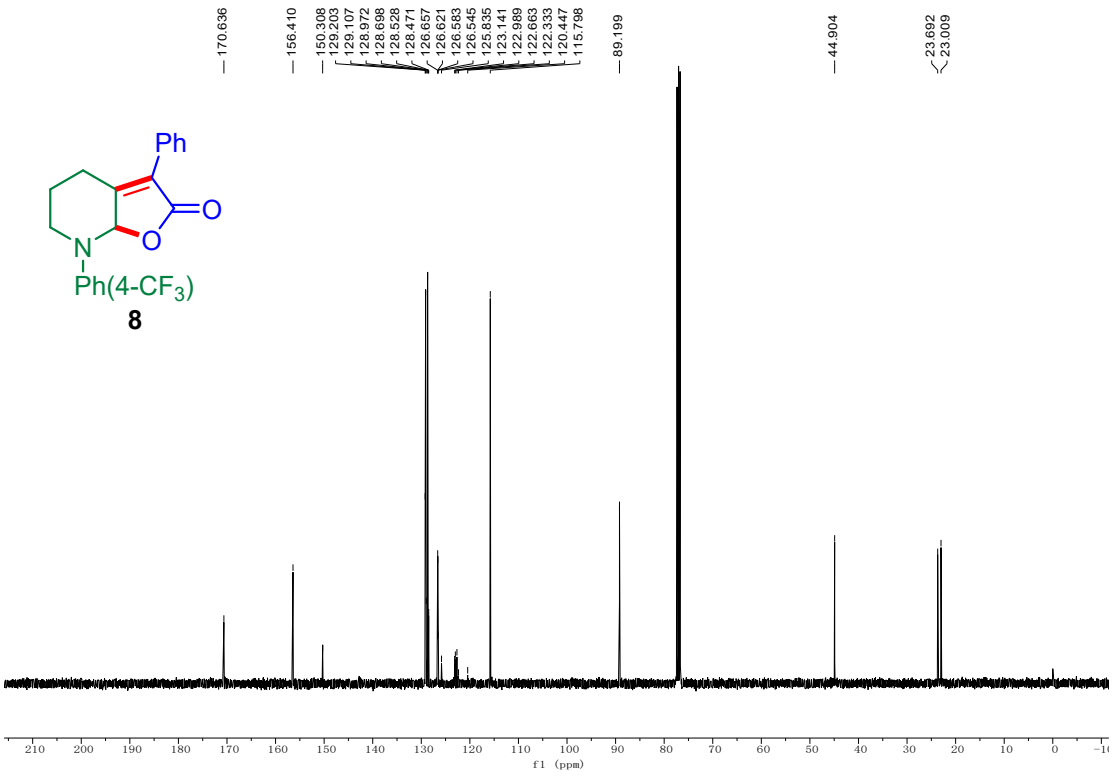
1.98
1.00
0.99
1.03
1.06
1.05
1.06
1.09
f1 (ppm)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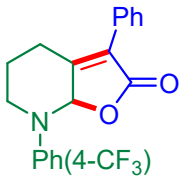
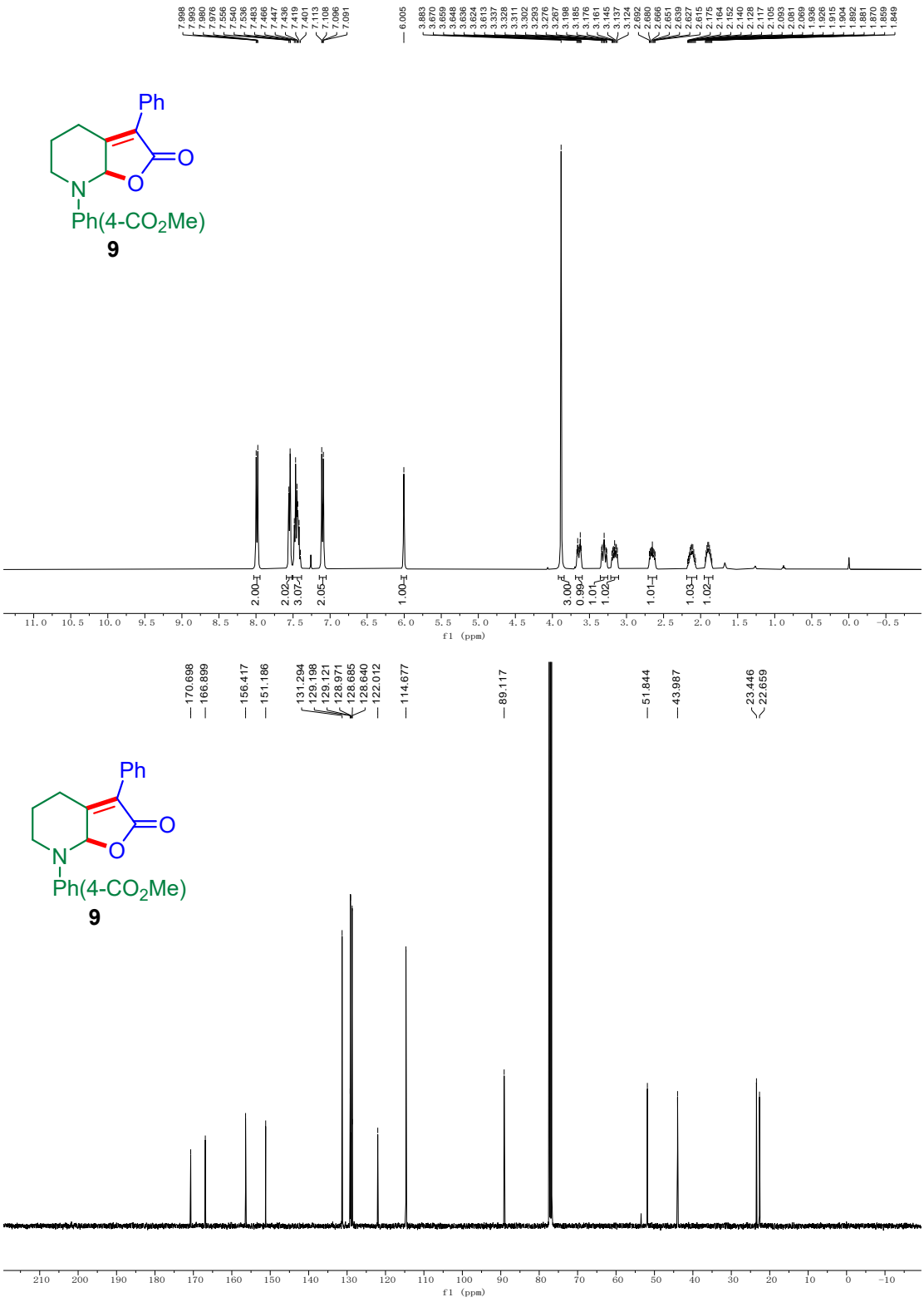
128.471
126.657
126.621
126.583
126.545
125.835
123.141
122.989
122.663
122.333
120.447
115.798
89.199
44.904
23.692
23.009
Ph
O
N
O
Ph(4-CF3)
8
f1 (ppm)



8


Ph
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N
O
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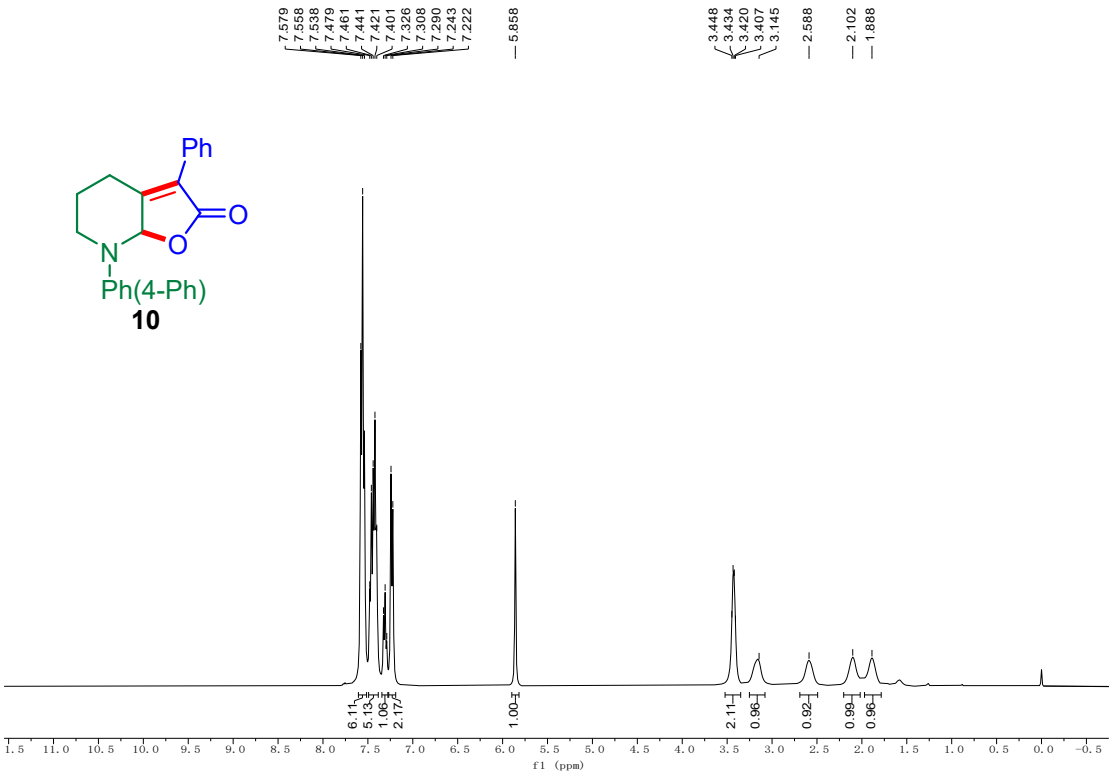
f1 (ppm)
Ph
O
N
O
Ph(4-CO2Me)
9
f1 (ppm)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7.441
7.421
7.401
7.326
7.308
7.290
7.243
7.222
5.858
3.448
3.434
3.420
3.407
3.145
2.588
2.102
1.888
Ph
O
O
N
Ph(4-Ph)
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5.13
1.06
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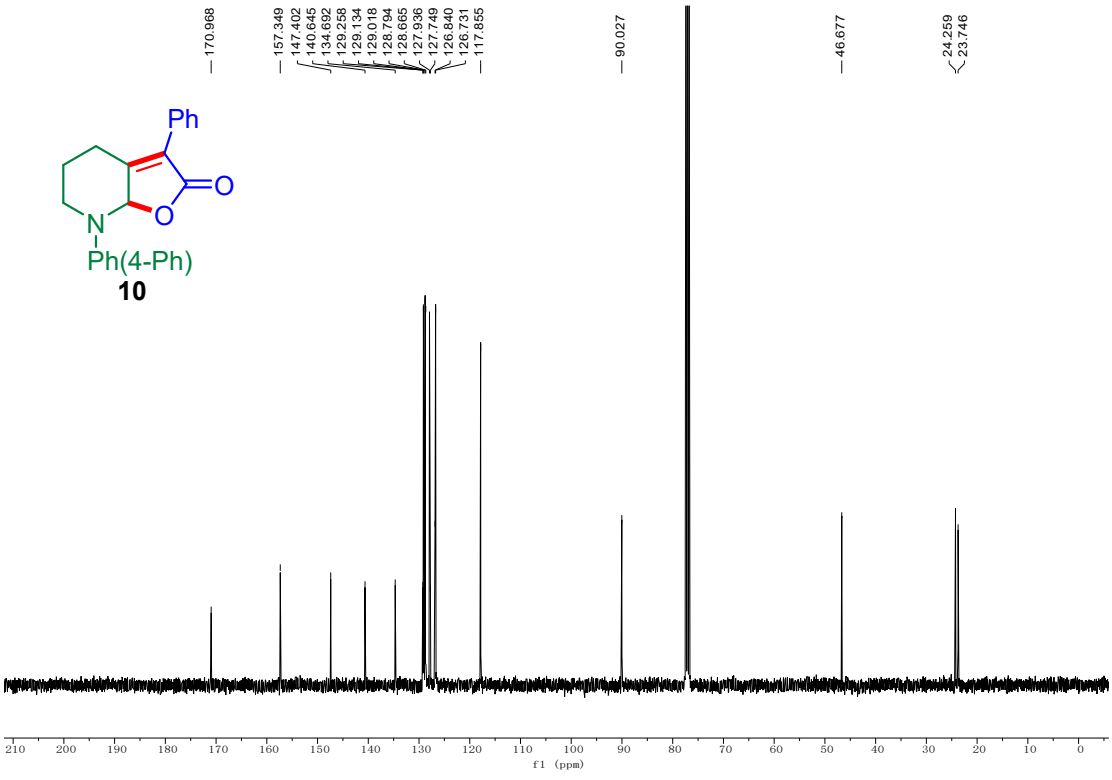
1.00
2.11
0.96
0.92
0.99
0.96
f1 (ppm)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128.665
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127.749
126.840
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Ph
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O
N
Ph(4-Ph)
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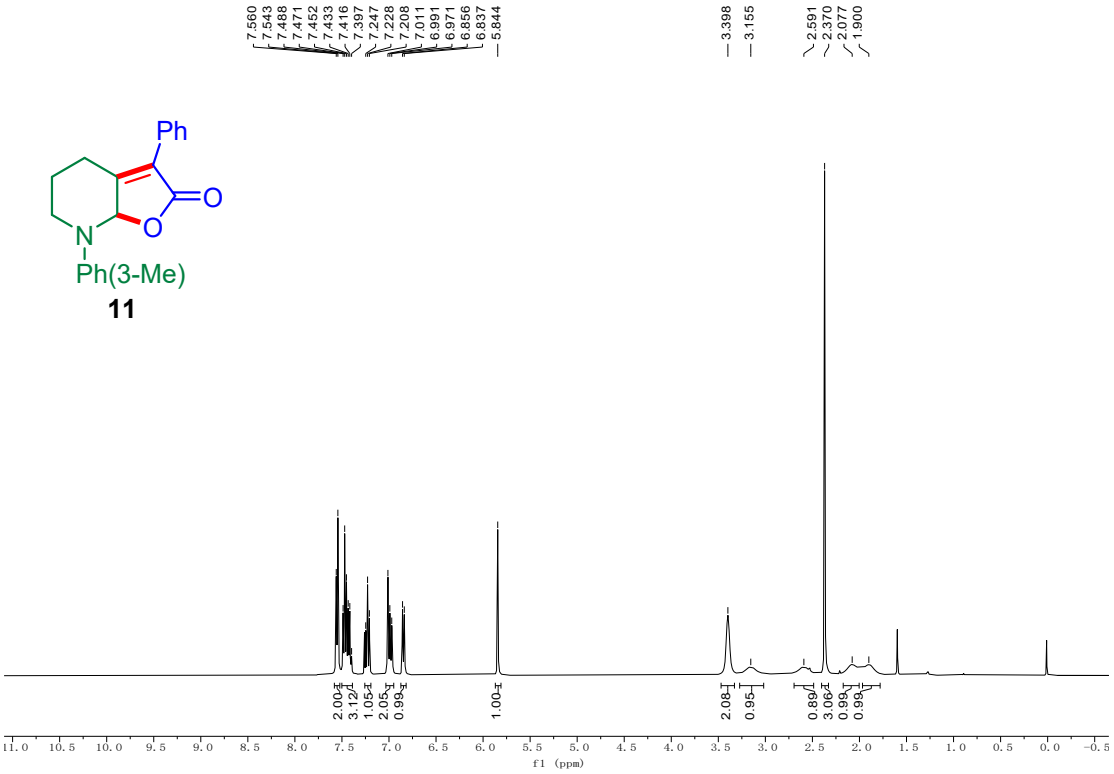
f1 (ppm)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7.433
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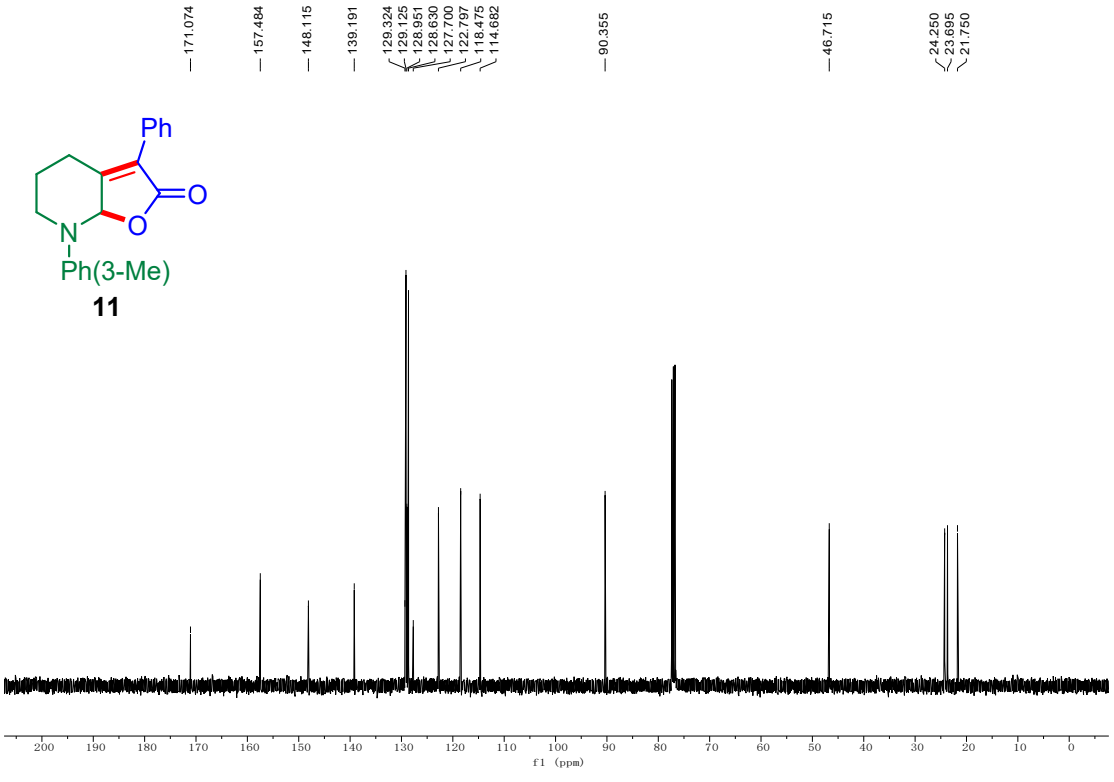
7.397
7.247
7.228
7.208
7.011
6.991
6.971
6.856
6.837
5.844
3.398
3.155
2.591
2.370
2.077
1.900
Ph
O
N
O
Ph(3-Me)
11
2.00
3.12
1.05
2.05
0.99
1.00
2.08
0.95
0.89
3.06
0.95
0.95
f1 (ppm)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24.250
23.695
21.750
Ph
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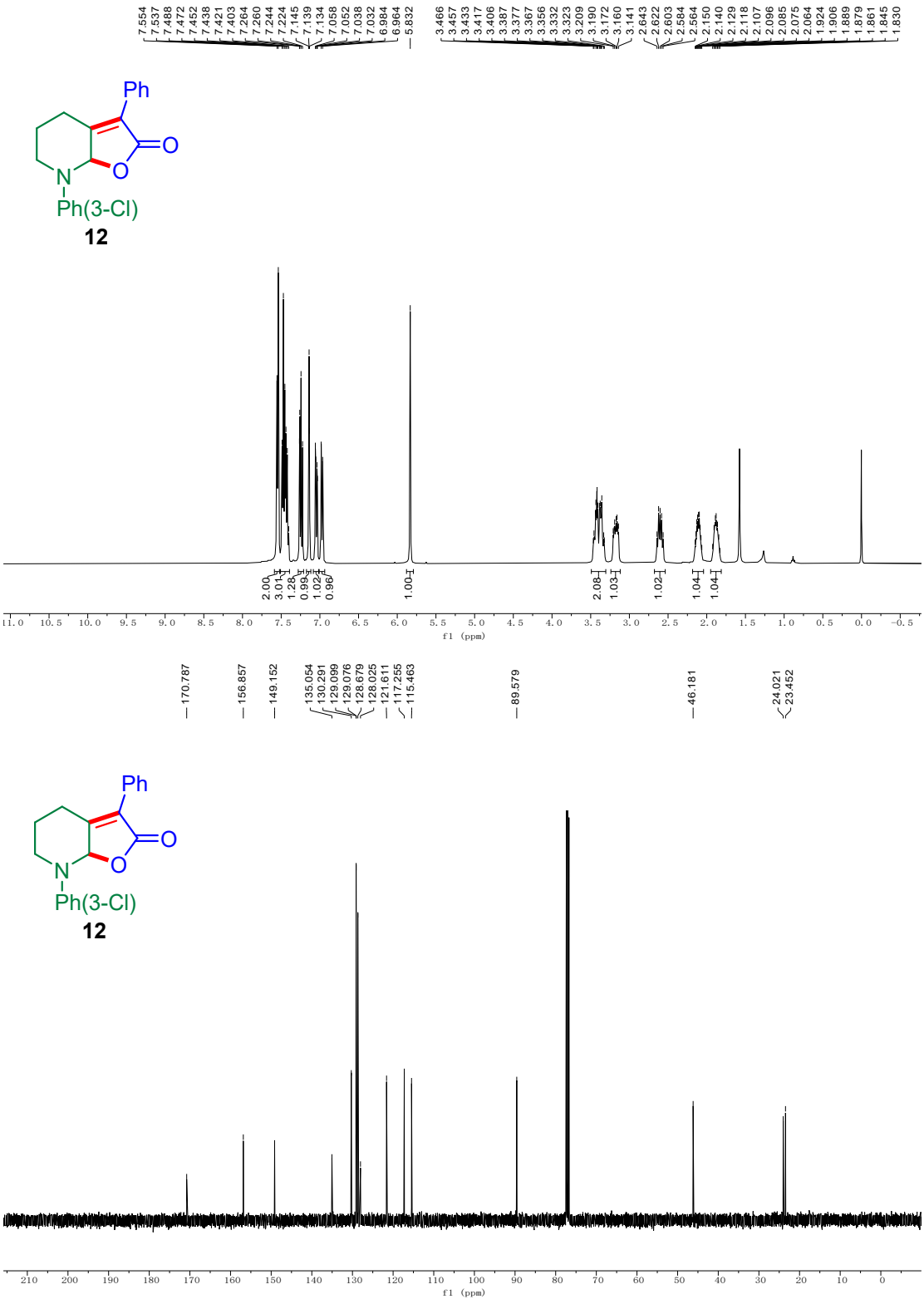
N
O
Ph(3-Me)
11
f1 (ppm)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7.260
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7.224
7.145
7.139
7.134
7.058
7.052
7.038
7.032
6.984
6.964
5.832
3.466
3.457
3.433
3.417
3.406
3.387
3.377
3.367
3.356
3.332
3.323
3.209
3.190
3.172
3.160
3.141
2.643
2.622
2.603
2.584
2.564
2.150
2.140
2.129
2.118
2.107
2.096
2.085
2.075
2.064
1.924
1.906
1.889
1.879
1.861
1.845
1.830
Ph
O
N
O
Ph(3-Cl)
12
2.00
3.01
1.28
0.99
1.02
0.96
1.00
2.08
1.03
1.02
1.04
1.04
f1 (ppm)
170.787
156.857
149.152
135.054
130.291
129.099
129.076
128.679
128.025
121.611
117.255
115.463
89.579
46.181
24.021
23.452
Ph
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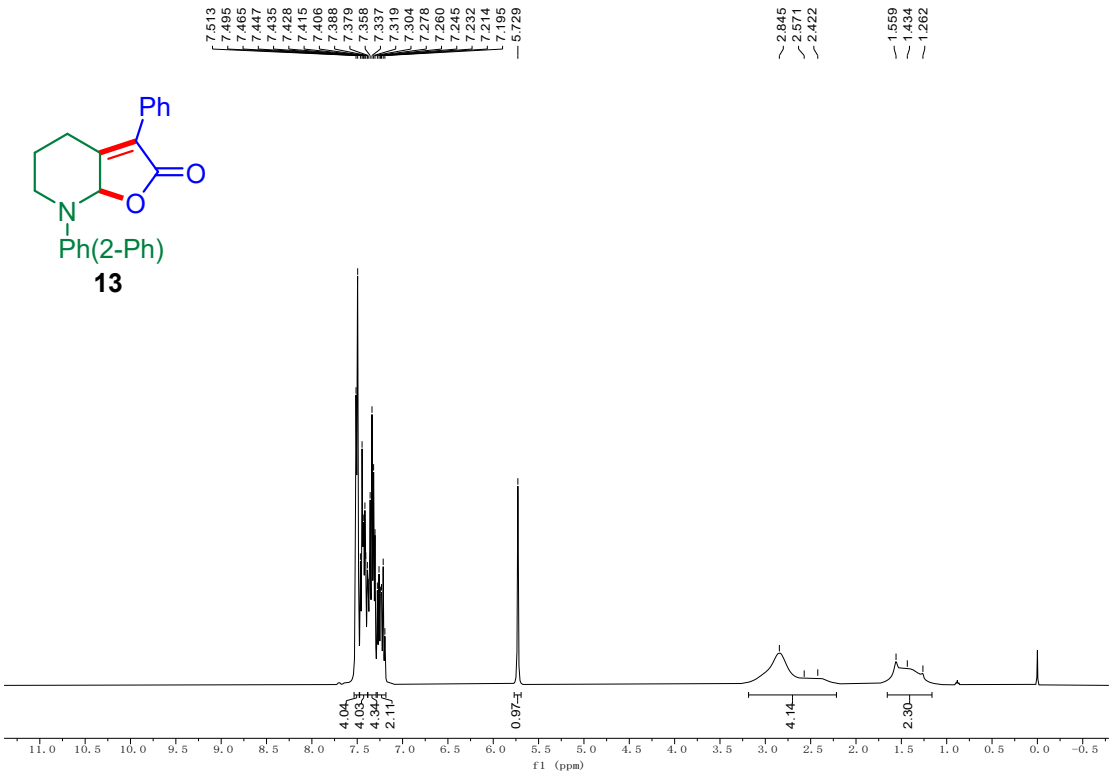
N
O
Ph(3-Cl)
12
f1 (ppm)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7.465
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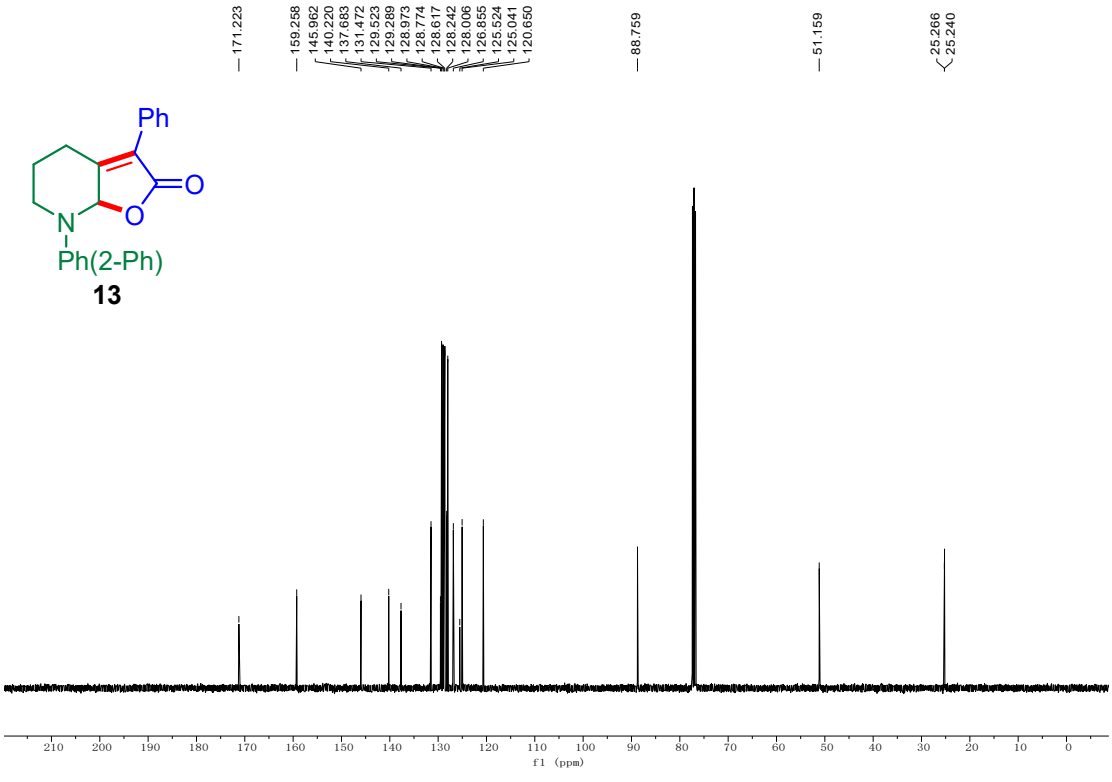
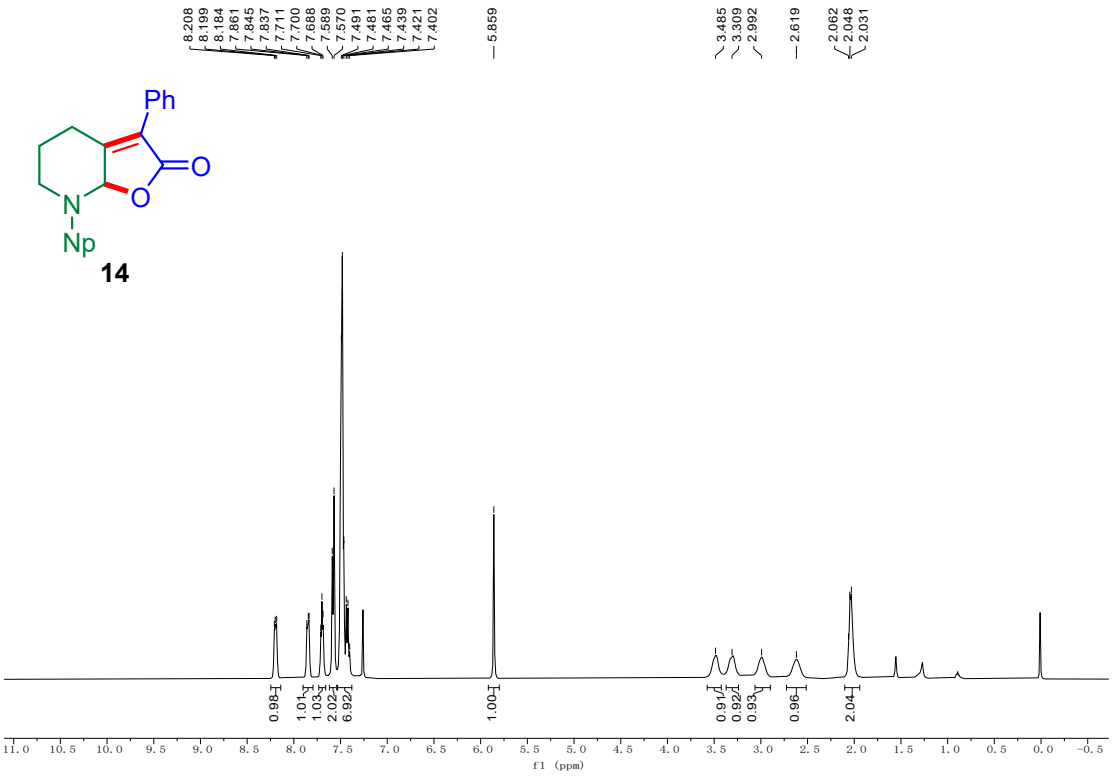
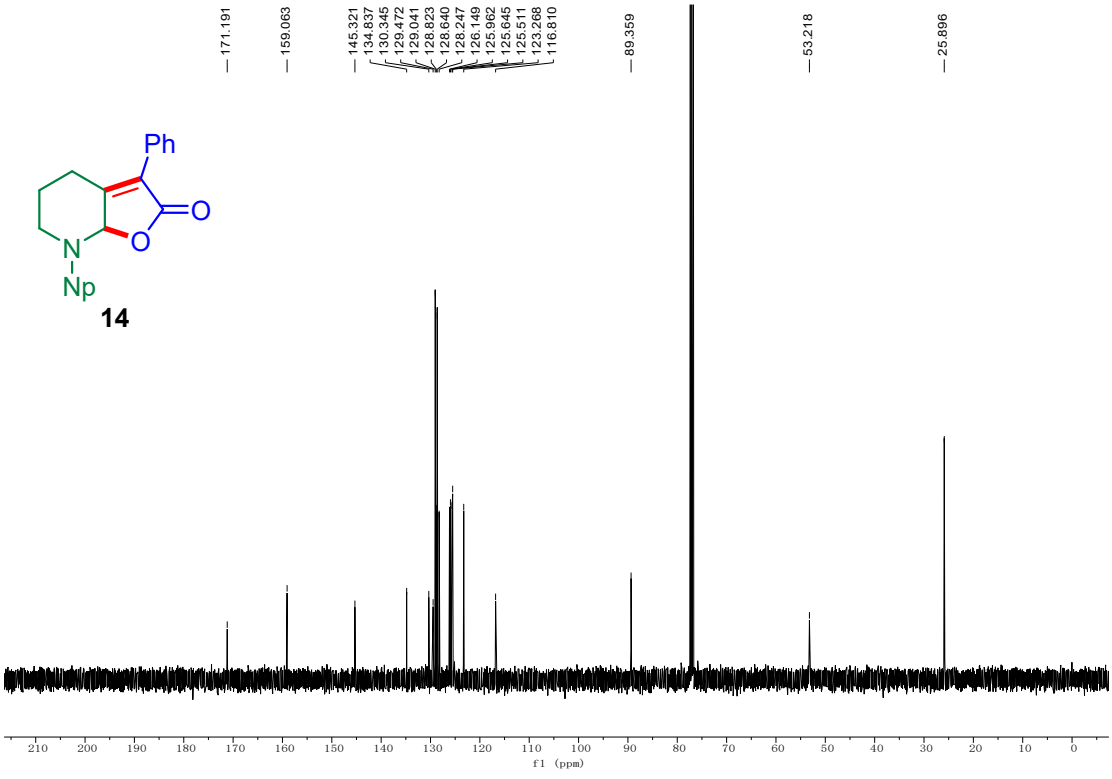
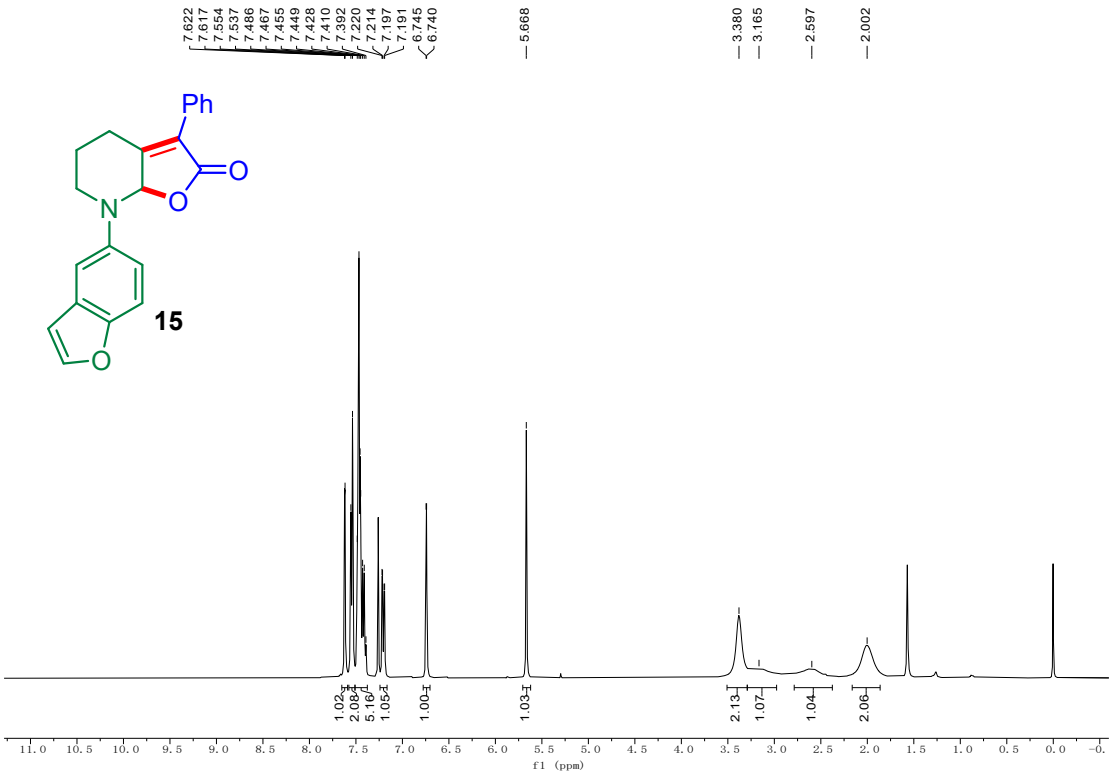
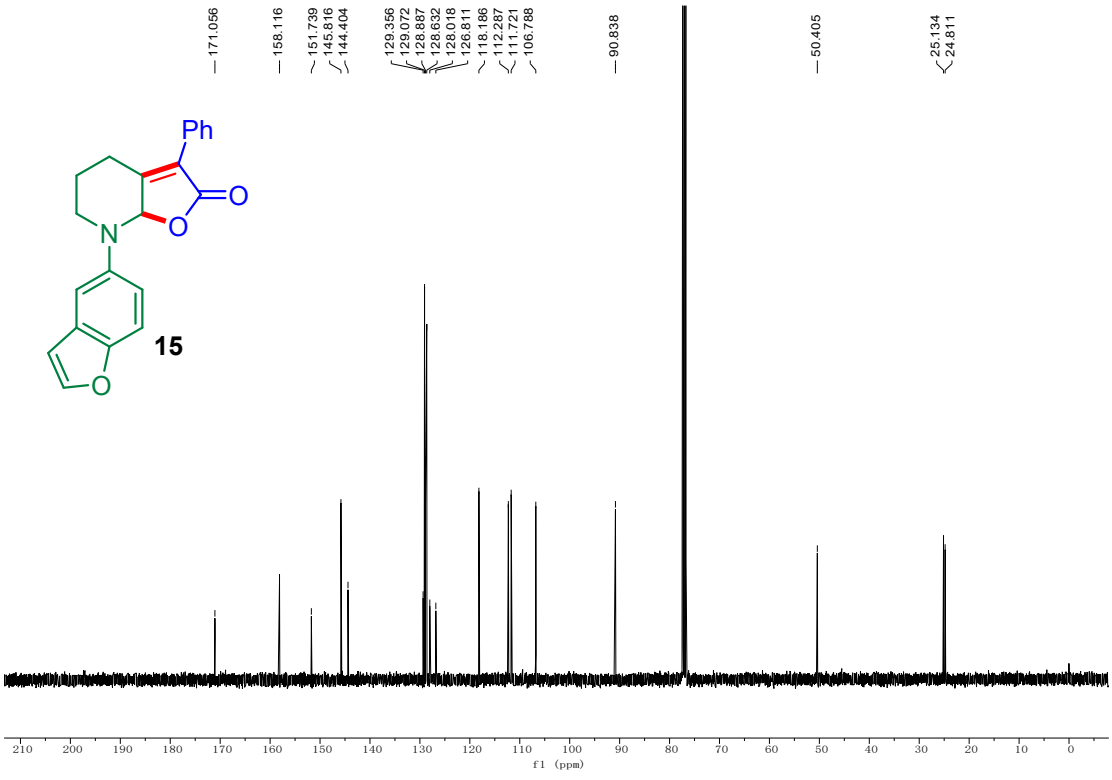
7.428
7.415
7.406
7.388
7.379
7.358
7.337
7.319
7.304
7.278
7.260
7.245
7.232
7.214
7.195
5.729
2.845
2.571
2.422
1.559
1.434
1.262
Ph
O
N
O
Ph(2-Ph)
13
4.04
4.03
4.34
2.11
0.97
4.14
2.30
f1 (ppm)

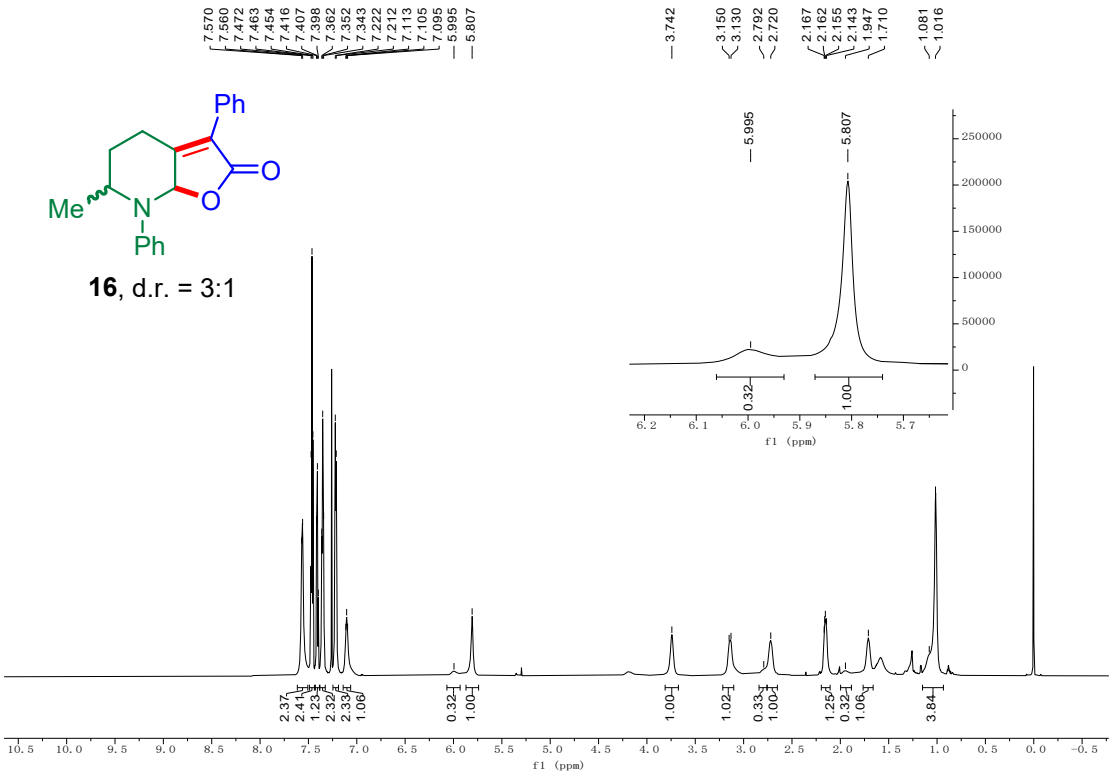

171.223
159.258
145.962
140.220
137.683
131.472
129.523
129.289
128.973
128.774
128.617
128.242
128.006
126.855
125.524
125.041
120.650
88.759
51.159
25.266
25.240
Ph
O
N
O
Ph(2-Ph)
13
f1 (ppm)

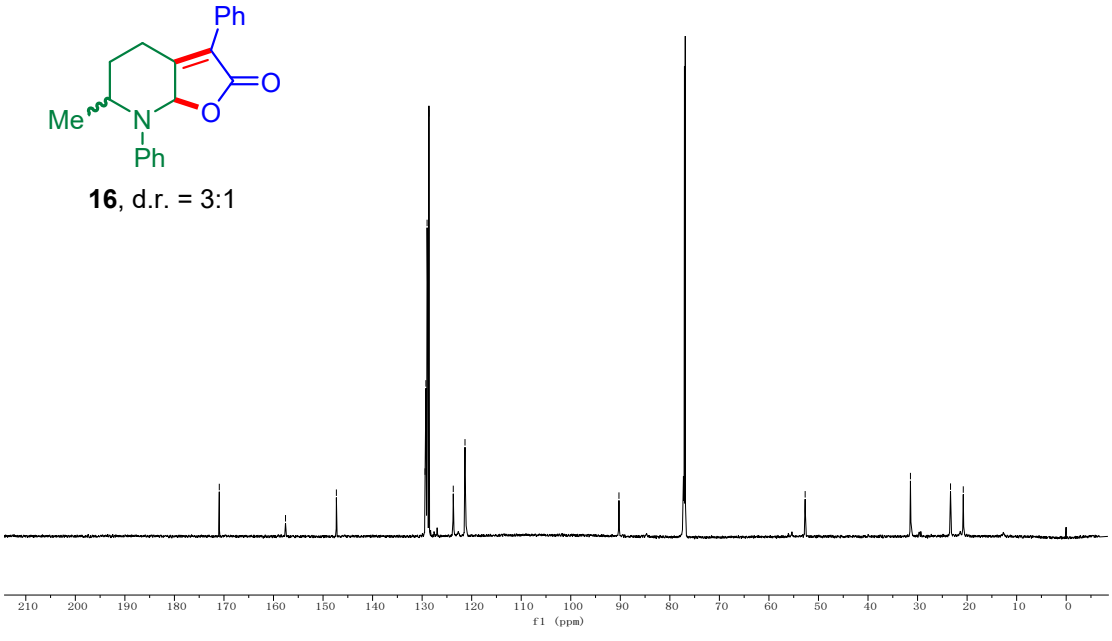

8.208
8.199
8.184
7.861
7.845
7.837
7.711
7.700
7.688
7.589
7.570
7.491
7.481
7.465
7.439
7.421
7.402
5.859
3.485
3.309
2.992
2.619
2.062
2.048
2.031
Ph
O
O
N
Np
14
0.98
1.01
1.03
2.02
6.92
1.00
0.91
0.92
0.93
0.96
2.04
f1 (ppm)

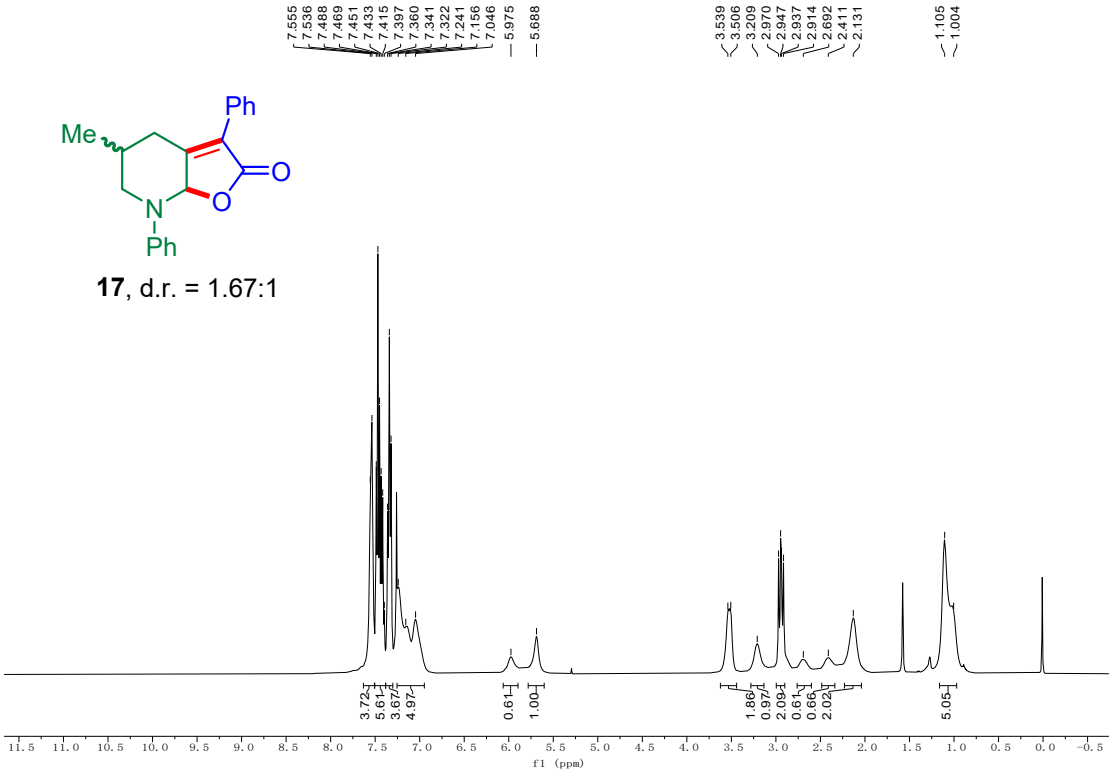

171.191
159.063
145.321
134.837
130.345
129.472
129.041
128.823
128.640
128.247
126.149
125.962
125.645
125.511
123.268
116.810
89.359
53.218
25.896
Ph
O
O
N
Np
14
f1 (ppm)


7.622
7.617
7.554
7.537
7.486
7.467
7.455
7.449
7.428
7.410
7.392
7.220
7.214
7.197
7.191
6.745
6.740
5.668
3.380
3.165
2.597
2.002
Ph
O
N
O
15
O
1.02
2.08
5.16
1.05
1.00
1.03
2.13
1.07
1.04
2.06
f1 (ppm)

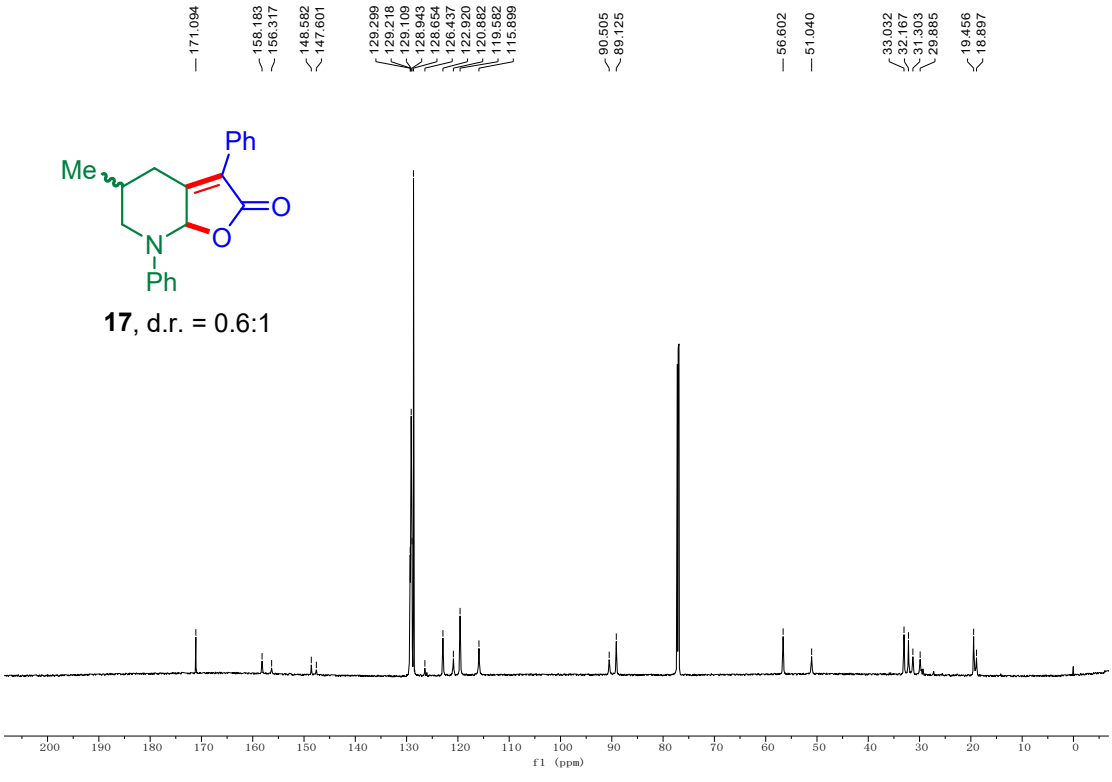

171.056
158.116
151.739
145.816
144.404
129.356
129.072
128.887
128.632
128.018
126.811
118.186
112.287
111.721
106.788
90.838
50.405
25.134
24.811
Ph
O
N
O
15
O
f1 (ppm)


Ph
Me
N
Ph
O
O
16, d.r. = 3:1
f1 (ppm)

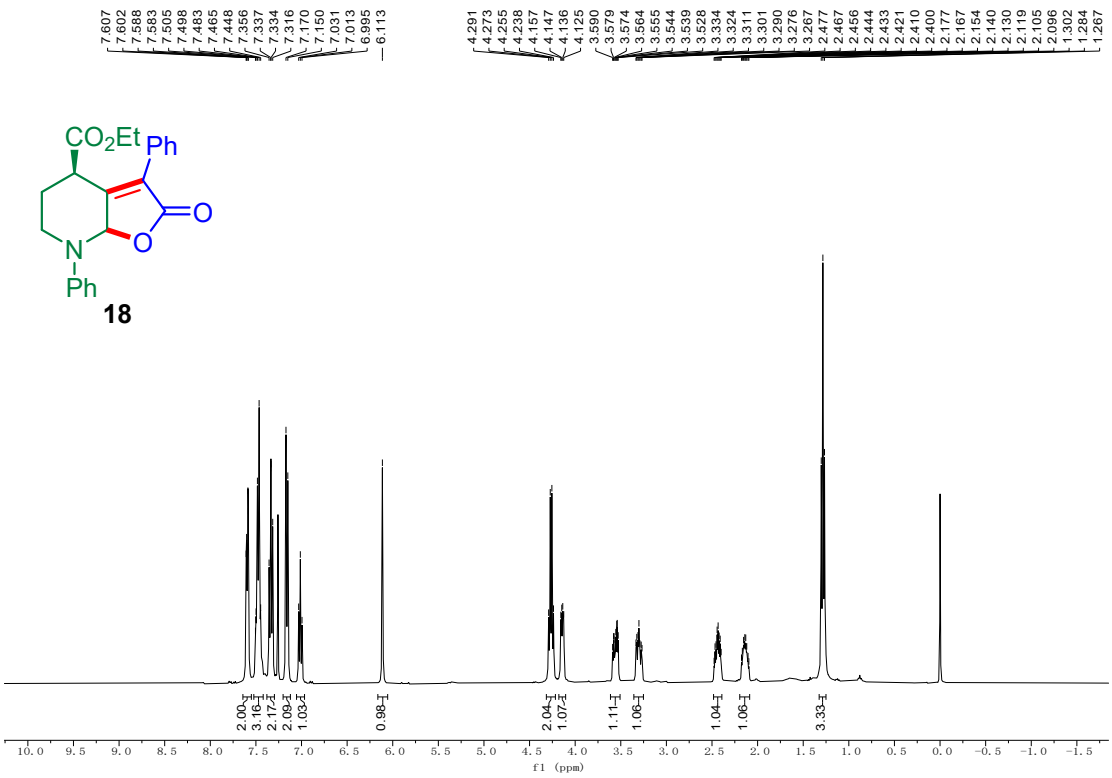

Ph
Me
N
Ph
O
O
16, d.r. = 3:1
f1 (ppm)

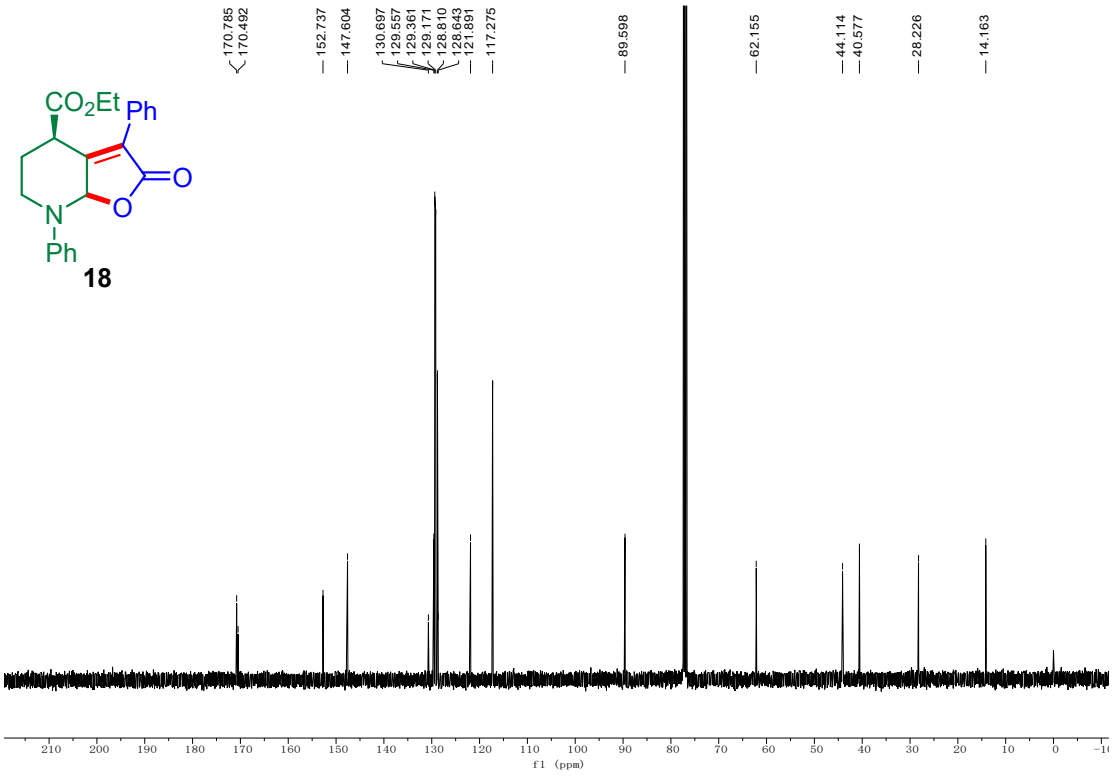


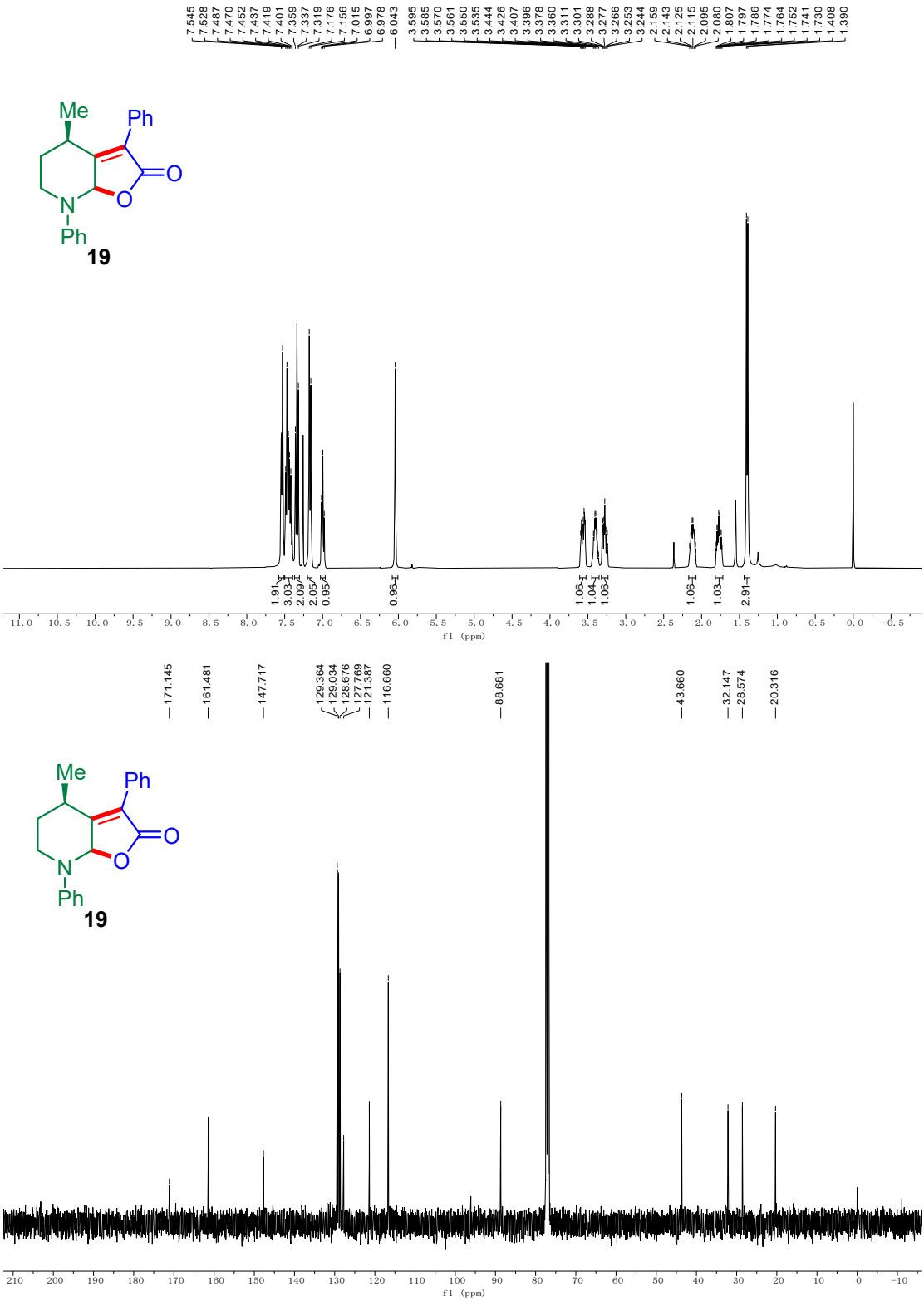
17, d.r. = 1.67:1

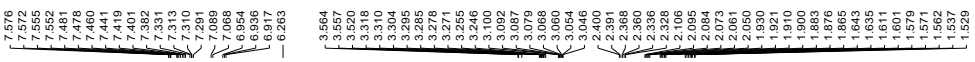


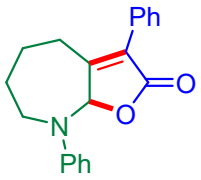
17, d.r. = 0.6:1


7.607
7.602
7.588
7.583
7.505
7.498
7.483
7.465
7.448
7.356
7.337
7.334
7.316
7.170
7.150
7.031
7.013
6.995
6.113
4.291
4.273
4.255
4.238
4.157
4.147
4.136
4.125
3.590
3.579
3.574
3.564
3.555
3.544
3.539
3.528
3.334
3.324
3.311
3.301
3.290
3.276
3.267
2.477
2.467
2.456
2.444
2.433
2.421
2.410
2.400
2.177
2.167
2.154
2.140
2.130
2.119
2.105
2.096
1.302
1.284
1.267
CO2Et
Ph
O
O
N
Ph
18
2.00
3.16
2.17
2.09
1.03
0.98
2.04
1.07
1.11
1.06
1.04
1.06
3.33
f1 (ppm)

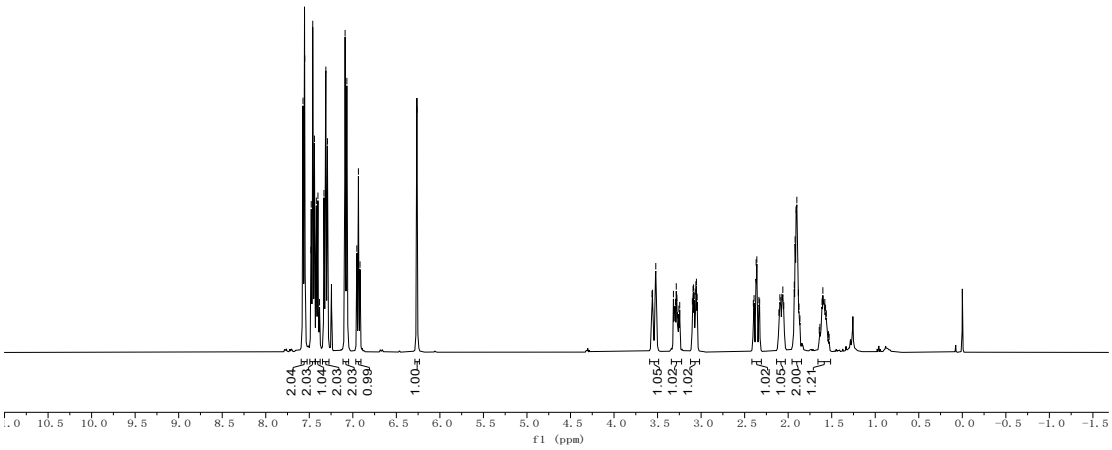

170.785
170.492
152.737
147.604
130.697
129.557
129.361
129.171
128.810
128.643
121.891
117.275
89.598
62.155
44.114
40.577
28.226
14.163
CO2Et
Ph
O
O
N
Ph
18
f1 (ppm)

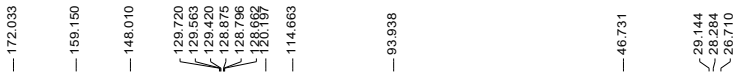

7.545
7.528
7.487
7.470
7.452
7.437
7.419
7.401
7.359
7.337
7.319
7.176
7.156
7.015
6.997
6.978
6.043
3.595
3.585
3.570
3.561
3.550
3.535
3.444
3.426
3.407
3.396
3.378
3.360
3.311
3.301
3.288
3.277
3.266
3.253
3.244
2.159
2.143
2.125
2.115
2.095
2.080
1.807
1.797
1.786
1.774
1.764
1.752
1.741
1.730
1.408
1.390
Me
Ph
O
O
N
Ph
19
1.91
3.03
2.09
2.05
0.95
0.96
1.06
1.04
1.06
1.06
1.03
2.91
f1 (ppm)
171.145
161.481
147.717
129.364
129.034
128.676
127.769
121.387
116.660
88.681
43.660
32.147
28.574
20.316
Me
Ph
O
O
N
Ph
19
f1 (ppm)

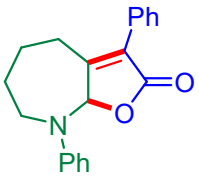

7.576
7.572
7.555
7.552
7.481
7.478
7.460
7.441
7.419
7.401
7.382
7.331
7.313
7.310
7.291
7.089
7.068
6.954
6.936
6.917
6.263
3.564
3.557
3.520
3.318
3.310
3.304
3.295
3.285
3.278
3.271
3.255
3.246
3.100
3.092
3.087
3.079
3.068
3.060
3.054
3.046
2.400
2.391
2.368
2.360
2.336
2.328
2.106
2.095
2.084
2.073
2.061
2.050
1.930
1.921
1.910
1.900
1.883
1.876
1.865
1.643
1.635
1.611
1.601
1.579
1.571
1.562
1.537
1.529


Ph
O
O
N
Ph

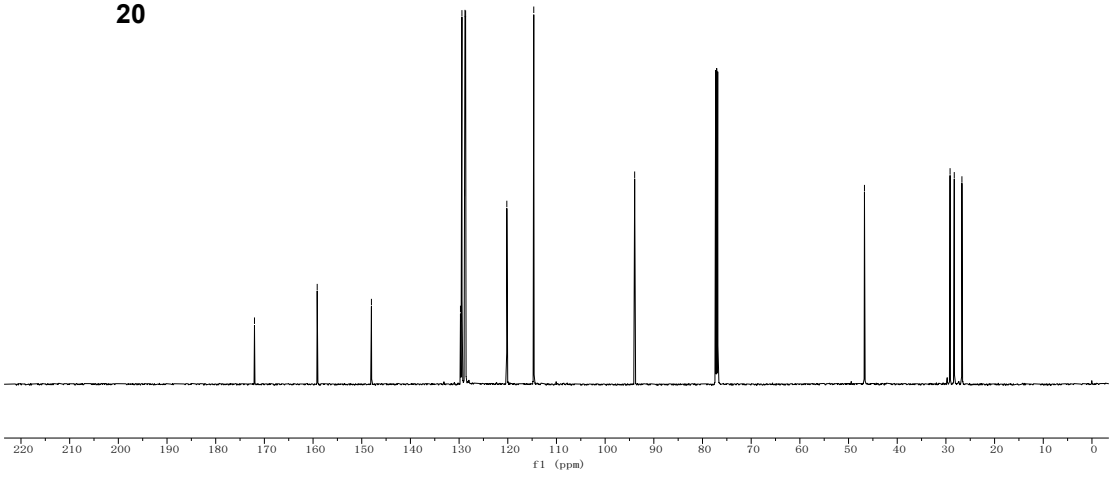
20

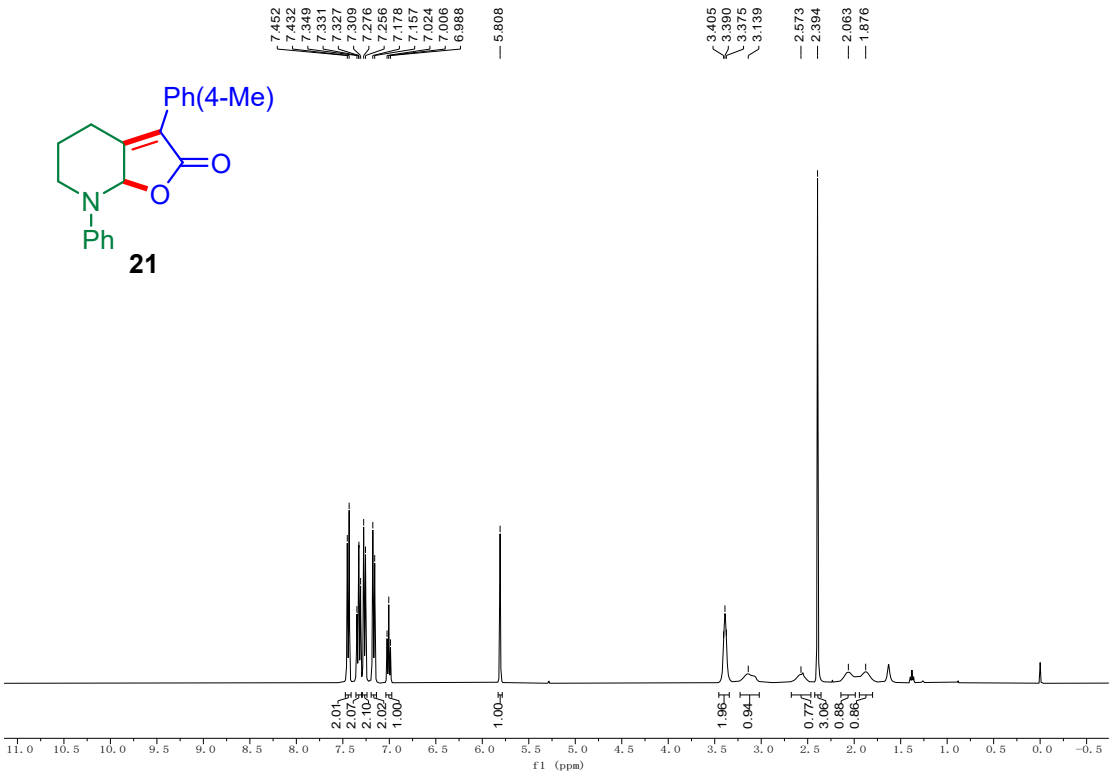

2.04
2.03
1.04
2.03
2.03
0.99
1.00
1.05
1.02
1.02
1.02
1.05
2.00
1.21
f1 (ppm)

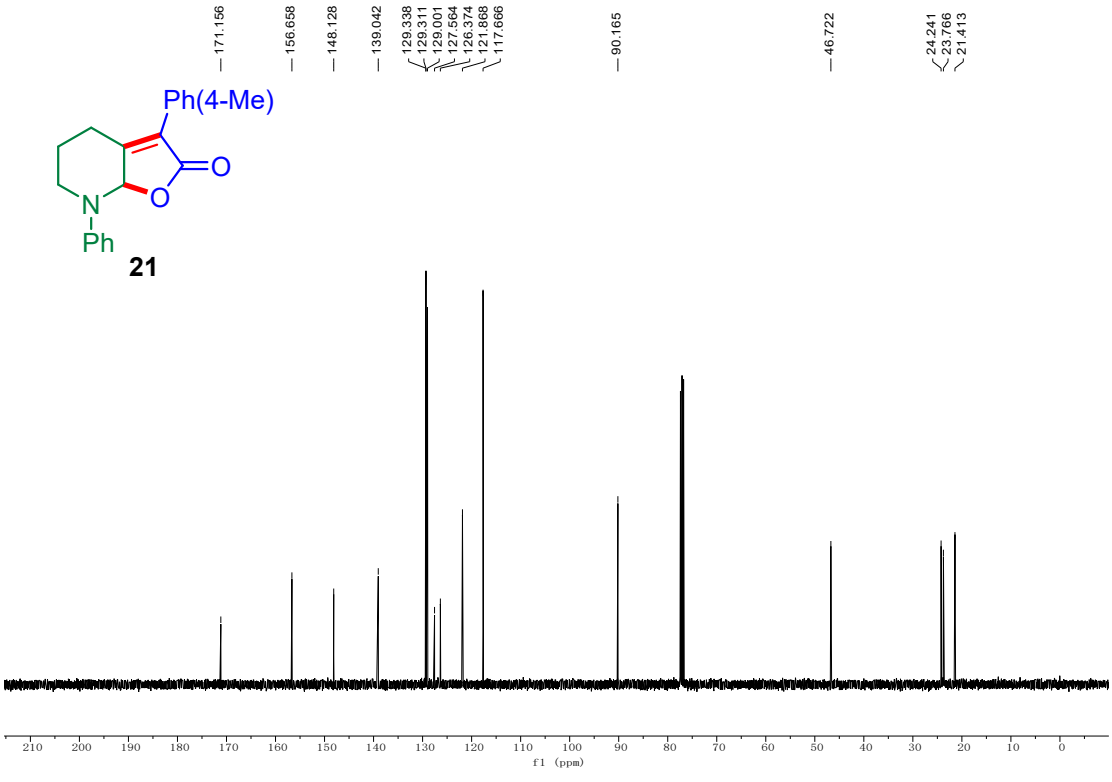

172.033
159.150
148.010
129.720
129.563
129.420
128.875
128.796
120.197
114.663
93.938
46.731
29.144
28.284
26.710

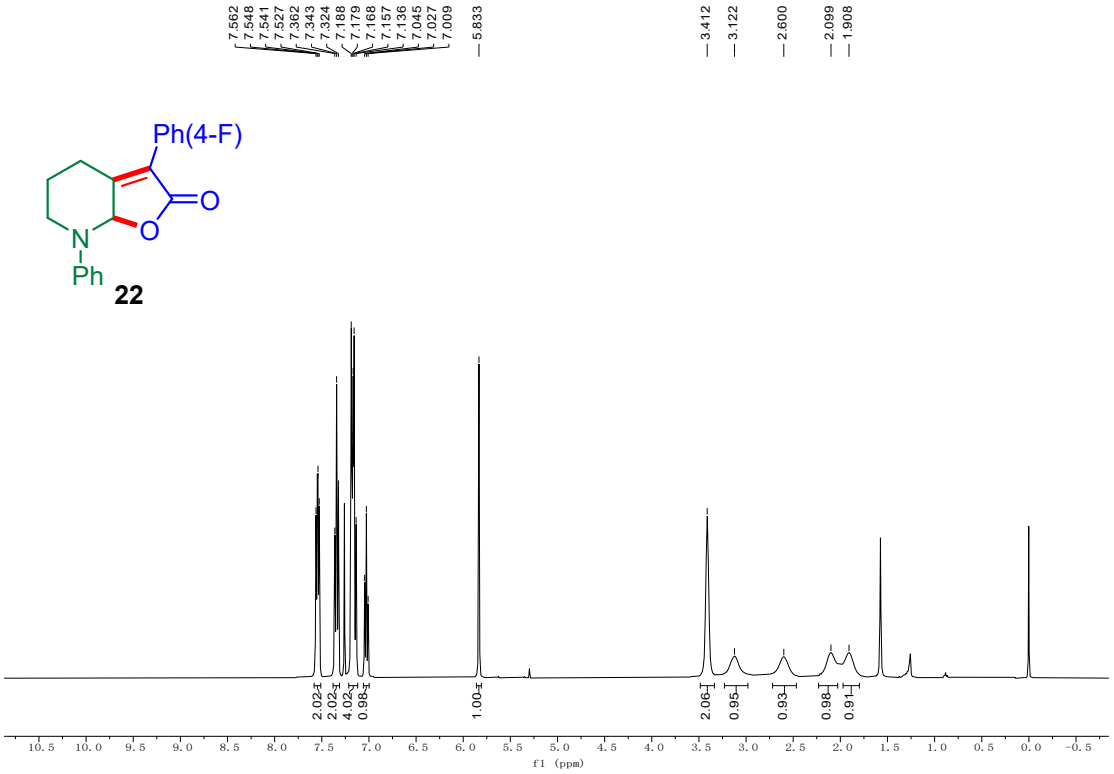

Ph
O
O
N
Ph

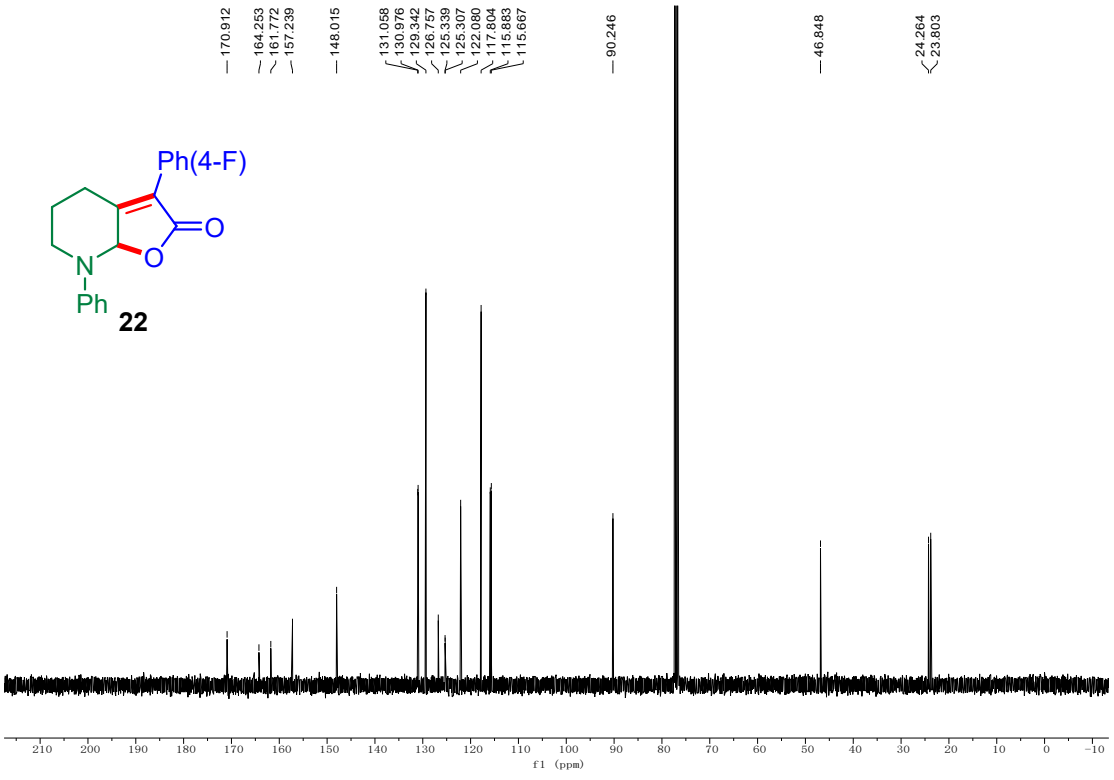
20

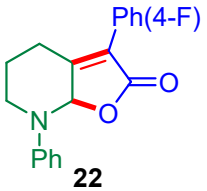

f1 (ppm)


7.452
7.432
7.349
7.331
7.327
7.309
7.276
7.256
7.178
7.157
7.024
7.006
6.988
5.808
3.405
3.390
3.375
3.139
2.573
2.394
2.063
1.876
Ph(4-Me)
O
O
N
Ph
21
2.01
2.07
2.10
2.02
1.00
1.00
1.96
0.94
0.77
3.06
0.88
0.86
f1 (ppm)

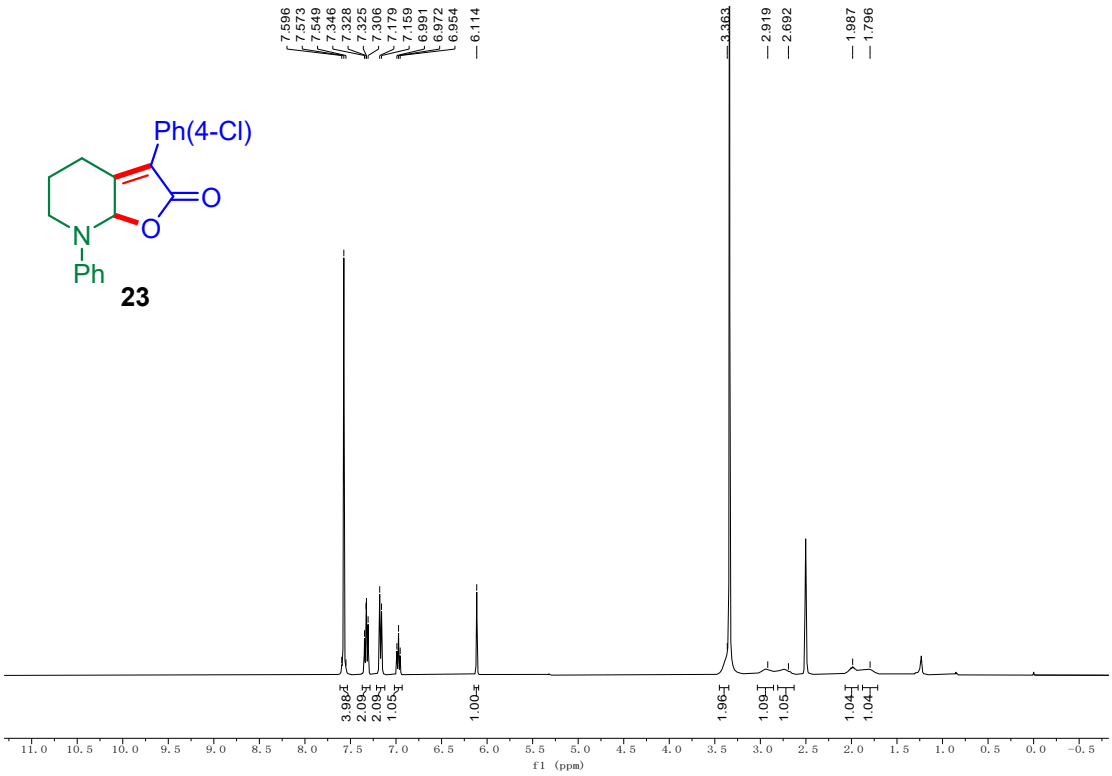

171.156
156.658
148.128
139.042
129.338
129.311
129.001
127.564
126.374
121.868
117.666
90.165
46.722
24.241
23.766
21.413
Ph(4-Me)
O
O
N
Ph
21
f1 (ppm)

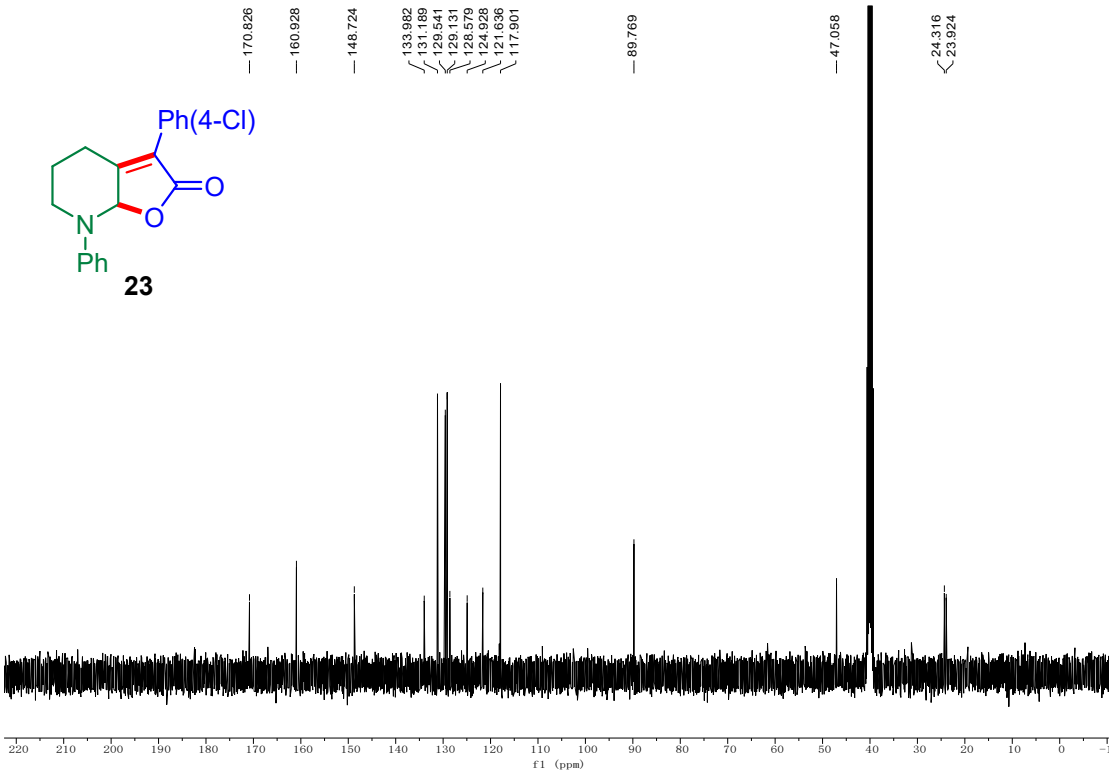

7.562
7.548
7.541
7.527
7.362
7.343
7.324
7.188
7.179
7.168
7.157
7.136
7.045
7.027
7.009
5.833
3.412
3.122
2.600
2.099
1.908
Ph(4-F)
O
O
N
Ph
22
2.02
2.02
4.02
0.98
1.00
2.06
0.95
0.93
0.98
0.91
f1 (ppm)

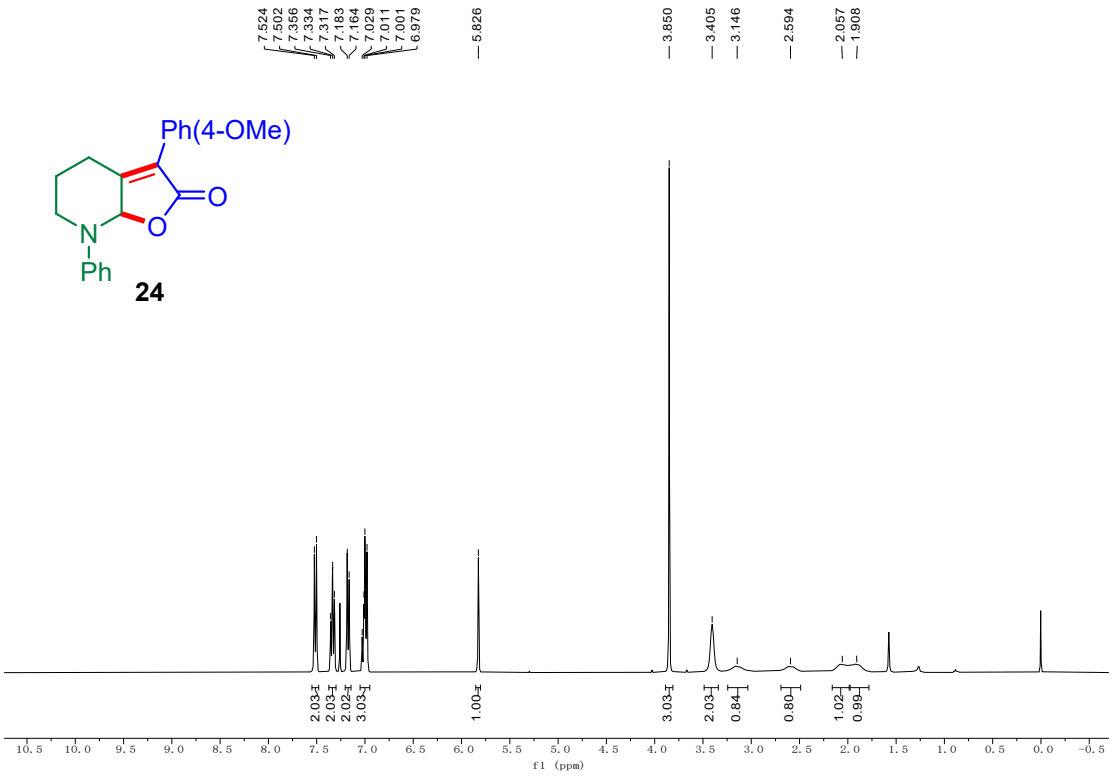

170.912
164.253
161.772
157.239
148.015
131.058
130.976
129.342
126.757
125.339
125.307
122.080
117.804
115.883
115.667
90.246
46.848
24.264
23.803
Ph(4-F)
O
O
N
Ph
22
f1 (ppm)

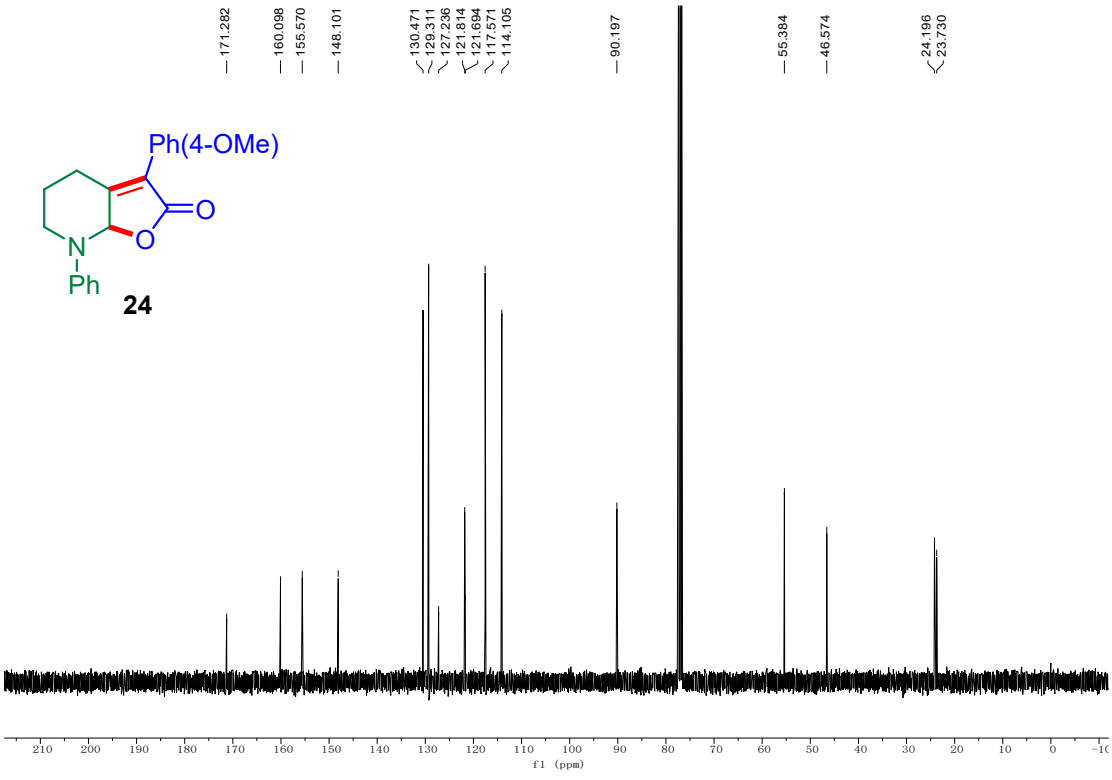


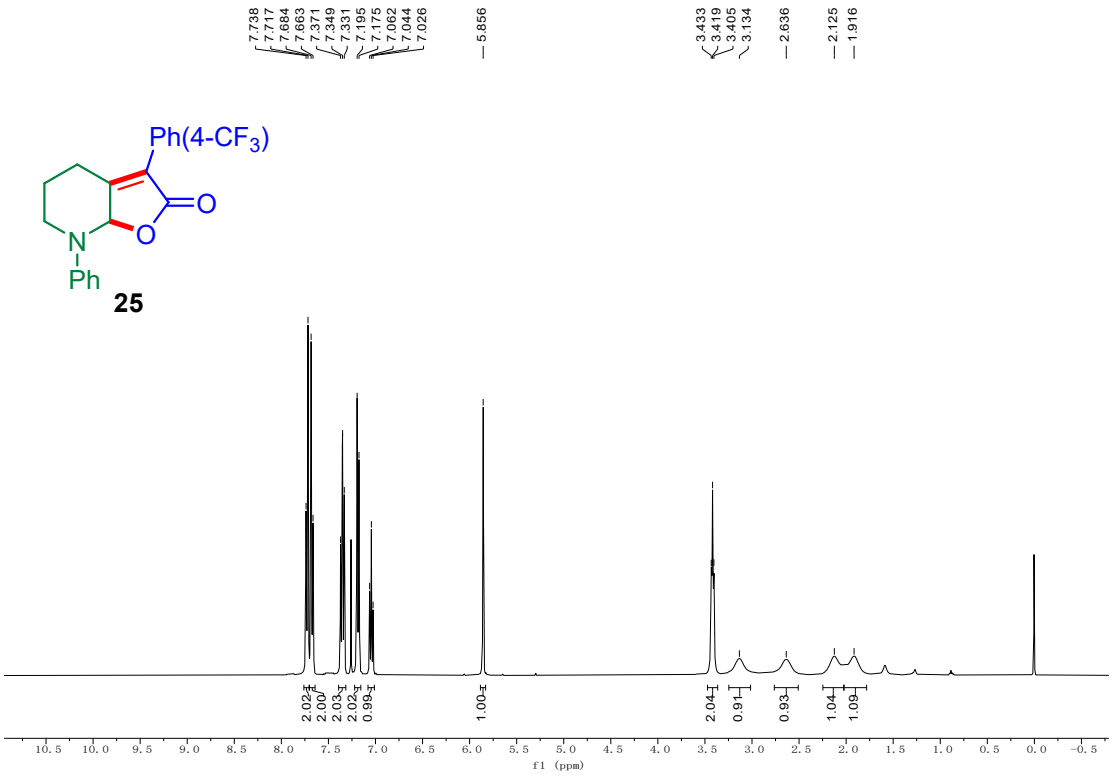
22

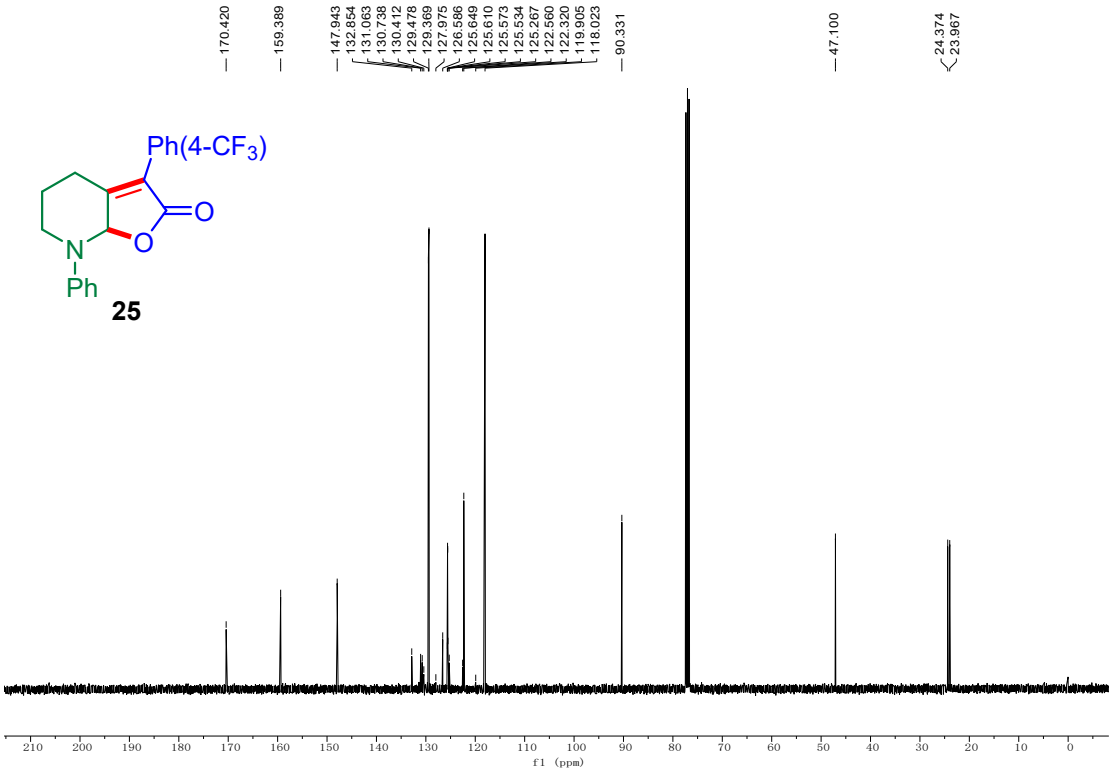

7.596
7.573
7.549
7.346
7.328
7.325
7.306
7.179
7.159
6.991
6.972
6.954
6.114
3.363
2.919
2.692
1.987
1.796
Ph(4-Cl)
O
O
N
Ph
23
3.98
2.09
2.09
1.05
1.00
1.96
1.09
1.05
1.04
1.04
f1 (ppm)

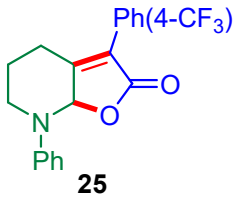

170.826
160.928
148.724
133.982
131.189
129.541
129.131
128.579
124.928
121.636
117.901
89.769
47.058
24.316
23.924
Ph(4-Cl)
O
O
N
Ph
23
f1 (ppm)


7.524
7.502
7.356
7.334
7.317
7.183
7.164
7.029
7.011
7.001
6.979
5.826
3.850
3.405
3.146
2.594
2.057
1.908
Ph(4-OMe)
O
N
O
Ph
24
2.03
2.03
2.02
3.03
1.00
3.03
2.03
0.84
0.80
1.02
0.99
f1 (ppm)

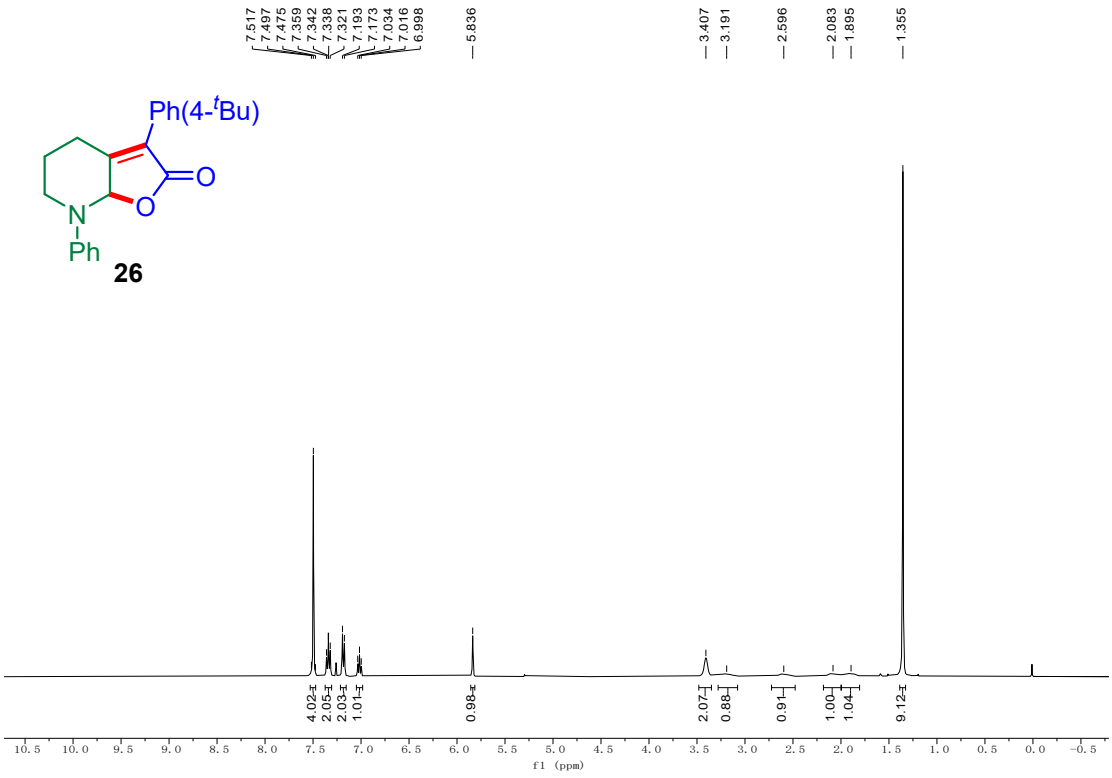

171.282
160.098
155.570
148.101
130.471
129.311
127.236
121.814
121.694
117.571
114.105
90.197
55.384
46.574
24.196
23.730
Ph(4-OMe)
O
N
O
Ph
24
f1 (ppm)

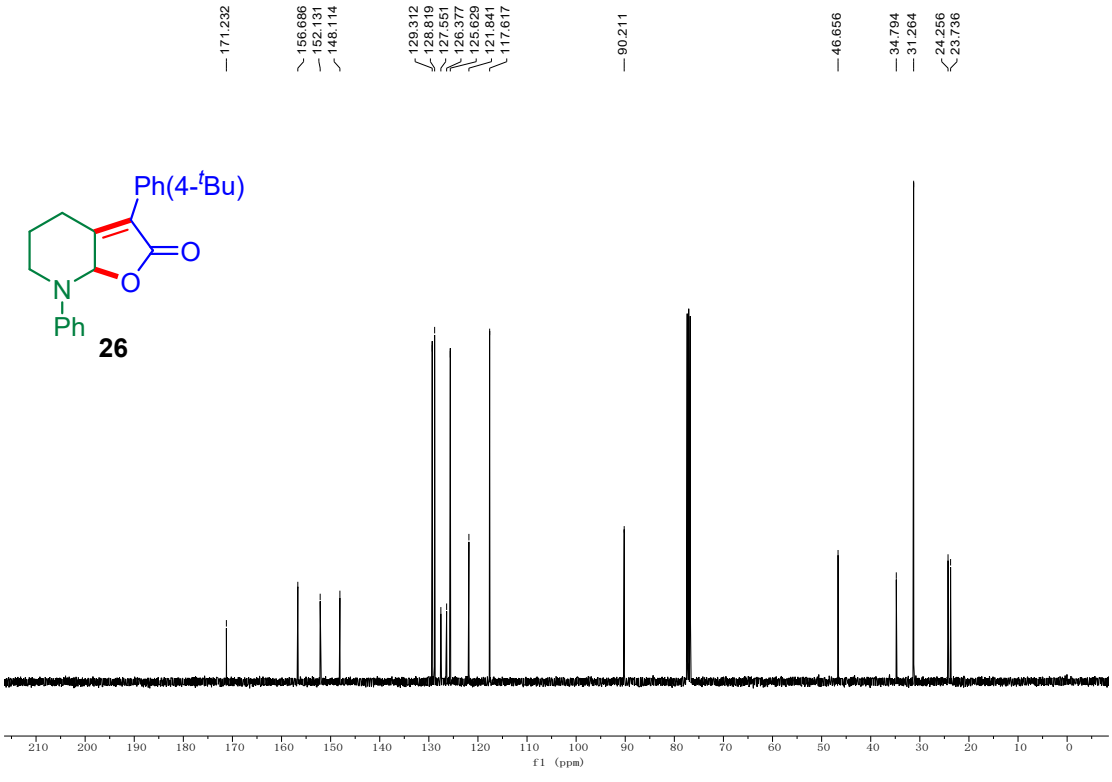

7.738
7.717
7.684
7.663
7.371
7.349
7.331
7.195
7.175
7.062
7.044
7.026
5.856
3.433
3.419
3.405
3.134
2.636
2.125
1.916
Ph(4-CF3)
O
O
N
Ph
25
2.02
2.00
2.03
2.02
0.99
1.00
2.04
0.91
0.93
1.04
1.09
f1 (ppm)

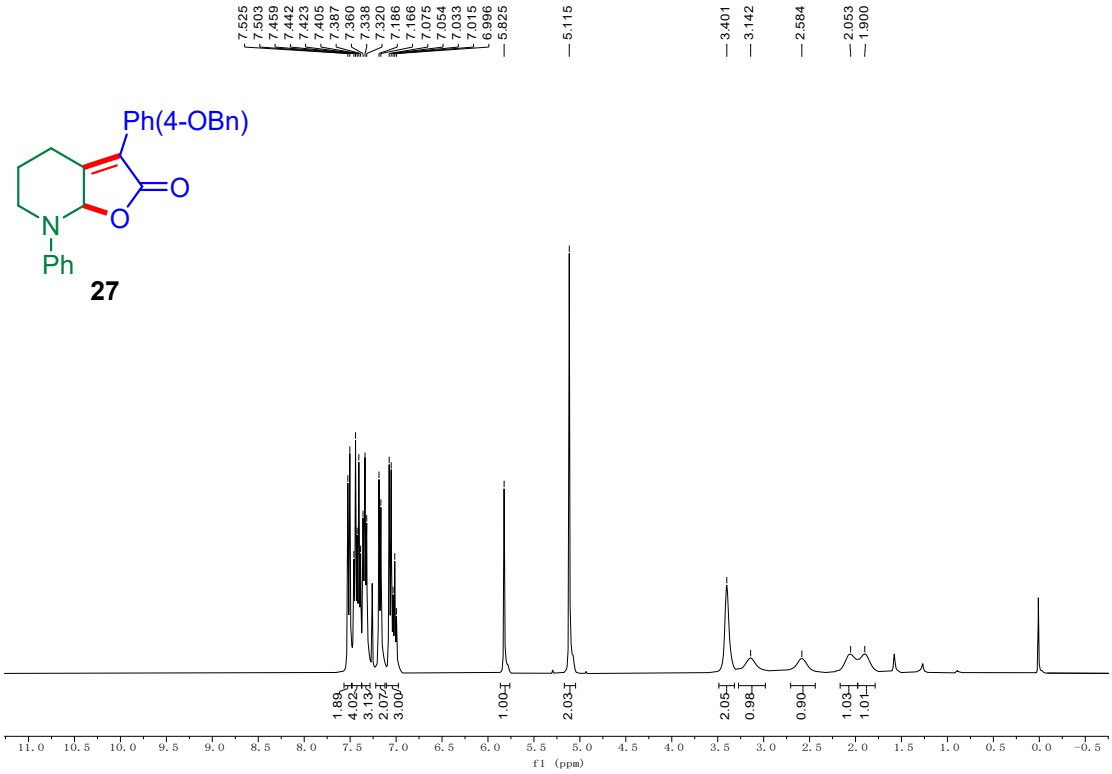

170.420
159.389
147.943
132.854
131.063
130.738
130.412
129.478
129.369
127.975
126.586
125.649
125.610
125.573
125.534
125.267
122.560
122.320
119.905
118.023
90.331
47.100
24.374
23.967
Ph(4-CF3)
O
O
N
Ph
25
f1 (ppm)

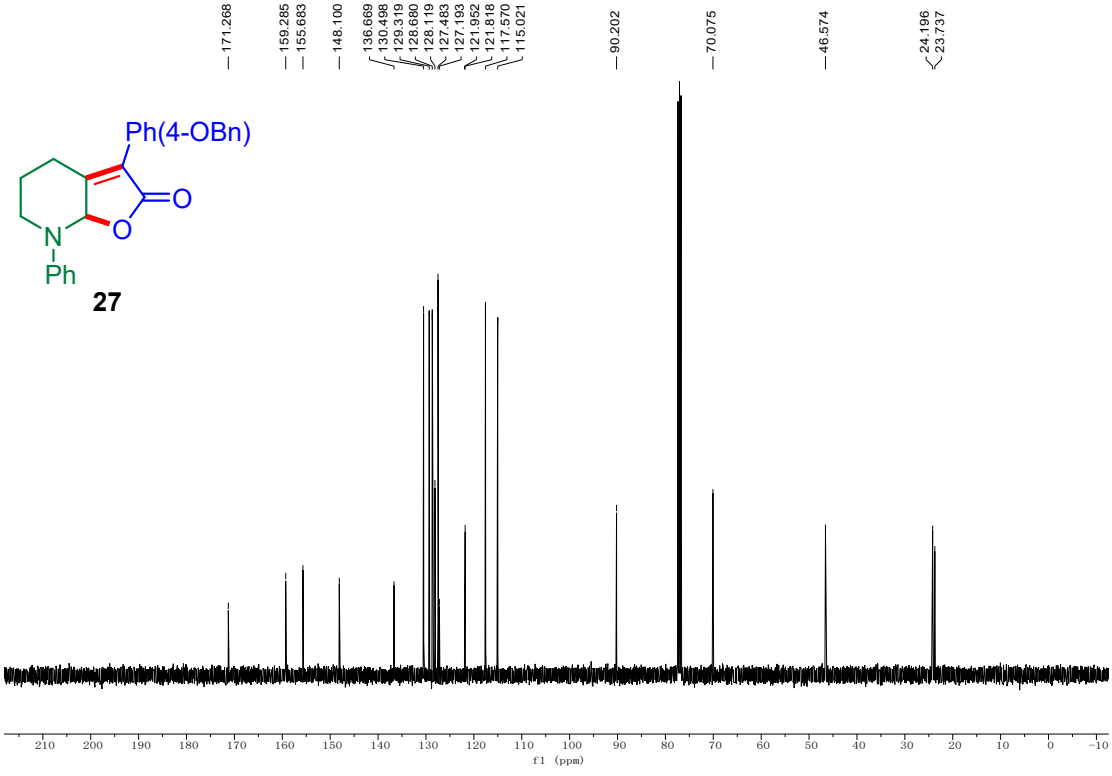


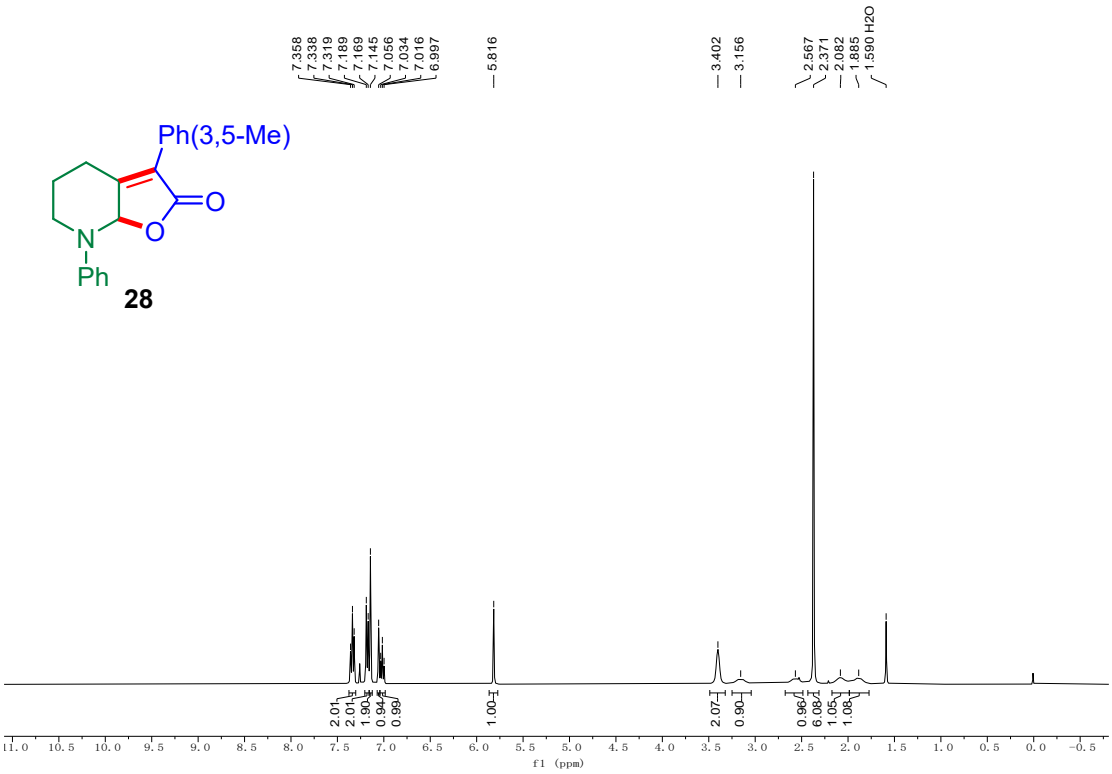
25

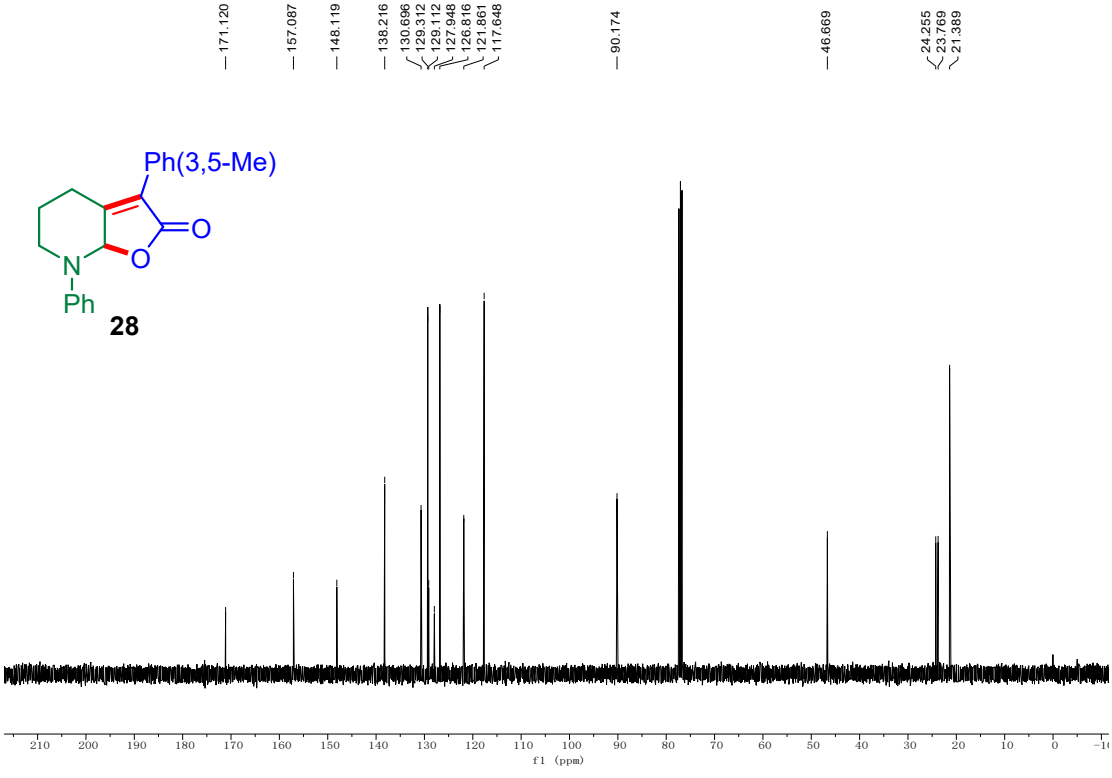

7.517
7.497
7.475
7.359
7.342
7.338
7.321
7.193
7.173
7.034
7.016
6.998
5.836
3.407
3.191
2.596
2.083
1.895
1.355
Ph(4-tBu)
O
O
N
Ph
26
4.02
2.05
2.03
1.01
0.98
2.07
0.88
0.91
1.00
1.04
9.12
f1 (ppm)

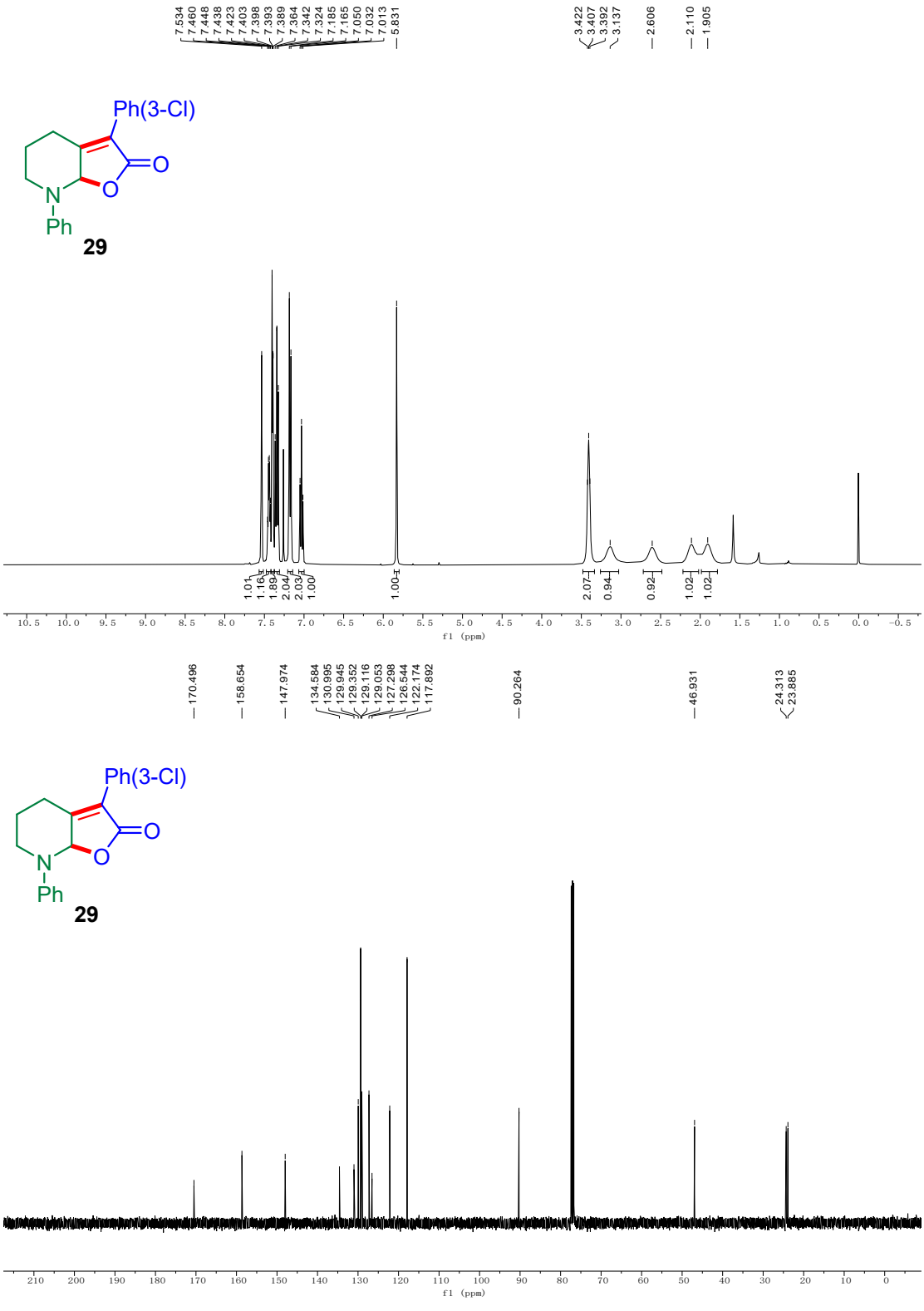

171.232
156.686
152.131
148.114
129.312
128.819
127.551
126.377
125.629
121.841
117.617
90.211
46.656
34.794
31.264
24.256
23.736
Ph(4-tBu)
O
O
N
Ph
26
f1 (ppm)

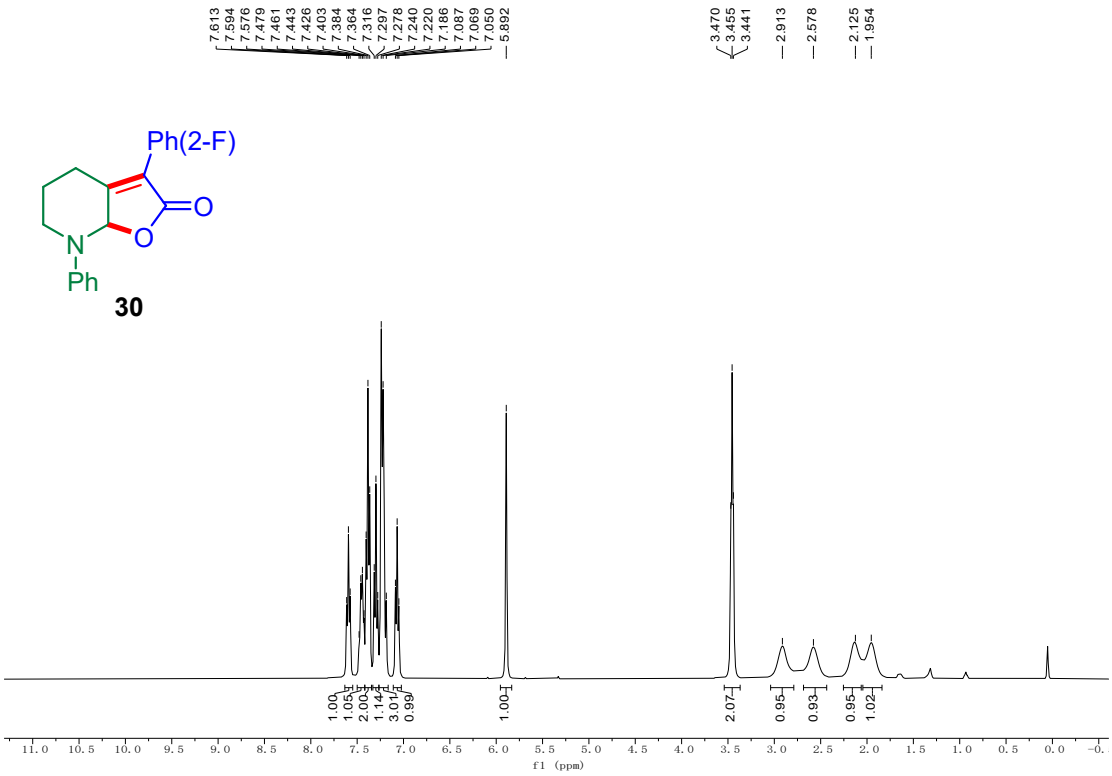

7.525
7.503
7.459
7.442
7.423
7.405
7.387
7.360
7.338
7.320
7.186
7.166
7.075
7.054
7.033
7.015
6.996
5.825
5.115
3.401
3.142
2.584
2.053
1.900
Ph(4-OBn)
O
N
O
Ph
27
1.89
4.02
3.13
2.07
3.00
1.00
2.03
2.05
0.98
0.90
1.03
1.01
f1 (ppm)

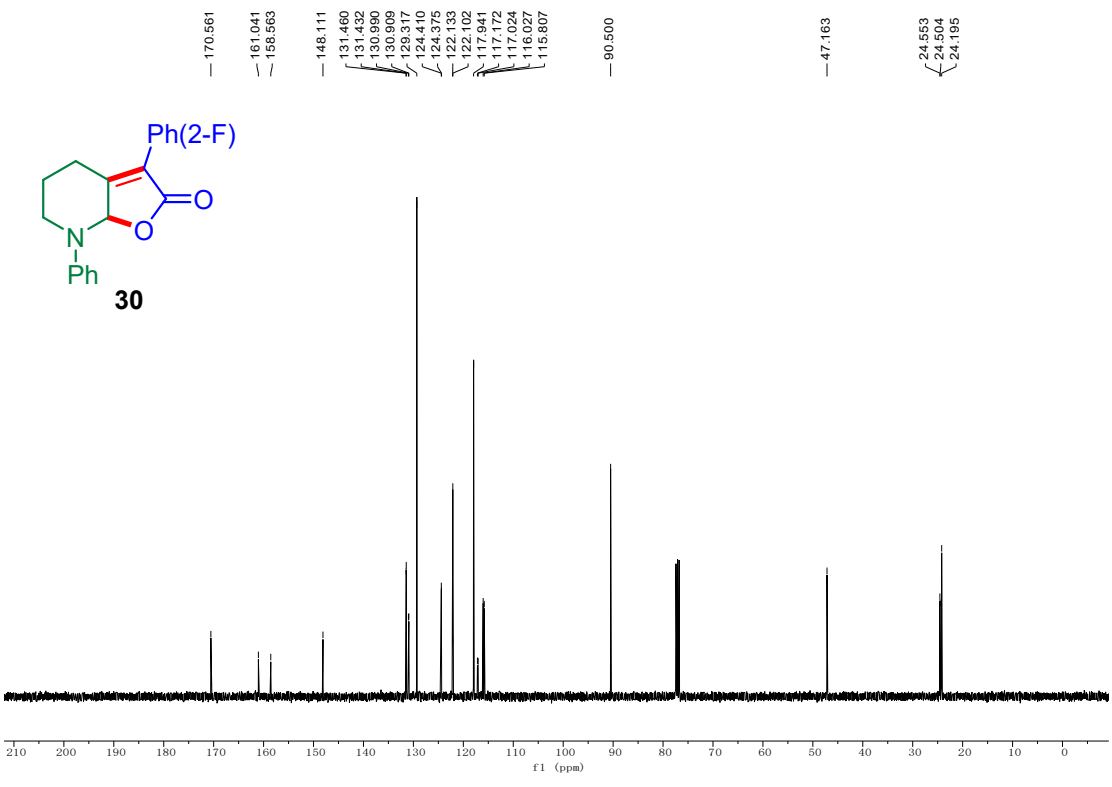

171.268
159.285
155.683
148.100
136.669
130.498
129.319
128.680
128.119
127.483
127.193
121.952
121.818
117.570
115.021
90.202
70.075
46.574
24.196
23.737
Ph(4-OBn)
O
N
O
Ph
27
f1 (ppm)

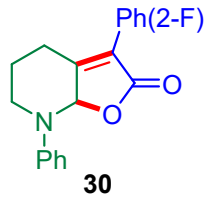

7.358
7.338
7.319
7.189
7.169
7.145
7.056
7.034
7.016
6.997
5.816
3.402
3.156
2.567
2.371
2.082
1.885
1.590 H2O
Ph(3,5-Me)
O
N
O
Ph
28
2.01
2.01
1.90
0.94
0.99
1.00
2.07
0.90
0.96
6.08
1.05
1.08
f1 (ppm)


171.120
157.087
148.119
138.216
130.696
129.312
129.112
127.948
126.816
121.861
117.648
90.174
46.669
24.255
23.769
21.389
Ph(3,5-Me)
O
N
O
Ph
28
f1 (ppm)


7.534
7.460
7.448
7.438
7.423
7.403
7.398
7.393
7.389
7.364
7.342
7.324
7.185
7.165
7.050
7.032
7.013
5.831
3.422
3.407
3.392
3.137
2.606
2.110
1.905
Ph(3-Cl)
O
N
O
Ph
29
1.01
1.16
1.89
2.04
2.03
1.00
1.00
2.07
0.94
0.92
1.02
1.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
170.496
158.654
147.974
134.584
130.995
129.945
129.352
129.116
129.053
127.298
126.544
122.174
117.892
90.264
46.931
24.313
23.885
Ph(3-Cl)
O
N
O
Ph
29
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

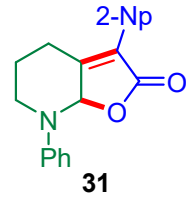

7.613
7.594
7.576
7.479
7.461
7.443
7.426
7.403
7.384
7.364
7.316
7.297
7.278
7.240
7.220
7.186
7.087
7.069
7.050
5.892
3.470
3.455
3.441
2.913
2.578
2.125
1.954
Ph(2-F)
O
N
O
Ph
30
1.00
1.05
2.00
1.14
3.01
0.99
1.00
2.07
0.95
0.93
0.95
1.02
f1 (ppm)


170.561
161.041
158.563
148.111
131.460
131.432
130.990
130.909
129.317
124.410
124.375
122.133
122.102
117.941
117.172
117.024
116.027
115.807
90.500
47.163
24.553
24.504
24.195
Ph(2-F)
O
N
O
Ph
30
f1 (ppm)

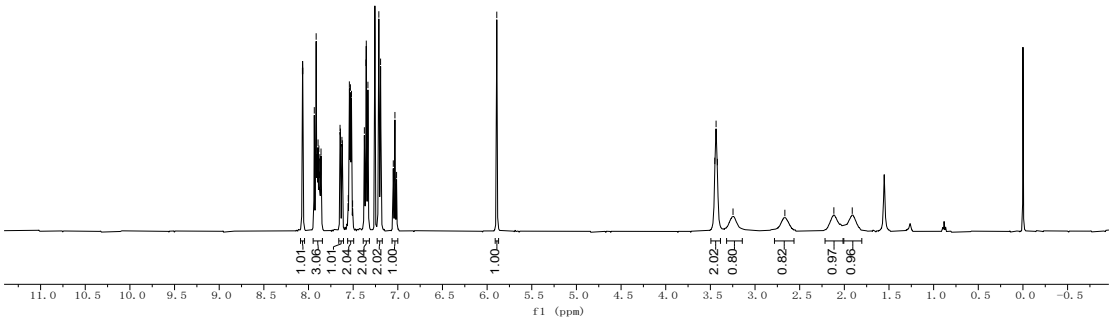


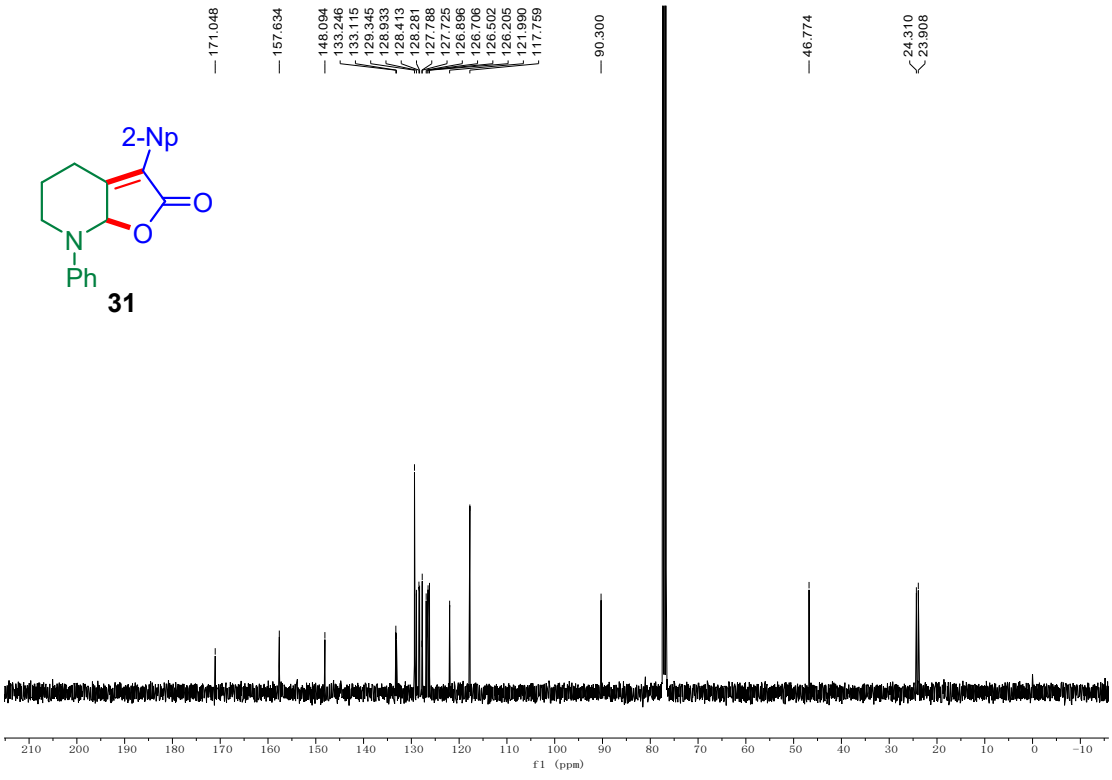
30


8.068
8.064
7.935
7.914
7.903
7.893
7.884
7.877
7.873
7.864
7.860
7.647
7.643
7.626
7.621
7.555
7.543
7.538
7.531
7.524
7.519
7.506
7.375
7.357
7.353
7.335
7.213
7.193
7.051
7.032
7.014
5.892
3.451
3.436
3.422
3.247
2.666
2.117
1.911


2-Np
O
N
O
Ph

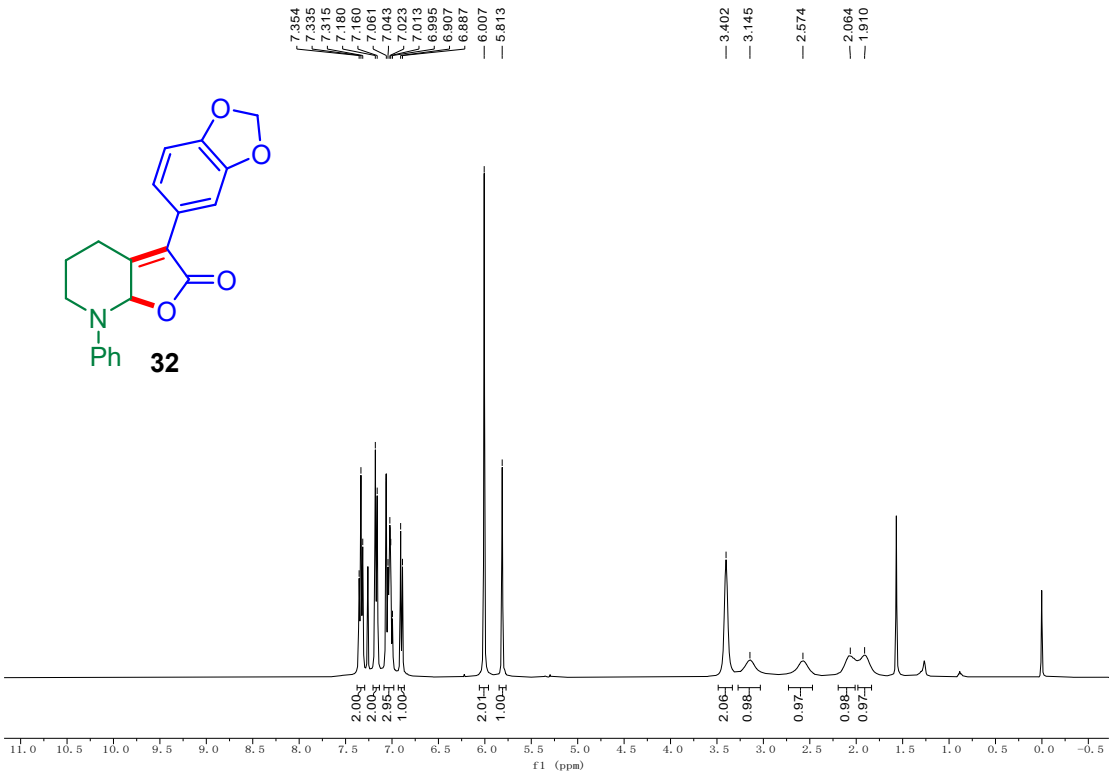
31

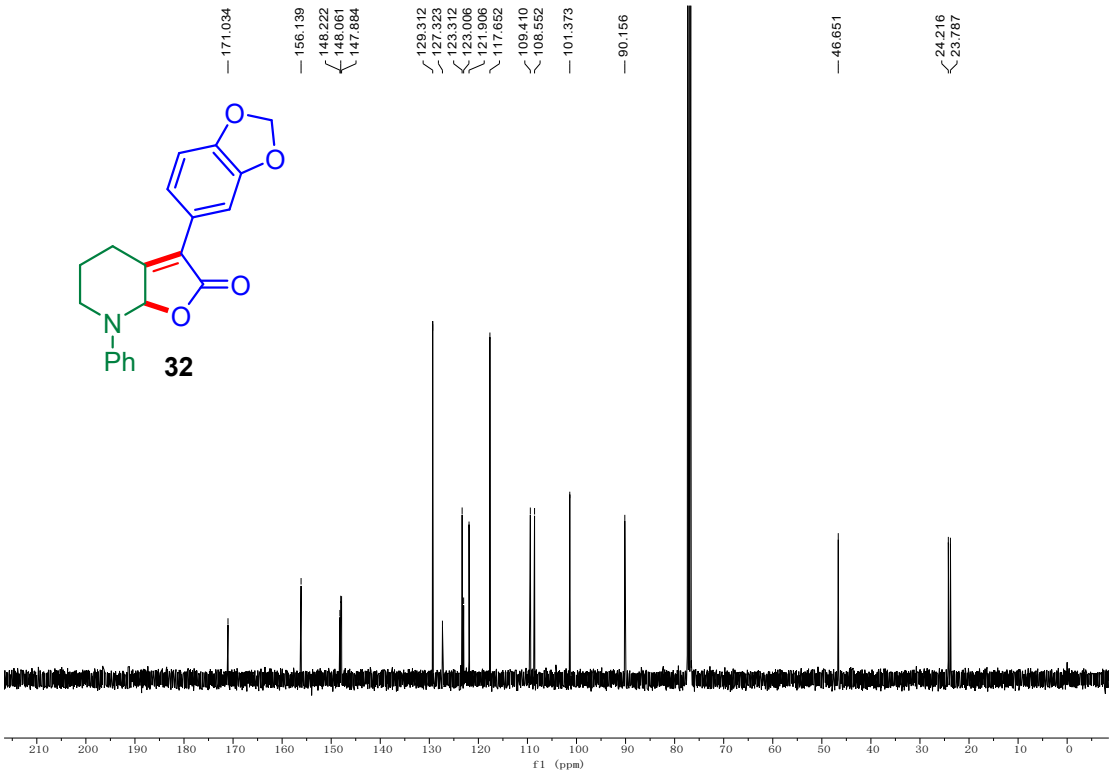

1.01
3.06
1.01
2.04
2.04
2.02
1.00
1.00
2.02
0.80
0.82
0.97
0.96
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)

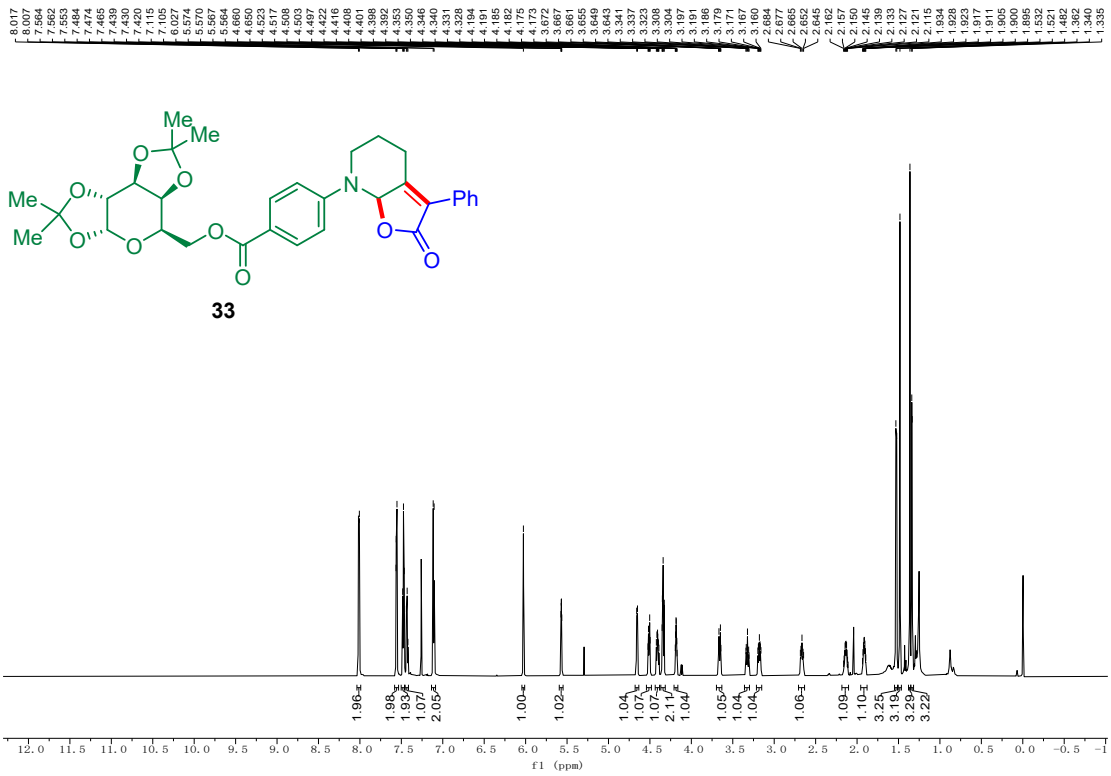

171.048
157.634
148.094
133.246
133.115
129.345
128.933
128.413
128.281
127.788
127.725
126.896
126.706
126.502
126.205
121.990
117.759
90.300
46.774
24.310
23.908
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

2-Np
O
N
O
Ph

31


7.354
7.335
7.315
7.180
7.160
7.061
7.043
7.023
7.013
6.995
6.907
6.887
6.007
5.813
3.402
3.145
2.574
2.064
1.910
O
O
O
O
N
Ph
32
2.00
2.00
2.95
1.00
2.01
1.00
2.06
0.98
0.97
0.98
0.97
f1 (ppm)


171.034
156.139
148.222
148.061
147.884
129.312
127.323
123.312
123.006
121.906
117.652
109.410
108.552
101.373
90.156
46.651
24.216
23.787
O
O
O
O
N
Ph
32
f1 (ppm)



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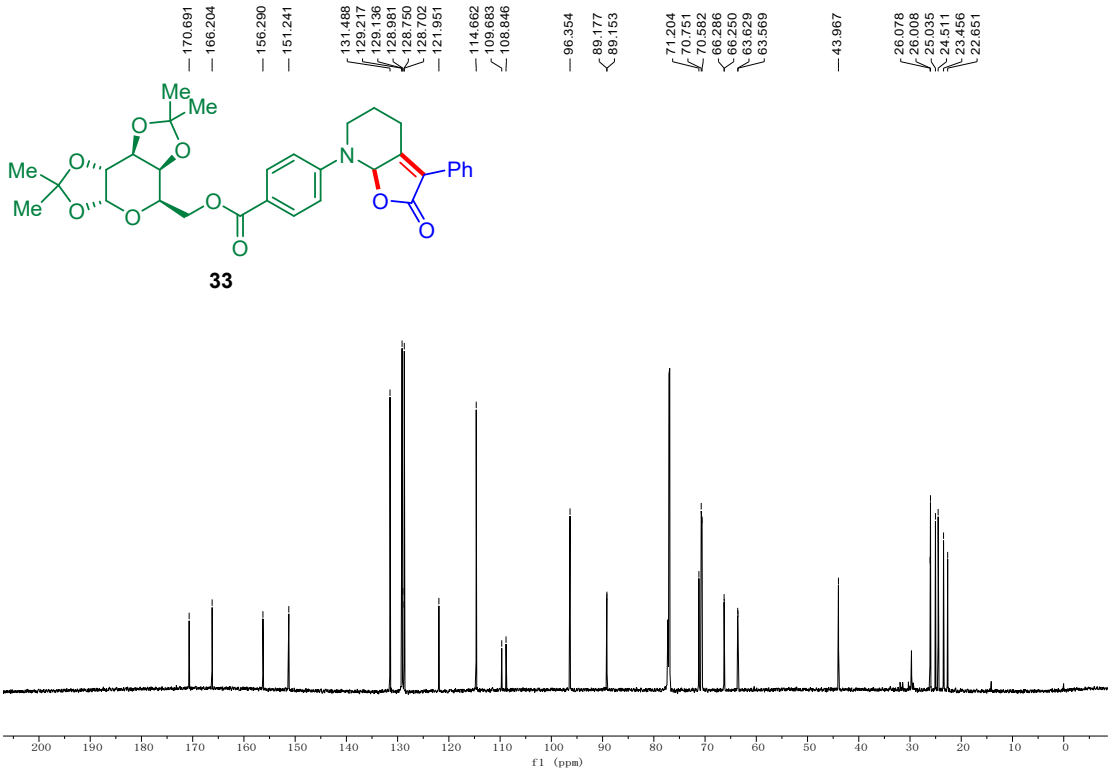

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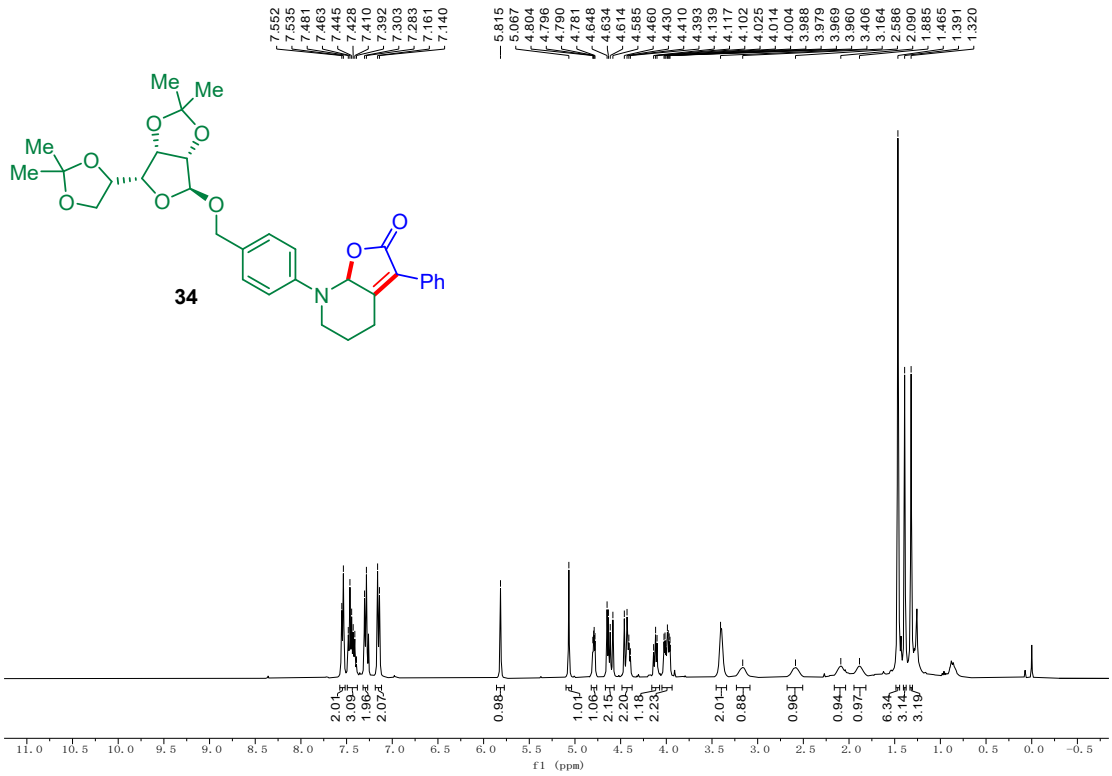
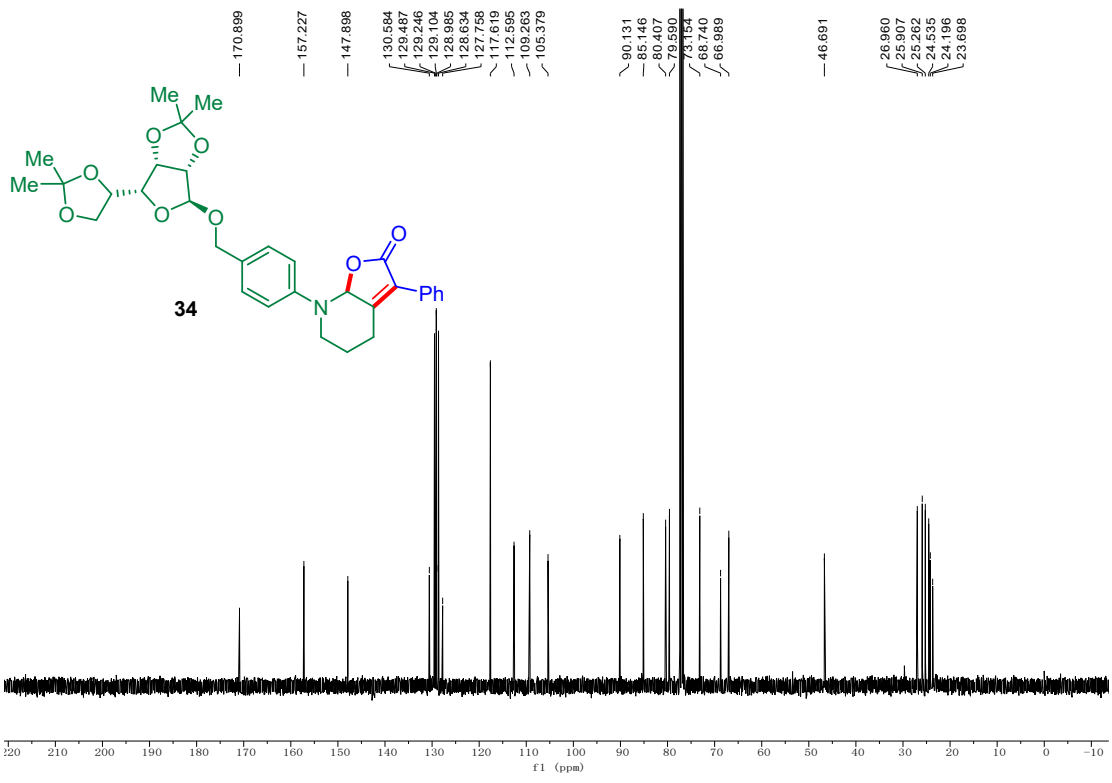
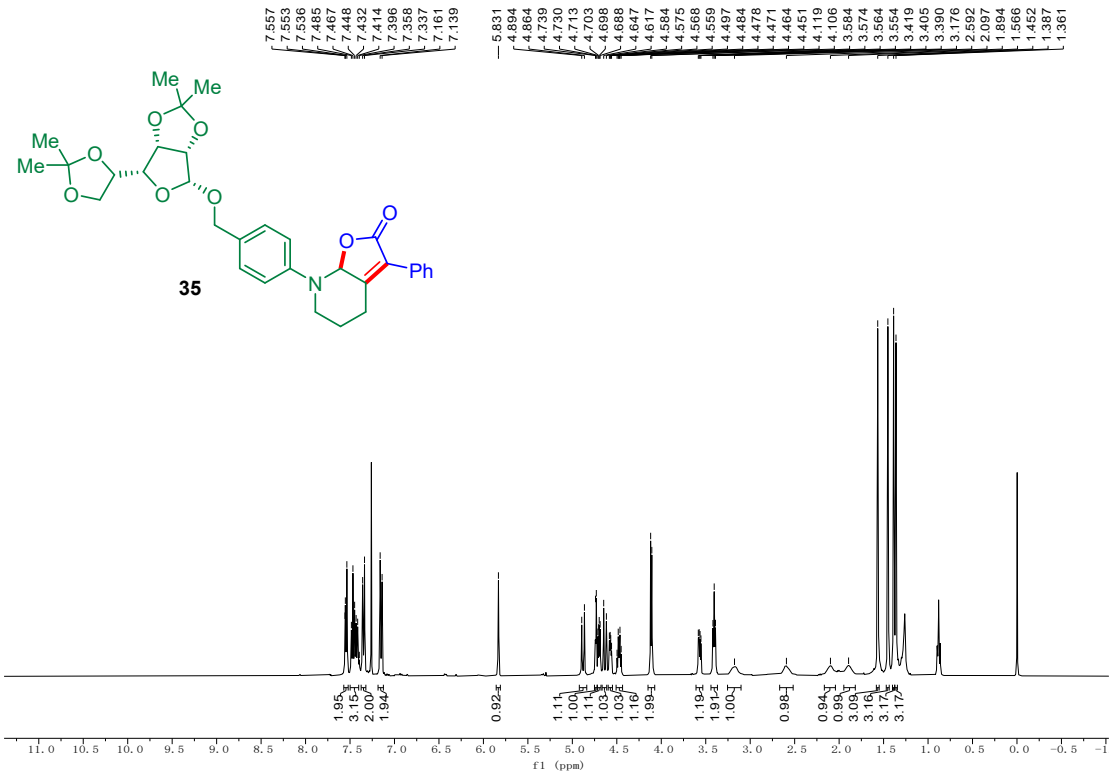
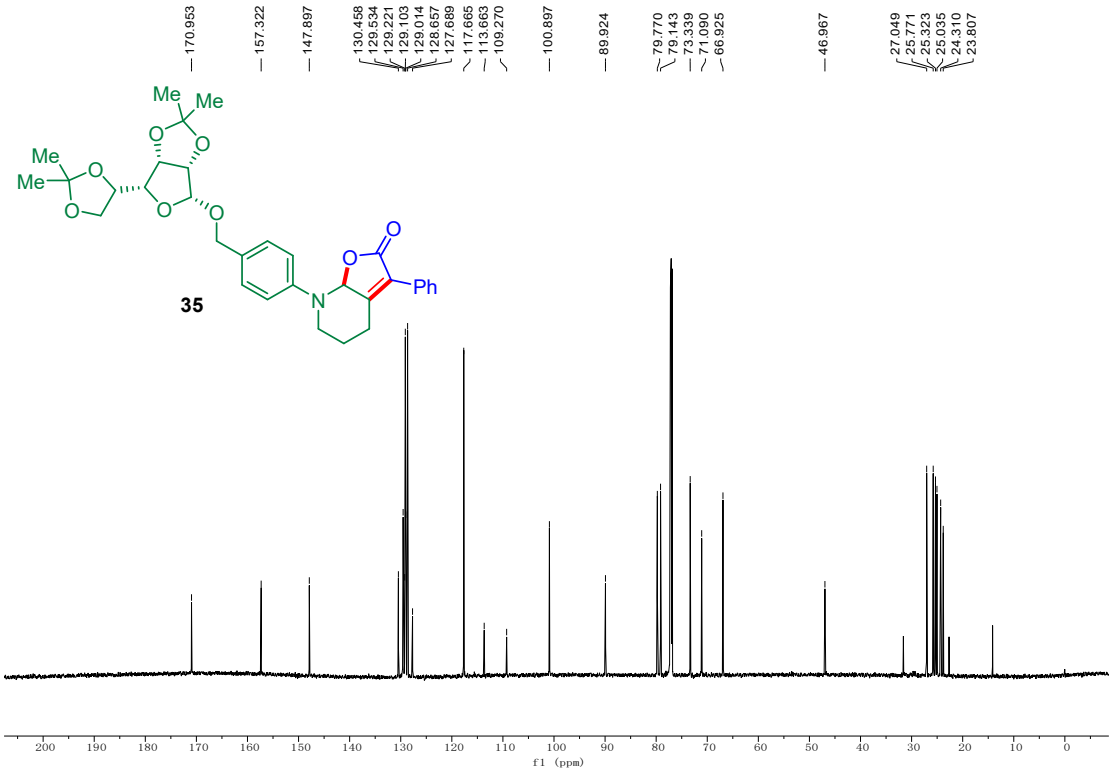

7.552
7.535
7.481
7.463
7.445
7.428
7.410
7.392
7.303
7.283
7.161
7.140
5.815
5.067
4.804
4.796
4.790
4.781
4.648
4.634
4.614
4.585
4.460
4.430
4.410
4.393
4.139
4.117
4.102
4.025
4.014
4.004
3.988
3.979
3.969
3.960
3.406
3.164
2.586
2.090
1.885
1.465
1.391
1.320
Me
Me
Me
Me
O
O
O
O
O
O
O
N
Ph
34
2.01
3.09
1.96
2.07
0.98
1.01
1.06
2.15
2.20
1.18
2.23
2.01
0.88
0.96
0.94
0.97
6.34
3.14
3.19
f1 (ppm)


170.899
157.227
147.898
130.584
129.487
129.246
129.104
128.985
128.634
127.758
117.619
112.595
109.263
105.379
90.131
85.146
80.407
79.590
73.154
68.740
66.989
46.691
26.960
25.907
25.262
24.535
24.196
23.698
Me
Me
Me
Me
O
O
O
O
O
O
O
N
Ph
34
f1 (ppm)


7.557
7.553
7.536
7.485
7.467
7.448
7.432
7.414
7.396
7.358
7.337
7.161
7.139
5.831
4.894
4.864
4.739
4.730
4.713
4.703
4.698
4.688
4.647
4.617
4.584
4.575
4.568
4.559
4.497
4.484
4.478
4.471
4.464
4.451
4.119
4.106
3.584
3.574
3.564
3.554
3.419
3.405
3.390
3.176
2.592
2.097
1.894
1.566
1.452
1.387
1.361
Me
Me
Me
Me
O
O
O
O
O
O
O
O
N
Ph
35
1.95
3.15
2.00
1.94
0.92
1.11
1.00
1.11
1.03
1.03
1.16
1.99
1.19
1.91
1.00
0.98
0.94
0.99
3.05
3.16
3.17
3.17
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)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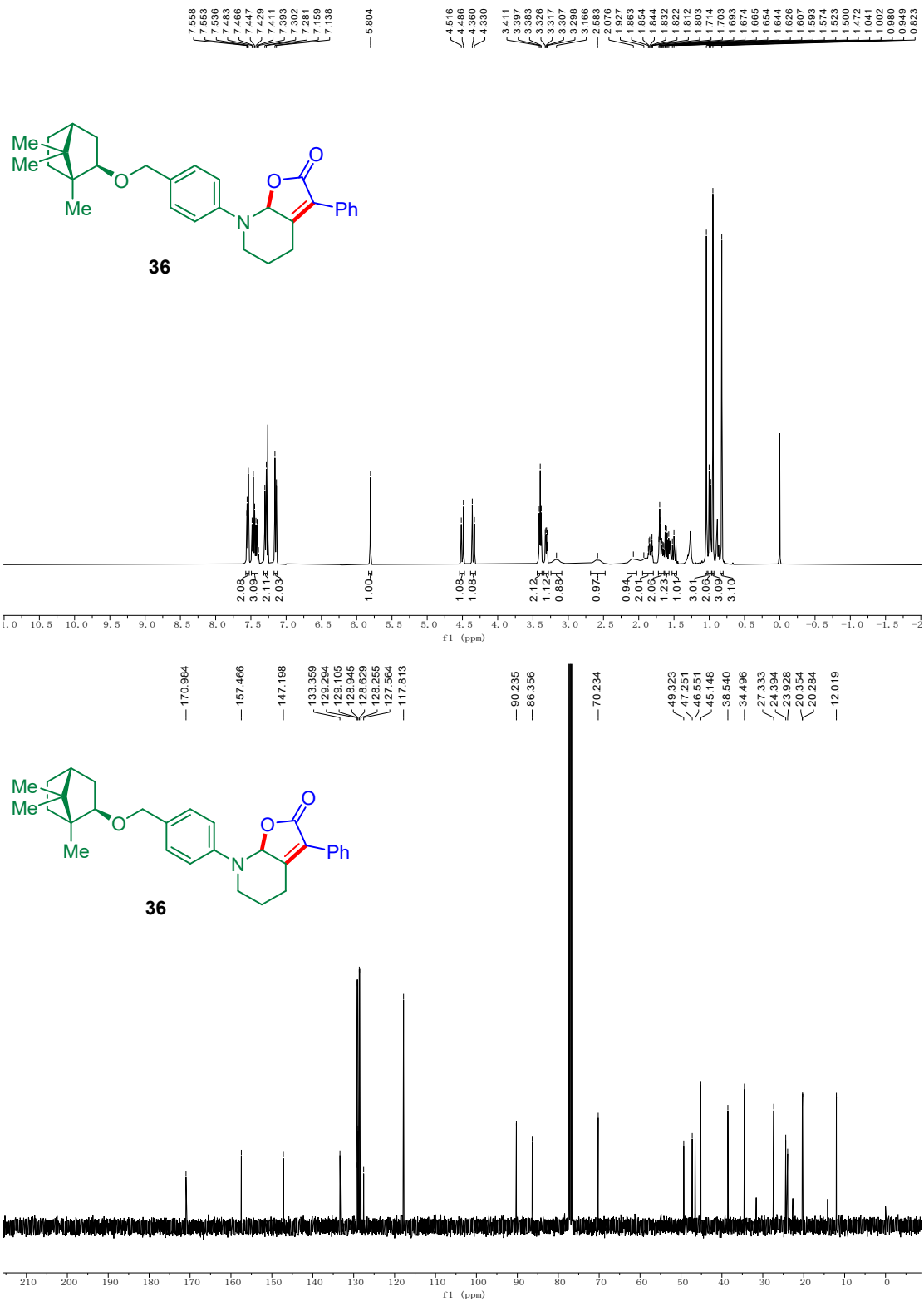
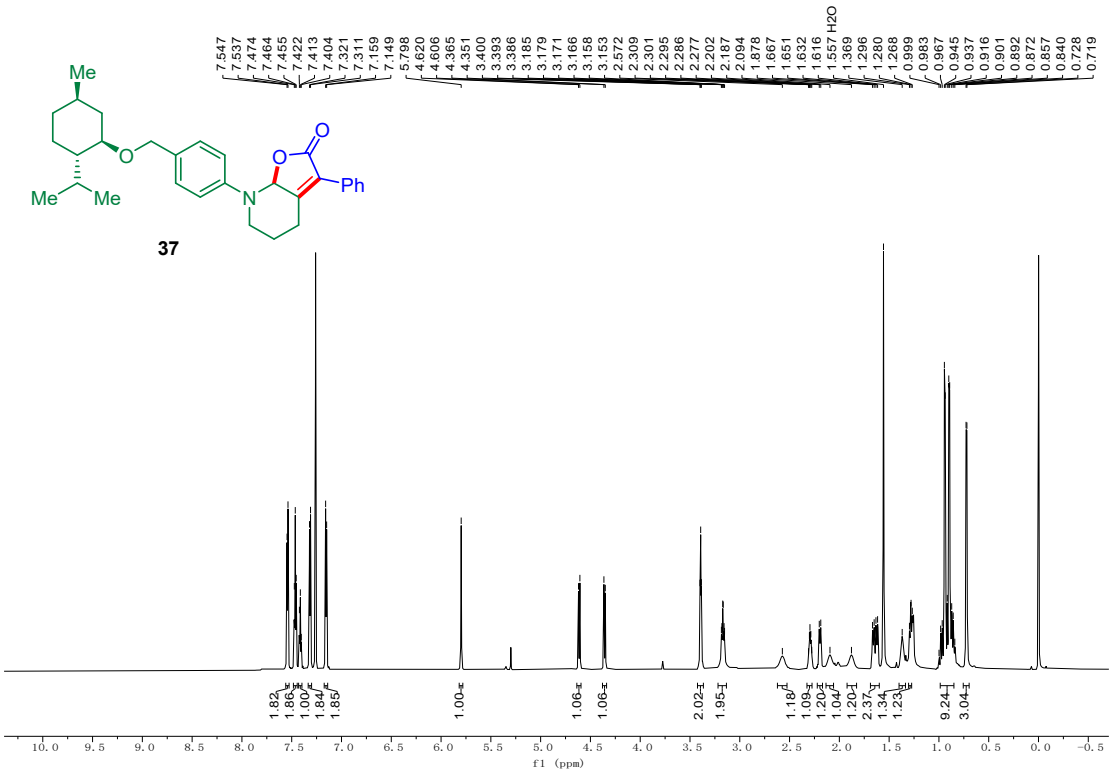
157.322
147.897
130.458
129.534
129.221
129.103
129.014
128.657
127.689
117.665
113.663
109.270
100.897
89.924
79.770
79.143
73.339
71.090
66.925
46.967
27.049
25.771
25.323
25.035
24.310
23.807
Me
Me
Me
Me
O
O
O
O
O
O
O
O
N
Ph
35
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Me
Me
Me
O
O
O
N
Ph
36
f1 (ppm)
Me
Me
Me
O
O
O
N
Ph
36
f1 (ppm)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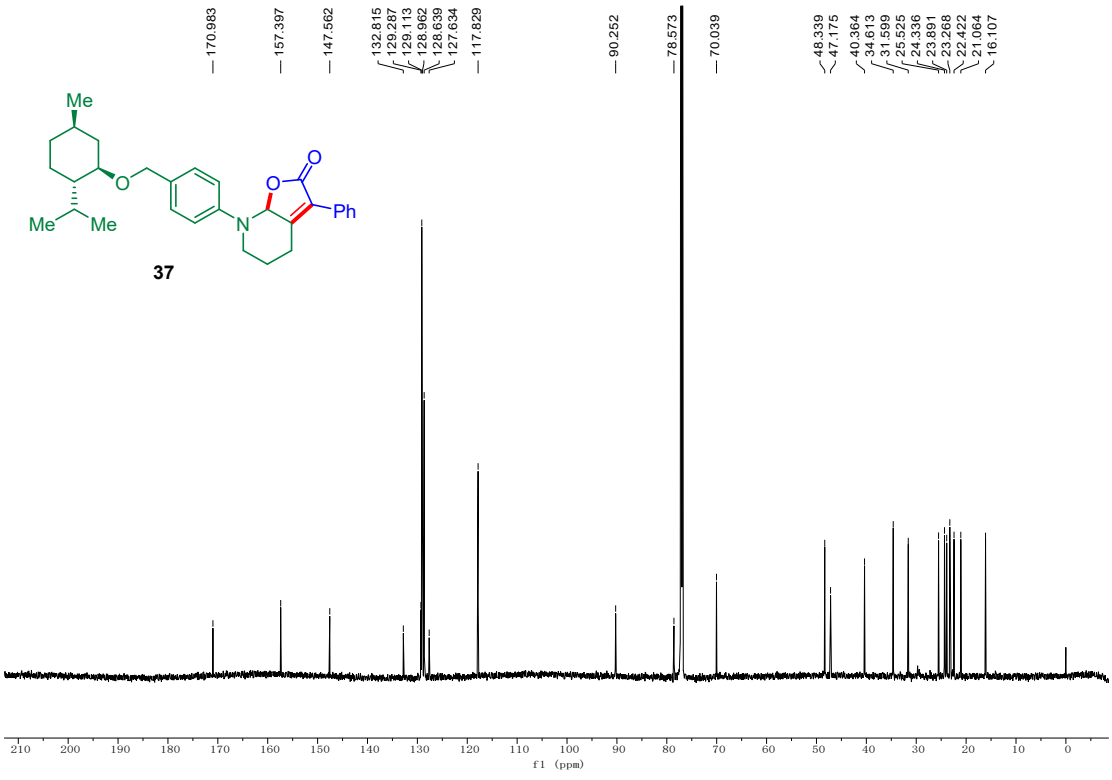
7.537
7.474
7.464
7.455
7.422
7.413
7.404
7.321
7.311
7.159
7.149
5.798
4.620
4.606
4.365
4.351
3.400
3.393
3.386
3.185
3.179
3.171
3.166
3.158
3.153
2.572
2.309
2.301
2.295
2.286
2.277
2.202
2.187
2.094
1.878
1.667
1.651
1.632
1.616
1.557 H2O
1.369
1.296
1.280
1.268
0.999
0.983
0.967
0.945
0.937
0.916
0.901
0.892
0.872
0.857
0.840
0.728
0.719
Me
O
Me
Me
O
Ph
N
37
1.82
1.86
1.00
1.84
1.85
1.00
1.06
1.06
2.02
1.95
1.18
1.09
1.20
1.04
1.20
2.37
1.34
1.23
9.24
3.04
f1 (ppm)


170.983
157.397
147.562
132.815
129.287
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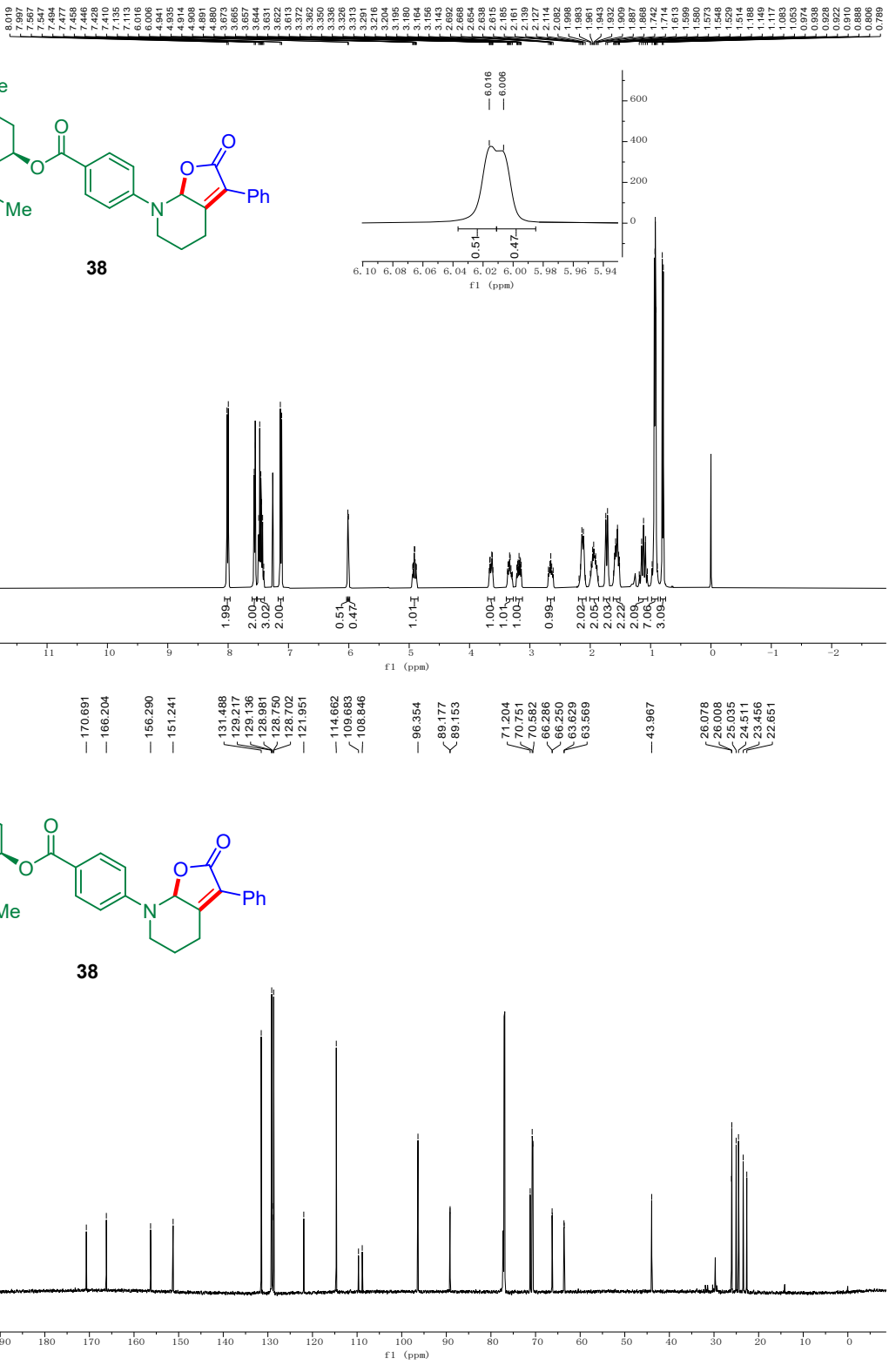
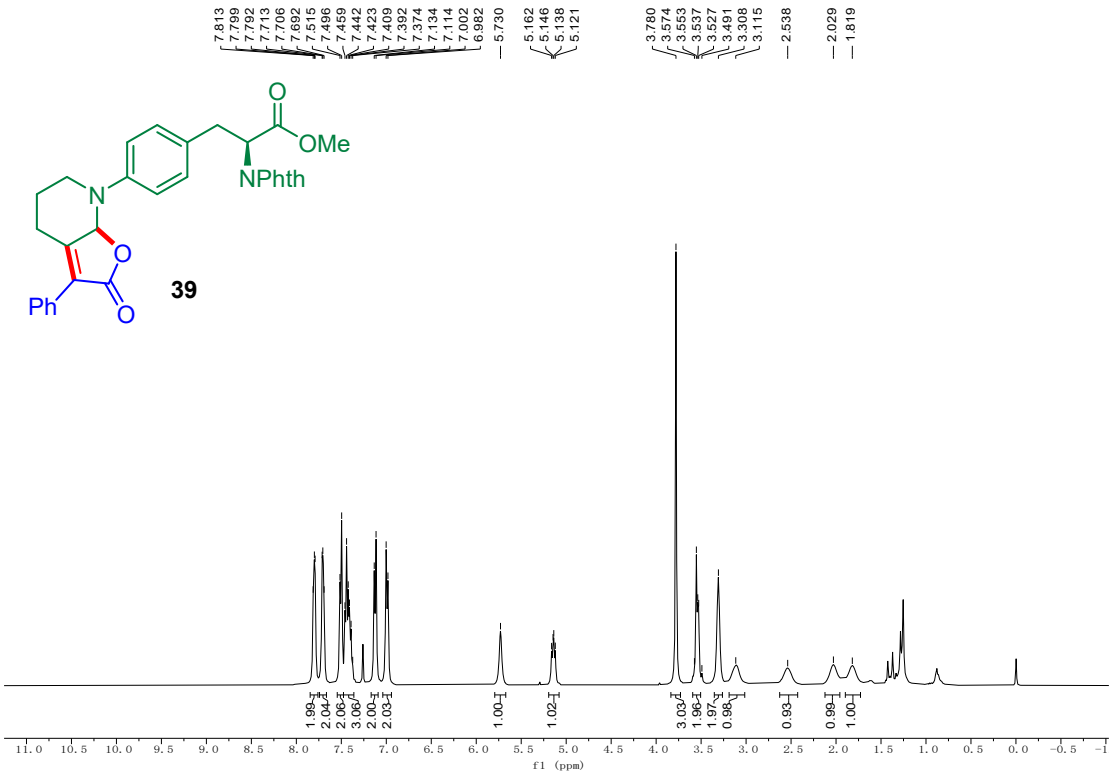
128.962
128.639
127.634
117.829
90.252
78.573
70.039
48.339
47.175
40.364
34.613
31.599
25.525
24.336
23.891
23.268
22.422
21.064
16.107
Me
O
Me
Me
O
Ph
N
37
f1 (ppm)


Me
O
O
O
Me
Me
O
N
Ph
38
6.016
6.006
0.51
0.47
f1 (ppm)
1.99
2.00
3.02
2.00
0.51
0.47
1.01
1.00
1.01
1.00
0.99
2.02
2.05
2.03
2.22
2.09
7.06
3.09
f1 (ppm)
170.691
166.204
156.290
151.241
131.488
129.217
129.136
128.981
128.750
128.702
121.951
114.662
109.683
108.846
96.354
89.177
89.153
71.204
70.751
70.582
66.286
66.250
63.629
63.569
43.967
26.078
26.008
25.035
24.511
23.456
22.651
Me
O
O
O
Me
Me
O
N
Ph
38
f1 (ppm)


7.813
7.799
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7.706
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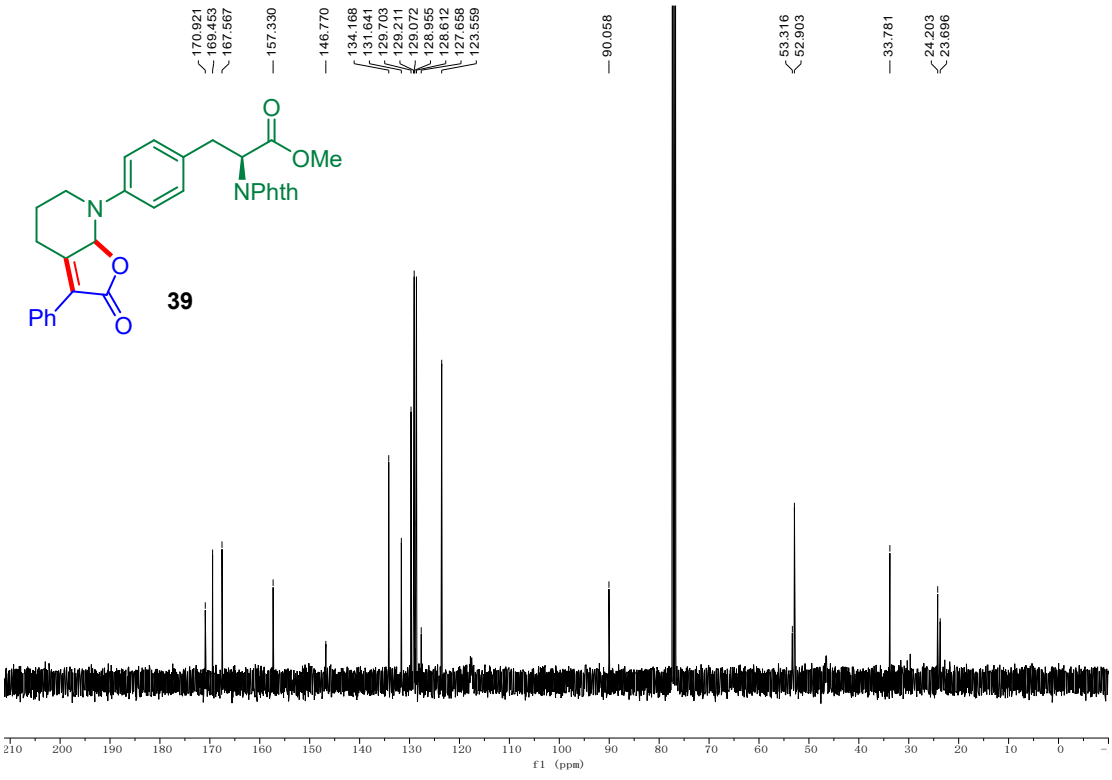
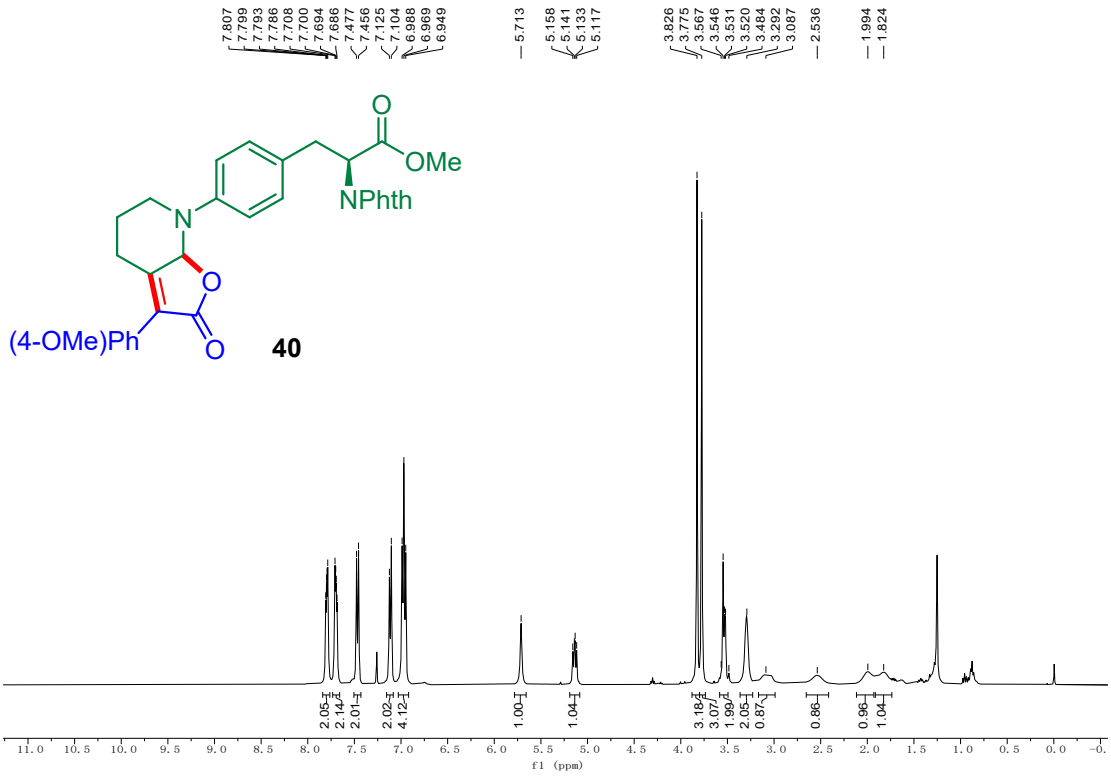
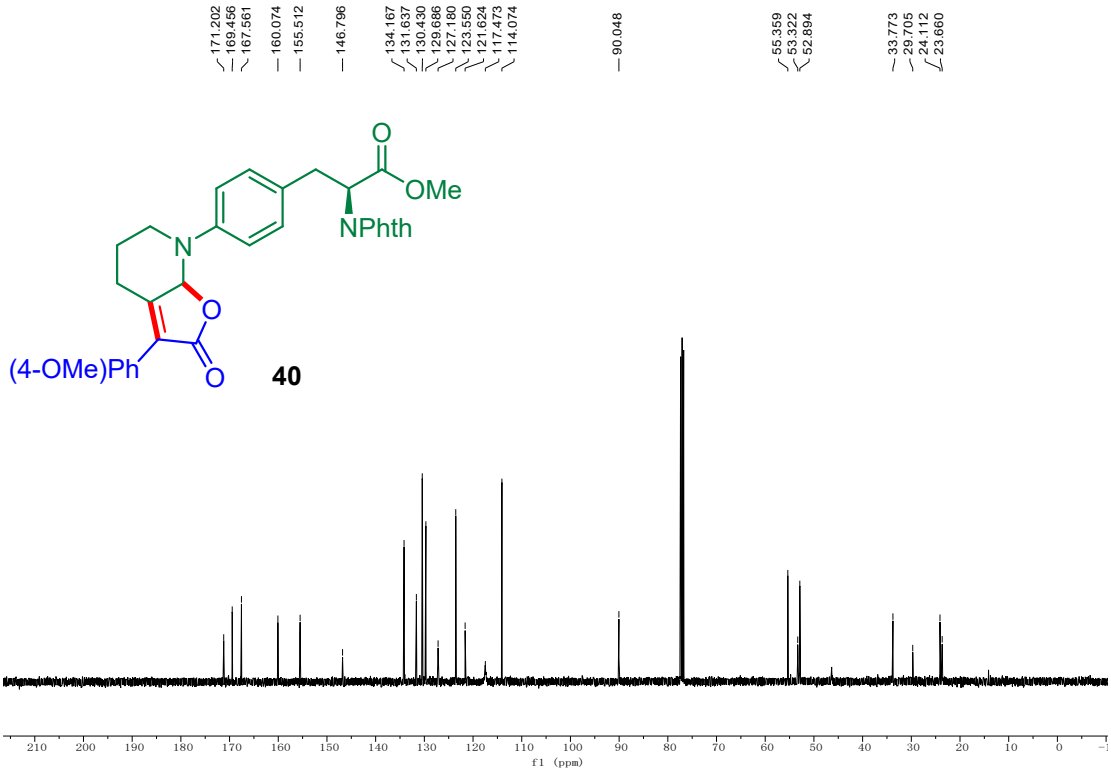
7.496
7.459
7.442
7.423
7.409
7.392
7.374
7.134
7.114
7.002
6.982
5.730
5.162
5.146
5.138
5.121
3.780
3.574
3.553
3.537
3.527
3.491
3.308
3.115
2.538
2.029
1.819
O
OMe
NPhth
N
O
Ph
O
39
1.99
2.04
2.06
3.06
2.00
2.03
1.00
1.02
3.03
1.96
1.97
0.98
0.93
0.99
1.00
f1 (ppm)


170.921
169.453
167.567
157.330
146.770
134.168
131.641
129.703
129.211
129.072
128.955
128.612
127.658
123.559
90.058
53.316
52.903
33.781
24.203
23.696
O
OMe
NPhth
N
O
Ph
O
39
f1 (ppm)


7.807
7.799
7.793
7.786
7.708
7.700
7.694
7.686
7.477
7.456
7.125
7.104
6.988
6.969
6.949
5.713
5.158
5.141
5.133
5.117
3.826
3.775
3.567
3.546
3.531
3.520
3.484
3.292
3.087
2.536
1.994
1.824
O
OMe
NPhth
N
O
O
(4-OMe)Ph
40
2.05
2.14
2.01
2.02
4.12
1.00
1.04
3.18
3.07
1.99
2.05
0.87
0.86
0.96
1.04
f1 (ppm)


171.202
169.456
167.561
160.074
155.512
146.796
134.167
131.637
130.430
129.686
127.180
123.550
121.624
117.473
114.074
90.048
55.359
53.322
52.894
33.773
29.705
24.112
23.660
O
OMe
NPhth
N
O
O
(4-OMe)Ph
40
f1 (ppm)