Supplementary Information for

Palladium-catalyzed domino cycloisomerization/double condensation of acetylenic acids with dinucleophiles

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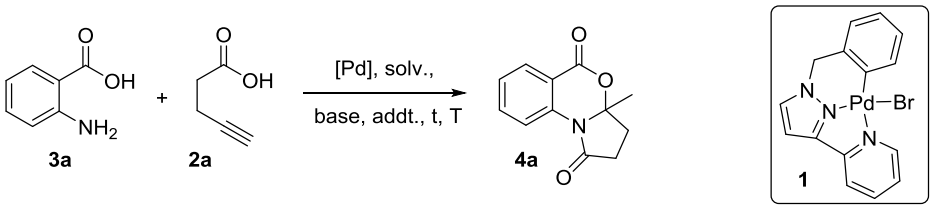
Synthesis of 5-phenylpent-4-ynoic acid. Chromium trioxide (2.5 g, 25 mmol) was dissolved in water (7.5 mL), and concentrated sulfuric acid (2.5 mL) was added dropwise with careful stirring and cooling in an ice-water bath. From this solution (Jones reagent), 4 mL were added dropwise to a solution of pent-4-yn-1-ol (204 mg, 1.27 mmol) in acetone (20 mL) at 0ºC. Stirring was continued for 4 h at the same temperature, and then *i*-PrOH (5 mL) was added. The mixture was acidified with 1 M aqueous HCl to pH = 1 and extracted with CH_2Cl_2 (3 × 20 mL). The combined organic layers were washed with water (20 mL), dried over anhydrous $NaSO_4$ and filtered, and the filtrate concentrated *in vacuo*. Purification by flash column chromatography (7:3 Hexanes:EtOAc) provided 5-phenylpent-4-ynoic acid (121.1 mg, 58%) as white prisms; m.p. 96-99 °C ($CHCl_3$) (Lit.[1] 103-107 ºC); ^{1}H-NMR ($CDCl_3$) δ 11.49 (s, 1H, COO*H*), 7.49-7.34 (m, 2H, H_{arom}), 7.34-7.16 (m, 3H, H_{arom}), 2.89-2.51 (m, 4H, CH_2); ^{13}C-NMR ($CDCl_3$) δ 178.4 (*C*OOH), 131.6, 128.2, 127.9 (C_{arom}), 123.4 (qC_{arom}), 87.6 (qC), 81.4 (qC), 33.5 (*C*H_2), 15.1 (*C*H_2).

Table S1. Palladium-catalyzed formation of benzo[*d*]pyrrolooxazine-1,5-dione **4a**. Initial experiments.[a]



Entry	solv. (0.1 M)	[Pd] (10^{-2} mol%)	Base	Additive	T (ºC)	t (h)	4a (%)[b]
1	PhMe	$Pd(OAc)_2$	-	-	100	96	-
2	MeOH	**1**	Et_3N	-	80	120	-
3	DMF	$PdCl_2$	Cs_2CO_3	-	120	120	-
4	THF	$Pd(PPh_3)_4$	DBU	$BF_3{\cdot}O(C_2H_5)_2$	80	120	-
5	H_2O	$Pd(OAc)_2$	pyridine	-	110	120	-
6	DMA	**1**	KO^{t}Bu	-	130	96	-
7	DMSO	$Pd(OAc)_2$	DMAP	$BF_3{\cdot}O(C_2H_5)_2$	120	96	-
8	MeCN	**1**	Cs_2CO_3	-	90	120	-
9	CH_2Cl_2	$Pd(OAc)_2$	LiOH		70	96	-
9	CH_2Cl_2	**1**	DIPEA		60	96	<5
10	THF	$Pd(PPh_3)_4$	Et_3N	$BF_3{\cdot}O(C_2H_5)_2$	80	120	-
11	MeOH	$Pd(PPh_3)_4$	NaOH		100	120	-
12	DMF	$PdCl_2$	KOH_3	-	120	96	-
13	$CHCl_3$ (0.1)	**1** (10^{-2})	Cs_2CO_3	-	60	96	-
14	CH_2Cl_2	$Pd(OAc)_2$	Et_3N		70	96	<5
15	$CHCl_3$ (0.1)	**1** (10^{-2})	Et_3N	-	60	96	14
16	CH_2Cl_2 (0.1)	**1** (10^{-2})	Et_3N	-	60	96	<5

[a] Reaction conditions: **2a** (0.2 mmol), **3a** (0.2 mmol), base (2 mol%), additive (10^{-2} mol%). [b] Isolated yields.

Benzopyrrolooxazine dione 4a. Structure factor table

Bond precision: C-C = 0.0016 A Wavelength=1.54184

Cell: a=12.0162(2) b=11.7139(2) c=14.3786(3)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2023.88(6)	2023.88(6)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C12 H11 N O3	C12 H11 N1 O3
Sum formula	C12 H11 N O3	C12 H11 N O3
Mr	217.22	217.22
Dx,g cm-3	1.426	1.426
Z	8	8
Mu (mm-1)	0.858	0.858
F000	912.0	912.0
F000'	915.03	
h,k,lmax	14,14,17	14,14,17
Nref	2003	2001
Tmin,Tmax	0.847,0.918	0.891,0.943
Tmin'	0.847	

Correction method= ANALYTICAL

Data completeness= 0.999 Theta(max)= 72.440

R(reflections)= 0.0322(1800) wR2(reflections)= 0.0833(2001)

S = 1.058 Npar= 146

Benzopyridothiadiazinone dioxide 4g. Structure factor table

Bond precision: C-C = 0.0020 A Wavelength=1.54184

Cell: a=11.5076(2) b=14.6631(2) c=7.0969(1)
alpha=90 beta=96.595(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1189.59(3)	1189.59(3)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C12 H14 N2 O3 S	C12 H14 N2 O3 S1
Sum formula	C12 H14 N2 O3 S	C12 H14 N2 O3 S
Mr	266.31	266.31
Dx,g cm-3	1.487	1.487
Z	4	4
Mu (mm-1)	2.460	2.460
F000	560.0	560.0
F000'	562.96	
h,k,lmax	14,18,8	14,18,8
Nref	2341[1175]	2286
Tmin,Tmax	0.625,0.754	0.602,0.829
Tmin'	0.438	

Correction method= ANALYTICAL

Data completeness= 1.95/0.98 Theta(max)= 71.980

R(reflections)= 0.0208(2277) wR2(reflections)= 0.0545(2286)

S = 1.078 Npar= 212

Benzopyridooxazine dione 4e. Structure factor table

Bond precision: C-C = 0.0017 A Wavelength=1.54184

Cell: a=6.5496(1) b=18.3428(3) c=23.7505(3)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2853.34(7)	2853.34(7)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C18 H15 N O3	C18 H15 N1 O3
Sum formula	C18 H15 N O3	C18 H15 N O3
Mr	293.31	293.31
Dx,g cm-3	1.366	1.366
Z	8	8
Mu (mm-1)	0.761	0.761
F000	1232.0	1232.0
F000'	1235.86	
h,k,lmax	8,22,29	8,22,29
Nref	2938	2934
Tmin,Tmax	0.827,0.874	0.861,0.900
Tmin'	0.827	

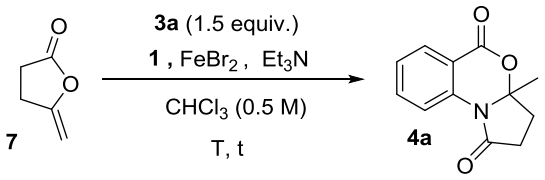
Correction method= ANALYTICAL

Data completeness= 0.999 Theta(max)= 74.930

R(reflections)= 0.0362(2796) wR2(reflections)= 0.0926(2934)

S = 1.058 Npar= 199

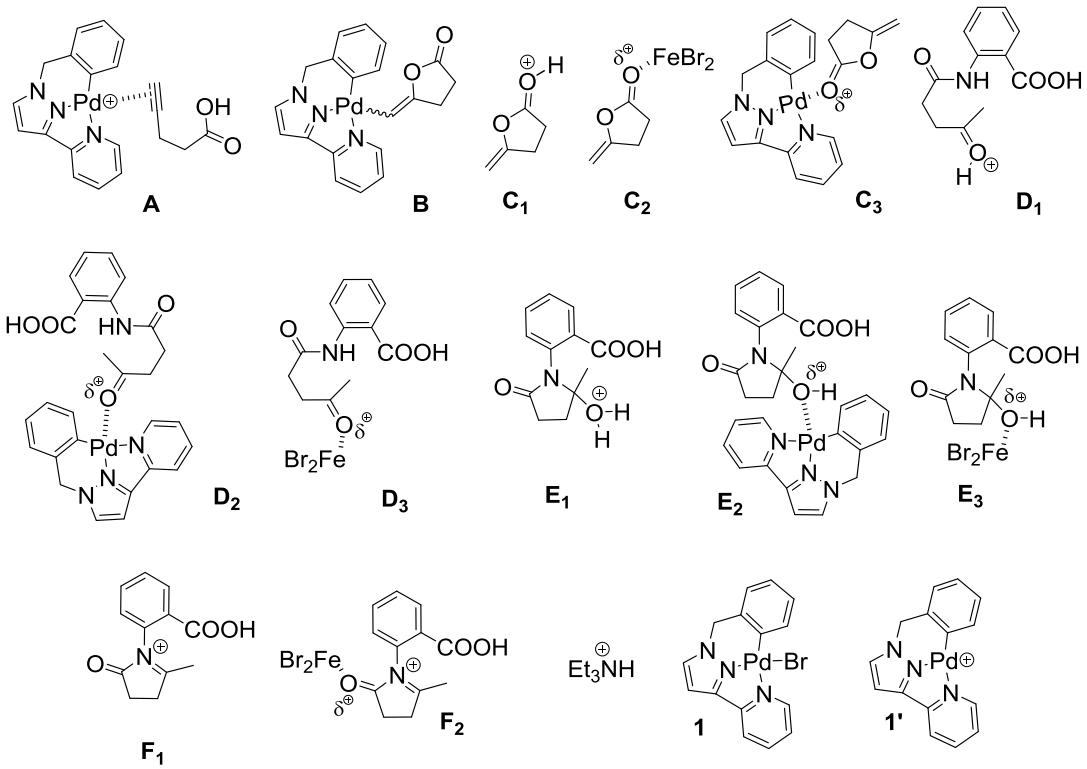
Table S2. Reaction of methylene lactone 7 with anthranilic acid 3a



Entry	**1** (mol%)	Et_3N (mol%)	$FeBr_3$ (mol%)	T (ºC)	t (h)	**4a** (%)[a]
1	**1** (10^{-2})	2	-	50	24	-
2	**1** (10^{-2})	2	-	120	96	14
3	**1** (10^{-2})	-	-	120	96	7
4	-	2	10^{-2}	80	96	-
5	-	2	10^{-2}	120	96	<5
6	-	-	10^{-2}	120	96	-
7[c]	**1** (10^{-4})	10^{-2}	10^{-4}	120	96	8
8[d]	**1** (10^{-4})	2	10^{-4}	120	96	10
9[e]	**1** (10^{-2})	2	10^{-2}	120	96	90

[a] Isolated yields.

Figure S1. Transient species and catalysts detected by ESI-mass spectrometry



ESI-MS analysis

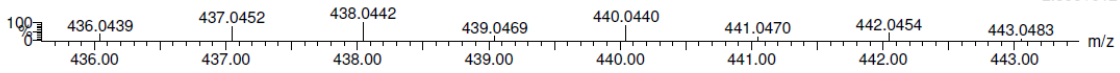
Pd(II) complex **A** (M^+)

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1719 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-18 N: 0-3 O: 0-2 Br: 0-2 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C20H18N3O2Pd
1: TOF MS ES+
2.59e+012



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
437.0452	437.0450	0.2	0.5	13.5	87.4	n/a	n/a	C20 H18 N3 O2 105Pd

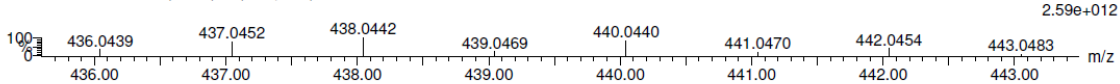
Pd(II) complex **B** (MH^+)

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1719 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-18 N: 0-3 O: 0-2 Br: 0-2 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C20H18N3O2Pd
1: TOF MS ES+
2.59e+012



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
437.0452	437.0450	0.2	0.5	13.5	87.4	n/a	n/a	C20 H18 N3 O2 105Pd

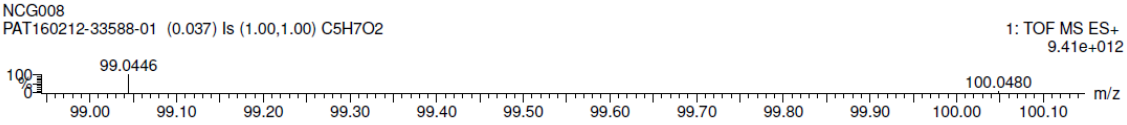
Intermediate **C₁** (M^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
54 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 Br: 0-10

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C5H7O2



Minimum:				-1.5				
Maximum:		1.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
99.0446	99.0446	0.0	0.0	2.5	82.0	n/a	n/a	C5 H7 O2

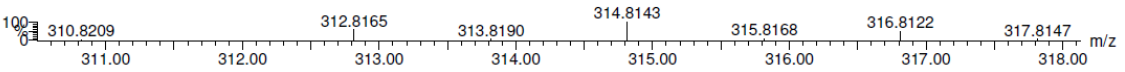
Fe complex **C₂** (MH^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 0.3 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
413 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-5 H: 0-7 N: 0-3 O: 0-2 54Fe: 0-1 56Fe: 0-1 57Fe: 0-1 58Fe: 0-1 Br: 0-2

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C5H7Br2FeO2



Minimum:				-1.5				
Maximum:		0.3	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
314.8143	314.8146	-0.3	-1.0	1.5	82.6	n/a	n/a	C5 H7 O2 58Fe Br2

Pd(II) complex **C₃** (M^+)

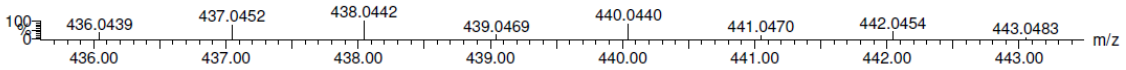
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 0.3 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1841 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-3 O: 0-2 Br: 0-2 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C20H18N3O2Pd

1: TOF MS ES+
2.59e+012



Minimum:				-1.5				
Maximum:		0.3	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
437.0452	437.0450	0.2	0.5	13.5	88.2	n/a	n/a	C20 H18 N3 O2 105Pd

Intermediate **D₁** (M^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 0.3 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
447 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-3 O: 0-4 Br: 0-2 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
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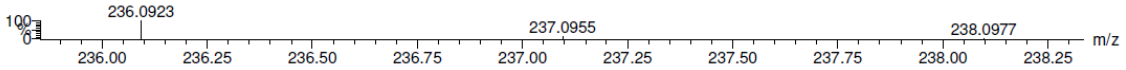
1: TOF MS ES+
8.62e+012



Minimum:				-1.5				
Maximum:		0.3	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
236.0923	236.0923	0.0	0.0	6.5	38.5	n/a	n/a	C12 H14 N O4

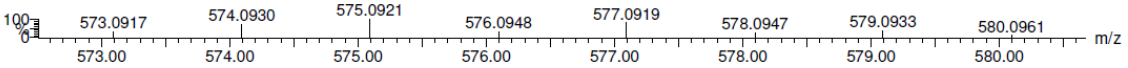
Pd(II) complex **D₂** (M^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
7598 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-27 H: 0-27 N: 0-4 O: 0-4 Br: 0-2 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C27H25N4O4Pd
1: TOF MS ES+
2.53e+012



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
574.0930	574.0927	0.3	0.5	17.5	86.9	n/a	n/a	C27 H25 N4 O4 105Pd

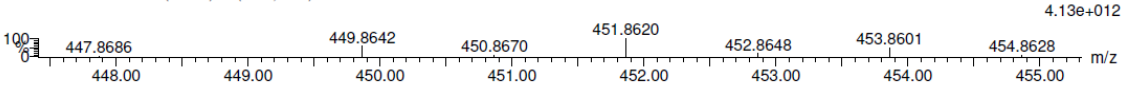
Fe complex **D₃** (MH^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 0.5 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
716 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-14 N: 0-2 O: 0-4 54Fe: 0-1 56Fe: 0-1 57Fe: 0-1 58Fe: 0-1 Br: 0-2

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C12H14Br2FeNO4
1: TOF MS ES+
4.13e+012



Minimum:				-1.5				
Maximum:		0.5	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
451.8620	451.8622	-0.2	-0.4	5.5	81.0	n/a	n/a	C12 H14 N O4 58Fe Br2

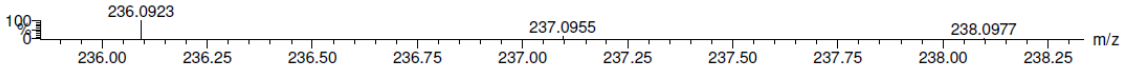
Intermediate **E₁** (M^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-14 N: 0-2 O: 0-4 Br: 0-2

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C12H14NO4 1: TOF MS ES+ 8.62e+012



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
236.0923	236.0923	0.0	0.0	6.5	38.3	n/a	n/a	C12 H14 N O4

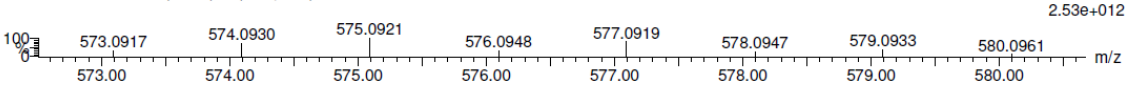
Pd(II) complex **E₂** (M^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
7598 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-27 H: 0-27 N: 0-4 O: 0-4 Br: 0-2 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C27H25N4O4Pd 1: TOF MS ES+ 2.53e+012



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
574.0930	574.0927	0.3	0.5	17.5	86.9	n/a	n/a	C27 H25 N4 O4 105Pd

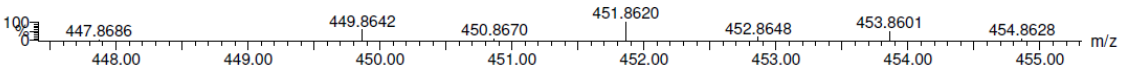
Fe complex **E3** (MH^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 0.5 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
716 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-14 N: 0-2 O: 0-4 54Fe: 0-1 56Fe: 0-1 57Fe: 0-1 58Fe: 0-1 Br: 0-2

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C12H14Br2FeNO4 1: TOF MS ES+ 4.13e+012



Minimum:				-1.5				
Maximum:		0.5	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
451.8620	451.8622	-0.2	-0.4	5.5	81.0	n/a	n/a	C12 H14 N O4 58Fe Br2

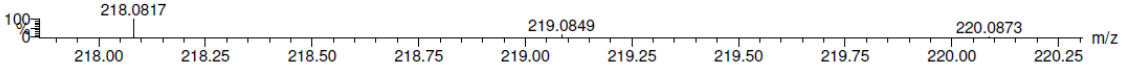
Intermediate **F1** (M^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
430 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-27 H: 0-27 N: 0-4 O: 0-4 Br: 0-2 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C12H12NO3 1: TOF MS ES+ 8.65e+012



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
218.0817	218.0817	0.0	0.0	7.5	42.3	n/a	n/a	C12 H12 N O3

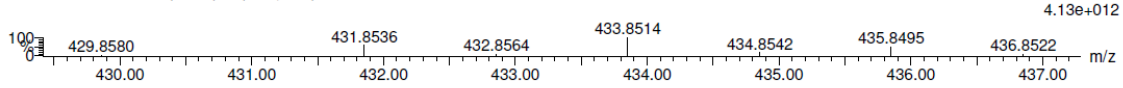
Fe complex **F₂** (M^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 0.5 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
453 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-12 N: 0-1 O: 0-4 54Fe: 0-1 56Fe: 0-1 57Fe: 0-1 58Fe: 0-1 Br: 0-2

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C12H12Br2FeNO3 1: TOF MS ES+ 4.13e+012



Minimum:				-1.5				
Maximum:		0.5	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
433.8514	433.8517	-0.3	-0.7	6.5	81.0	n/a	n/a	C12 H12 N O3 58Fe Br2

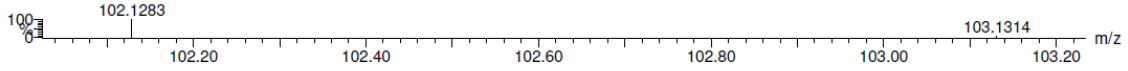
Et_3NH (MH^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-18 N: 0-3 O: 0-2 Br: 0-2 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C6H16N 1: TOF MS ES+ 9.30e+012



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
102.1283	102.1283	0.0	0.0	-0.5	81.3	n/a	n/a	C6 H16 N

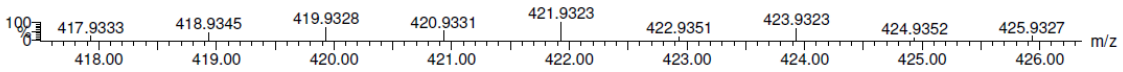
Pd(II) complex **1** (MH^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
623 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-13 N: 0-3 O: 0-1 Br: 0-1 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1
110Pd: 0-1

NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C15H13BrN3Pd 1: TOF MS ES+
2.44e+012



Minimum:				-1.5				
Maximum:		1.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
419.9328	419.9328	0.0	0.0	10.5	84.8	n/a	n/a	C15 H13 N3 Br 106Pd

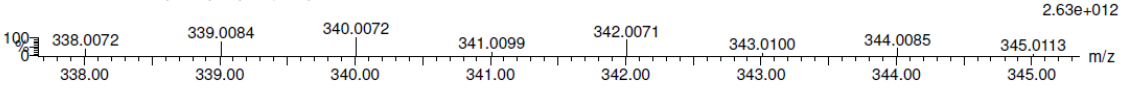
Pd(II) complex **1'** (M^+)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
279 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-13 N: 0-4 Br: 0-1 102Pd: 0-1 104Pd: 0-1 105Pd: 0-1 106Pd: 0-1 108Pd: 0-1 110Pd: 0-1

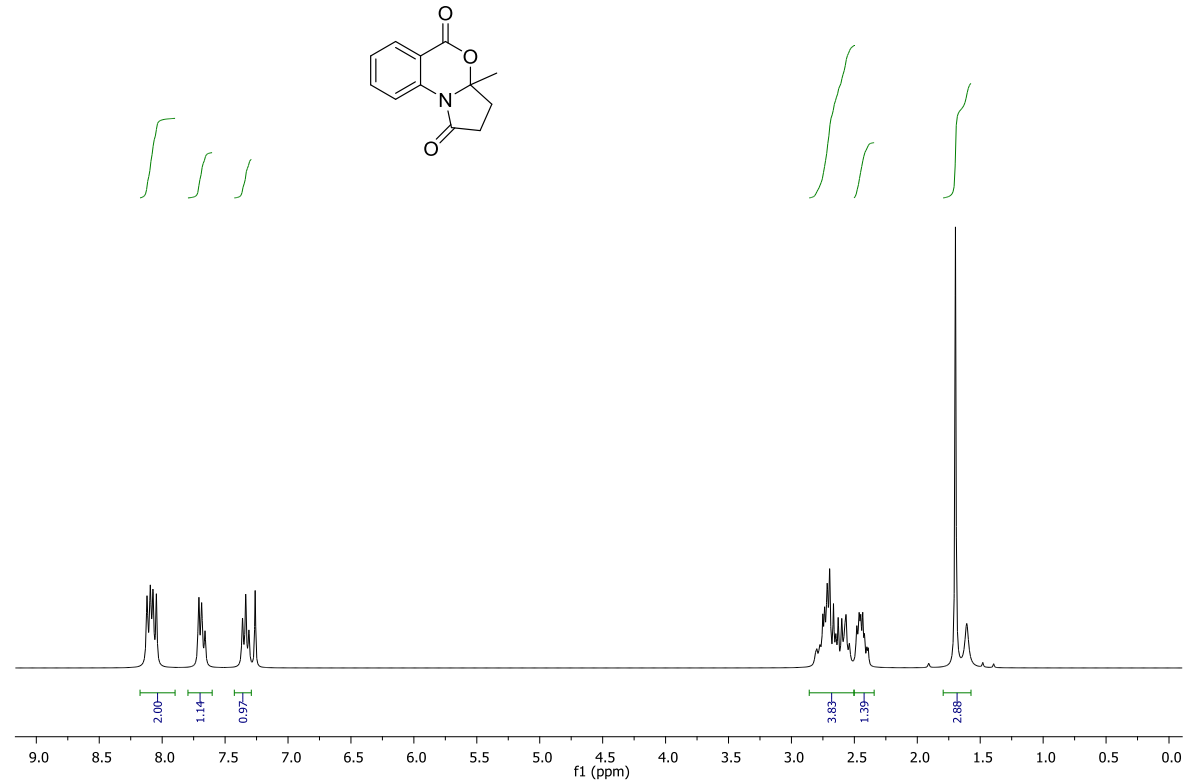
NCG008
PAT160212-33588-01 (0.037) Is (1.00,1.00) C15H12N3Pd 1: TOF MS ES+
2.63e+012

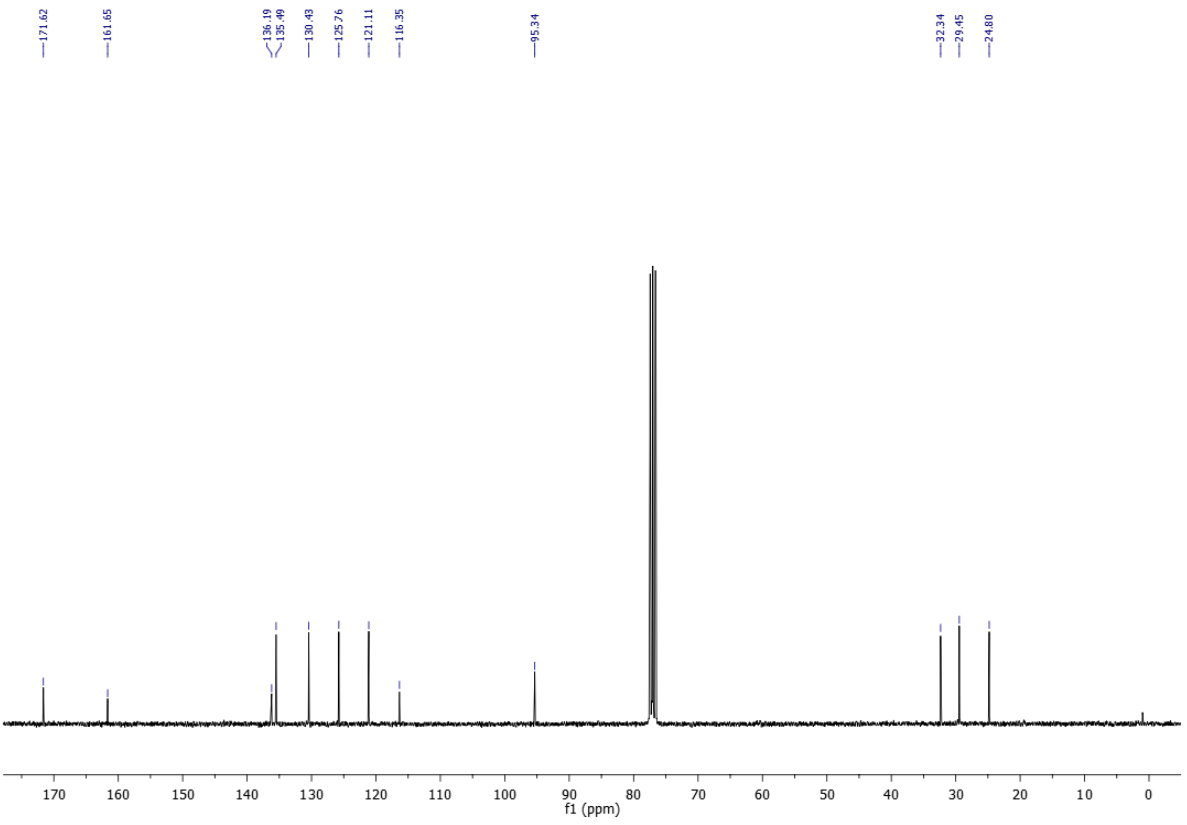


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
339.0084	339.0082	0.2	0.6	11.5	87.9	n/a	n/a	C15 H12 N3 105Pd

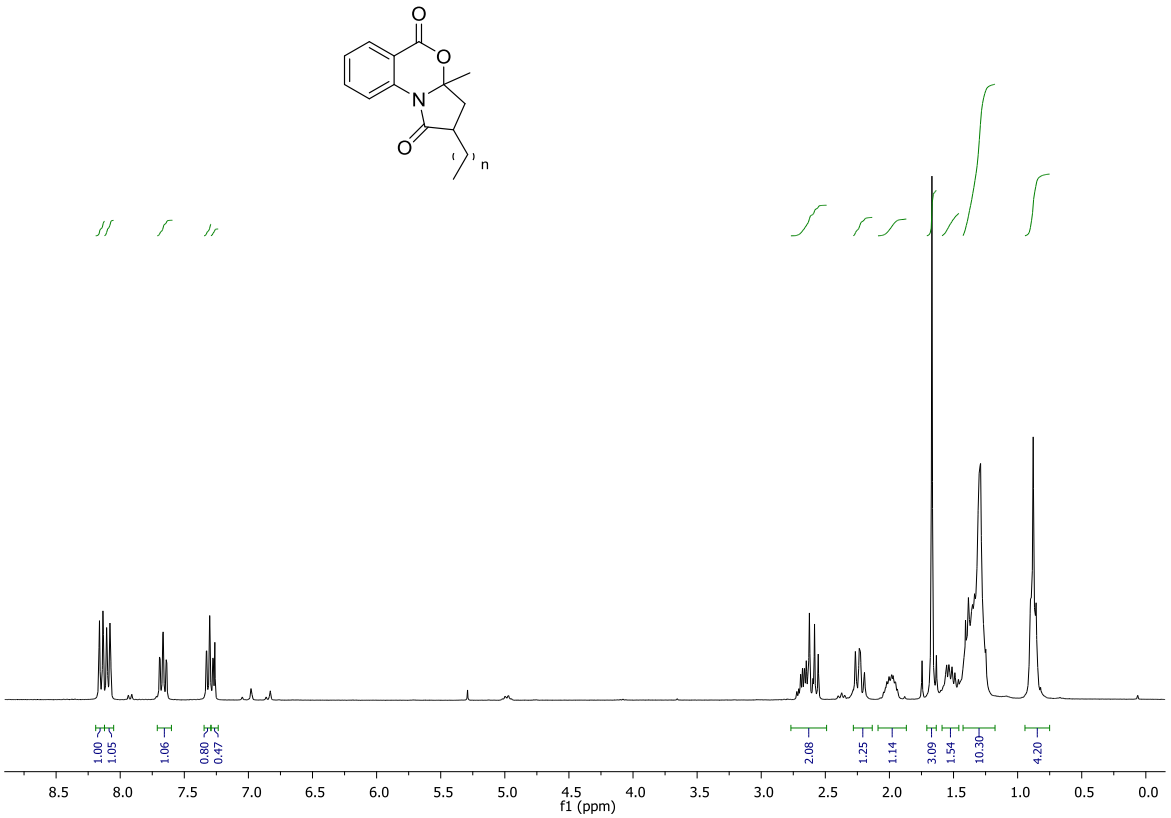
NMR Spectra

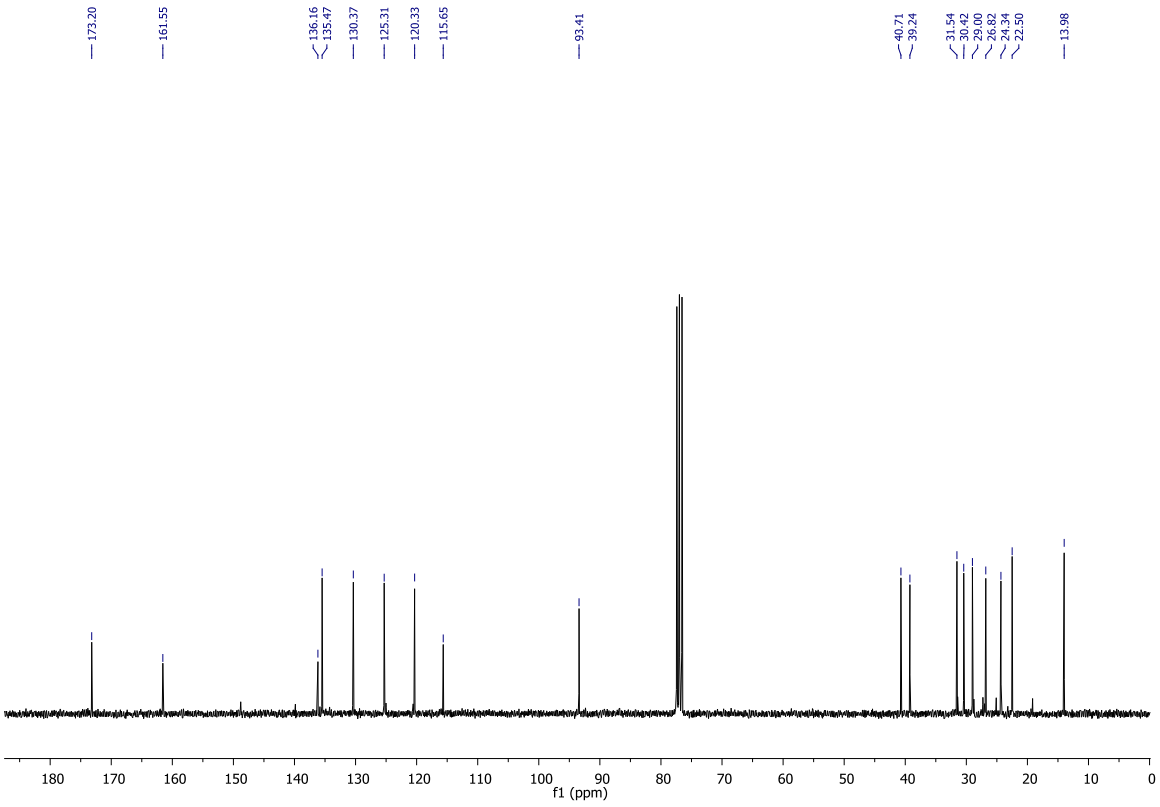
3a-methyl-3,3*a*-dihydro-5*H*-benzo[*d*]pyrrolo[2,1-*b*][1,3]oxazine-1,5(2*H*)-dione **(4a)**



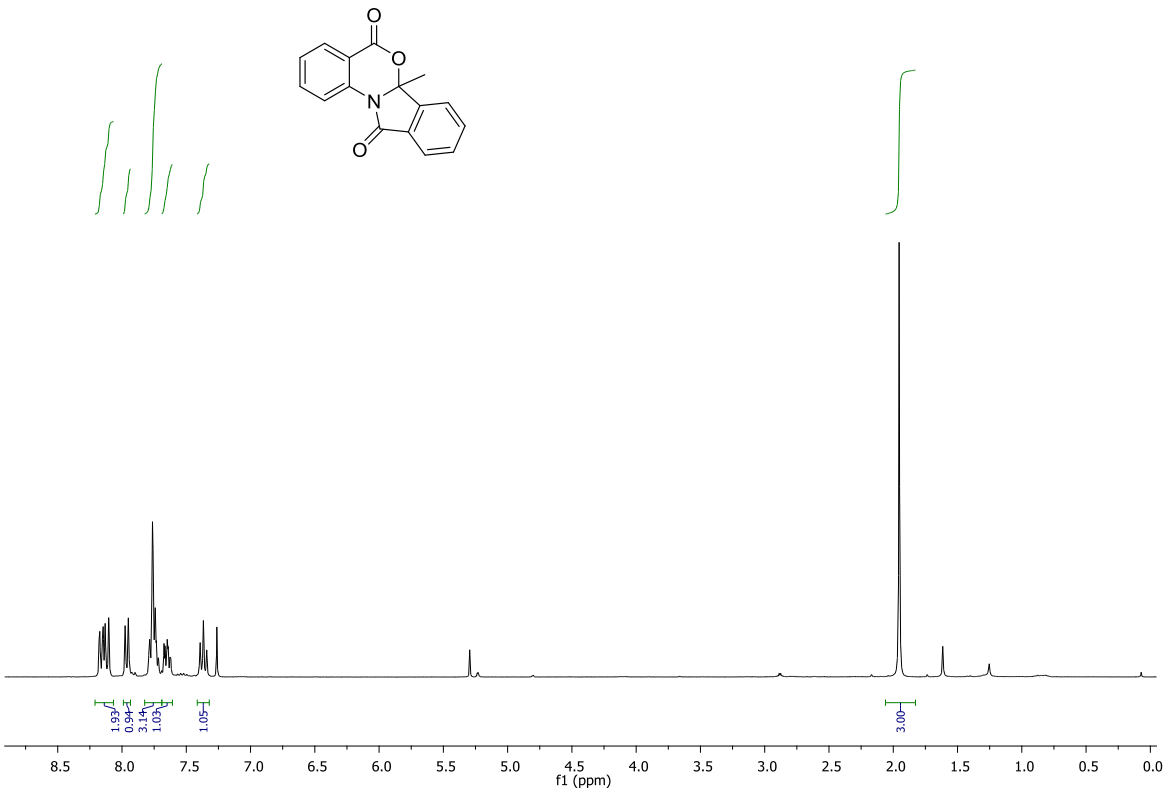


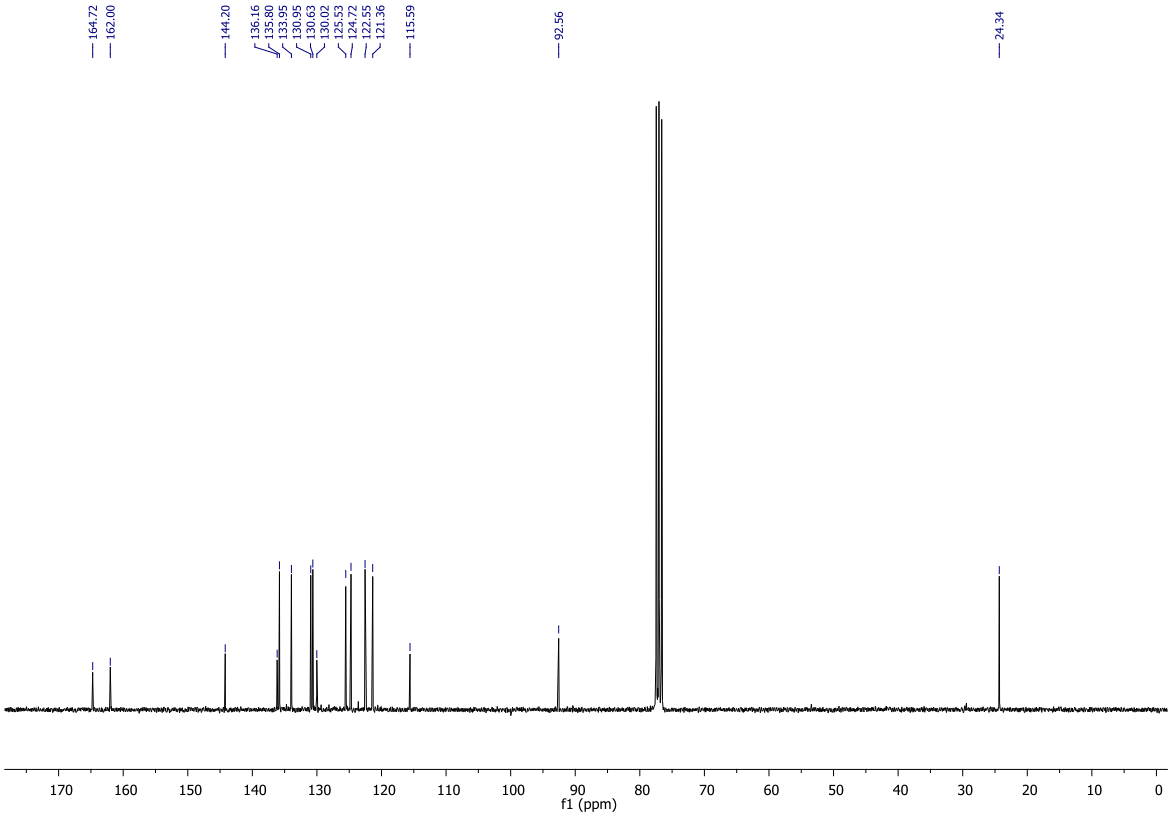
2-hexyl-3a-methyl-3,3a-dihydro-1*H*-benzo[*d*]pyrrolo[2,1-*b*][1,3]oxazine-1,5(2*H*)-dione **(4b)**



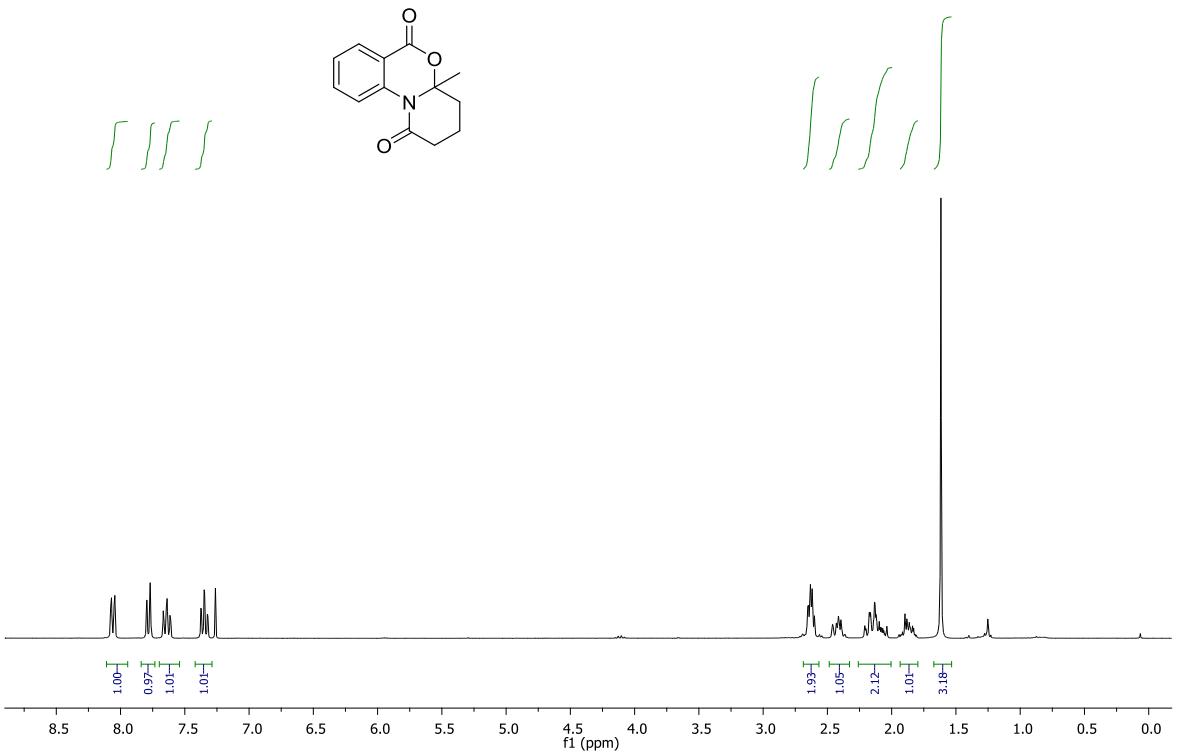


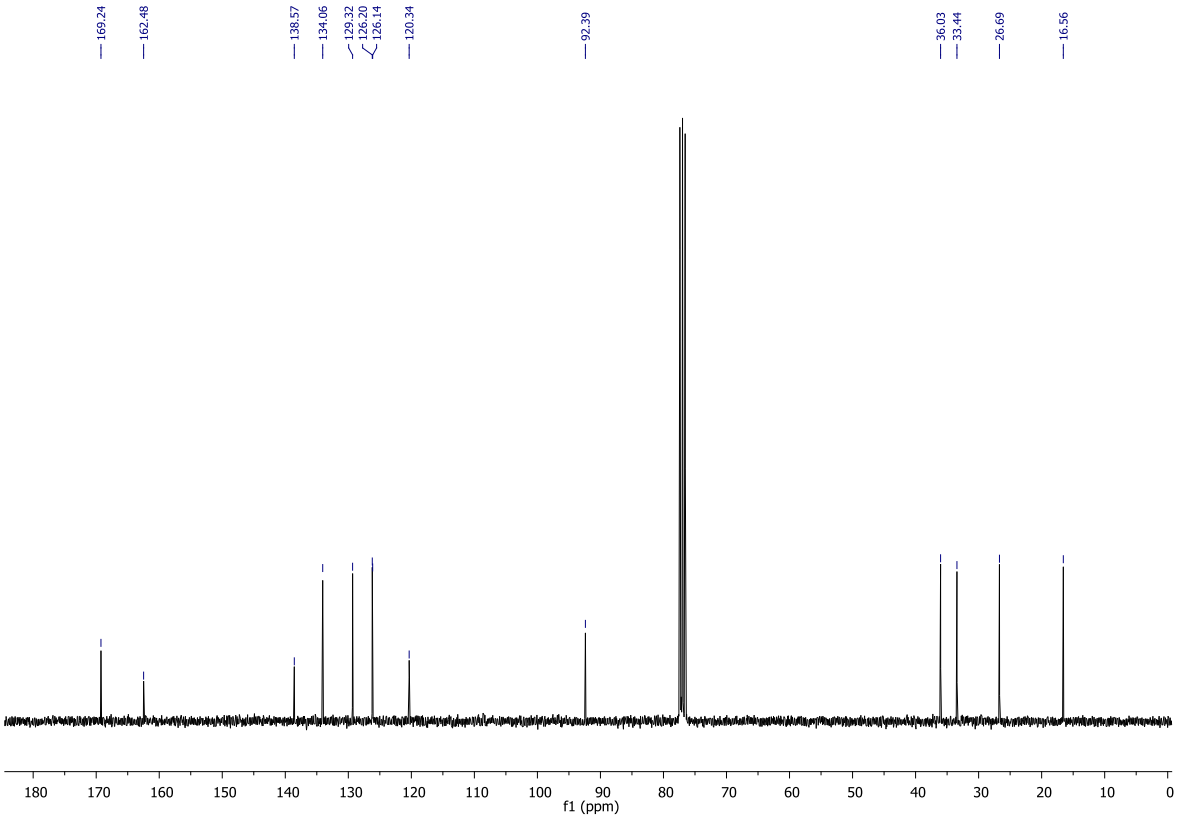
6a-methyl-5*H*-benzo[4,5][1,3]oxazino[2,3-*a*]isoindole-5,11(6a*H*)-dione **(6c)**



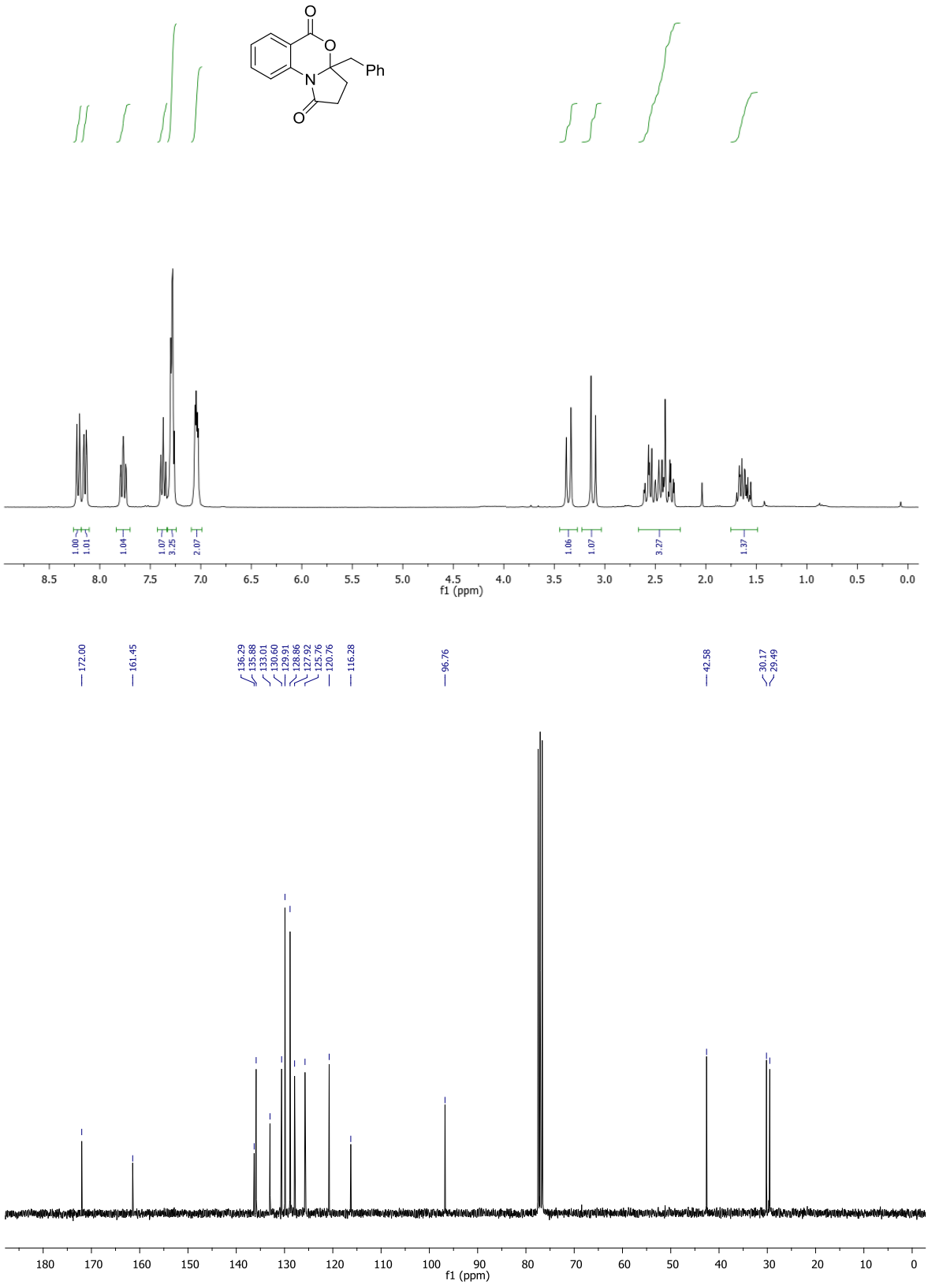


4a-methyl-2,3,4,4a-tetrahydro-1*H*,6*H*-benzo[d]pyrido[2,1-*b*][1,3]oxazine-1,6-dione **(4d)**

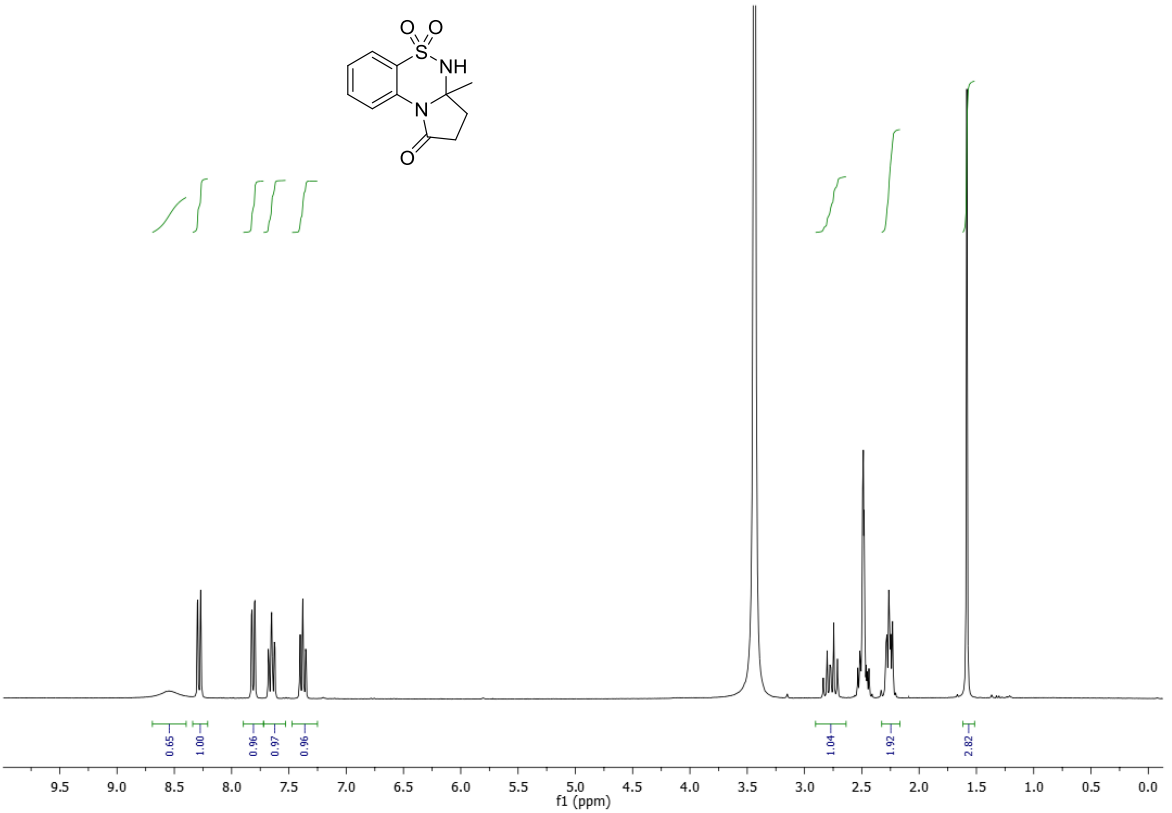


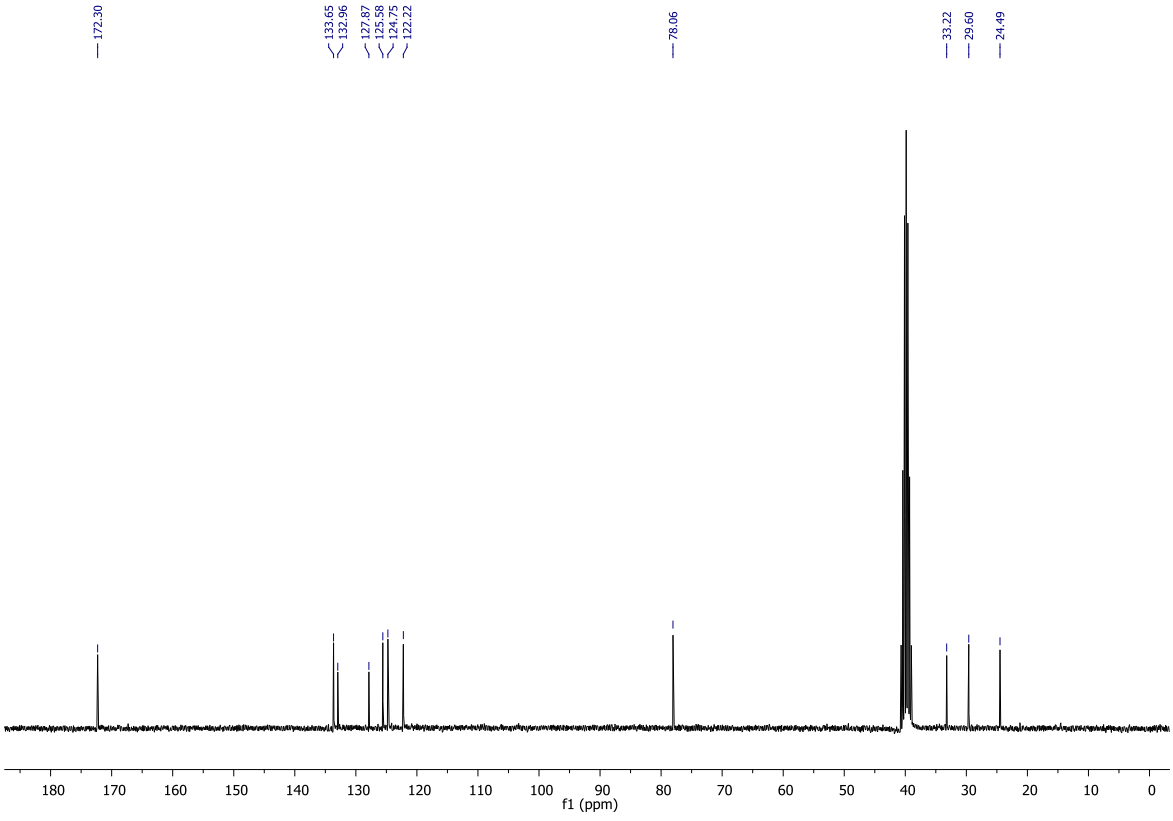


3a-benzyl-3,3a-dihydro-5*H*-benzo[*d*]pyrrolo[2,1-*b*][1,3]oxazine-1,5(2*H*)-dione **(4e)**

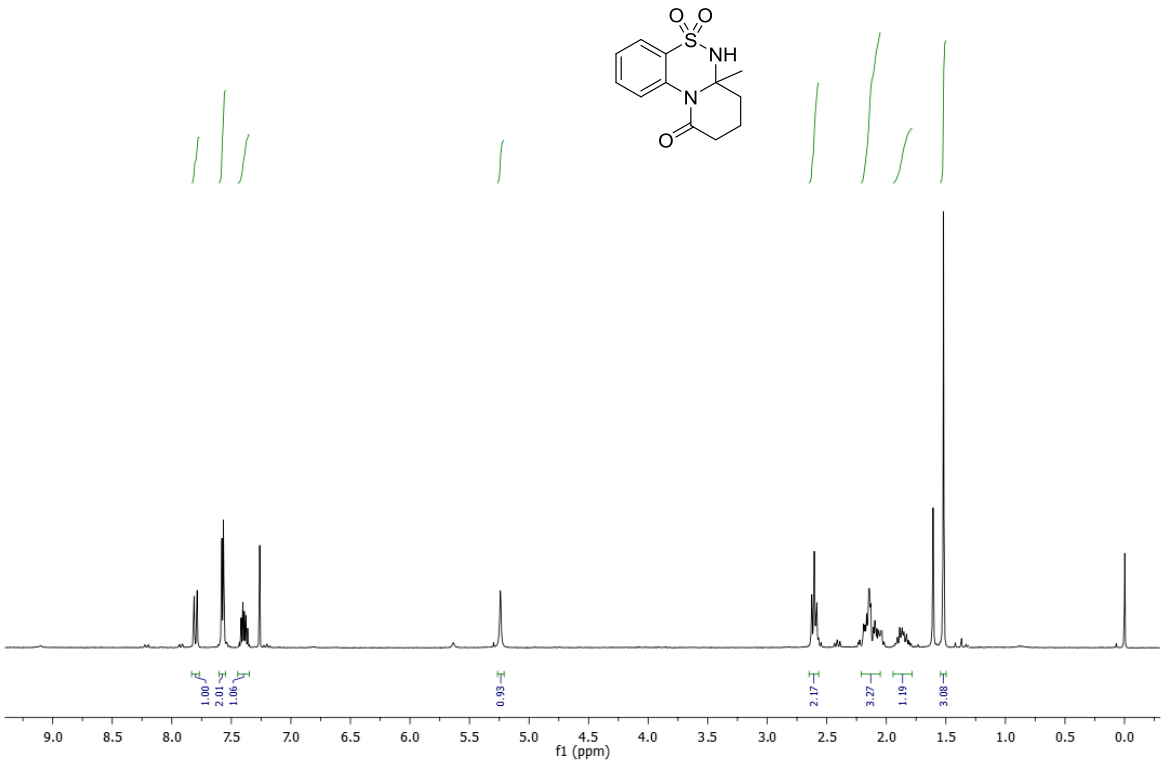


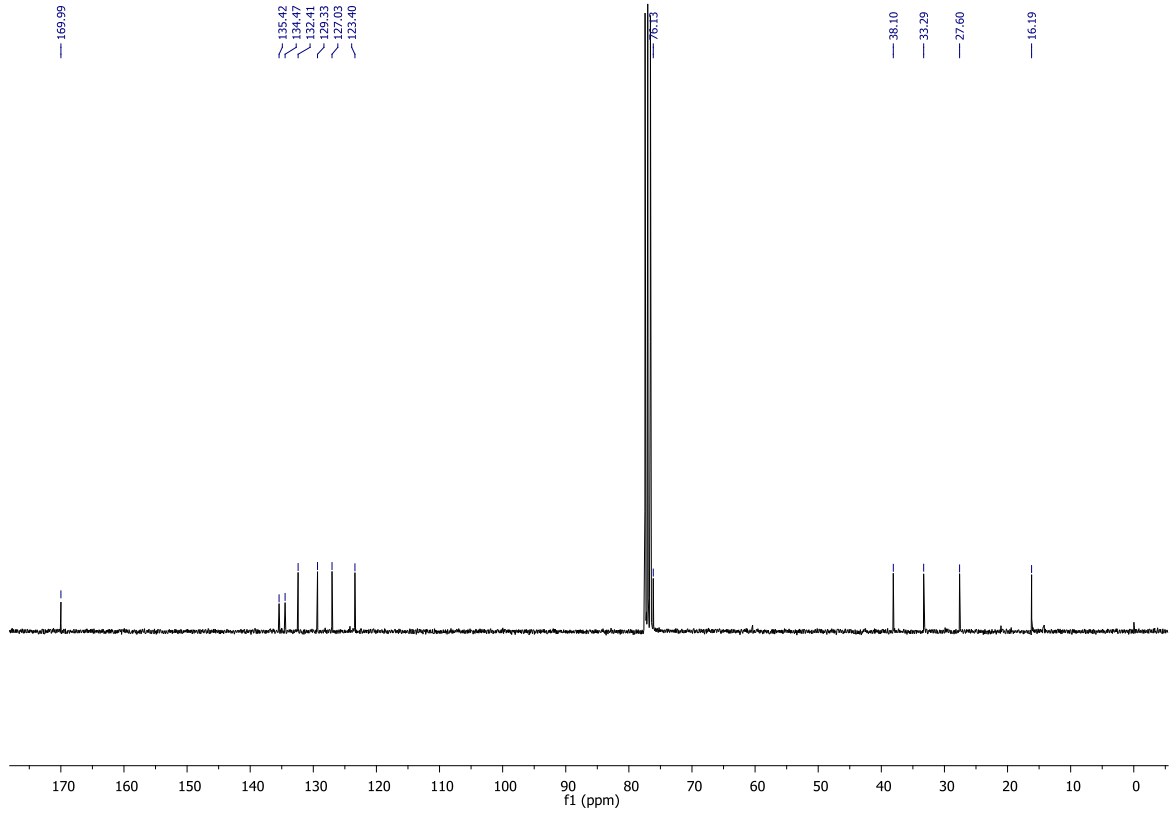
3a-methyl-2,3,3a,4-tetrahydro-1*H*-benzo[*e*]pyrrolo[2,1-*c*][1,2,4]thiadiazin-1-one 5,5-dioxide **(4f)**



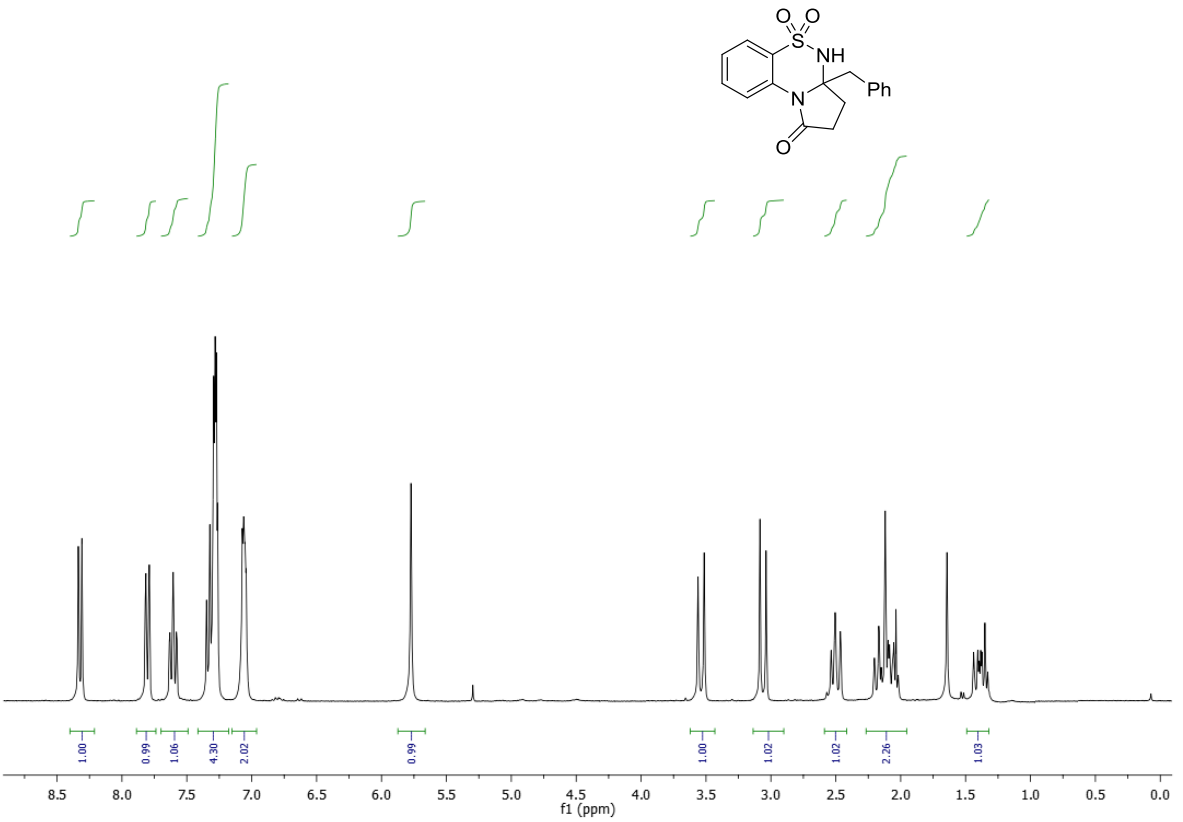


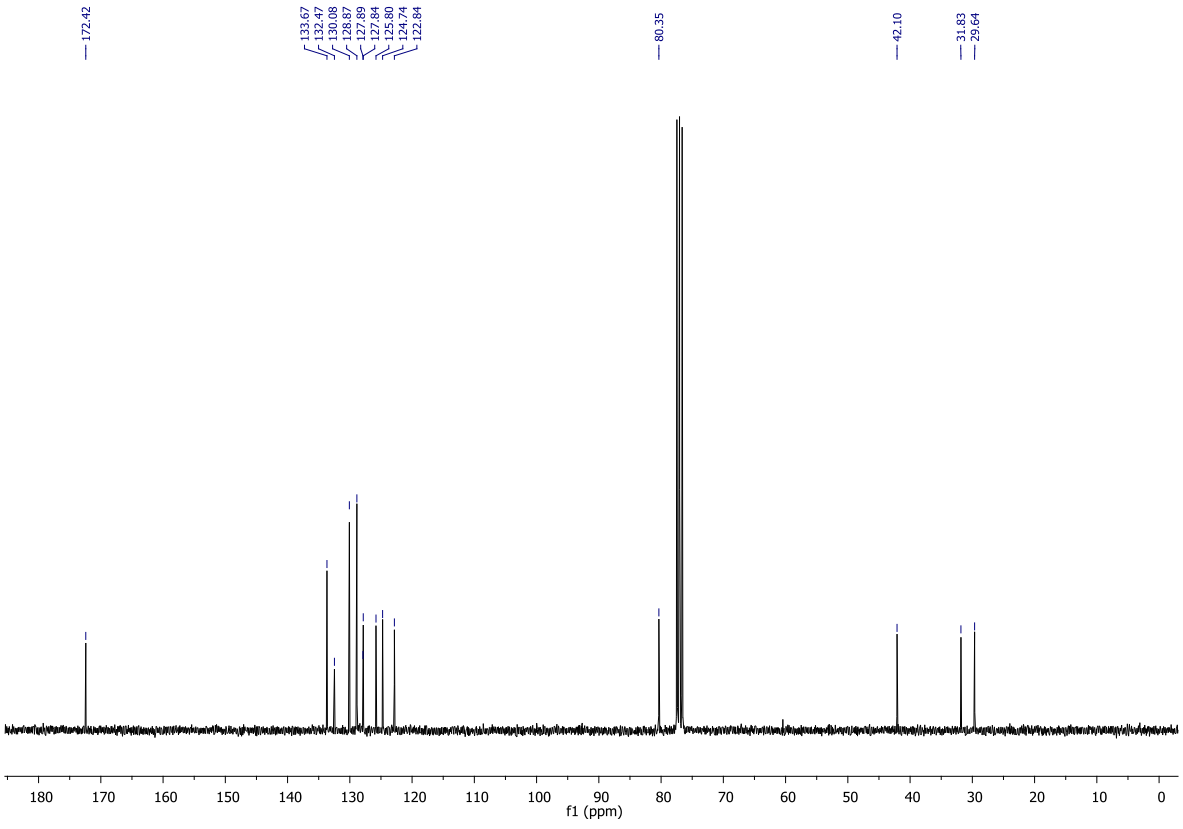
6a-methyl-6a,7,8,9-tetrahydrobenzo[*e*]pyrido[2,1-*c*][1,2,4]thiadiazin-10(6*H*)-one 5,5-dioxide **(4g)**



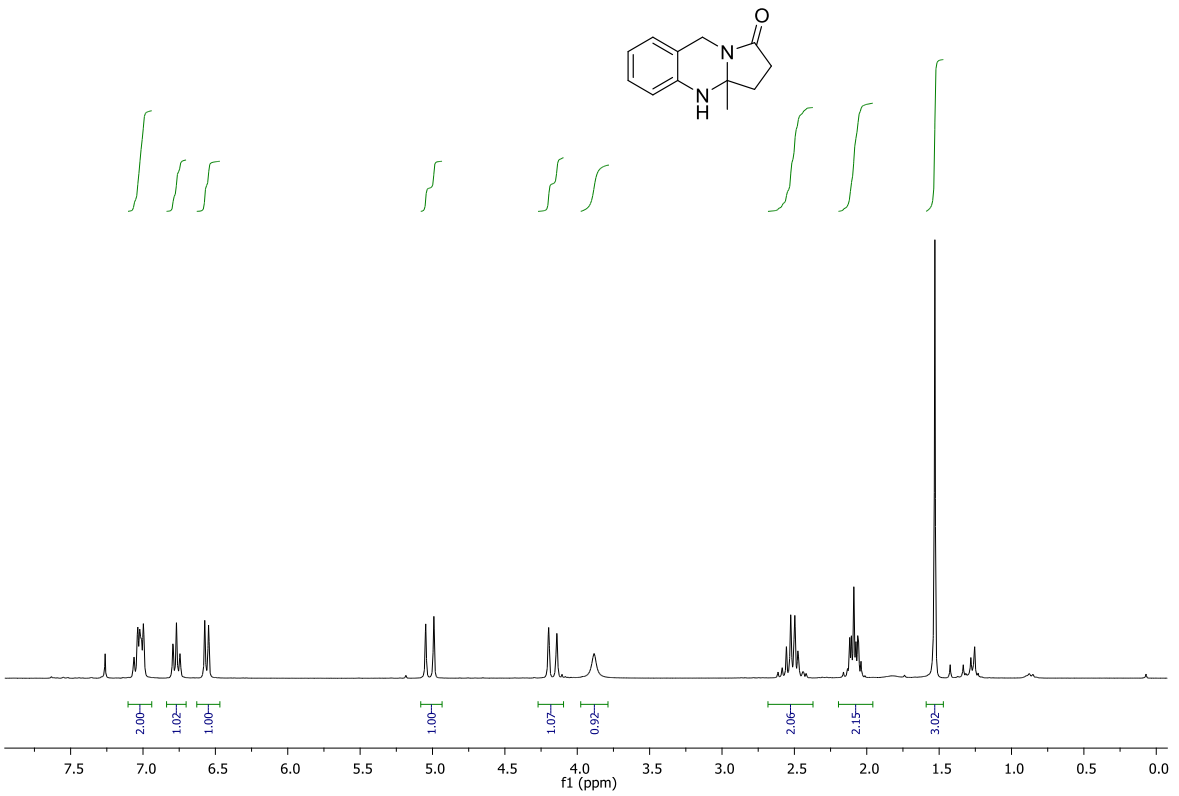


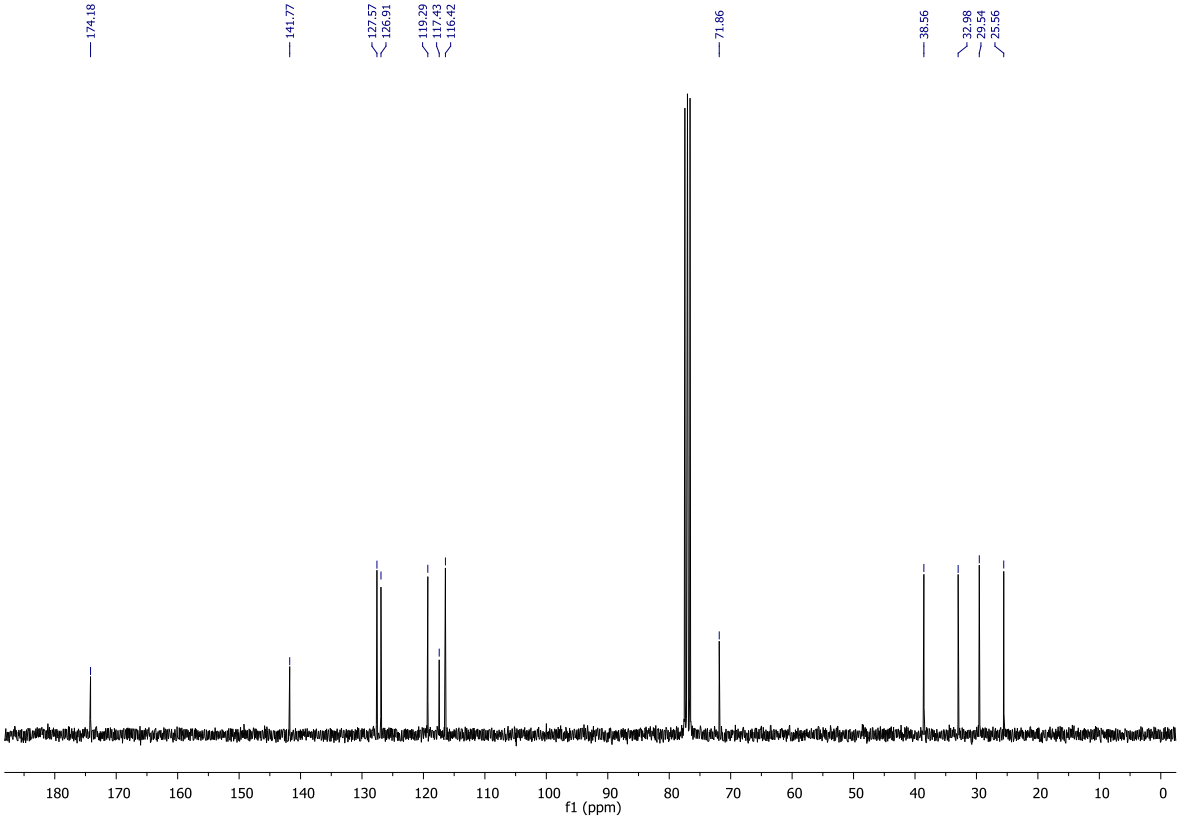
3a-benzyl-2,3,3a,4-tetrahydro-1*H*-benzo[*e*]pyrrolo[2,1-*c*][1,2,4]thiadiazin-1-one 5,5-dioxide **(4h)**



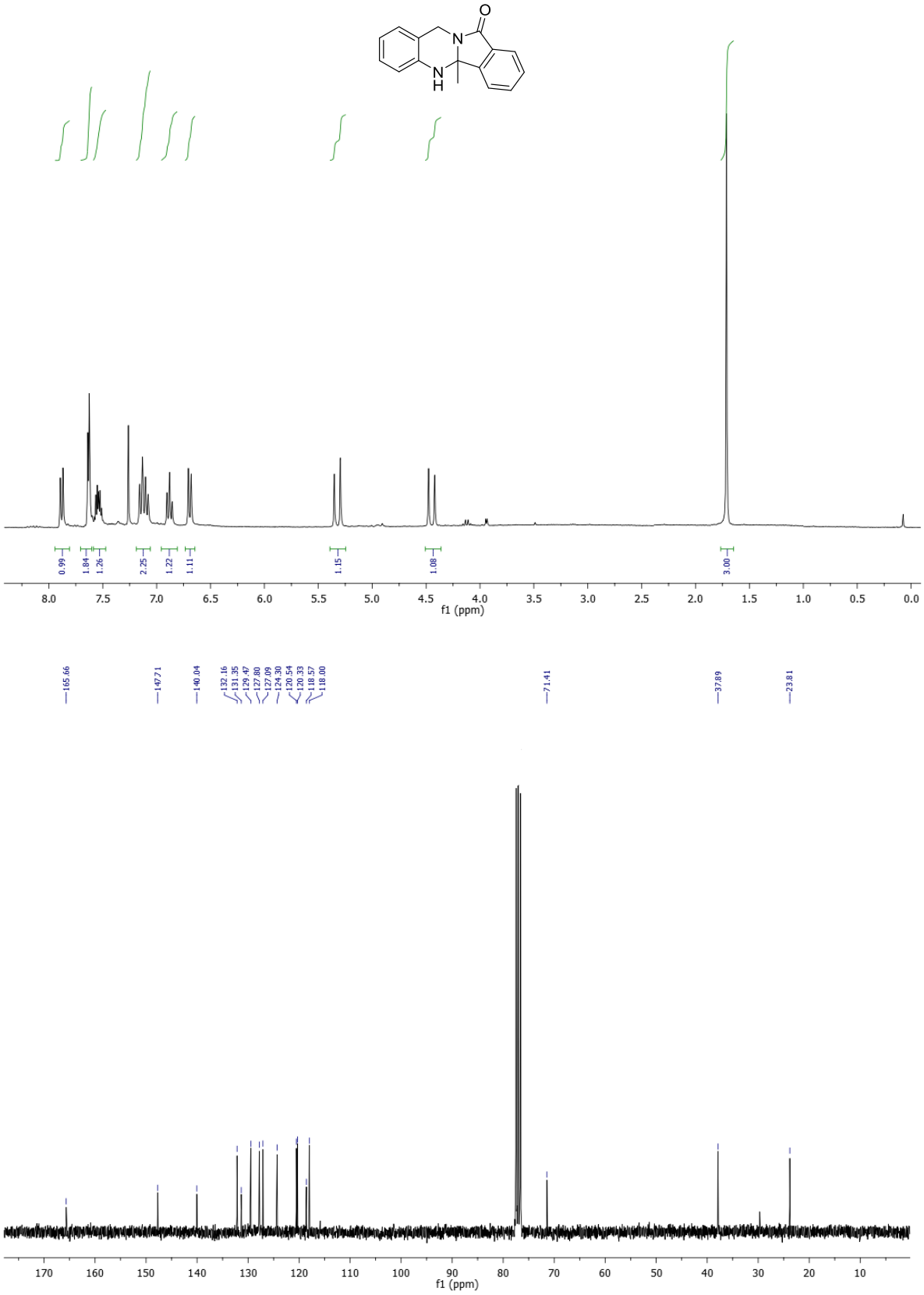


3a-methyl-3,3a,4,9-tetrahydropyrrolo[2,1-*b*]quinazolin-1(2*H*)-one **(6a)**

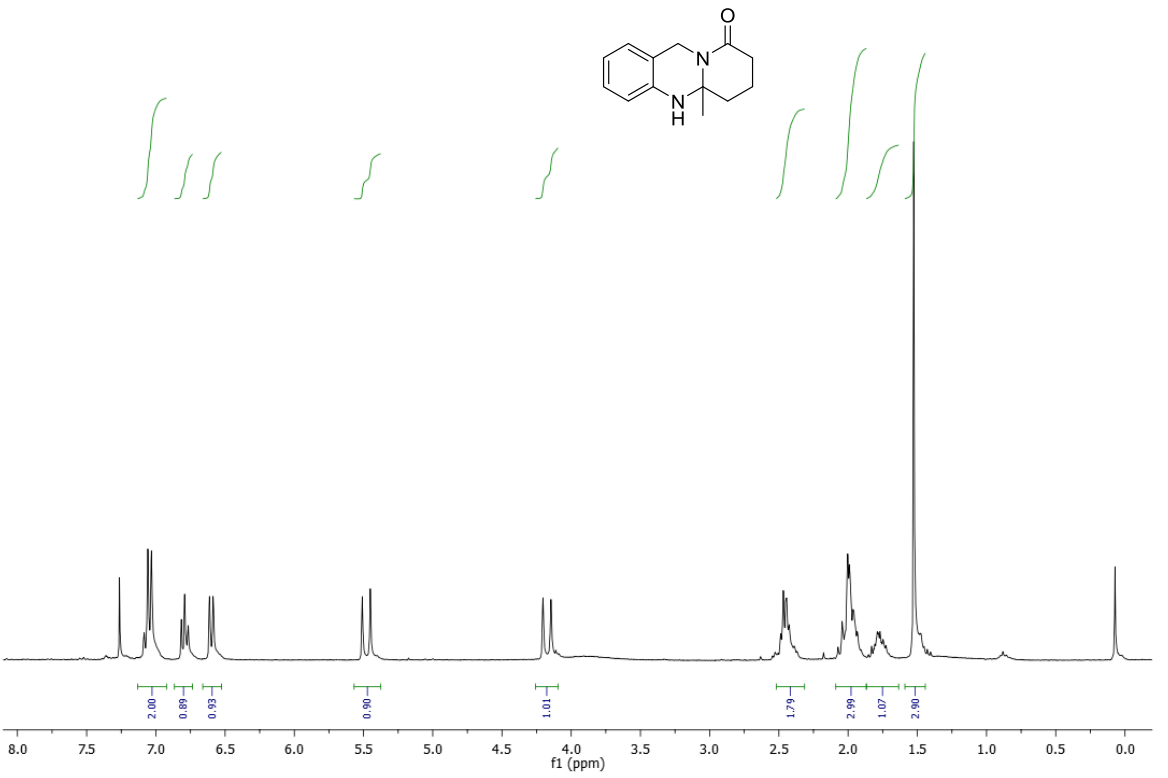


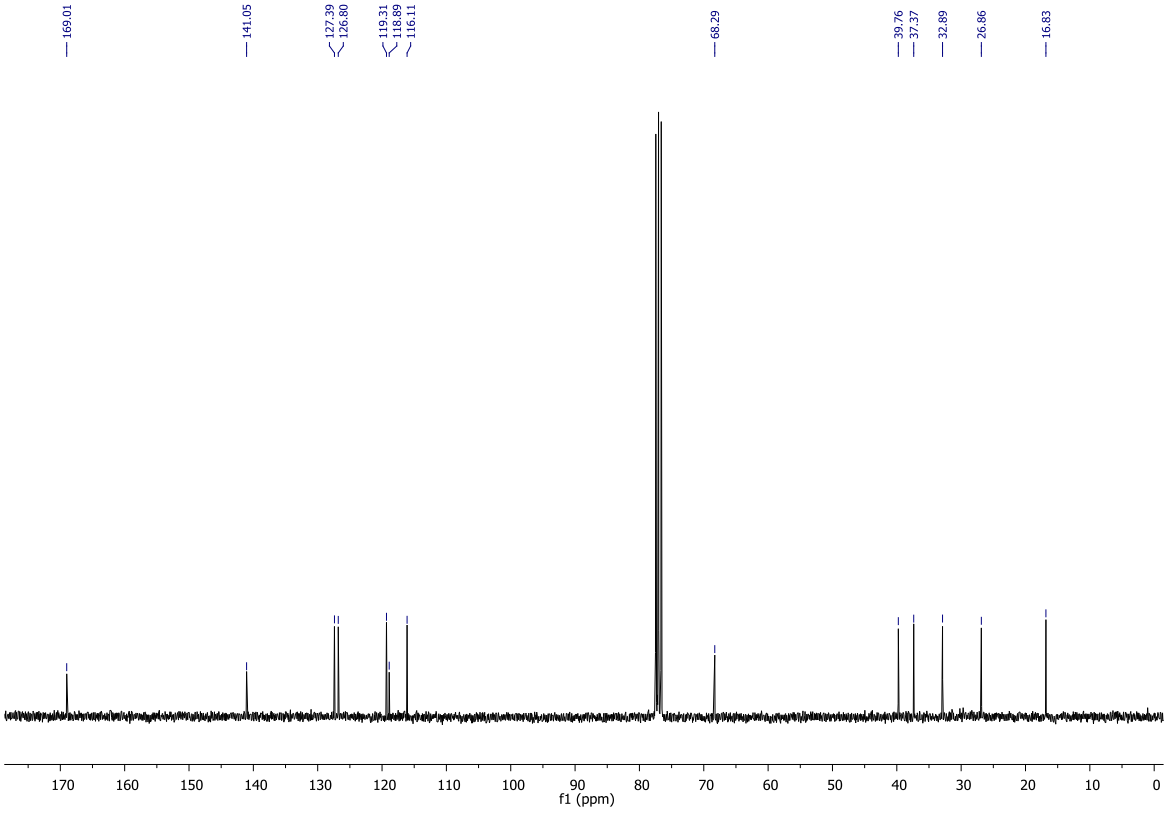


4b-methyl-5,10-dihydroisoindolo[1,2-*b*]quinazolin-12(4b*H*)-one **(6b)**

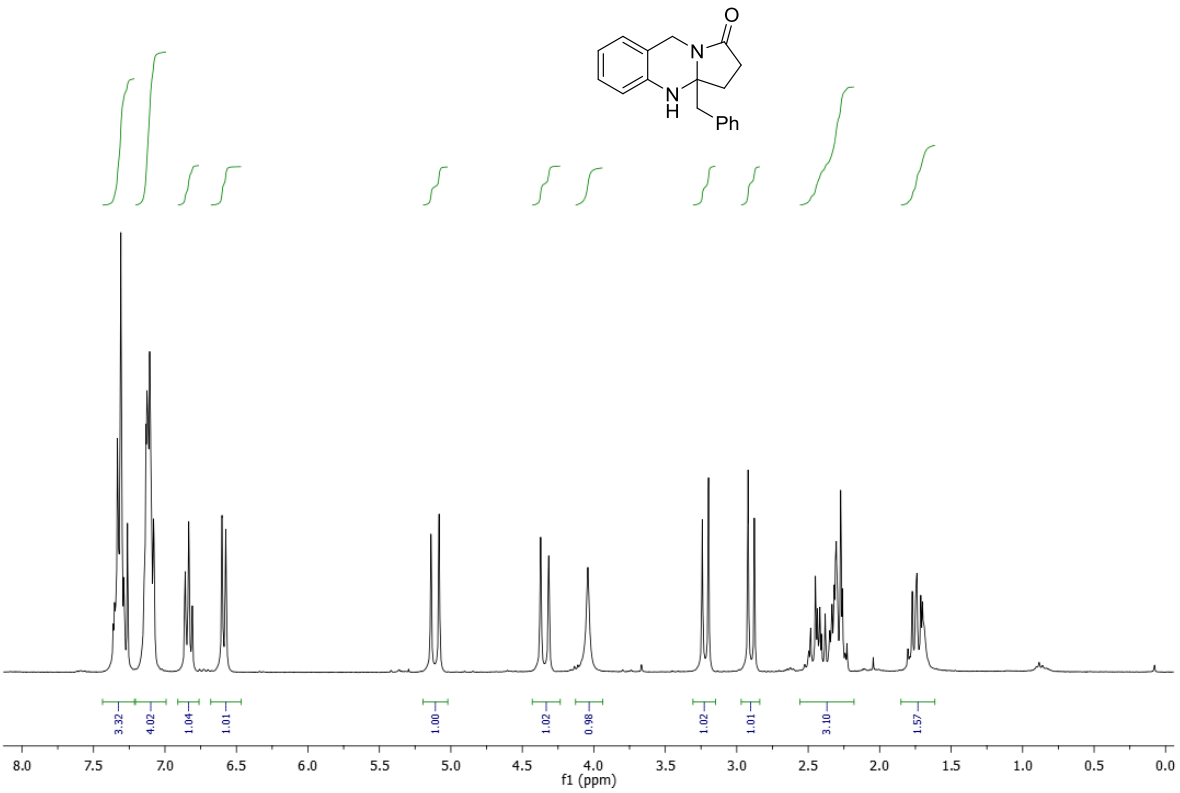


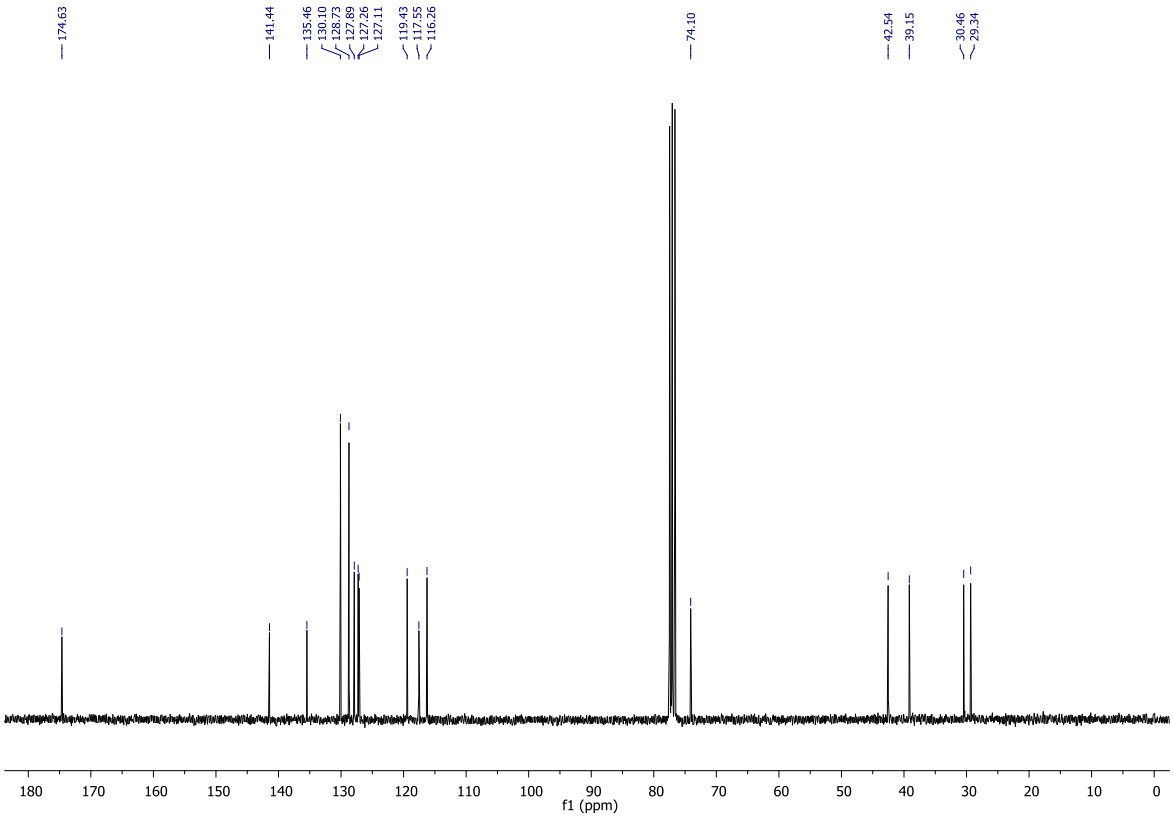
5a-methyl-5,5a,6,7,8,11-hexahydro-9*H*-pyrido[2,1-*b*]quinazolin-9-one **(6c)**



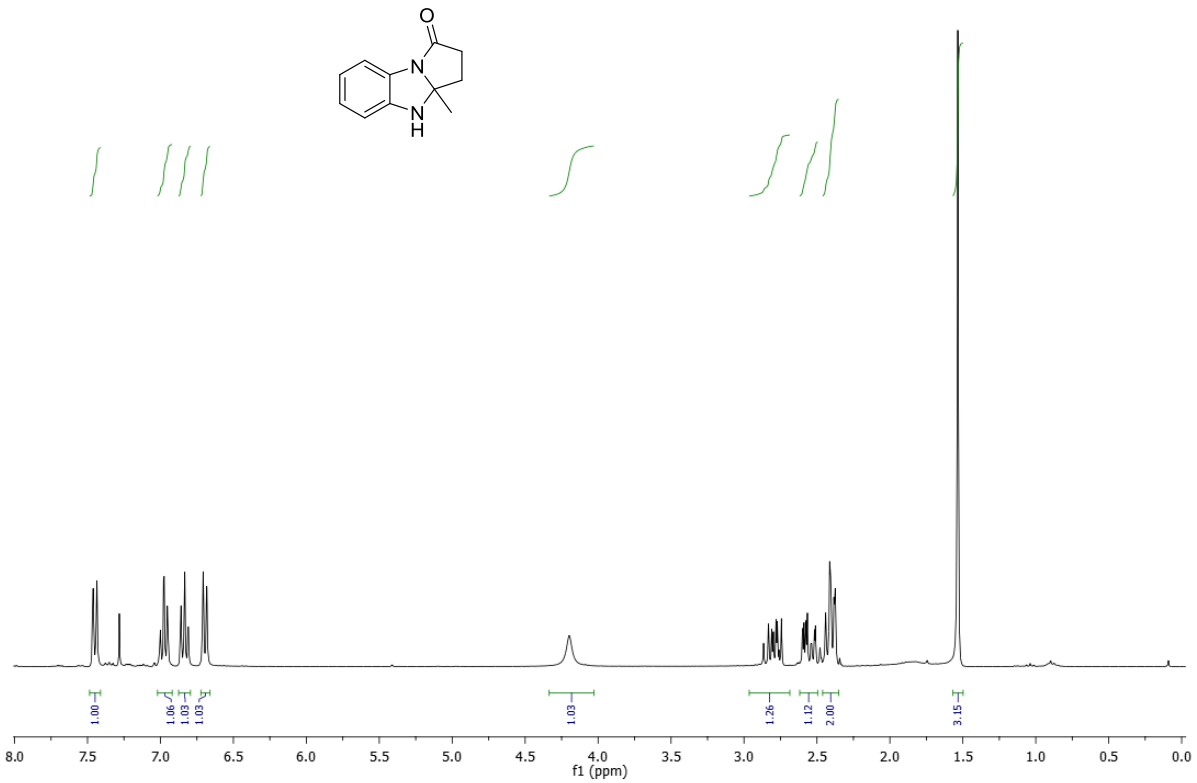


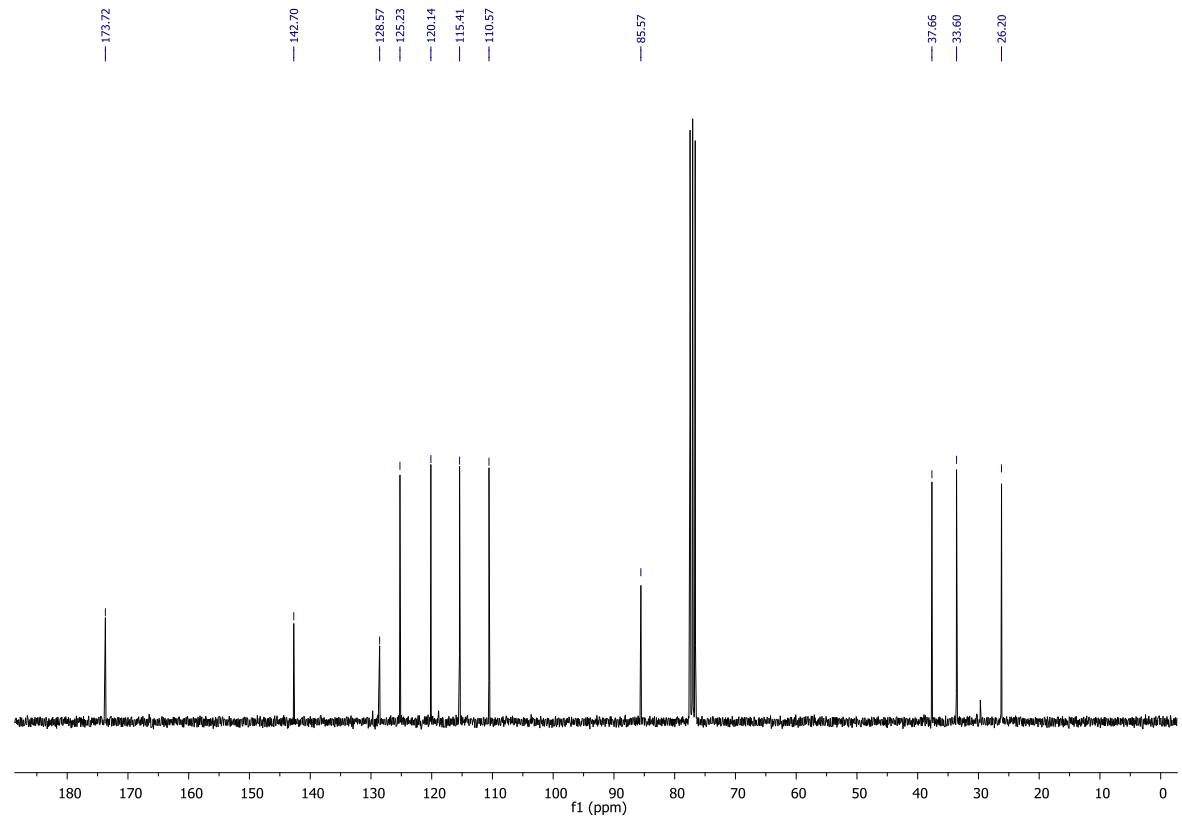
3a-benzyl-3,3a,4,9-tetrahydropyrrolo[2,1-*b*]quinazolin-1(2*H*)-one **(6d)**



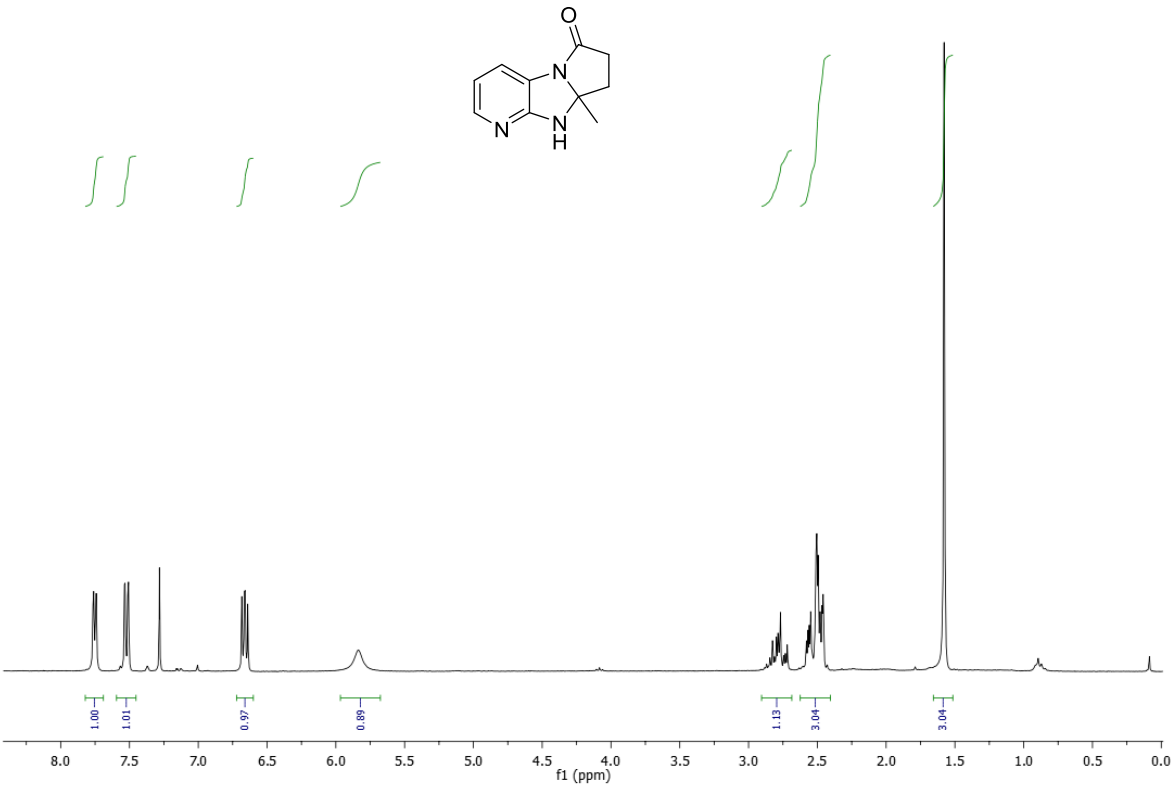


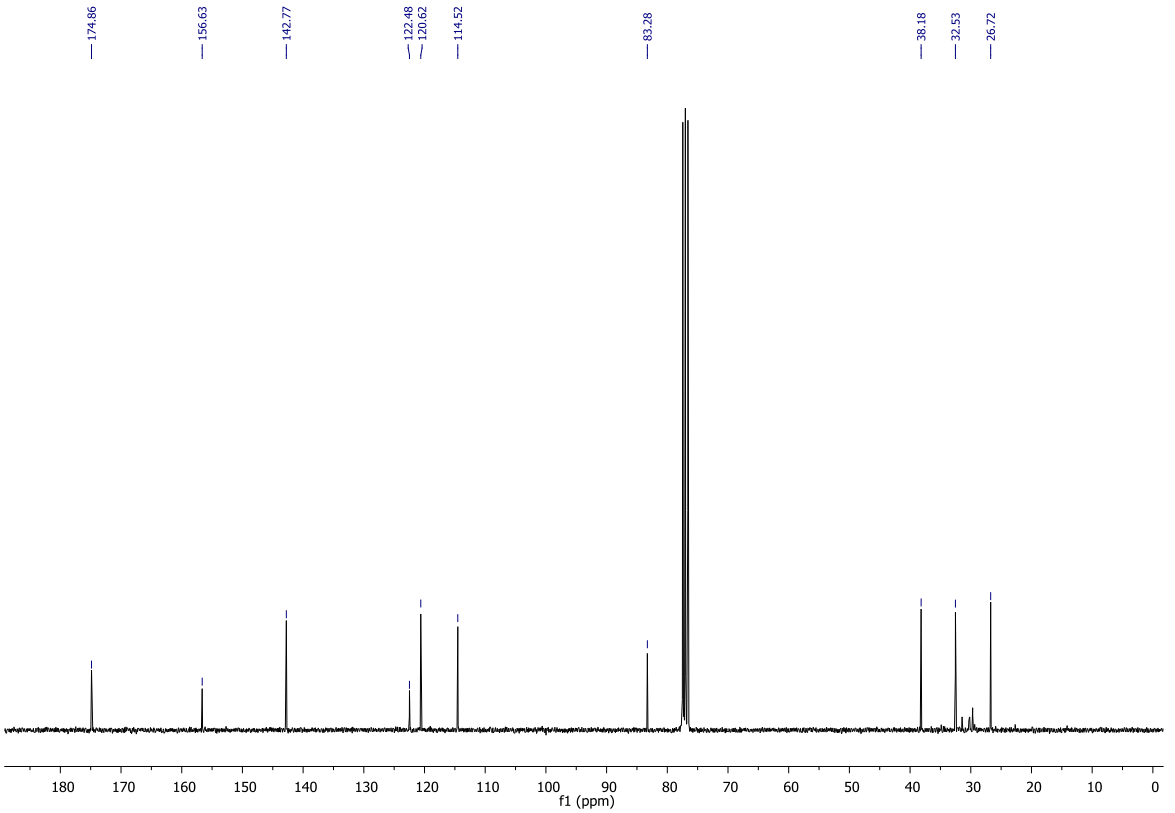
3a-methyl-2,3,3a,4-tetrahydro-1*H*-benzo[*d*]pyrrolo[1,2-*a*]imidazol-1-one **(6e)**





8a-methyl-7,8,8a,9-tetrahydro-6*H*-pyrrolo[1',2':1,2]imidazo[4,5-*b*]pyridin-6-one **(6g)**





References

1 H. Harkat, A. Y. Dembele, J.-M. Weibel, A. Blanc, P. Pale *Tetrahedron* **2009,** *65*, 1871-1879.