Supporting Information

Synthesis of ω-functionalized ketones from strained cyclic alcohols by ring-opening and cross-recombination between alkyl and *N*-oxyl radicals

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1. General information

In all experiments RT stands for 22–25 °C. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE II 300 and Bruker Fourier 300HD (300.13 MHz for ^{1}H and 75.47 MHz for ^{13}C, respectively) spectrometers in $CDCl_3$. Chemical shifts were reported in parts per million(ppm), and the residual solvent peak was used as an internal reference: ^{1}H ($CDCl_3$ δ = 7.26 ppm), ^{13}C ($CDCl_3$ δ = 77.16 ppm). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), m (multiplet). Coupling constants were reported in Hertz (Hz). FT-IR spectra were recorded on Bruker Alpha instrument. High resolution mass spectra (HR-MS) were measured on a Bruker maXis instrument using electrospray ionization (ESI). The measurements were performed in a positive ion mode (interface capillary voltage – 4500 V); mass range from m/z 50 to m/z 3000 Da; external calibration with Electrospray Calibrant Solution (Fluka). A syringe injection was used for all acetonitrile solutions (flow rate 3 μL/min). Nitrogen was applied as a dry gas; interface temperature was set at 180 °C.

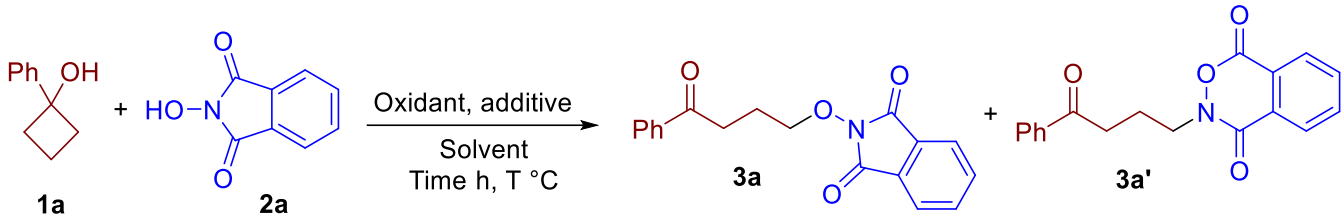
$Pb(OAc)_4$ 95%, $PhI(OAc)_2$ (PIDA) 98%, $K_2S_2O_8$ 99%, potassium peroxymonosulfate (Oxone®, extra pure, min. 4.5% active oxygen), $NaBrO_3$ 99%, KIO_4 99%, $KMnO_4$ 99%, $Mn(OAc)_3{\cdot}2H_2O$ 95%, $Mn(OAc)_2{\cdot}4H_2O$ 99%, $Mn(ClO_4)_2{\cdot}6H_2O$ 99%, $Mn(NO_3)_2{\cdot}4H_2O$ 99%, $MnCl_2{\cdot}4H_2O$ 99%, $Mn(hfacac)_2{\cdot}3H_2O$ 95%, 2,2-bipyridine 99%+, $AgNO_3$ 99%, $(NH_4)_2[Ce(NO_3)_6]$ (CAN) 98%+, $CeCl_3{\cdot}3H_2O$ 99%, $Mo(CO)_6$ 98%, Et_3N 99%, benzyltriethylammonium chloride (TEBAC) 99%, cyclobutanone 98%, *N*-hydroxyphthalimide (NHPI) 98%, *N*-hydroxysuccinimide 98%, 2,2,6,6-tetramethylpiperidinooxy (TEMPO) 98%, 2,6-di-tert-butyl-4-methylphenol (BHT) 99.8%, 1,1-diphenylethylene 97%, $NH_2OH{\cdot}HCl$ 99%, and $NaHCO_3$ 99% were used as is from commercial sources. CH_2Cl_2 and $C_2H_4Cl_2$ were distilled prior to use. MeCN was distilled over P_2O_5, acetone was distilled over $KMnO_4$, MeOH was distilled over magnesium and iodine, THF was distilled over sodium. Glacial acetic acid, 1,1,1,3,3,3-hexafluoro-2-propanol and 2,2,2-trifluoroethanol were used as is from commercial sources.

Tertiary cyclobutanol substrates **1a–g** were prepared by the addition of organometallic reagents to cyclobutanone according to the published literature procedures.[1–5] 1-phenylcyclopropanol **1h** was prepared from acetophenone silyl enol ether by Simmons–Smith cyclopropanation.[6,7] Tetrachloro-*N*-hydroxyphthalimide **2b**,[8] *N*-hydroxynaphthalimide **2c**,[9] and 4-hydroxy-2-hydroxyhexahydro-1H-4,7-methanoisoindole-1,3(2H)-dione **2d**[10] were prepared according to the published literature procedures. $PhI(OCOCF_3)_2$ (PIFA)[11] and $Ag(bpy)_2NO_3$[12] were prepared according to the published literature procedures.

2. Experimental Data

2.1 Optimization of reaction conditions of oxidative C–O coupling between 1-phenylcyclobutanol 1a and NHPI 2a (additional experimental data for Table 1).

Table S1. Optimization of the reaction conditions [a]



1a **2a** **3a** **3a'**

Run	Oxidant	Additive, mol %	Molar ratio **1a:2a:**oxidant	Solvent	Time, h	T, °C	Yield **3a/3a'**, %[b]	Conversion **1a**, %
1	$Pb(OAc)_4$	-	1:1:2	MeCN	2.5	RT	0	0
2	$Pb(OAc)_4$	-	1:1:2	DCM	2.5	RT	<5	10
3	$Pb(OAc)_4$	-	1:1:1.1	DCE	2.5	80	0	<5
4	PIDA	-	1:1:1.1	DCM	2.5	RT	0	<5
5	PIDA	-	1:1:1.5	HFIP	2.5	RT	0	100
6	PIDA	-	1:1:1.1	DCE	2.5	80	<5	20
7	PIDA	$Mn(OAc)_3$, 20 mol% bpy, 22 mol%	1:1:1.5	MeCN	2.5	80	<5	100
8	PIFA	-	1:1:1.1	DCM	2.5	RT	0	100
9	$K_2S_2O_8$	$AgNO_3$, 20 mol%	1:1:1.1	DCM/H_2O	2.5	RT	0	<5
10	$K_2S_2O_8$	$AgNO_3$, 20 mol%	1:1:1.1	$MeCN/H_2O$ = 1/1	2.5	RT	0	0
11	$K_2S_2O_8$	$Ag(bpy)_2NO_3$, 20 mol%	1:1:1.1	$MeCN/H_2O$ = 1/1	2.5	RT	<5	5-10
12	$K_2S_2O_8$	$AgNO_3$, 20 mol%	1:1:1.1	$MeCN/H_2O$ = 1/1	1	60	0	<5
13	$K_2S_2O_8$	$AgNO_3$, 20 mol%	1:2:1.1	$MeCN/H_2O$ = 1/1	1	60	0	0
14	$K_2S_2O_8$	$AgNO_3$, 20 mol%	1:1:1.2	$MeCN/H_2O$ = 1/1	3	80	12	20
15	$K_2S_2O_8$	$AgNO_3$, 20 mol% py, 5 equiv	1:1:1.2	$MeCN/H_2O$ = 1/1	3	80	0	0
16	$K_2S_2O_8$	$Mn(OAc)_2{\cdot}4H_2O$, 20 mol%	1:1:1.2	AcOH	1	60	0	0
17	Oxone	-	1:1:1.1	$MeCN/H_2O$ = 1/1	2.5	RT	0	0
18	$NaBrO_3$	CAN, 20 mol%	1:1: 2.5	$MeCN/H_2O$ = 1/1	2.5	RT	<5	5-10
19	KIO_4	$CeCl_3$, 20 mol%	1:1:2.5	$MeCN/H_2O$ = 1/1	2.5	RT	0	0
20	$Mn(OAc)_3$	-	1:1:2	AcOH	2.5	60	41	
21	$Mn(OAc)_3$	-	1:2:3	AcOH	2.5	60	42	
22	$Mn(OAc)_3$	-	1:1:2.5	AcOH	1	60	36	
23	**$Mn(OAc)_3$**	**$Mn(OAc)_2{\cdot}4H_2O$, 20 mol%**	**1:1:2**	**AcOH**	**1**	**60**	**56/12**	**100**
24	$KMnO_4$	-	1:1:0.4	AcOH	1	60	40/11	86
25	$KMnO_4$	-	1:2:0.4	AcOH	1	60	37/10	74
26	$KMnO_4$	-	1:2:0.6	AcOH	1	60	40/10	100
27	$KMnO_4$	$Mn(OAc)_2{\cdot}4H_2O$, 20 mol%	1:1:0.4	AcOH	1	60	34/9	100
28	**$KMnO_4$**	**$Mn(OAc)_2{\cdot}4H_2O$, 20 mol%**	**1:1:0.5**	**AcOH**	**1**	**60**	**54/11**	**100**
29	$KMnO_4$	$Mn(OAc)_2{\cdot}4H_2O$, 20 mol%	1:1:0.5	AcOH	1	60	56/14	100

30	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1.5:1:0.5	AcOH	1	60	53/12	~130%
31	$KMnO_4$	$MnCl_2 \cdot 4H_2O$, 20 mol%	1:1:0.5	AcOH	1	60	43/21	100
32	$KMnO_4$	$Mn(ClO_4)_2 \cdot 6H_2O$, 20 mol%	1:1:0.5	AcOH	1	60	0/0	100
33	$KMnO_4$	$Mn(hfacac)_2 \cdot 3H_2O$, 20 mol%	1:1:0.5	AcOH	1	60	46/13	100
34	$KMnO_4$	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:0.5	AcOH	1	60	55/9	100
35[c]	**$KMnO_4$**	**$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%**	**1:1:0.5**	**AcOH**	**1**	**60**	**61/14**	**100**
36	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1:1:0.6	AcOH	1	60	40/9	100
37	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1:1.5:0.5	AcOH	1	60	48/10	100
38	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1:2:0.6	AcOH	1	60	50/11	100
39	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 60 mol%	1:2:0.6	AcOH	1	60	41/12	100
40	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 100 mol%	1:2:0.6	AcOH	1	60	43/11	100
41	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 140 mol%	1:2:0.6	AcOH	1	60	46/12	100
42	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 10 mol%	1:2:0.6	AcOH	1	60	50/10	100
43	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1:1:0.5	AcOH	1	40	36/7	100
44	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1:1:0.5	AcOH	30	60	27/12	100
45	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1:1:0.5	AcOH	1	80	44/10	100
46	$KMnO_4$	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1:1:0.5	AcOH	1	100	57/13	100
47	$NaBrO_3$	CAN, 20 mol%	1:1: 2.5	MeCN/H_2O = 1/1	2.5	80	7/0	15
48	CAN	-	1:1:2.1	MeCN	2.5	RT	30/4	100
49[d]	CAN	-	1:1:2.1	MeCN	2.5	RT	35	100
50	CAN	-	1:1:2.1	MeCN/H_2O = 1/1	2.5	RT	49/16	81
51	CAN	-	1:1:3	MeCN/H_2O = 1/1	3	RT	53/16	100
52	CAN	-	1:1:2.1	DCM/H_2O = 1/1	2.5	RT	21	54
53	CAN	-	1:1:3	MeCN/H_2O = 1/1	2.5	5/RT	39	100
54	CAN	-	1:1:2.2	AcOH	2.5	60	28/<5	100
55[d]	CAN	-	1:1:3	MeCN/H_2O = 1/1	3	RT	55/<5	100
56	CAN	$MnCl_2 \cdot 4H_2O$, 20 mol%	1:1:3	MeCN/H_2O = 1/1	3	RT	59/15	100
57	CAN	$MnCl_2 \cdot 4H_2O$, 20 mol%	1:2:3	MeCN/H_2O = 1/1	3	RT	63/18	100
58	CAN	$MnCl_2 \cdot 4H_2O$, 20 mol%	1:2:3	Acetone/H_2O	2.5	RT	35	72
59	CAN	$MnCl_2 \cdot 4H_2O$, 20 mol%	1:2:3	AcOH	1	60	22	100
60	CAN	$MnCl_2 \cdot 4H_2O$, 20 mol%	1:2:2	MeCN/H_2O = 1/1	3	RT	36/10	60
61	CAN	$MnCl_2 \cdot 4H_2O$, 20 mol%	1:1:2.2	MeCN/H_2O = 1/1	3	RT	57/19	90
62	CAN	$MnCl_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	MeCN/H_2O = 1/1	3	RT	59/19	100
63	CAN	$Mn(ClO_4)_2 \cdot 6H_2O$, 20 mol%	1:1:2.5	MeCN/H_2O = 1/1	3	RT	56/17	100
64	CAN	$Mn(OAc)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	MeCN/H_2O = 1/1	3	RT	64/14	100

65	**CAN**	**$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%**	**1:1:2.5**	**MeCN/H_2O = 1/1**	**3**	**RT**	**69/27**	**100**
66	CAN	$Mn(hfacac)_2 \cdot 3H_2O$, 20 mol%	1:1:2.5	MeCN/H_2O = 1/1	3	RT	53/19	100
67	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1.5:1:2.5	MeCN/H_2O = 1/1	3	RT	56/14	100
68	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	THF/H_2O = 1/1	3	RT	0/0	<5
69	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	MeOH	3	RT	23/0	30
70	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	Acetone/H_2O = 1/1	3	RT	66/21	100
71	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	DCM/H_2O = 1/1	3	RT	30/10	47
72	**CAN**	**$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%**	**1:1:2.5**	**MeCN/H_2O = 1/1**	**1**	**RT**	**67/20**	**100**
73	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	MeCN/H_2O = 1/1	0.5	RT	61/15	100
74	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	MeCN/H_2O = 1/1	1	60	68/18	100
75	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	MeCN/H_2O = 1/1	1	0-5 => RT	59/25	100
76[c]	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	MeCN/H_2O = 1/1	1	RT	64/17	100
77	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 10 mol%	1:1:2.5	MeCN/H_2O = 1/1	1	RT	65/19	100
78	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 40 mol%	1:1:2.5	MeCN/H_2O = 1/1	1	RT	67/17	100
79	CAN	$Mn(NO_3)_2 \cdot 4H_2O$, 20 mol%	1:1:2.5	MeCN	1	RT	46/11	100
80	CAN	-	1:1:2.5	MeCN/H_2O = 1/1	1	RT	52/13	100

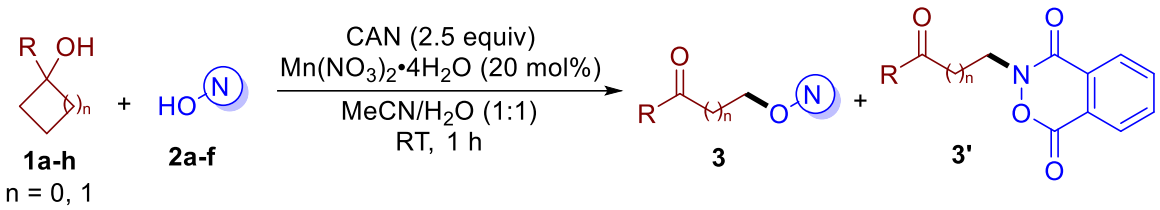
[a] **General procedure**: an oxidant (0.2–1.2 mmol) was added to a stirred mixture of 1-phenylcyclobutanol **1a** (60 mg, 0.4 mmol), NHPI **2a** (66.5 mg, 0.4 mmol), an additive (0–140 mol%), and solvent (2.5 mL) at a given temperature; the stirring was continued at the same temperature for appropriate time. Reaction mixture was diluted with CH_2Cl_2 (10 mL) and water (10 mL) and shaken. The organic layer was separated and the aqueous was extracted with CH_2Cl_2 (2×10 mL). All organic extracts were combined, washed successively with saturated solution of $NaHCO_3$ (10 mL), brine (10 mL), dried over Na_2SO_4, and rotary evaporated under water-jet vacuum. Reaction products **3aa** and **3aa'** were isolated by column chromatography on silica gel using the CH_2Cl_2/EtOAc = 80/1 eluent.

[b] Isolated yield

[c] Ar atmosphere

[d] Reaction mixture was irradiated for 2.5 h with 36W 400 nm LED

2.2 General reaction conditions for oxidative C–O coupling reaction of cycloalkanols 1 with *N*-hydroxyimides 2 (experimental data for Scheme 2).



General procedure: CAN (548 mg, 1 mmol) was added to a stirred mixture of cycloalkanol **1** (35–91 mg, 0.4 mmol), *N*-hydroxyimide **2** (46–120 mg, 0.4 mmol), $Mn(NO_3)_2 \cdot 4H_2O$ (20 mg, 0.08 mmol, 20 mol%), and MeCN/H_2O (2.5 mL, 1:1) at room temperature; the stirring was continued at room temperature for 1 hour. Reaction products **3** and **3'** were isolated as described above for **3a** and **3a'** in experiments of Table S1.

2.3 Gram-scale synthesis of 3aa (Scheme 3, a).

CAN (8.22 g, 15 mmol) was added to a stirred mixture of 1-phenylcyclobutanol **1a** (889 mg, 6 mmol), NHPI **2a** (998 mg, 6 mmol), $Mn(NO_3)_2 \cdot 4H_2O$ (301 mg, 1.2 mmol, 20 mol%), and MeCN/H_2O (37.5 mL, 1:1) at room temperature; the stirring was continued at room temperature for 1 hour. Reaction mixture was diluted with CH_2Cl_2 (150 mL) and water (150 mL) and shaken. Organic layer was separated and aqueous was extracted with CH_2Cl_2 (2×150 mL). All organic extracts were combined, washed successively with saturated solution of $NaHCO_3$ (150 mL), brine (150 mL), dried over Na_2SO_4, and rotary evaporated under water-jet vacuum. Reaction products **3aa** (1.05 g, 3.39 mmol, 57%) and **3aa'** (352 mg, 1.1 mmol, 19%) were isolated by column chromatography on silica gel using the CH_2Cl_2/EtOAc = 80/1 as eluent.

2.4 Synthesis of γ-hydroxy ketone 4 (Scheme 3, b).

A mixture of **3aa** (185 mg, 0.6 mmol), Et_3N (919 mg, 9 mmol), and $Mo(CO)_6$ (158 mg, 0.6 mmol) in MeCN/H_2O (5 mL, 15:1) was stirred at 80 °C for 9 h. The reaction mixture was cooled to room temperature and rotatory evaporated under water-jet vacuum. 4-Hydroxy-1-phenylbutan-1-one **4** (90%, 88 mg, 0.54 mmol) was isolated by column chromatography on silica gel using the PE/EtOAc = 1/1 as eluent.

2.5 Synthesis of dihydro-1,2-oxazine 5 (Scheme 3, b).

$NaHCO_3$ (84 mg, 1.0 mmol) was added to a stirred mixture of compound **3aa** (154 mg, 0.5 mmol) and $NH_2OH \cdot HCl$ (70 mg, 1.0 mmol) in MeCN (3 mL) and H_2O (0.5 mL) at room temperature; the stirring

was continued for 1 h. The mixture was rotatory evaporated to dryness, and the residue was extracted with CH_2Cl_2 (3x10 mL). The organic extracts were combined, washed with saturated aqueous $NaHCO_3$ (2x10 mL), dried over $MgSO_4$, and rotary evaporated under water-jet vacuum. 3-Phenyl-5,6-dihydro-4H-1,2-oxazine **5** (94%, 75 mg, 0.47 mmol) obtained as a white powder was analytically pure and was not further purified.

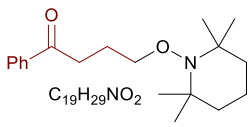
2.6 Synthesis of cyclic nitrone 6 (Scheme 3, b).

$NaHCO_3$ (109 mg, 1.3 mmol) was added to a stirred mixture of compound **3aa'** (204 mg, 0.66 mmol) and $NH_2OH{\cdot}HCl$ (90 mg, 1.3 mmol) in MeCN (4 mL) and H_2O (0.6 mL) at room temperature; stirring was continued for 1 h. The mixture was rotatory evaporated to dryness, and the residue was extracted with CH_2Cl_2 (3x10 mL). The organic extracts were combined, washed with saturated aqueous $NaHCO_3$ (2x10 mL), dried over $MgSO_4$, and rotary evaporated under water-jet vacuum. 5-Phenyl-3,4-dihydro-2H-pyrrole-1-oxide **6** (68%, 73 mg, 0.45 mmol) obtained as a slightly yellow solid was analytically pure and was not further purified.

2.7 Reaction of 1-phenylcyclobutanol 1a with *N*-hydroxyphthalimide 2a in Standard Conditions in the Presence of Radical Scavengers (Scheme 4).

CAN (8.22 g, 15 mmol) was added to a stirred mixture of 1-phenylcyclobutanol **1a** (60 mg, 0.4 mmol), NHPI **2a** (66.5 mg, 0.4 mmol), $Mn(NO_3)_2{\cdot}4H_2O$ (20 mg, 0.08 mmol, 20 mol%), radical scavenger – TEMPO, BHT or 1,1-diphenylethylene (125–176 mg, 0.8 mmol) and MeCN/H_2O (2.5 mL, 1:1) at room temperature; the stirring was continued at room temperature for 1 hour.

TEMPO-adduct derived from primary C-radical was detected by HRMS (HR-MS (ESI): m/z = 304.2271, calcd. for $C_{19}H_{29}NO_2+H^+$: 304.2271.):



Display Report

Analysis Info

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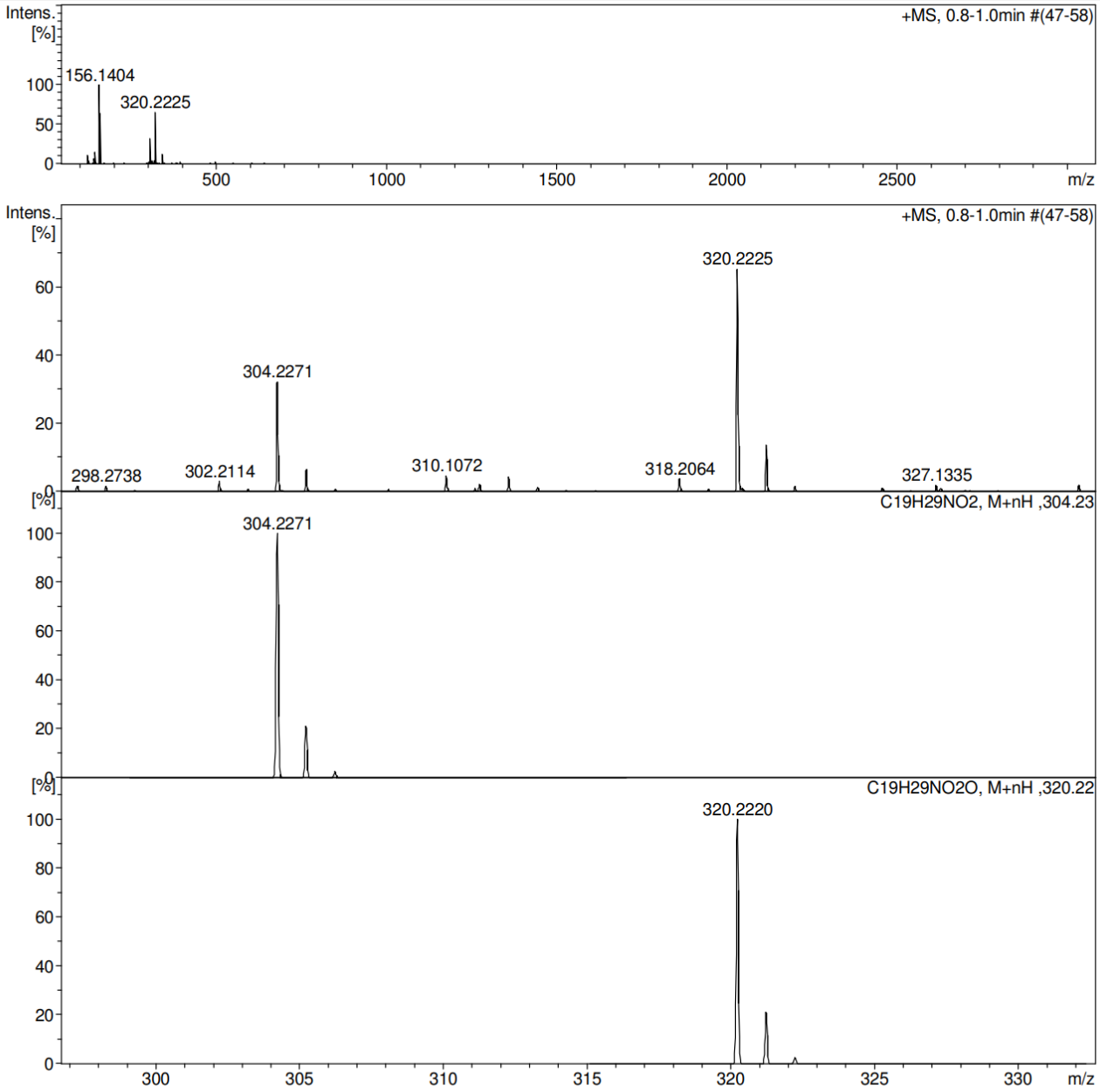
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN BUD-1218	Instrument / Ser#	micrOTOF 10248
Comment	C19H29NO2 mH304.2271 clb added CH3CN		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



3. X-ray single-crystal diffraction: Structure determination of compound 3aa'

X-ray diffraction data were collected at 100K on a Bruker Quest D8 diffractometer equipped with a Photon-III area-detector (shutterless φ- and ω-scan technique), using graphite-monochromatized Mo K_α-radiation. The intensity data were integrated by the SAINT program[13] and corrected for absorption and decay using SADABS.[14] The structure was solved by direct methods using SHELXT[15] and refined on F^2 using SHELXL-2018.[16] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters. The SHELXTL program suite[13] was used for molecular graphics. Crystal data and structure refinement for **3aa'** are summarized in Table S2. Compound **3aa'** crystallizes in orthorhombic space group $P2_12_12_1$ (Figure S1).

Table S2. Crystal data and structure refinement for **3aa'**.

Empirical formula	$C_{18}H_{15}NO_4$	
Formula weight	309.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 5.22790(10) Å	α = 90°
	b = 13.8547(4) Å	β = 90°
	c = 20.1340(6) Å	γ = 90°
Volume	1458.33(7) $Å^3$	
Z	4	
Density (calculated)	1.409 g/cm^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	648	
Crystal size	0.590 x 0.120 x 0.090 mm^3	
Theta range for data collection	1.784 to 30.528°	
Index ranges	-7<=h<=7, -19<=k<=19, -28<=l<=28	
Reflections collected	45414	
Independent reflections	4467 [R(int) = 0.0341]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.7121	

Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4467 / 0 / 208	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0316, wR2 = 0.0823	
R indices (all data)	R1 = 0.0342, wR2 = 0.0845	
Absolute structure parameter	-0.1(2)	
Largest diff. peak and hole	0.302 and -0.197 e.Å^{-3}	

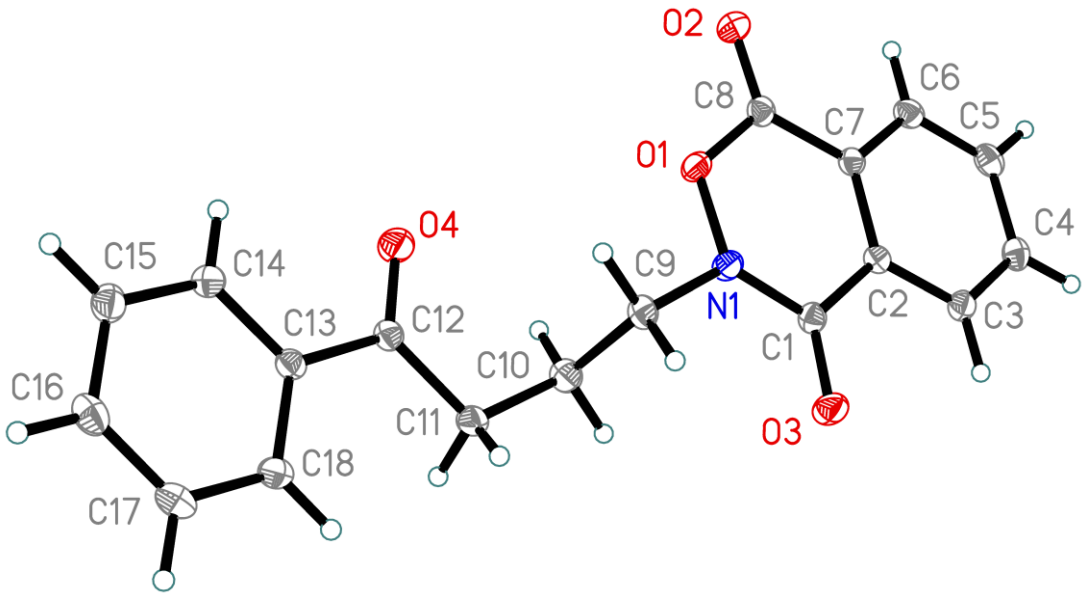
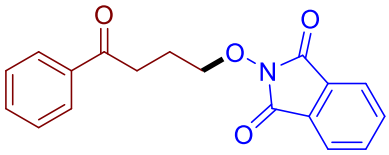
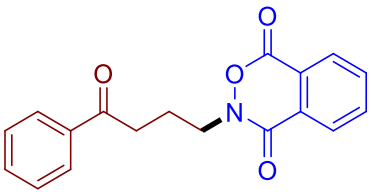


Figure S1. Crystal structure of compound **3aa'**, showing the atomic numbering and 50% probability displacement ellipsoids

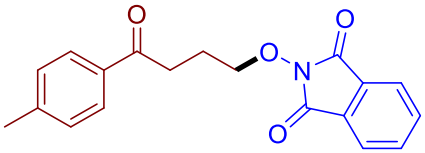
4. Characterization data of synthesized compounds



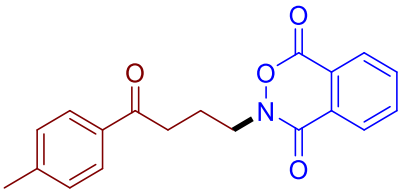
2-(4-oxo-4-phenylbutoxy)isoindoline-1,3-dione, **3aa** was isolated as pale yellow solid (67%, purified by column chromatography with CH_2Cl_2/EtOAc = 80/1 as eluent). Mp = 79–80 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.08 – 7.94 (m, 2H), 7.86 – 7.77 (m, 2H), 7.77 – 7.68 (m, 2H), 7.61 – 7.51 (m, 1H), 7.51 – 7.40 (m, 2H), 4.33 (t, *J* = 5.9 Hz, 2H), 3.37 (t, *J* = 7.0 Hz, 2H), 2.28 – 2.09 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 199.5, 163.8, 137.0, 134.6, 133.2, 129.0, 128.7, 128.2, 123.6, 77.9, 34.6, 22.7. **FT-IR** (thin layer): ν_{max} = 1784, 1731, 1681, 1186, 979, 877, 763, 701. **HR-MS (ESI):** *m/z* = 327.1338, calcd. for $C_{18}H_{15}NO_4$+NH_4^+: 327.1339.



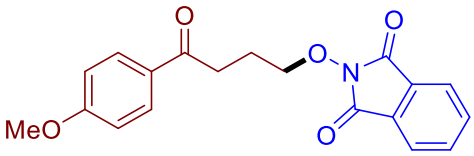
3-(4-Oxo-4-phenylbutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, **3aa'** was isolated as pale yellow solid (20%, purified by column chromatography with CH_2Cl_2/EtOAc = 80/1 as eluent). Mp = 114–117 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.28 – 8.11 (m, 2H), 7.93 – 7.83 (m, 3H), 7.83 – 7.75 (m, 1H), 7.54 – 7.45 (m, 1H), 7.44 – 7.33 (m, 2H), 4.17 (t, *J* = 6.7 Hz, 2H), 3.09 (t, *J* = 7.1 Hz, 2H), 2.35 – 2.18 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.7, 159.9, 156.9, 136.7, 135.8, 133.9, 133.1, 129.7, 129.5, 128.6, 128.0, 127.7, 123.7, 47.8, 35.4, 21.7. **FT-IR** (thin layer): ν_{max} = 1752, 1736, 1679, 1652, 1284, 1262, 700, 687. **HR-MS (ESI):** *m/z* = 348.0639, calcd. for $C_{18}H_{15}NO_4$+K^+: 348.0633.



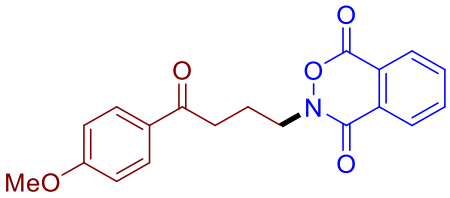
2-(4-Oxo-4-(*p*-tolyl)butoxy)isoindoline-1,3-dione, **3ba** was isolated as white crystals (50%, purified by column chromatography with PE/EtOAc = 2.5/1 as eluent). Mp = 115–116 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.94 (d, *J* = 8.0 Hz, 2H), 7.87 – 7.80 (m, 2H), 7.79 – 7.71 (m, 2H), 7.32 – 7.25 (m, 2H), 4.35 (t, *J* = 5.8 Hz, 2H), 3.34 (t, *J* = 7.0 Hz, 1H), 2.42 (s, 3H), 2.27 – 2.13 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 199.1, 163.8, 143.9, 134.6, 129.4, 129.1, 128.4, 123.6, 78.0, 34.5, 22.9, 21.8. **FT-IR** (thin layer): ν_{max} = 1785, 1733, 1676, 1606, 1185, 1133, 978, 877, 814, 701. **HR-MS** (ESI): *m/z* = 324.1223, calcd. for $C_{19}H_{17}NO_4$+H^+: 324.1230.



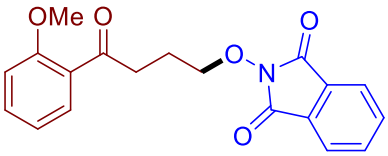
3-(4-Oxo-4-(*p*-tolyl)butyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ba' was isolated as yellow solid (11%, purified by column chromatography with PE/EtOAc = 2.5/1 as eluent). Mp = 117–119 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.25 (t, *J* = 7.4 Hz, 2H), 7.92 (t, *J* = 7.5 Hz, 1H), 7.88 – 7.78 (m, 3H), 7.23 (d, *J* = 7.9 Hz, 2H), 4.21 (t, *J* = 6.6 Hz, 2H), 3.10 (t, *J* = 7.1 Hz, 2H), 2.39 (s, 3H), 2.35 – 2.23 (m, 2H). **^{13}C NMR** (75.47 MHz, яCDCl$_3$): δ = 198.4, 160.0, 157.1, 144.0, 135.9, 134.4, 134.0, 129.9, 129.7, 129.4, 128.3, 127.9, 123.8, 48.1, 35.4, 22.0, 21.8. **FT-IR** (thin layer): ν_{max} = 1735, 1682, 1654, 1603, 1465, 1413, 1287, 1121, 698. **HR-MS** (ESI): *m/z* = 346.1038, calcd. for $C_{19}H_{17}NO_4$+Na^+: 346.1050.



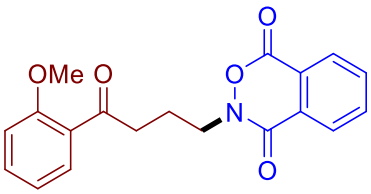
2-(4-(4-Methoxyphenyl)-4-oxobutoxy)isoindoline-1,3-dione, **3ca** was isolated as yellow crystals (49%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 98–100 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.98 (d, *J* = 7.9 Hz, 2H), 7.84 – 7.77 (m, 2H), 7.76 – 7.69 (m, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 4.31 (t, *J* = 5.9 Hz, 2H), 3.86 (s, 3H), 3.29 (t, J = 7.1 Hz, 2H), 2.24 – 2.11 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.0, 163.8, 163.6, 134.6, 130.5, 130.2, 129.0, 123.6, 113.8, 78.0, 55.6, 34.2, 22.9. **FT-IR** (thin layer): ν_{max} = 1726, 1675, 1598, 1171, 985, 875, 704. **HR-MS** (ESI): *m/z* = 340.1169, calcd. for $C_{19}H_{17}NO_5$+H^+: 340.1179.



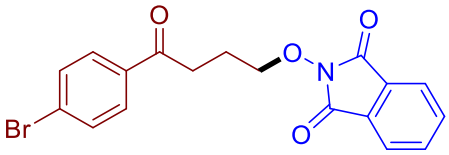
3-(4-(4-Methoxyphenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ca' was isolated as pale yellow solid (13%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 115–116 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.25 (t, *J* = 7.2 Hz, 2H), 7.97 – 7.79 (m, 4H), 6.90 (d, *J* = 8.6 Hz, 2H), 4.21 (t, *J* = 6.6 Hz, 2H), 3.85 (s, 3H), 3.07 (t, *J* = 7.0 Hz, 2H), 2.36 – 2.22 (m, 2H).**^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 197.3, 163.6, 160.0, 157.1, 135.8, 133.9, 130.4, 130.0, 129.9, 129.7, 127.9, 123.9, 113.9, 55.6, 48.1, 35.2, 22.1. **FT-IR** (thin layer): ν_{max} = 1757, 1734, 1672, 1649, 1601, 1281, 1262, 1167, 826, 698. **HR-MS** (ESI): *m/z* = 340.1177, calcd. for $C_{19}H_{17}NO_5$+H^+: 340.1179.



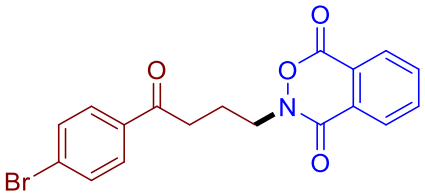
2-(4-(2-Methoxyphenyl)-4-oxobutoxy)isoindoline-1,3-dione, **3da** was isolated as pale green solid (53%, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). Mp = 74–76 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.84 – 7.76 (m, 2H), 7.76 – 7.66 (m, 3H), 7.44 (dd, *J* = 11.4, 4.2 Hz, 1H), 7.03 – 6.89 (m, 2H), 4.29 (t, *J* = 6.2 Hz, 2H), 3.92 (s, 3H), 3.29 (t, J = 7.1 Hz, 2H), 2.23 – 2.08 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 201.4, 163.6, 158.7, 134.40, 133.39, 130.2, 129.0, 128.2, 123.4, 120.6, 111.6, 78.0, 55.5, 39.7, 22.9. **FT-IR** (thin layer): ν_{max} = 1729, 1658, 1596, 1486, 1286, 1185, 1025, 878, 763, 705. **HR-MS** (ESI): *m/z* = 340.1182, calcd. for $C_{19}H_{17}NO_5$+H^+: 340.1179.



3-(4-(2-Methoxyphenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3da' was isolated as gray solid (13%, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). Mp = 106–108 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.27 (dd, *J* = 10.5, 8.0 Hz, 2H), 7.94 (t, *J* = 7.4 Hz, 1H), 7.85 (t, *J* = 7.5 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.05 – 6.90 (m, 2H), 4.18 (t, *J* = 6.6 Hz, 2H), 3.87 (s, 3H), 3.12 (t, *J* = 7.0 Hz, 2H), 2.31 – 2.17 (m, 2H).**^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 201.0, 160.1, 158.7, 156.9, 135.8, 133.9, 133.6, 130.5, 130.0, 129.7, 128.2, 127.9, 123.9, 120.8, 111.7, 55.6, 48.2, 40.9, 22.2. **FT-IR** (thin layer): ν_{max} = 1751, 1735, 1657, 1484, 1467, 1436, 1284, 699. **HR-MS** (ESI): *m/z* = 362.0999, calcd. for $C_{19}H_{17}NO_5$+Na: 362.0999.

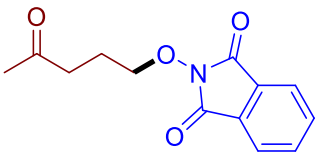


2-(4-(4-Bromophenyl)-4-oxobutoxy)isoindoline-1,3-dione, 3ea was isolated as white crystals (58%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 105–108 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.90 (d, *J* = 8.5 Hz, 2H), 7.86 – 7.78 (m, 2H), 7.78 – 7.70 (m, 2H), 7.62 (d, *J* = 8.5 Hz, 2H), 4.32 (t, *J* = 5.8 Hz, 2H), 3.34 (t, J = 7.0 Hz, 2H), 2.27 – 2.12 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.5, 163.8, 135.8, 134.7, 132.1, 129.8, 129.0, 128.4, 123.7, 77.8, 34.6, 22.7. **FT-IR** (thin layer): ν_{max} = 1786, 1735, 1680, 1583, 1398, 1186, 979, 878, 700. **HR-MS** (ESI): *m/z* = 388.0170, 390.0153, calcd. for $C_{18}H_{14}BrNO_4$+H^+: 388.0179, 390.0159.

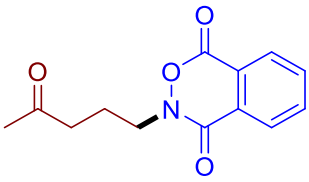


3-(4-(4-Bromophenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ea' was isolated as pale yellow solid (12%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 101-103 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.28 – 8.20 (m, 2H), 7.92 (td, *J* = 7.6, 1.3 Hz, 1H), 7.84 (td, *J* = 7.6, 1.3 Hz, 1H), 7.77 (d, *J* = 8.6 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 4.21 (t, *J* = 6.6 Hz, 2H), 3.09 (t, *J* = 7.2 Hz, 2H), 2.37 – 2.24 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 197.7, 160.0, 157.1, 135.9, 135.5, 134.0, 132.0, 129.8, 129.7, 129.65, 128.4, 127.9, 123.8, 47.9, 35.4, 21.8. **FT-IR** (thin layer): ν_{max}

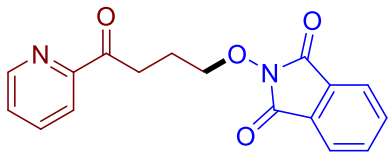
= 1752, 1734, 1683, 1657, 1584, 998, 695. **HR-MS** (ESI): *m/z* = 388.0170, 390.0153, calcd. for $C_{18}H_{14}BrNO_4$+H^+: 388.0179, 390.0159.



2-((4-Oxopentyl)oxy)isoindoline-1,3-dione, 3fa was isolated as white crystals (52%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 to 10/1 as eluent). Mp = 64–65 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.85 – 7.76 (m, 2H), 7.76 – 7.68 (m, 2H), 4.19 (t, *J* = 5.9 Hz, 2H), 2.80 (t, *J* = 7.0 Hz, 2H), 2.20 (s, 3H), 2.04 – 1.93 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 208.0, 163.7, 134.6, 129.0, 123.6, 77.6, 39.3, 30.3, 22.3. **FT-IR** (thin layer): ν_{max} = 1787, 1735, 1707, 1375, 1186, 1134, 993, 878, 700 **HR-MS** (ESI): *m/z* = 286.0476, calcd. for $C_{13}H_{13}NO_4$+K^+: 286.0476.

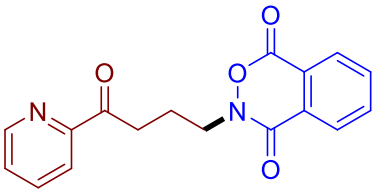


3-(4-Oxopentyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3fa' was isolated as brown gum (11%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 to 10/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.26 (d, *J* = 8.1 Hz, 1H), 8.23 (d, *J* = 7.9 Hz, 1H), 7.92 (t, *J* = 7.1 Hz, 1H), 7.83 (t, *J* = 7.6 Hz, 1H), 4.09 (t, *J* = 6.6 Hz, 2H), 2.57 (t, *J* = 7.1 Hz, 2H), 2.13 (s, 3H), 2.16– 2.04 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 207.4, 160.0, 157.0, 135.9, 134.0, 129.75, 129.69, 127.8, 123.7, 47.8, 40.3, 30.1, 21.3. **FT-IR** (thin layer): ν_{max} = 1758, 1737, 1714, 1659, 1437, 1411, 1287, 1121, 699. **HR-MS** (ESI): *m/z* = 265.1183, calcd. for $C_{13}H_{13}NO_4$+NH_4^+: 265.1183.

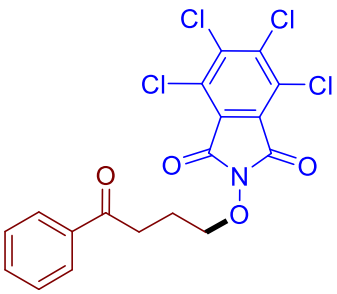


2-(4-Oxo-4-(pyridin-2-yl)butoxy)isoindoline-1,3-dione, 3ga was isolated as pale yellow solid (48%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 to 5/1 as eluent). Mp = 67–68 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.67 (d, *J* = 4.6 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.86 – 7.76 (m, 3H), 7.76 – 7.67 (m, 2H), 7.45 (ddd, *J* = 7.6, 4.6, 1.2 Hz, 1H), 4.31 (t, *J* = 6.4 Hz, 2H), 3.51 (t, *J* = 7.2 Hz, 2H), 2.29 – 2.11 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 200.9, 163.7, 153.2, 149.1, 137.0, 134.5, 134.3, 129.0, 127.3, 123.6, 121.8, 77.8, 33.9, 22.6. **FT-IR** (thin layer): ν_{max} = 1787, 1730, 1696,

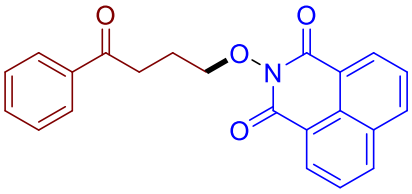
1466, 1375, 1187, 1127, 978, 877, 702. **HR-MS** (ESI): *m/z* = 333.0844, calcd. for $C_{17}H_{14}N_2O_4$+Na^+: 333.0846.



3-(4-Oxo-4-(pyridin-2-yl)butyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ga' was isolated as pale yellow solid (12%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 to 5/1 as eluent). Mp = 124–125 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.71 – 8.56 (m, 1H), 8.34 – 8.16 (m, 2H), 8.06 – 7.97 (m, 1H), 7.96 – 7.87 (m, 1H), 7.87 – 7.78 (m, 2H), 7.53 – 7.39 (m, 1H), 4.22 (t, *J* = 6.9 Hz, 2H), 3.37 (t, *J* = 7.1 Hz, 2H), 2.43 – 2.19 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 200.5, 160.1, 157.0, 153.1, 149.0, 137.2, 135.9, 134.0, 129.9, 129.7, 127.9, 127.4, 123.9, 122.0, 48.0, 34.7, 21.6. **FT-IR** (thin layer): ν_{max} = 1758, 1736, 1696, 1661, 1297, 745, 711, 696. **HR-MS** (ESI): *m/z* = 333.0844, calcd. for $C_{17}H_{14}N_2O_4$+Na^+: 333.0846.

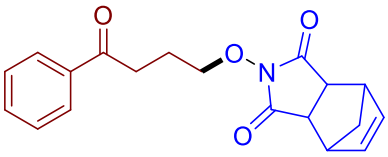


4,5,6,7-Tetrachloro-2-(4-oxo-4-phenylbutoxy)isoindoline-1,3-dione, **3ab** was isolated as pale yellow solid (20%, purified by column chromatography with CH_2Cl_2/EtOAc = 80/1 as eluent). Mp = 148–149 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.07 – 7.97 (m, 2H), 7.63 – 7.52 (m, 1H), 7.52 – 7.42 (m, 2H), 4.34 (t, *J* = 5.9 Hz, 2H), 3.35 (t, *J* = 7.0 Hz, 2H), 2.35 – 2.10 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 199.3, 159.3, 140.8, 136.9, 133.1, 130.2, 128.8, 128.2, 124.7, 78.3, 34.5, 22.7. **FT-IR** (thin layer): ν_{max} = 1737, 1684, 1370, 1040, 730, 689. **HR-MS (ESI):** *m/z* = 445.9515, calcd. for $C_{18}H_{11}Cl_4NO_4$+H^+: 445.9515.

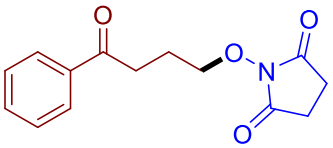


2-(4-Oxo-4-phenylbutoxy)-1H-benzo[de]isoquinoline-1,3(2H)-dione, **3ac** was isolated as pale brown solid (29%, purified by column chromatography with CH_2Cl_2/EtOAc = 80/1 as eluent). Mp = 134–136 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.69 – 8.48 (m, 2H), 8.30 – 8.14 (m, 2H), 8.11 – 7.99 (m,

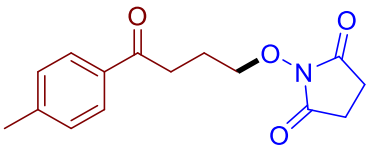
2H), 7.82 – 7.65 (m, 2H), 7.61 – 7.51 (m, 1H), 7.51 – 7.42 (m, 2H), 4.38 (t, *J* = 5.8 Hz, 2H), 3.45 (t, *J* = 7.1 Hz, 2H), 2.42 – 2.14 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 199.8, 161.2, 137.1, 134.7, 133.1, 131.7, 128.7, 128.3, 127.2, 122.9, 76.2, 35.1, 22.9. **FT-IR** (thin layer): ν_{max} = 1714, 1689, 1235, 778. **HR-MS (ESI):** *m/z* = 398.0791, calcd. for $C_{22}H_{17}NO_4$+K^+: 398.0791.



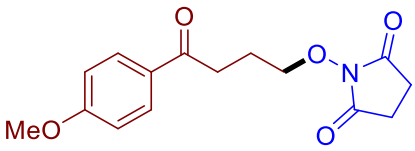
2-(4-Oxo-4-phenylbutoxy)-3a,4,7,7a-tetrahydro-1H-4,7-methanoisoindole-1,3(2H)-dione, **3ad** was isolated as pale yellow solid (33%, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). Mp = 85–86 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.10 – 7.82 (m, 2H), 7.63 – 7.49 (m, 1H), 7.49 – 7.35 (m, 2H), 6.14 (s, 2H), 4.06 (t, *J* = 5.9 Hz, 2H), 3.39 (s, 2H), 3.24 (t, *J* = 7.0 Hz, 2H), 3.16 (s, 2H), 2.12 – 1.99 (m, 2H), 1.74 (d, *J* = 8.9 Hz, 1H), 1.48 (d, *J* = 8.9 Hz, 1H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 199.4, 172.3, 137.0, 134.7, 133.1, 128.7, 128.1, 76.8, 51.5, 44.8, 42.7, 34.6, 22.6. **FT-IR** (thin layer): ν_{max} = 1727, 1715, 1686, 1373, 1205, 748, 723, 602. **HR-MS (ESI):** *m/z* = 348.1207, calcd. for $C_{19}H_{19}NO_4$+Na^+: 348.1206.



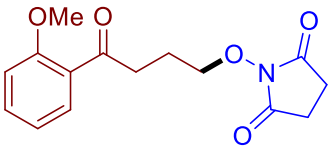
1-(4-Oxo-4-phenylbutoxy)pyrrolidine-2,5-dione, **3ae** was isolated as pale yellow solid (70%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 82–83 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.99 – 7.86 (m, 2H), 7.56 – 7.46 (m, 1H), 7.46 – 7.36 (m, 2H), 4.15 (t, *J* = 6.0 Hz, 2H), 3.23 (t, *J* = 7.0 Hz, 2H), 2.63 (s, 4H), 2.16 – 1.99 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 199.3, 171.4, 136.8, 133.1, 128.6, 128.0, 76.6, 34.4, 25.5, 22.4. **FT-IR** (thin layer): ν_{max} = 1717, 1681, 1214, 745, 693, 654. **HR-MS (ESI):** *m/z* = 284.0894, calcd. for $C_{14}H_{15}NO_4$+Na^+: 284.0893.



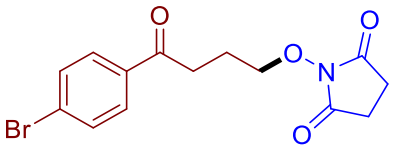
1-(4-Oxo-4-(*p*-tolyl)butoxy)pyrrolidine-2,5-dione, **3be** was isolated as white solid (73%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 95–96°C **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.88 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 4.20 (t, *J* = 5.9 Hz, 2H), 3.25 (t, *J* = 7.0 Hz, 2H), 2.69 (s, 4H), 2.39 (s, 3H), 2.22 – 2.01 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 199.1, 171.4, 144.0, 134.5, 129.4, 128.3, 76.9, 34.4, 25.6, 22.7, 21.7. **FT-IR** (thin layer): ν_{max} = 1719, 1676, 1605, 1216, 1202, 814 cm^{-1}. **HR-MS** (ESI): *m/z* = 298.1042, calcd. for $C_{15}H_{17}NO_4$+Na^+: 298.1050.



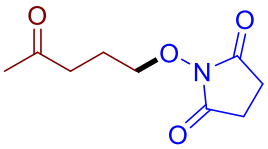
1-(4-(4-Methoxyphenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, 3ce was isolated as white solid (47%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 71–72°C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.01 – 7.93 (m, 2H), 6.96 – 6.88 (m, 2H), 4.19 (t, *J* = 5.9 Hz, 2H), 3.85 (s, *3*H), 3.22 (t, *J* = 7.0 Hz, 2H), 2.68 (s, 4H), 2.18 – 2.03 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.0, 171.4, 163.6, 130.4, 130.1, 113.8, 76.9, 55.6, 34.1, 25.6, 22.8. **FT-IR** (thin layer): ν_{max} = 1726, 1672, 1600, 1256, 1240, 1205, 1175 cm^{-1}; **HR-MS** (ESI): *m/z* = 314.0995, calcd. for $C_{15}H_{17}NO_5$+Na^+: 314.0999.



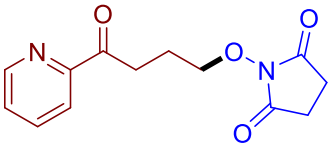
1-(4-(2-Methoxyphenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, **3de** was isolated as yellow oil (64%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.70 – 7.60 (m, 1H), 7.47 – 7.36 (m, 1H), 7.02 – 6.86 (m, 2H), 4.14 (t, *J* = 6.2 Hz, 2H), 3.87 (s, 3H), 3.19 (t, *J* = 7.0 Hz, 2H), 2.65 (s, 4H), 2.15 – 2.01 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 201.4, 171.3, 158.7, 133.5, 130.2, 128.1, 120.6, 111.7, 76.9, 55.6, 39.7, 25.5, 22.8. **FT-IR** (thin layer): ν_{max} = 1727, 1671, 1597, 1486, 1437, 1287, 1246, 1207 cm^{-1}; **HR-MS** (ESI): *m/z* = 314.0997, calcd. for $C_{15}H_{17}NO_5$+Na^+: 314.0999.



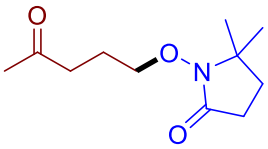
1-(4-(4-Bromophenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, **3ee** was isolated as pale brown gum (82%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.91 – 7.81 (m, 2H), 7.63 – 7.56 (m, 2H), 4.20 (t, *J* = 5.8 Hz, 2H), 3.27 (t, *J* = 7.0 Hz, 2H), 2.70 (s, 4H), 2.20 – 2.06 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 198.5, 171.3, 135.7, 132.0, 129.8, 128.4, 76.7, 34.5, 25.6, 22.6. **FT-IR** (thin layer): ν_{max} = 1722, 1682 cm^{-1}. **HR-MS** (ESI): *m/z* = 361.9990, calcd. for $C_{14}H_{14}BrNO_4$+Na^+: 361.9998.



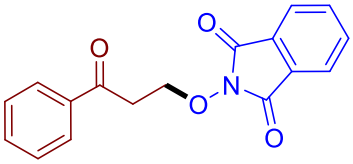
1-((4-Oxopentyl)oxy)pyrrolidine-2,5-dione, **3fe** was isolated as brown oil (70%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 4.09 (t, *J* = 5.9 Hz, 2H), 2.74 (t, *J* = 7.0 Hz, 2H), 2.69 (s, 4H), 2.18 (s, 3H), 2.01 – 1.84 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 208.1, 171.3, 76.5, 39.2, 30.2, 22.6, 22.1. **FT-IR** (thin layer): ν_{max} = 1785, 1715, 1429, 1401, 1373, 1208, 1171, 1075, 653 cm^{-1}. **HR-MS** (ESI): *m/z* = 222.0733, calcd. for $C_9H_{13}NO_4$+Na^+: 222.0737.



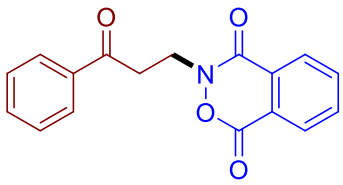
1-(4-Oxo-4-(pyridin-2-yl)butoxy)pyrrolidine-2,5-dione, 3ge was isolated as brown solid. (20%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 112-113°C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): 8.64 (d, *J* = 4.3 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.85 – 7.76 (m, 1H), 7.49 – 7.40 (m, 1 H), 4.18 (t, *J* = 6.4 Hz, 2H), 3.44 (t, *J* = 7.1 Hz, 2H), 2.67 (s, 4H), 2.20 – 2.03 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 200.9, 171.4, 153.2, 149.0, 137.0, 127.3, 121.8, 76.7, 33.8, 25.5, 22.4. **FT-IR** (thin layer): ν_{max} = 1714, 1698, 1204 cm^{-1}. **HR-MS** (ESI): *m/z* = 285.0849, calcd. for $C_{13}H_{14}N_2O_4$+Na^+: 285.0846.



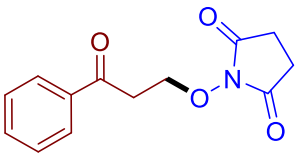
5,5-Dimethyl-1-((4-oxopentyl)oxy)pyrrolidin-2-one, **3ff** was isolated as yellow gum (35%, purified by column chromatography with CH_2Cl_2/EtOAc = 40/1 as eluent). **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 3.97 (t, *J* = 6.1 Hz, 2H), 2.66 (t, *J* = 7.1 Hz, 2H), 2.27 (t, *J* = 7.8 Hz, 2H), 2.14 (s, 3H), 1.97 – 1.85 (m, 2H), 1.81 (t, *J* = 7.7 Hz, 2H), 1.24 (s, 6H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 208.4, 171.5, 76.0, 60.9, 39.9, 30.8, 30.0, 26.5, 25.4, 22.8. **FT-IR** (thin layer): ν_{max} = 2970, 1714, 1368, 1206, 1170, 1093, 1049. **HR-MS** (ESI): *m/z* = 252.0098, calcd. for $C_{11}H_{19}NO_3$+K^+: 252.0097.



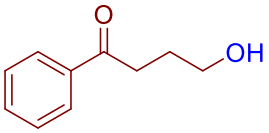
2-(3-Oxo-3-phenylpropoxy)isoindoline-1,3-dione, **3ha** was isolated as white solid (54%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 138–140 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.98 – 7.91 (m, 2H), 7.85 – 7.77 (m, 2H), 7.76 – 7.70 (m, 2H), 7.60 – 7.52 (m, 1H), 7.50 – 7.41 (m, 2H), 4.68 (t, *J* = 6.7 Hz, 2H), 3.53 (t, *J* = 6.7 Hz, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 196.6, 163.6, 136.5, 134.6, 133.5, 128.93, 128.76, 128.2, 123.7, 73.6, 37.5. **FT-IR** (thin layer): ν_{max} = 1728, 1688, 1210, 1185, 1136, 975, 876, 752, 694. **HR-MS** (ESI): *m/z* = 334.0476, calcd. for $C_{17}H_{13}NO_4$+K^+: 334.0476.



3-(3-Oxo-3-phenylpropyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ha' was isolated as white solid (13%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 91-94 °C. **^{1}H NMR** (300.13 MHz, CDCl3): δ = 8.35 – 8.20 (m, 2H), 8.01 – 7.90 (m, 3H), 7.85 7.90 – 7.81 (m, 1H), 7.62 – 7.53 (m, 1H), 7.51 – 7.42 (m, 2H), 4.54 (t, *J* = 7.2 Hz, 2H), 3.56 (t, *J* = 7.2 Hz, 2H). **^{13}C NMR** (75.47 MHz, CDCl3): δ = 197.0, 160.0, 157.1, 136.4, 136.0, 134.1, 133.7, 129.83, 129.76, 128.9, 128.2, 127.9, 123.8, 44.2, 35.8. **FT-IR** (thin layer): ν_{max} = 3440, 1731, 1678, 1657, 1286, 743, 694. **HR-MS** (ESI): m/z = 296.0916, calcd. for $C_{17}H_{13}NO_4$+H: 296.0917.

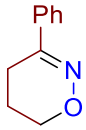


1-(3-Oxo-3-phenylpropoxy)pyrrolidine-2,5-dione, **3he** was isolated as white solid (60%, purified by column chromatography with CH_2Cl_2/EtOAc = 20/1 as eluent). Mp = 115–116 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): 7.97 – 7.87 (m, 2H), 7.63 – 7.53 (m, 1H), 7.50 – 7.41 (m, 2H), 4.57 (t, *J* = 6.4 Hz, 2H), 3.48 (t, *J* = 6.4 Hz, 2H), 2.67 (s, 4H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 196.9, 171.4, 136.5, 133.6, 128.8, 128.2, 72.2, 37.7, 25.6. **FT-IR** (thin layer): ν_{max} = 3486, 1719, 1681, 1210, 754, 690, 649 cm^{-1}; **HR-MS** (ESI): *m/z* = 270.0737, calcd. for $C_{13}H_{13}NO_4$+Na^+: 270.0737.

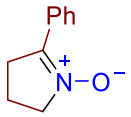


4-Hydroxy-1-phenylbutan-1-one, 4 was isolated as yellow oil (90%, purified by column chromatography with PE/EtOAc = 1/1 as eluent).[17] **^{1}H NMR** (300.13 MHz, DMSO-d_6): δ = 8.01 – 7.90 (m, 2H), 7.68 – 7.57 (m, 1H), 7.57 – 7.46 (m, 2H), 3.66 (bs, 1H), 3.46 (t, *J* = 6.4 Hz, 2H), 3.05 (t, *J* = 7.2

Hz, 2H), 1.85 – 1.69 (m, 2H). **^{13}C NMR** (75.47 MHz, DMSO-d_6): δ = 200.0, 136.8, 133.0, 128.7, 127.8, 60.1, 34.6, 27.2. **FT-IR** (thin layer): ν_{max} = 2951, 2882, 1720, 1684, 1598, 1449, 1368, 1321, 1276, 1236, 1206, 1054, 1030, 1002, 759, 742, 692 cm^{-1}. **HR-MS** (ESI): *m/z* = 187.0733, calcd. for $C_{10}H_{12}O_2$+Na^+: 187.0730.



3-Phenyl-5,6-dihydro-4H-1,2-oxazine, 5 was isolated as white solid (93%). Mp = 66–67 °C. **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 7.76 – 7.60 (m, 2H), 7.46 – 7.31 (m, 3H), 4.07 (t, *J* = 5.2 Hz, 2H), 2.60 (t, *J* = 6.9 Hz, 2H), 2.20 – 2.00 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 155.1, 136.2, 129.6, 128.6, 125.4, 65.8, 21.0, 19.5. **FT-IR** (thin layer): ν_{max} = 1448, 1016, 905, 842, 758, 694, 550. **HR-MS (ESI):** *m/z* = 162.0913, calcd. for $C_{10}H_{11}NO$+H^+: 162.0907.



5-Phenyl-3,4-dihydro-2H-pyrrole-1-oxide, 6 was isolated as slightly yellow solid (68%). Mp = 98–100 °C (Lit. Mp = 100–102 °C).[18] **^{1}H NMR** (300.13 MHz, $CDCl_3$): δ = 8.45 – 8.15 (m, 2H), 7.57 – 7.31 (m, 3H), 4.26 (t, *J* = 8.1 Hz, 2H), 3.19 (t, *J* = 7.6 Hz, 2H), 2.36 – 2.07 (m, 2H). **^{13}C NMR** (75.47 MHz, $CDCl_3$): δ = 141.5, 130.6, 129.1, 128.6, 127.5, 65.0, 31.2, 16.8. **FT-IR** (thin layer): ν_{max} = 1574, 1560, 1448, 1376, 1220, 768, 693. **HR-MS (ESI):** *m/z* = 162.0913, calcd. for $C_{10}H_{11}NO$+H^+: 162.0915.

5. References

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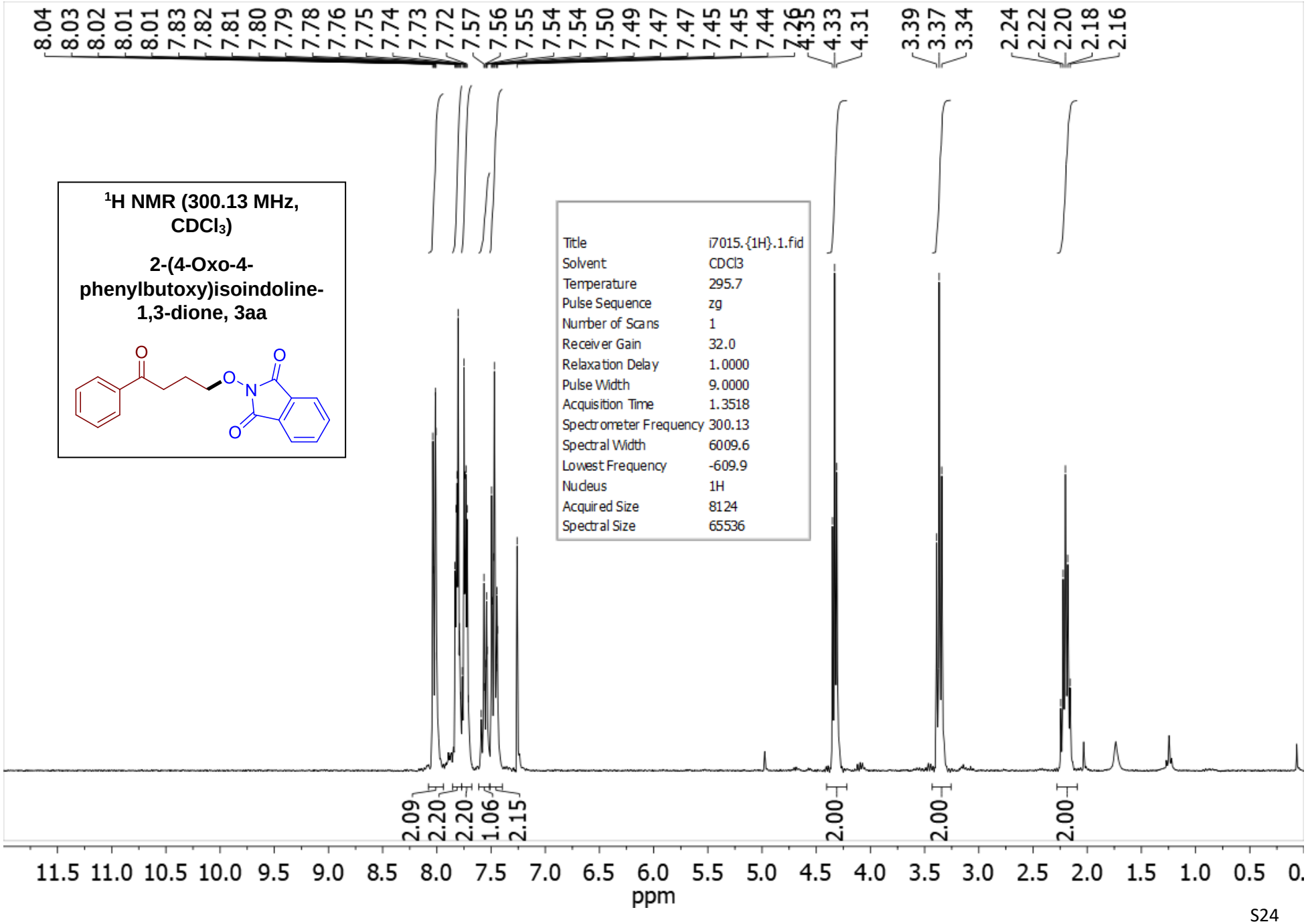
6. The ^{1}H and ^{13}C spectra of synthesized compounds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¹H NMR (300.13 MHz, CDCl₃)
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Title i7015.{1H}.1.fid
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Relaxation Delay 1.0000
Pulse Width 9.0000
Acquisition Time 1.3518
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.9
Nucleus 1H
Acquired Size 8124
Spectral Size 65536
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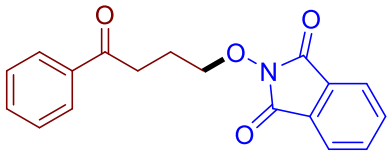
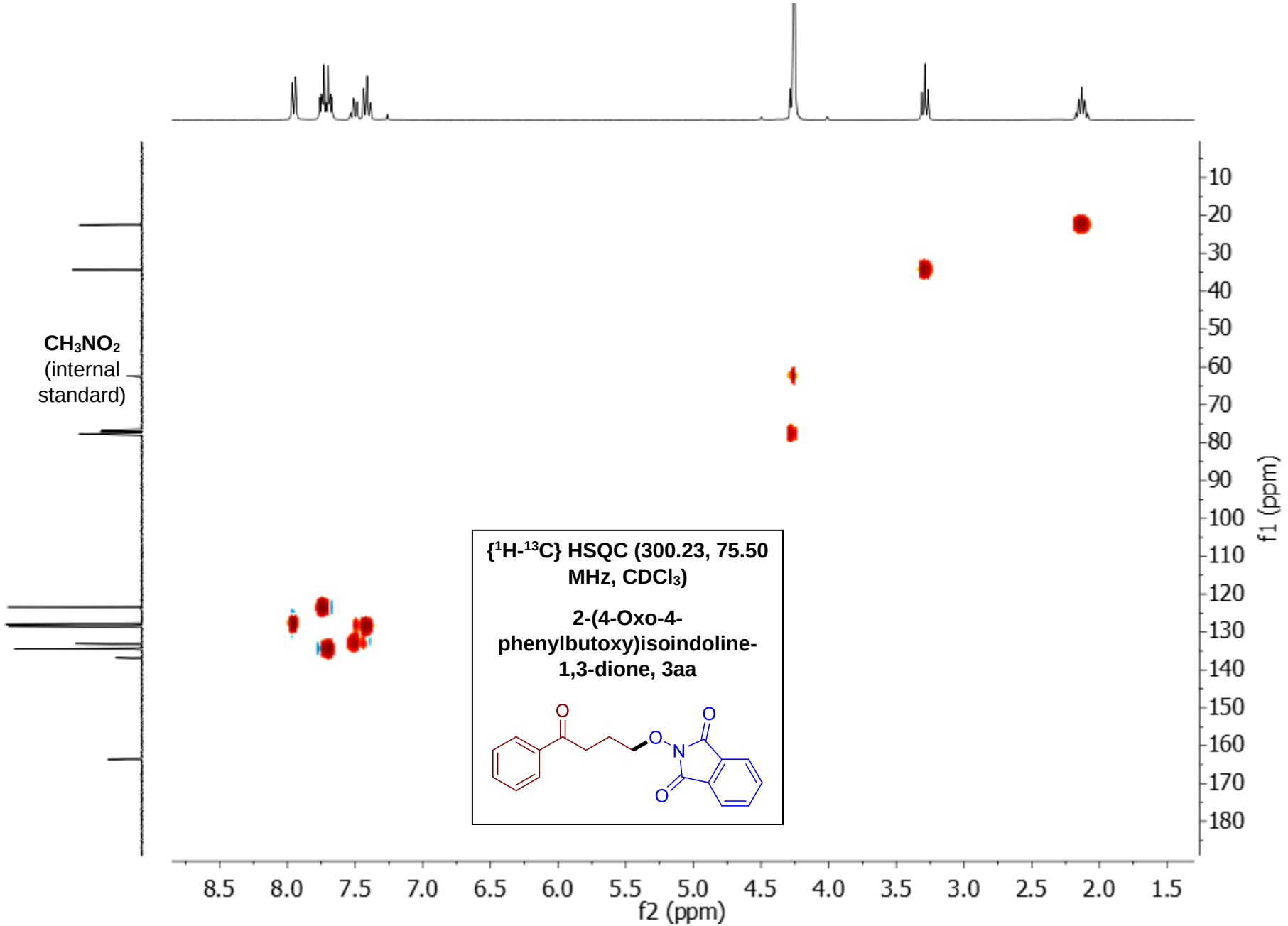
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
ppm

{^{1}H-^{13}C} HSQC (300.23, 75.50 MHz, $CDCl_3$)

2-(4-Oxo-4-phenylbutoxy)isoindoline-1,3-dione, 3aa

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(internal
standard)
{1H-13C} HSQC (300.23, 75.50 MHz, CDCl3)
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O
O
O
N
O
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
f2 (ppm)
10
20
30
40
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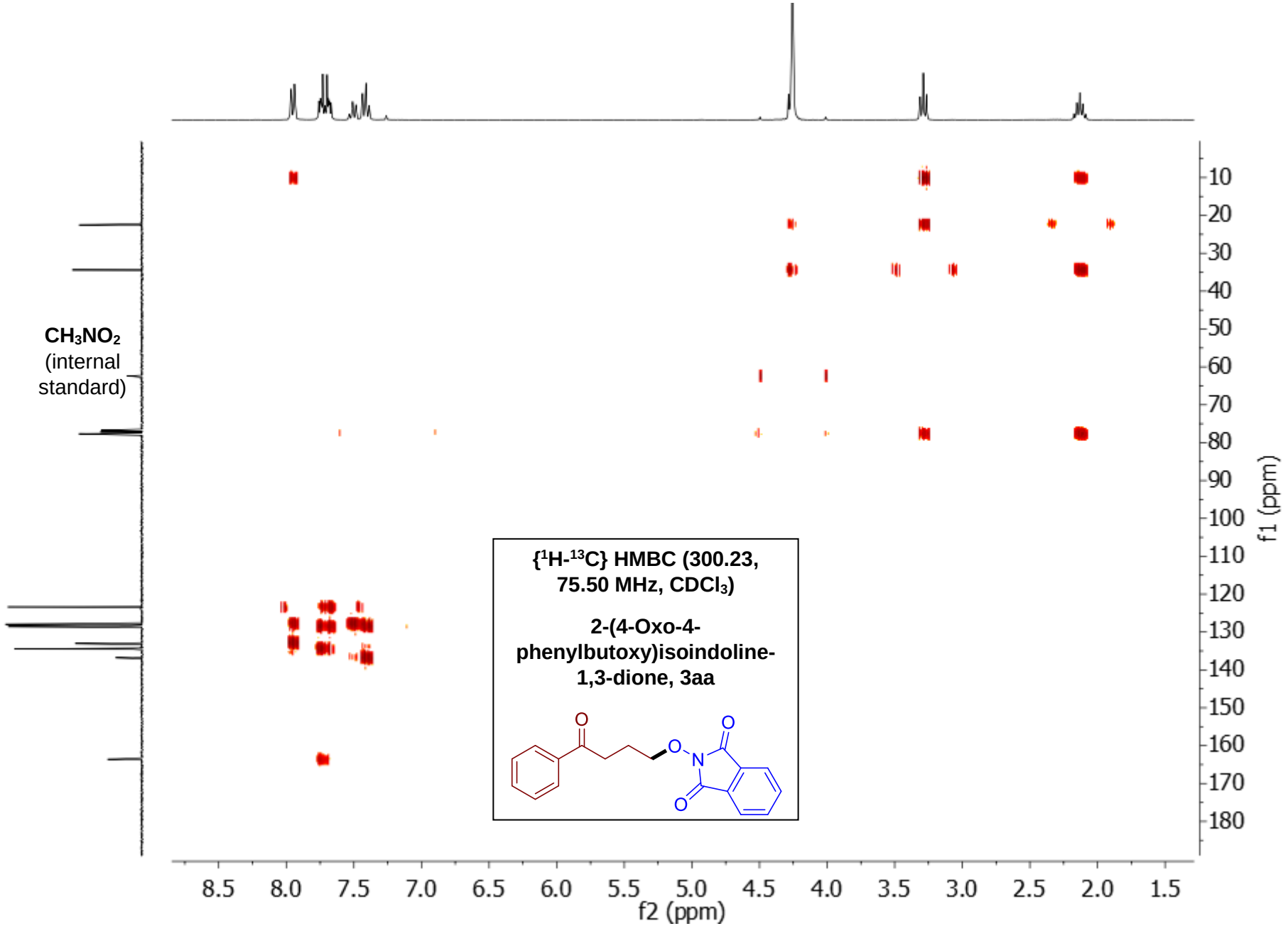
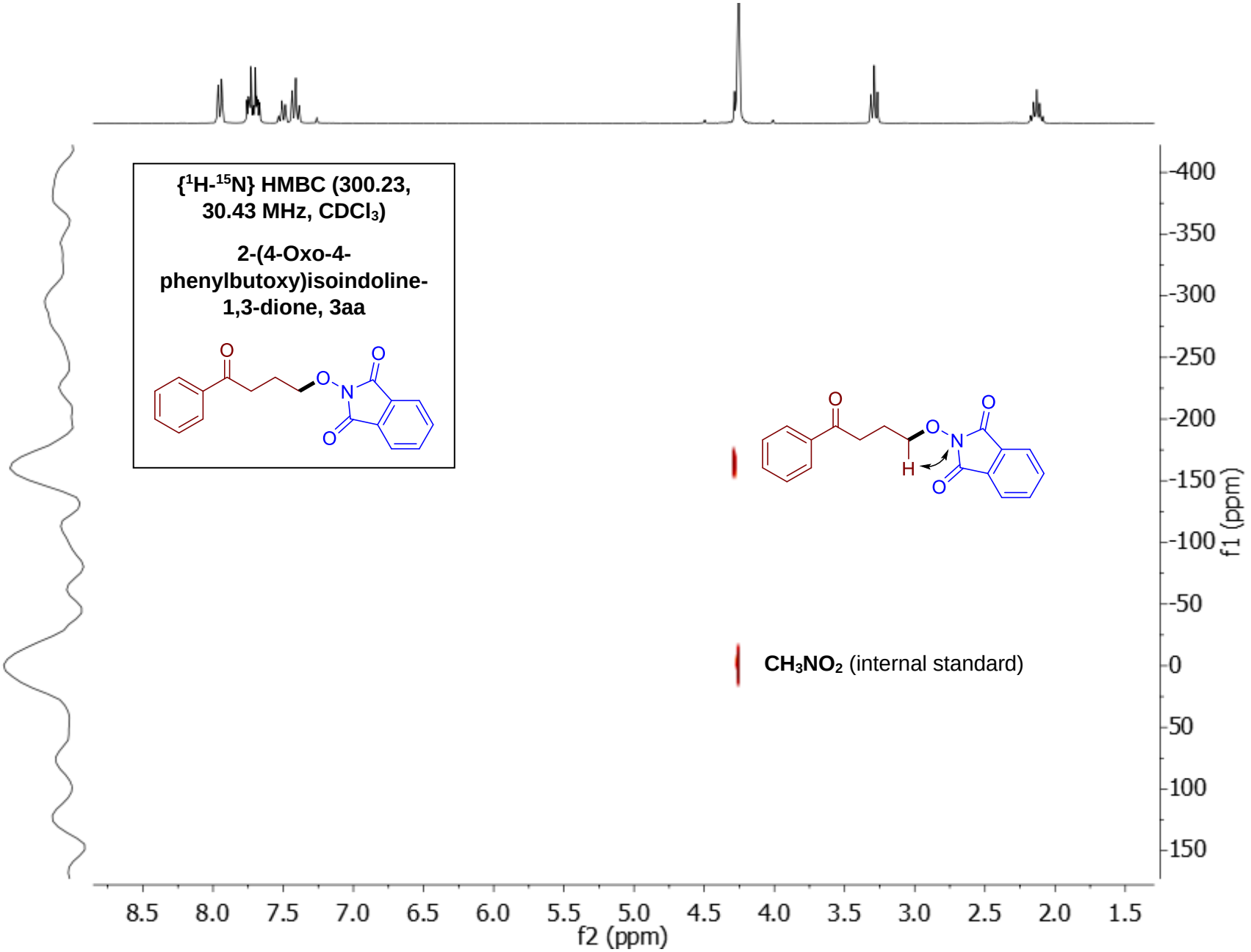
120
130
140
150
160
170
180
f1 (ppm)


CH3NO2
(internal
standard)
{1H-13C} HMBC (300.23,
75.50 MHz, CDCl3)
2-(4-Oxo-4-
phenylbutoxy)isoindoline-
1,3-dione, 3aa
O
O
N
O
O
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
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
f1 (ppm)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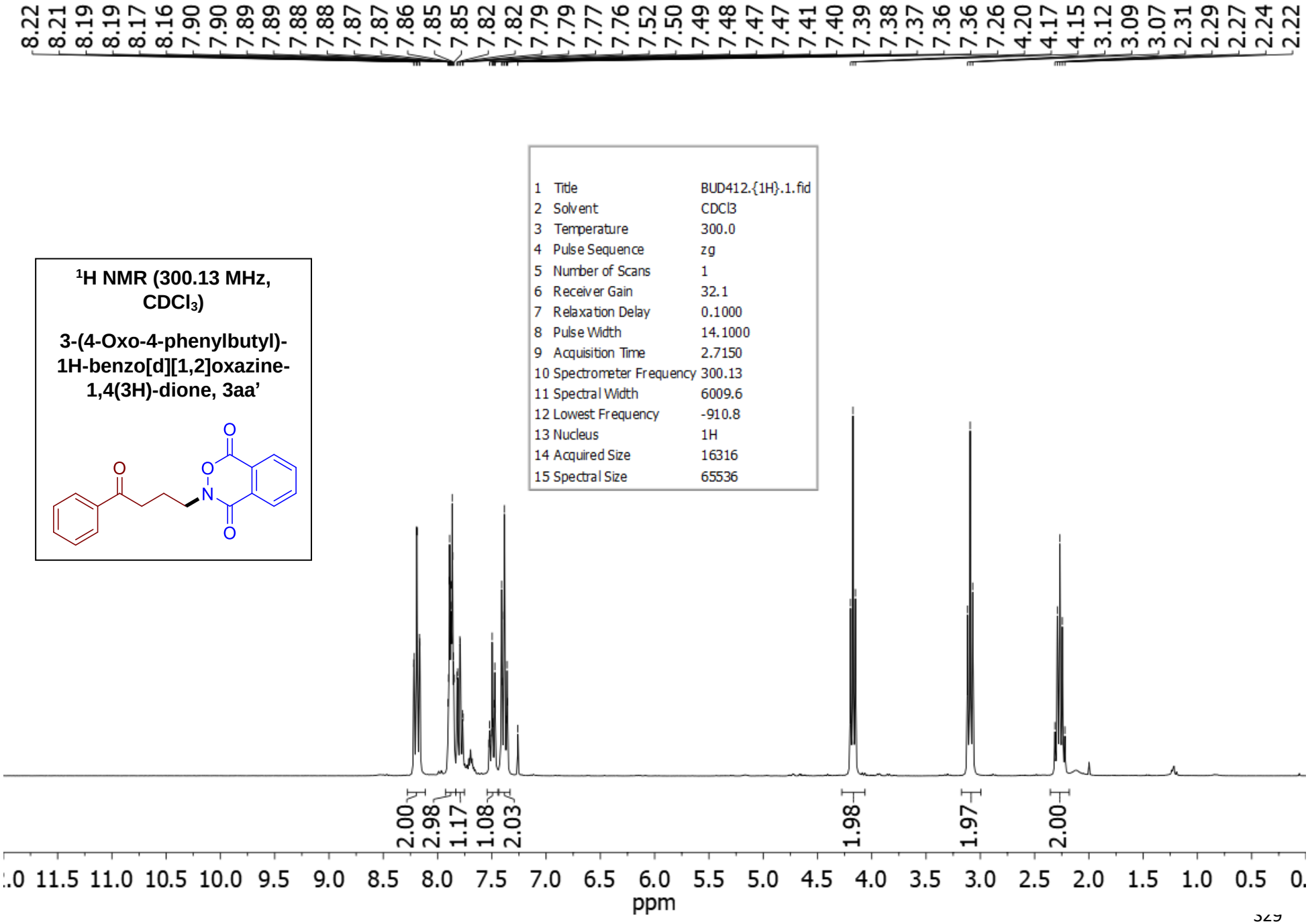
CH_3NO_2 (internal standard)
f2 (ppm)
f1 (ppm)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1H NMR (300.13 MHz, CDCl3)
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11 Spectral Width 6009.6
12 Lowest Frequency -910.8
13 Nucleus 1H
14 Acquired Size 16316
15 Spectral Size 65536
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11.5 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
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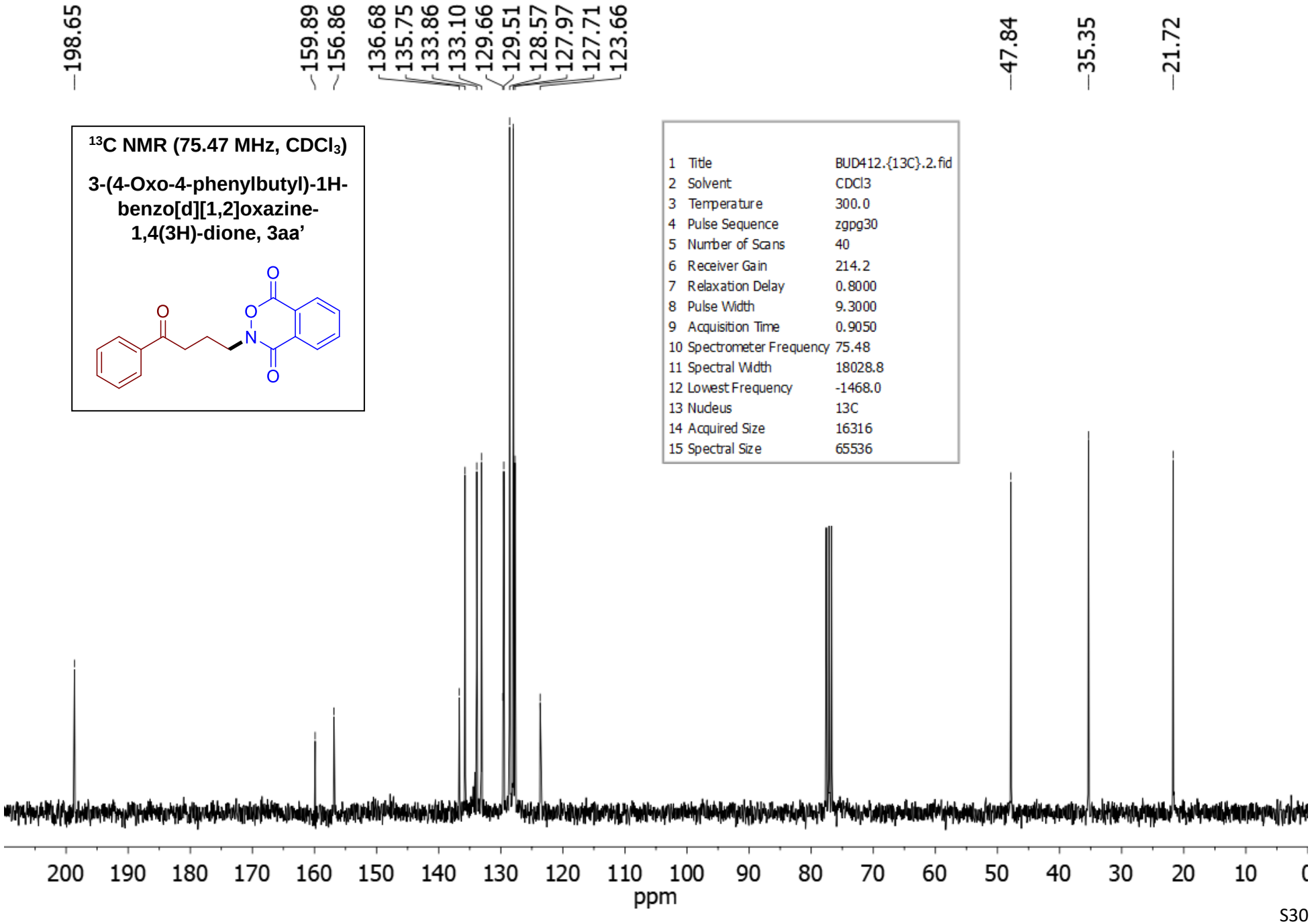
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135.75
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128.57
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123.66
47.84
35.35
21.72
13C NMR (75.47 MHz, CDCl3)
3-(4-Oxo-4-phenylbutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3aa'
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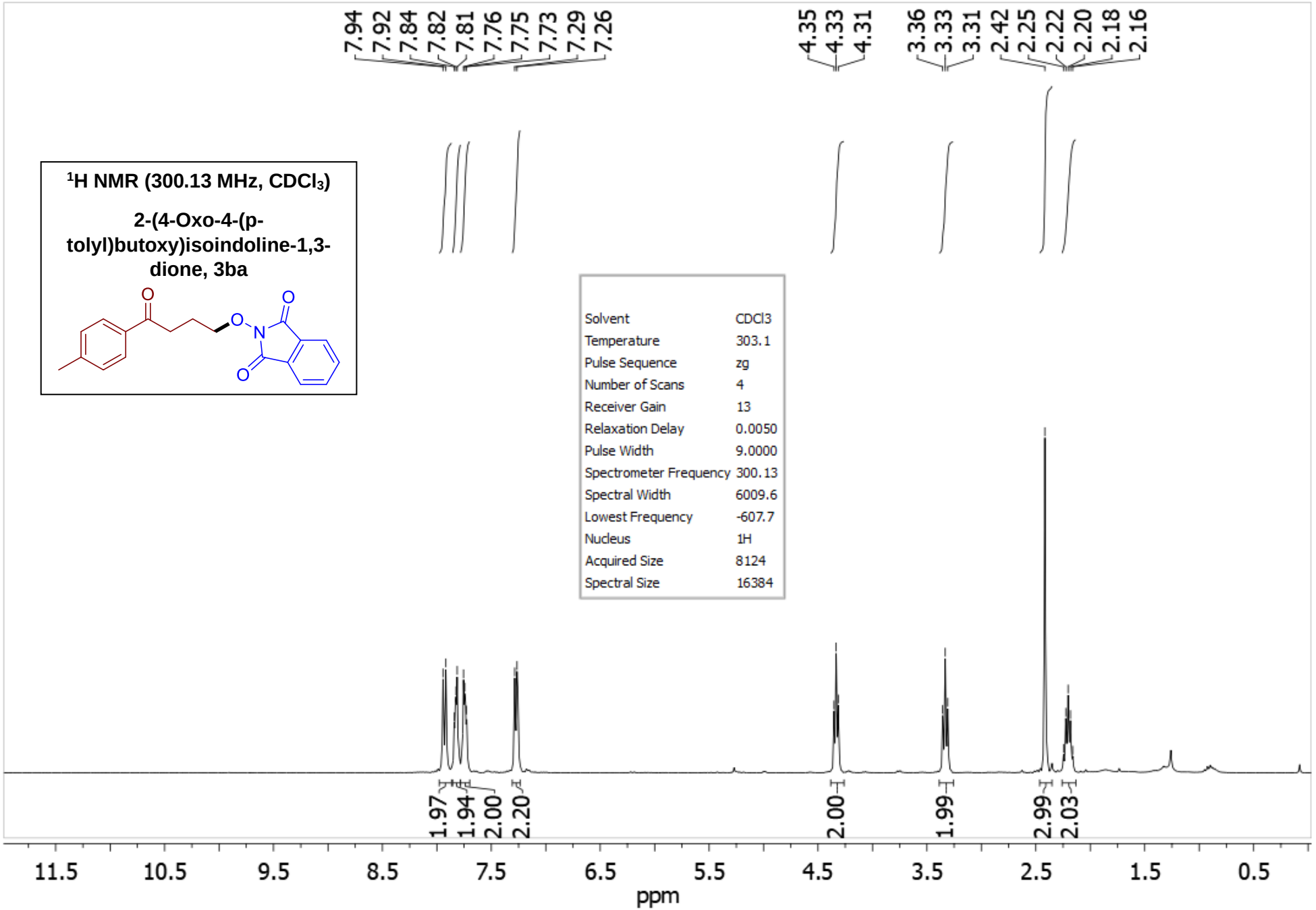
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7.26
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4.31
3.36
3.33
3.31
2.42
2.25
2.22
2.20
2.18
2.16
1H NMR (300.13 MHz, CDCl3)
2-(4-Oxo-4-(p-tolyl)butoxy)isoindoline-1,3-dione, 3ba
Solvent CDCl3
Temperature 303.1
Pulse Sequence zg
Number of Scans 4
Receiver Gain 13
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Lowest Frequency -607.7
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
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2.00
1.99
2.99
2.03
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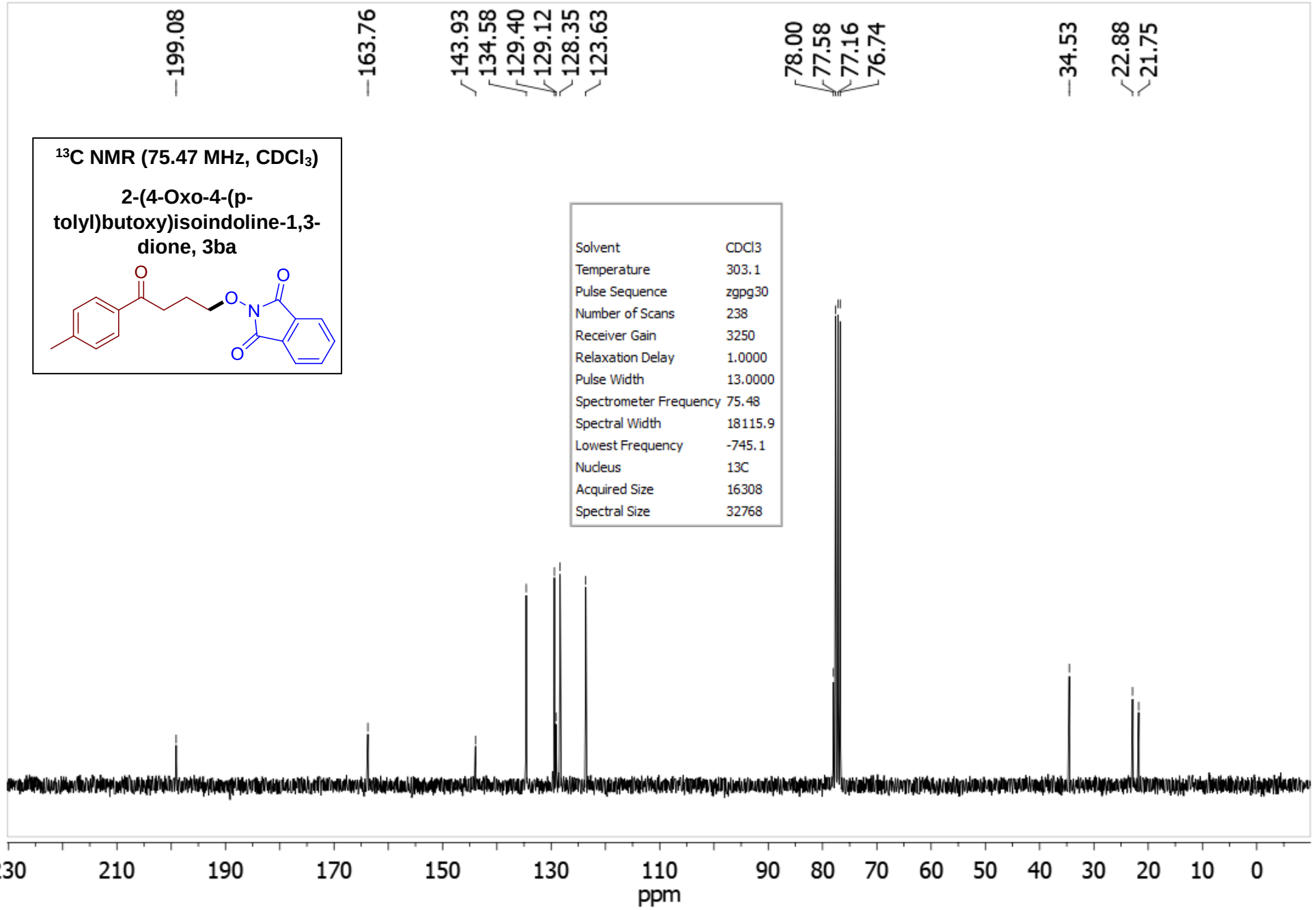
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34.53
22.88
21.75
13C NMR (75.47 MHz, CDCl3)
2-(4-Oxo-4-(p-tolyl)butoxy)isoindoline-1,3-dione, 3ba
Solvent CDCl3
Temperature 303.1
Pulse Sequence zgpg30
Number of Scans 238
Receiver Gain 3250
Relaxation Delay 1.0000
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Lowest Frequency -745.1
Nucleus 13C
Acquired Size 16308
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20
10
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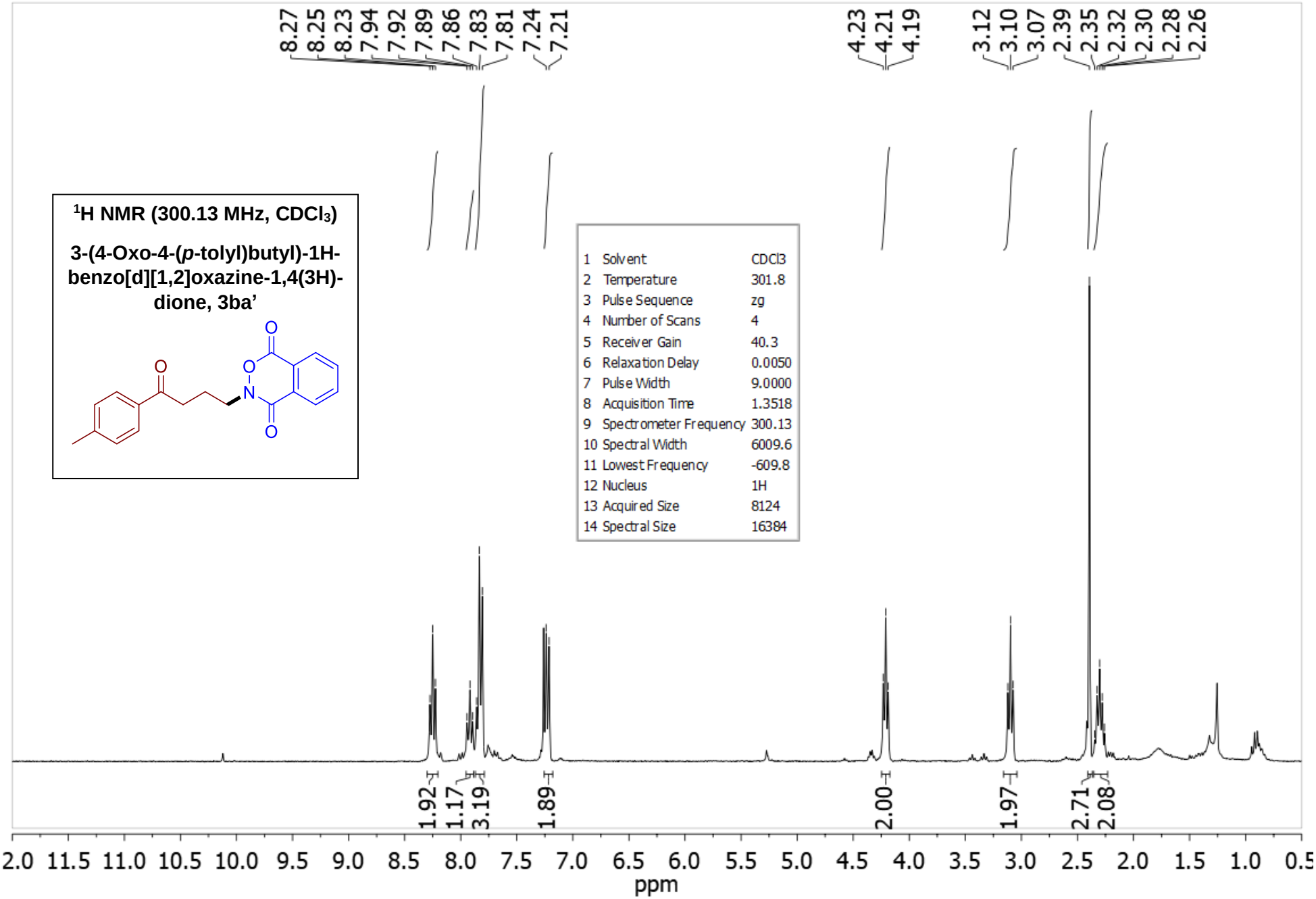
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7.24
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4.21
4.19
3.12
3.10
3.07
2.39
2.35
2.32
2.30
2.28
2.26
^{1}H NMR (300.13 MHz, CDCl$_3$)
3-(4-Oxo-4-(p-tolyl)butyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ba'
1 Solvent CDCl3
2 Temperature 301.8
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4 Number of Scans 4
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12 Nucleus 1H
13 Acquired Size 8124
14 Spectral Size 16384
1.92
1.17
3.19
1.89
2.00
1.97
2.71
2.08
2.0 11.5 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
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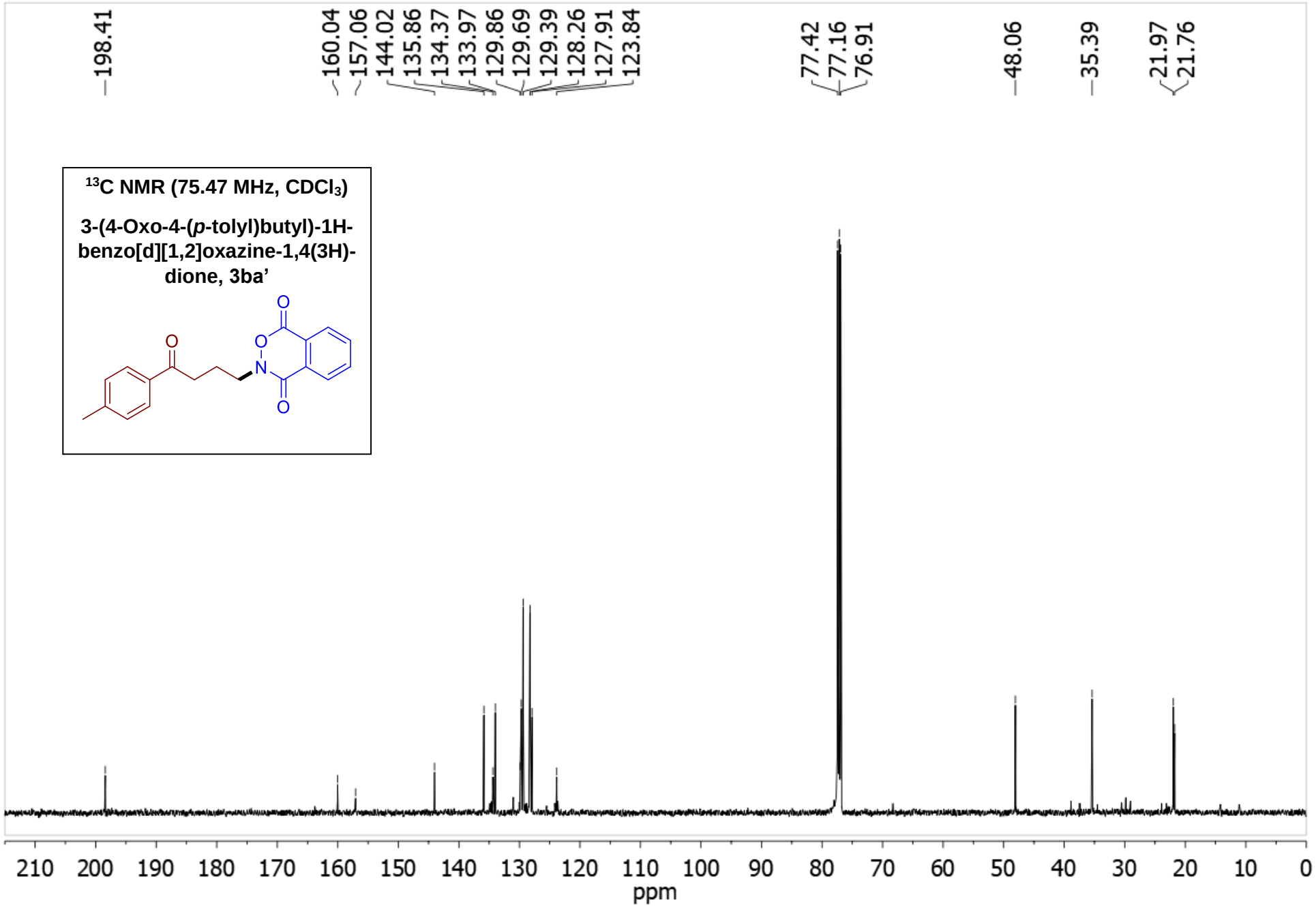
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123.84
77.42
77.16
76.91
48.06
35.39
21.97
21.76
^{13}C NMR (75.47 MHz, $CDCl_3$)
3-(4-Oxo-4-(*p*-tolyl)butyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ba'
O
O
O
N
O
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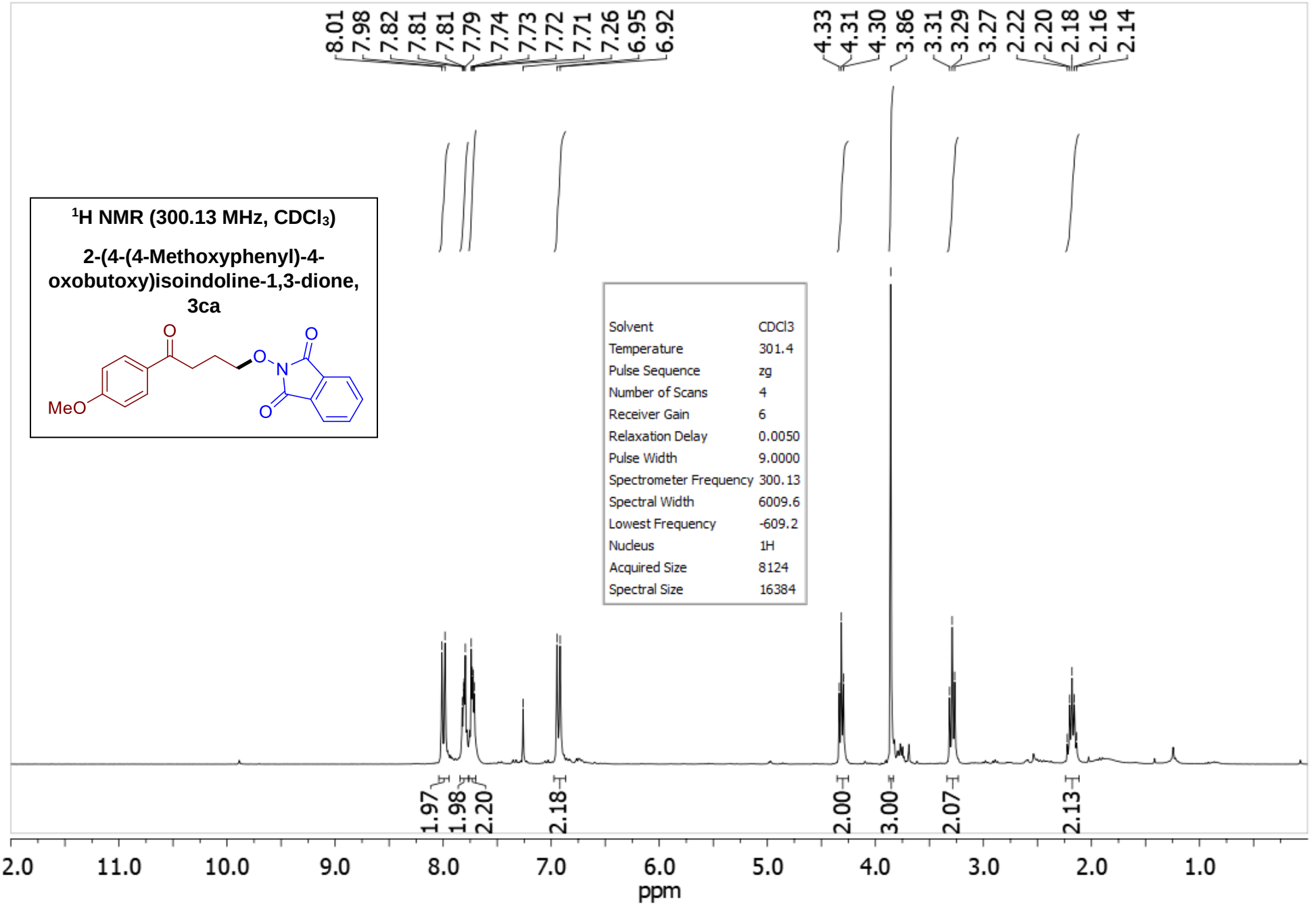
ppm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6.92
4.33
4.31
4.30
3.86
3.31
3.29
3.27
2.22
2.20
2.18
2.16
2.14
1H NMR (300.13 MHz, CDCl3)
2-(4-(4-Methoxyphenyl)-4-oxobutoxy)isoindoline-1,3-dione, 3ca
MeO
O
O
N
O
O
Solvent CDCl3
Temperature 301.4
Pulse Sequence zg
Number of Scans 4
Receiver Gain 6
Relaxation Delay 0.0050
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.2
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
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1.98
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2.18
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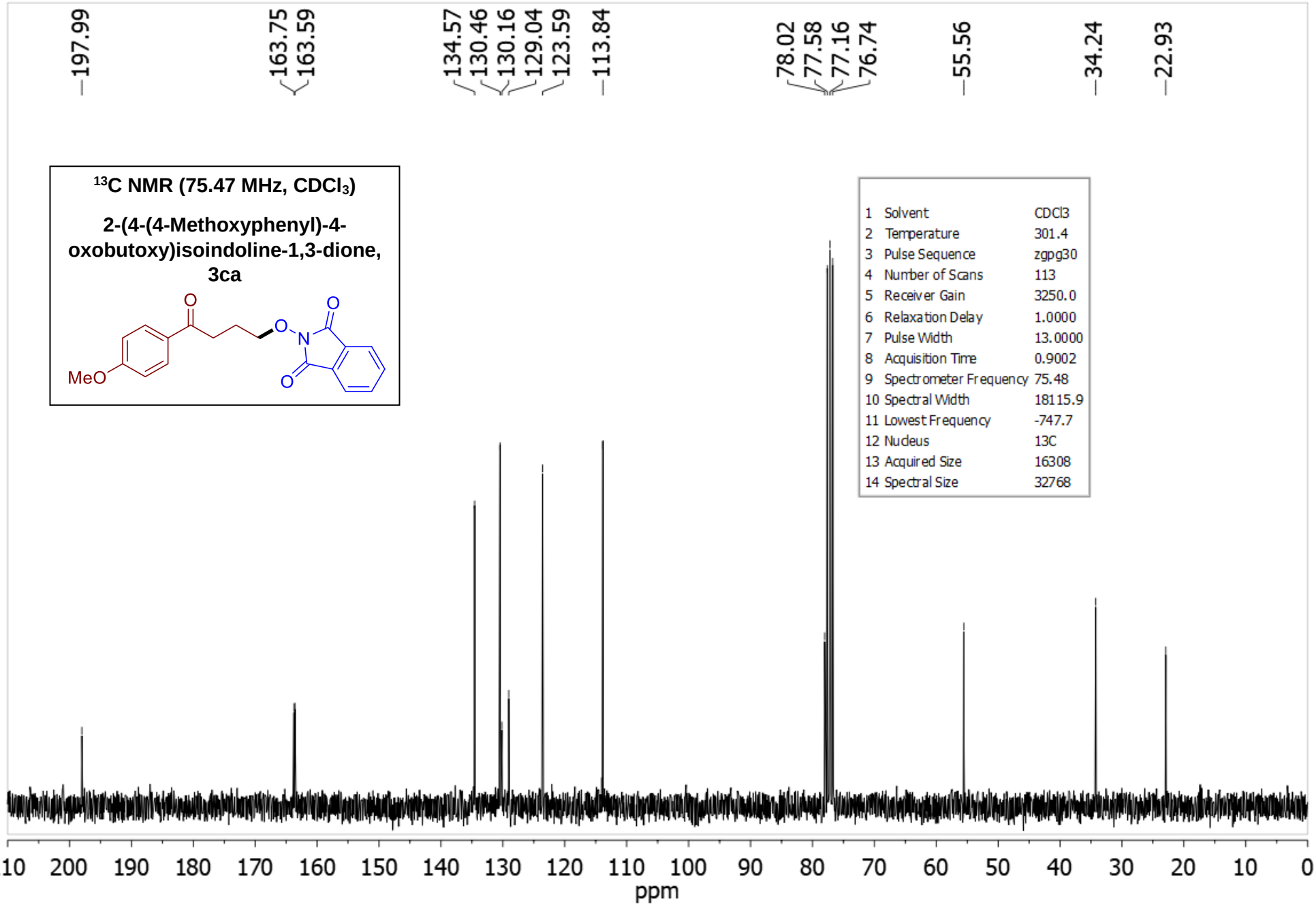
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76.74
55.56
34.24
22.93
13C NMR (75.47 MHz, CDCl3)
2-(4-(4-Methoxyphenyl)-4-oxobutoxy)isoindoline-1,3-dione, 3ca
MeO
O
O
O
N
O
O
1 Solvent CDCl3
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8 Acquisition Time 0.9002
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10 Spectral Width 18115.9
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12 Nucleus 13C
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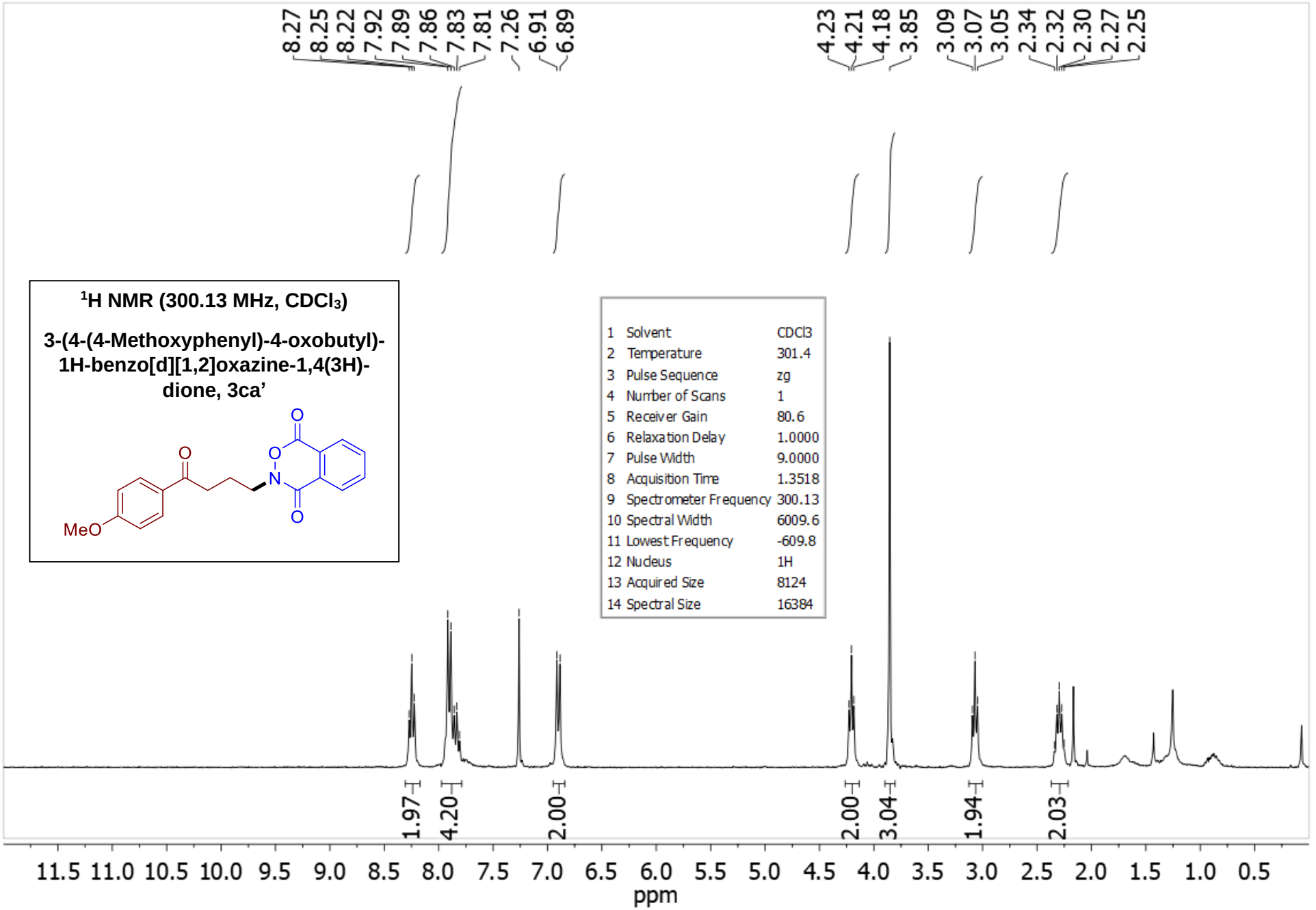
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4.21
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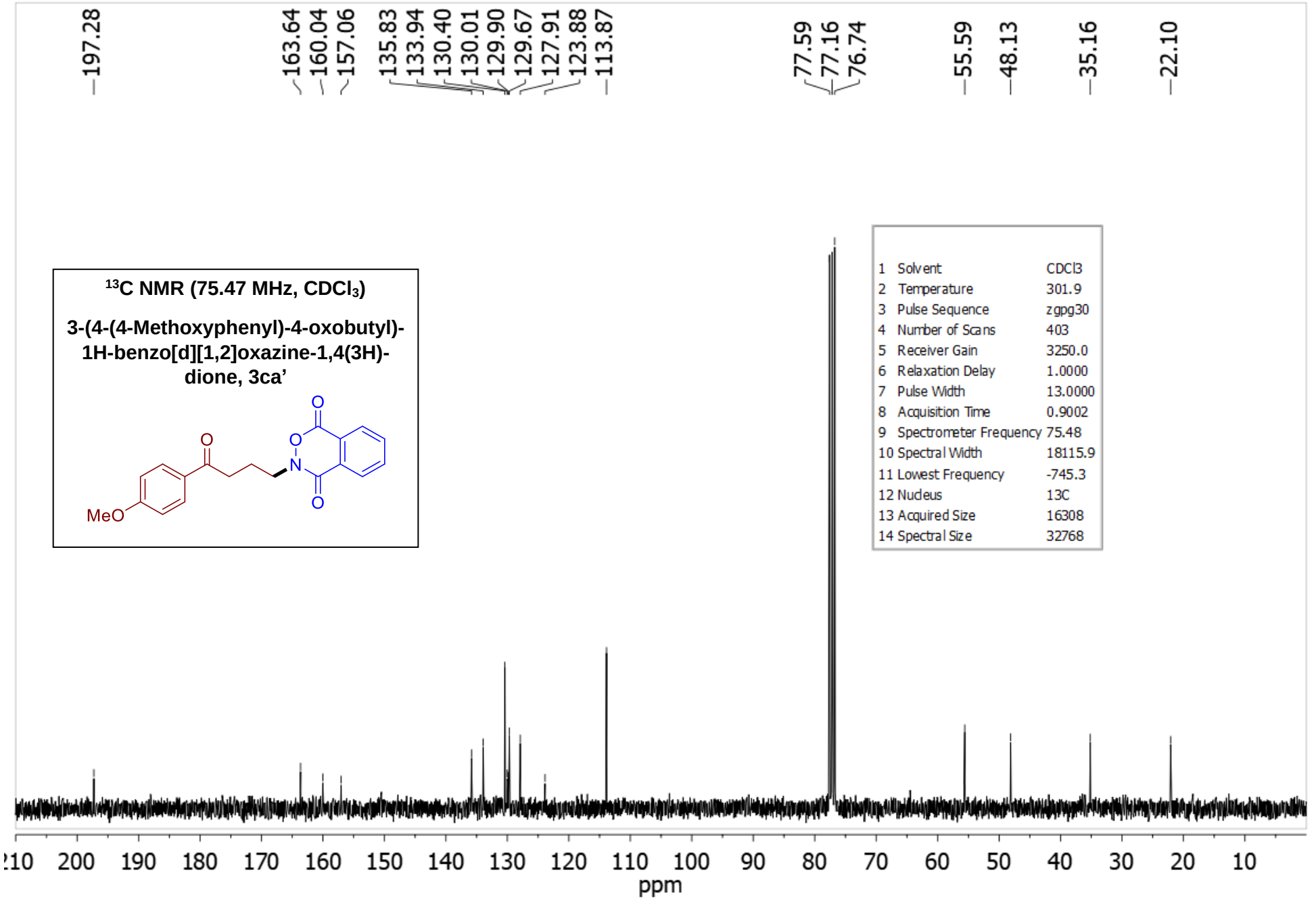
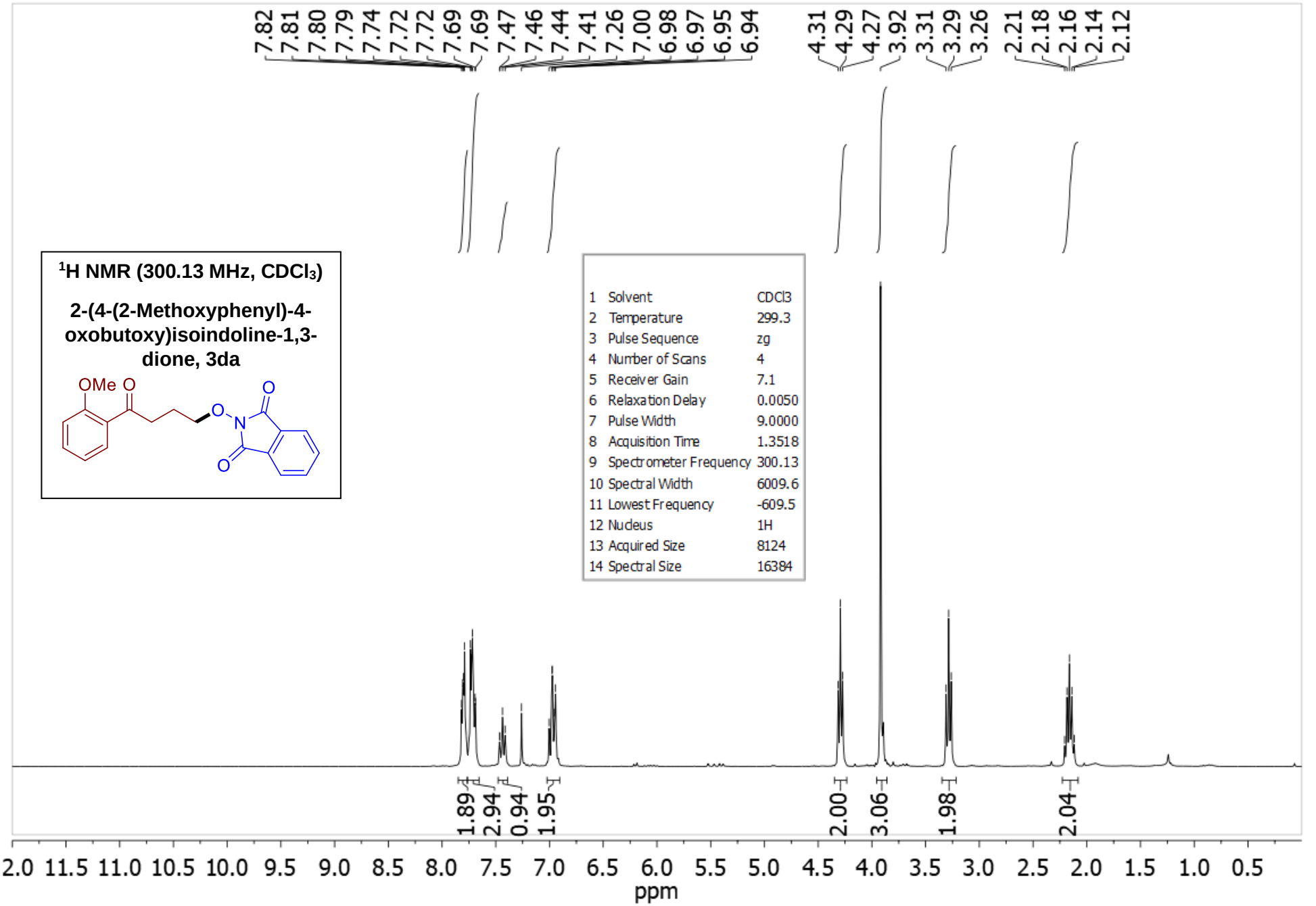
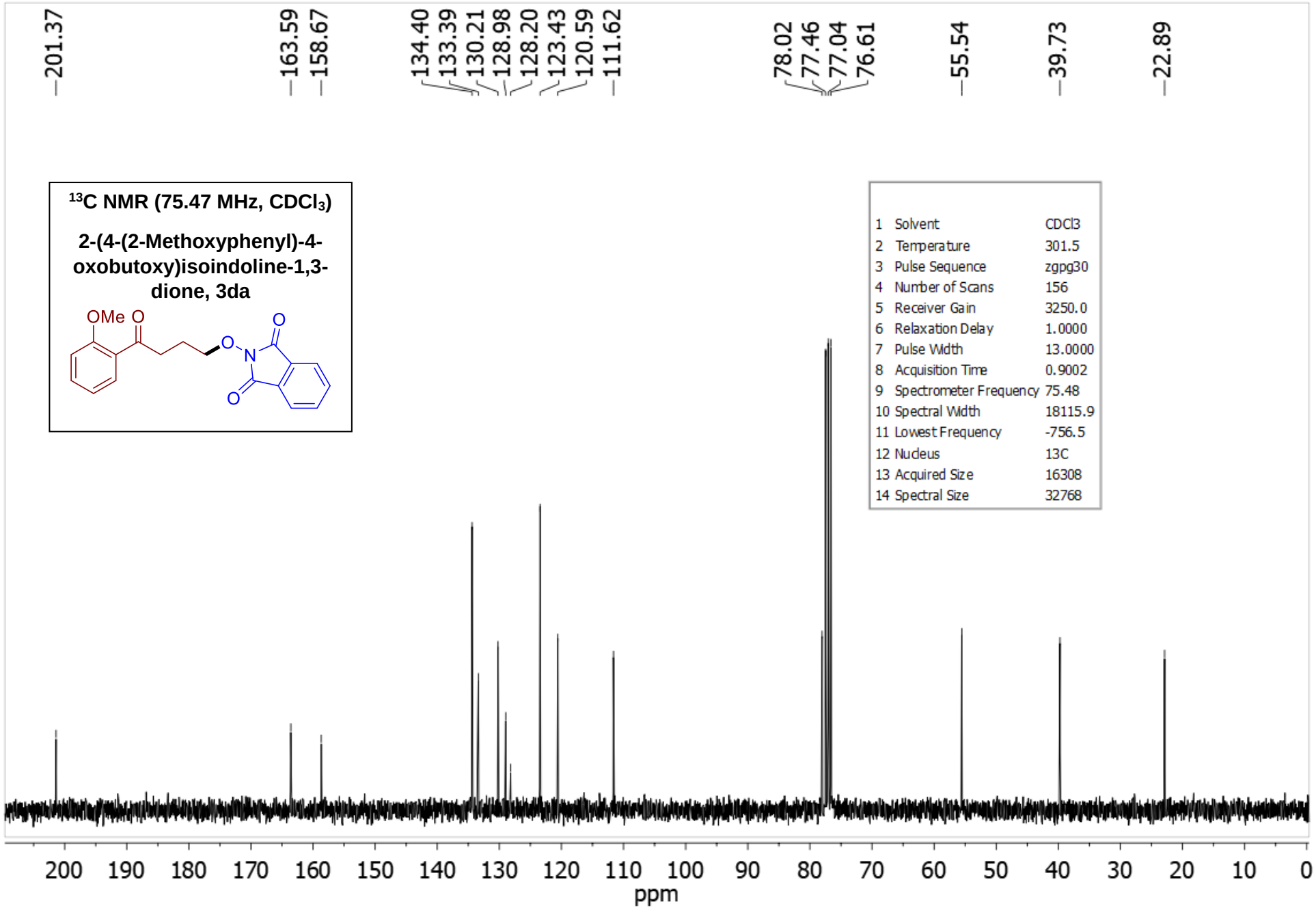
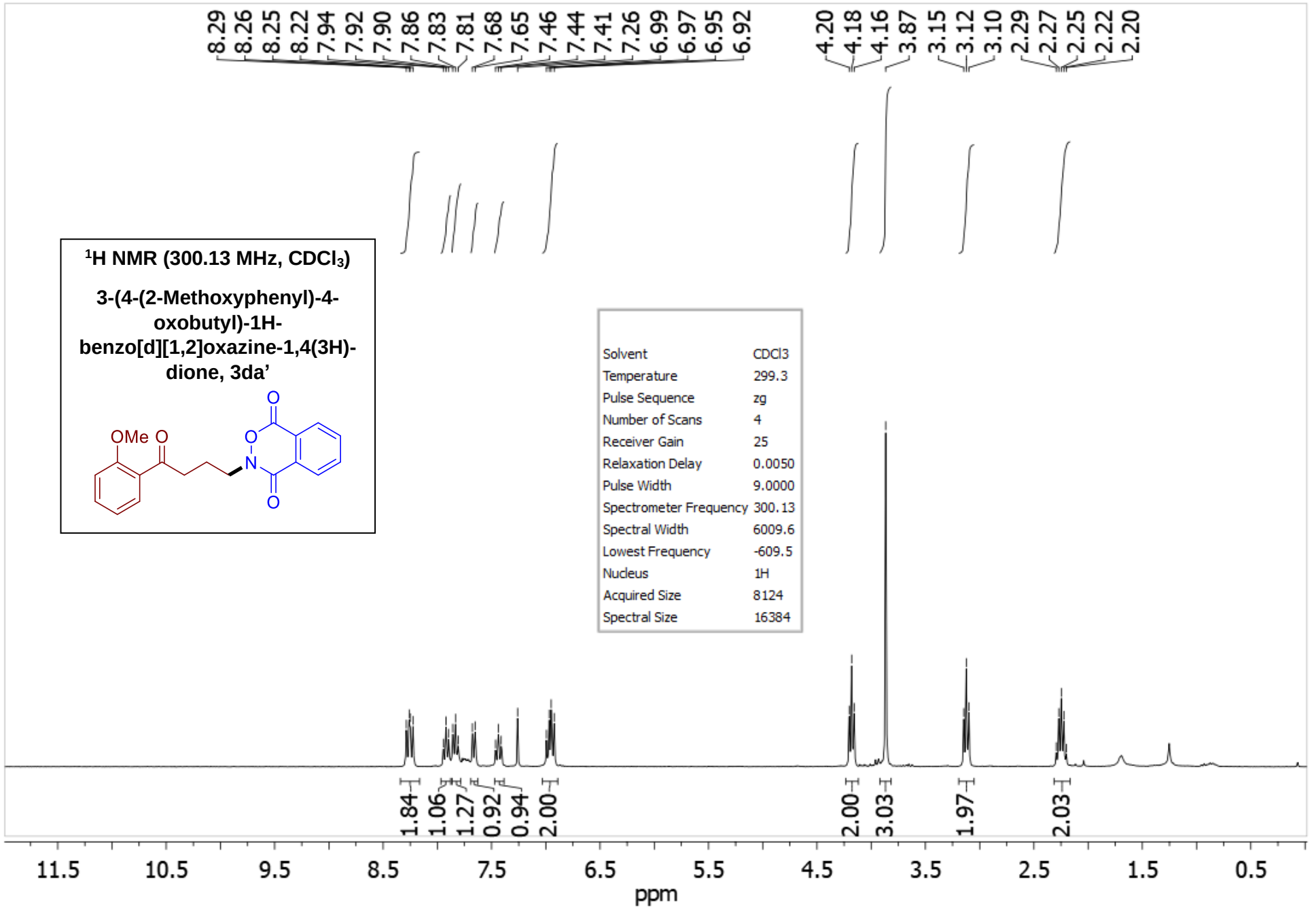
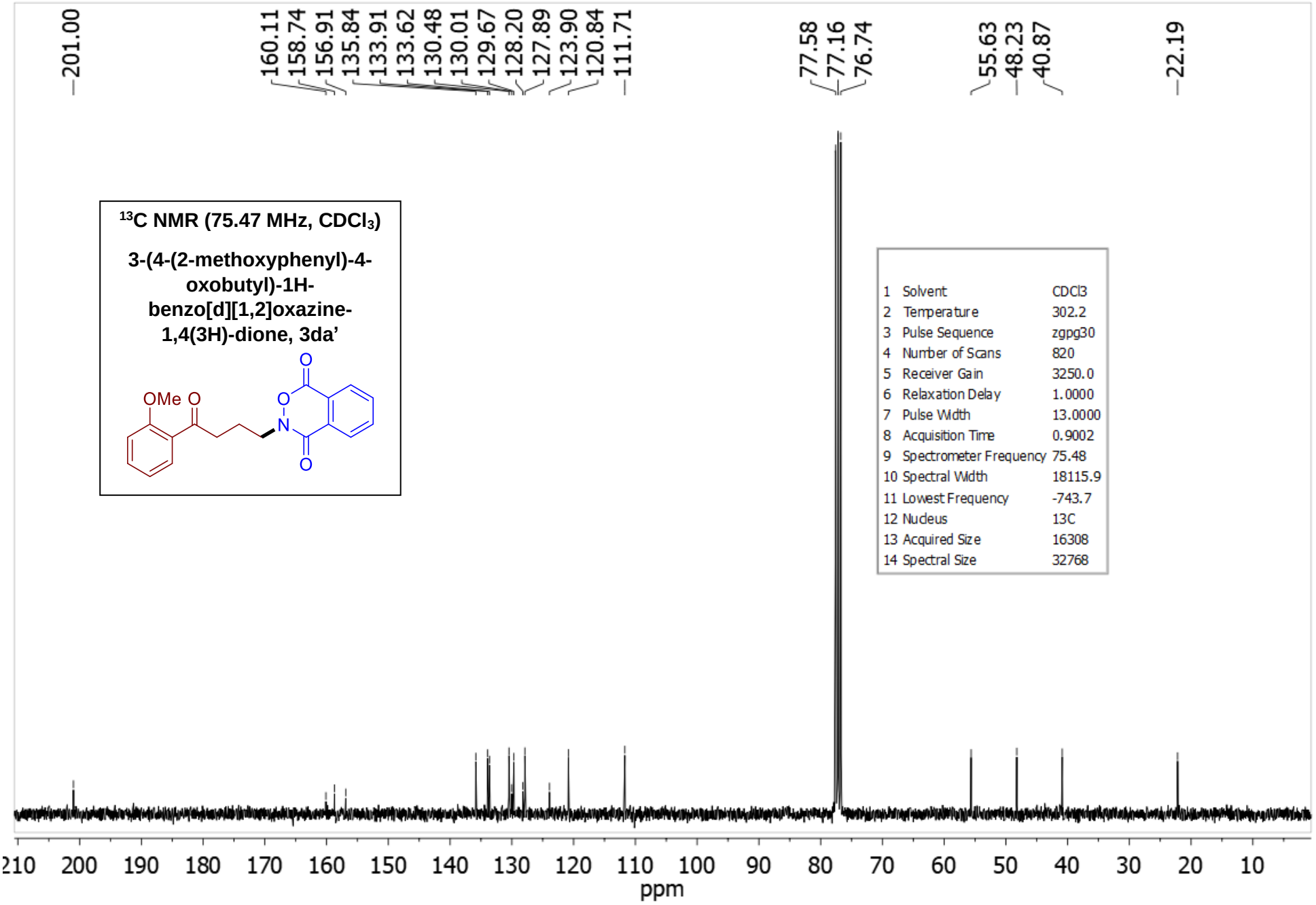
3.07
3.05
2.34
2.32
2.30
2.27
2.25
1H NMR (300.13 MHz, CDCl3)
3-(4-(4-Methoxyphenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ca'
MeO
1 Solvent CDCl3
2 Temperature 301.4
3 Pulse Sequence zg
4 Number of Scans 1
5 Receiver Gain 80.6
6 Relaxation Delay 1.0000
7 Pulse Width 9.0000
8 Acquisition Time 1.3518
9 Spectrometer Frequency 300.13
10 Spectral Width 6009.6
11 Lowest Frequency -609.8
12 Nucleus 1H
13 Acquired Size 8124
14 Spectral Size 16384
1.97
4.20
2.00
2.00
3.04
1.94
2.03
11.5 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
ppm

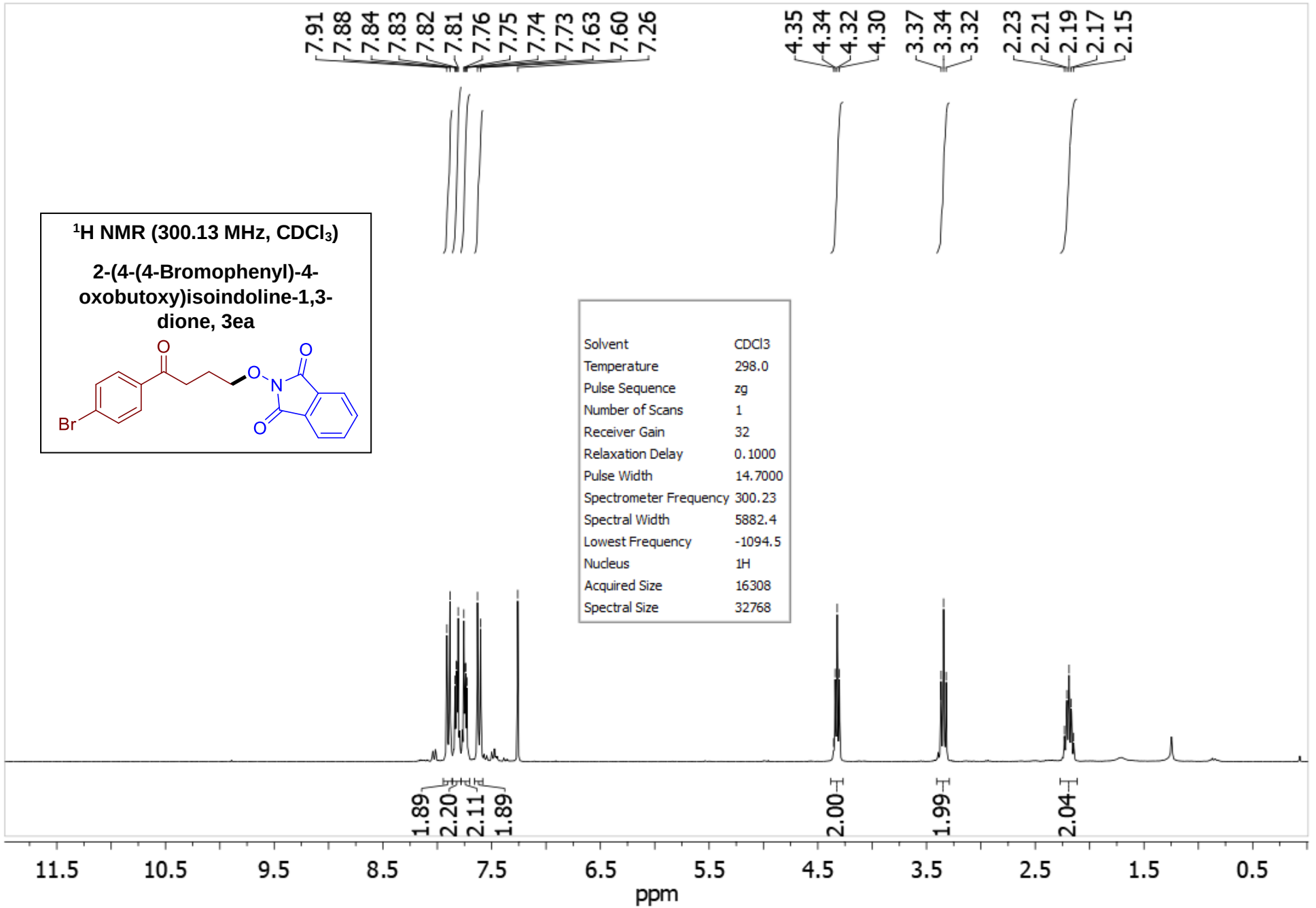

197.28
163.64
160.04
157.06
135.83
133.94
130.40
130.01
129.90
129.67
127.91
123.88
113.87
77.59
77.16
76.74
55.59
48.13
35.16
22.10
13C NMR (75.47 MHz, CDCl3)
3-(4-(4-Methoxyphenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ca'
MeO
1 Solvent CDCl3
2 Temperature 301.9
3 Pulse Sequence zgpg30
4 Number of Scans 403
5 Receiver Gain 3250.0
6 Relaxation Delay 1.0000
7 Pulse Width 13.0000
8 Acquisition Time 0.9002
9 Spectrometer Frequency 75.48
10 Spectral Width 18115.9
11 Lowest Frequency -745.3
12 Nucleus 13C
13 Acquired Size 16308
14 Spectral Size 32768
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

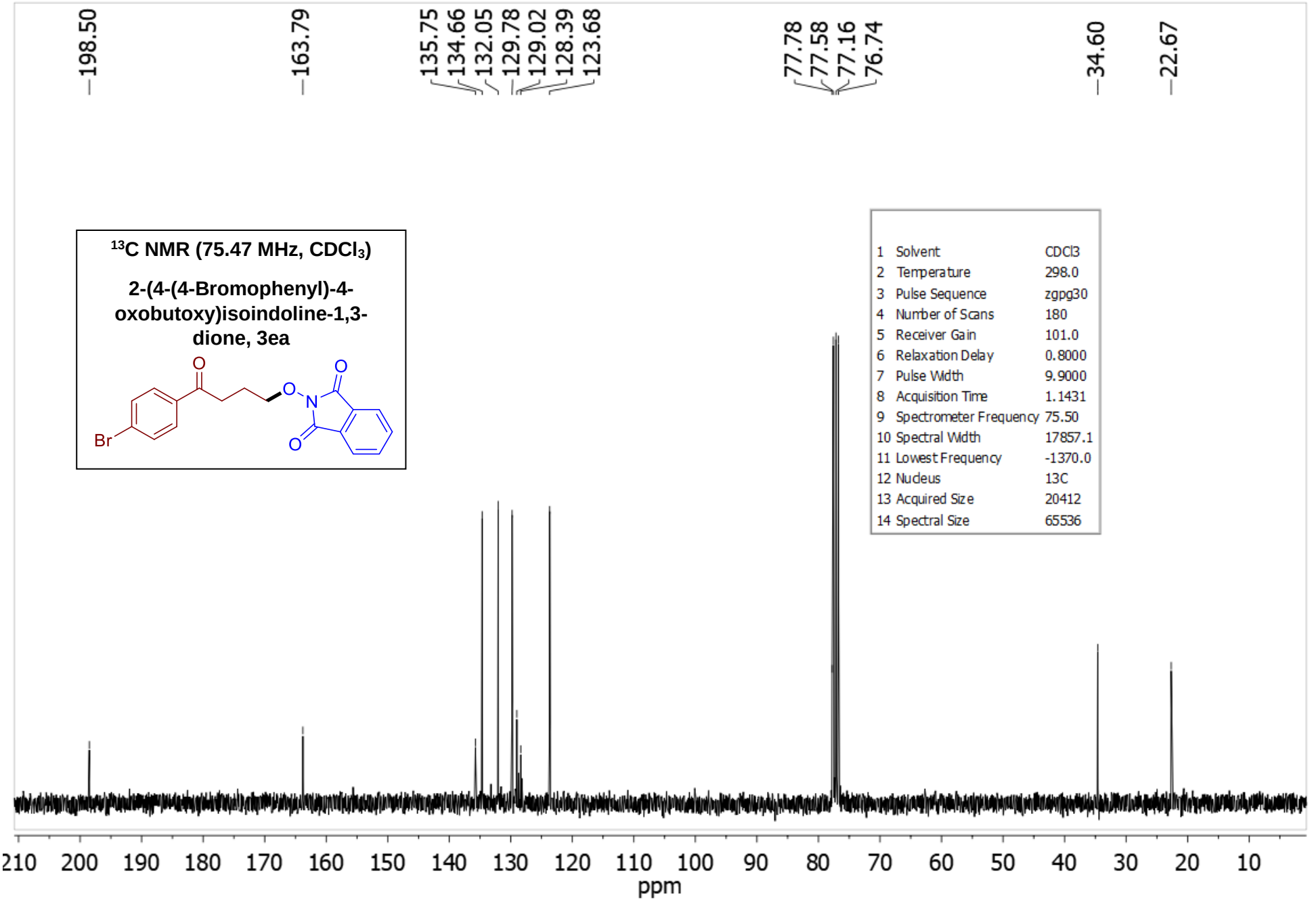

7.82 7.81 7.80 7.79 7.74 7.72 7.72 7.69 7.69 7.47 7.46 7.44 7.41 7.26 7.00 6.98 6.97 6.95 6.94
4.31 4.29 4.27 3.92 3.31 3.29 3.26 2.21 2.18 2.16 2.14 2.12
1H NMR (300.13 MHz, CDCl3)
2-(4-(2-Methoxyphenyl)-4-oxobutoxy)isoindoline-1,3-dione, 3da
OMe O
O
O
N
O
1 Solvent CDCl3
2 Temperature 299.3
3 Pulse Sequence zg
4 Number of Scans 4
5 Receiver Gain 7.1
6 Relaxation Delay 0.0050
7 Pulse Width 9.0000
8 Acquisition Time 1.3518
9 Spectrometer Frequency 300.13
10 Spectral Width 6009.6
11 Lowest Frequency -609.5
12 Nucleus 1H
13 Acquired Size 8124
14 Spectral Size 16384
1.89 2.94 0.94 1.95 2.00 3.06 1.98 2.04
2.0 11.5 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
ppm

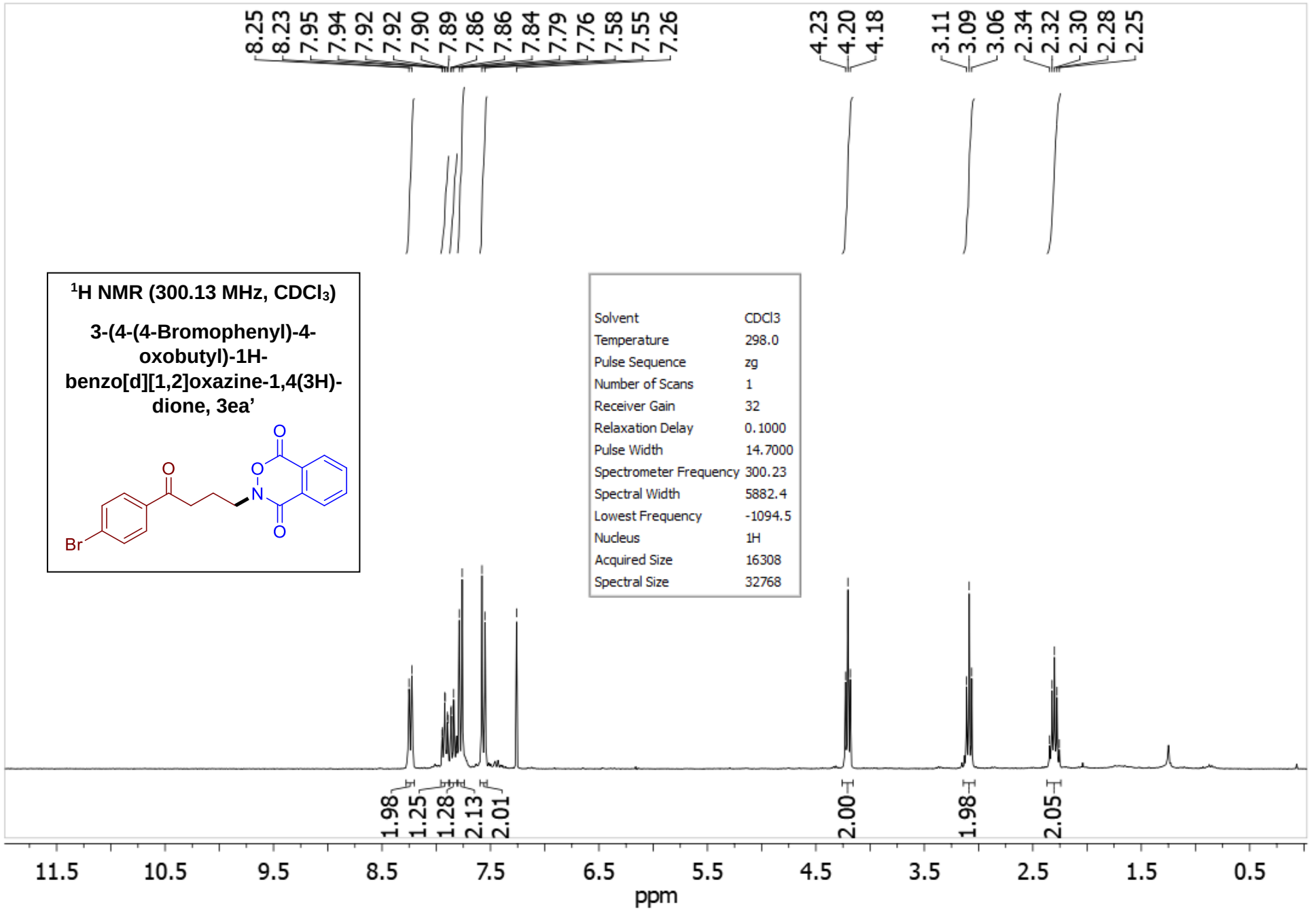

201.37
163.59
158.67
134.40
133.39
130.21
128.98
128.20
123.43
120.59
111.62
78.02
77.46
77.04
76.61
55.54
39.73
22.89
13C NMR (75.47 MHz, CDCl3)
2-(4-(2-Methoxyphenyl)-4-oxobutoxy)isoindoline-1,3-dione, 3da
OMe
O
N
O
O
O
1 Solvent CDCl3
2 Temperature 301.5
3 Pulse Sequence zgpg30
4 Number of Scans 156
5 Receiver Gain 3250.0
6 Relaxation Delay 1.0000
7 Pulse Width 13.0000
8 Acquisition Time 0.9002
9 Spectrometer Frequency 75.48
10 Spectral Width 18115.9
11 Lowest Frequency -756.5
12 Nucleus 13C
13 Acquired Size 16308
14 Spectral Size 32768
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

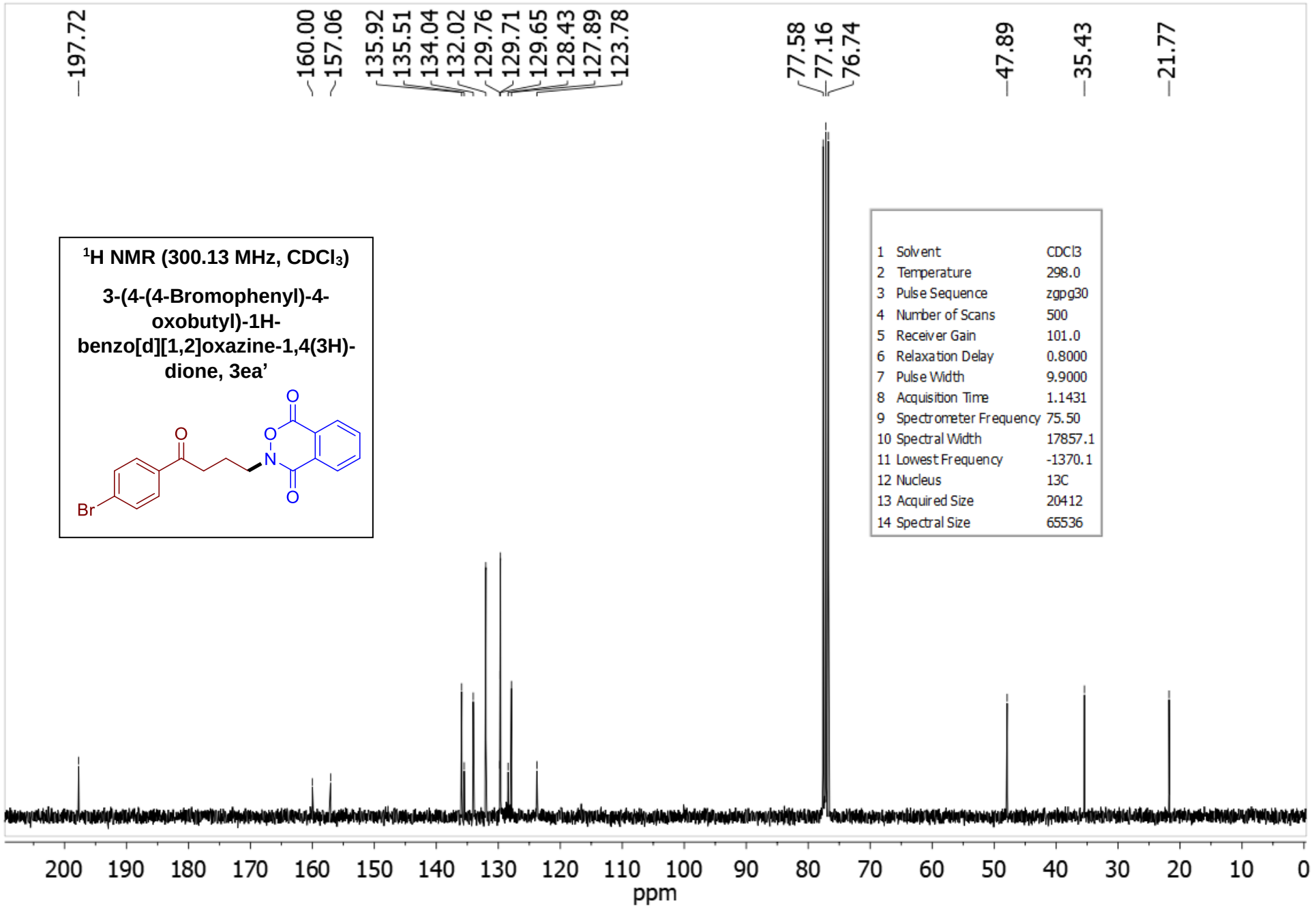

8.29
8.26
8.25
8.22
7.94
7.92
7.90
7.86
7.83
7.81
7.68
7.65
7.46
7.44
7.41
7.26
6.99
6.97
6.95
6.92
4.20
4.18
4.16
3.87
3.15
3.12
3.10
2.29
2.27
2.25
2.22
2.20
1H NMR (300.13 MHz, CDCl3)
3-(4-(2-Methoxyphenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3da'
OMe O
O
O
N
O
Solvent CDCl3
Temperature 299.3
Pulse Sequence zg
Number of Scans 4
Receiver Gain 25
Relaxation Delay 0.0050
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.5
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
1.84
1.06
1.27
0.92
0.94
2.00
2.00
3.03
1.97
2.03
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
ppm

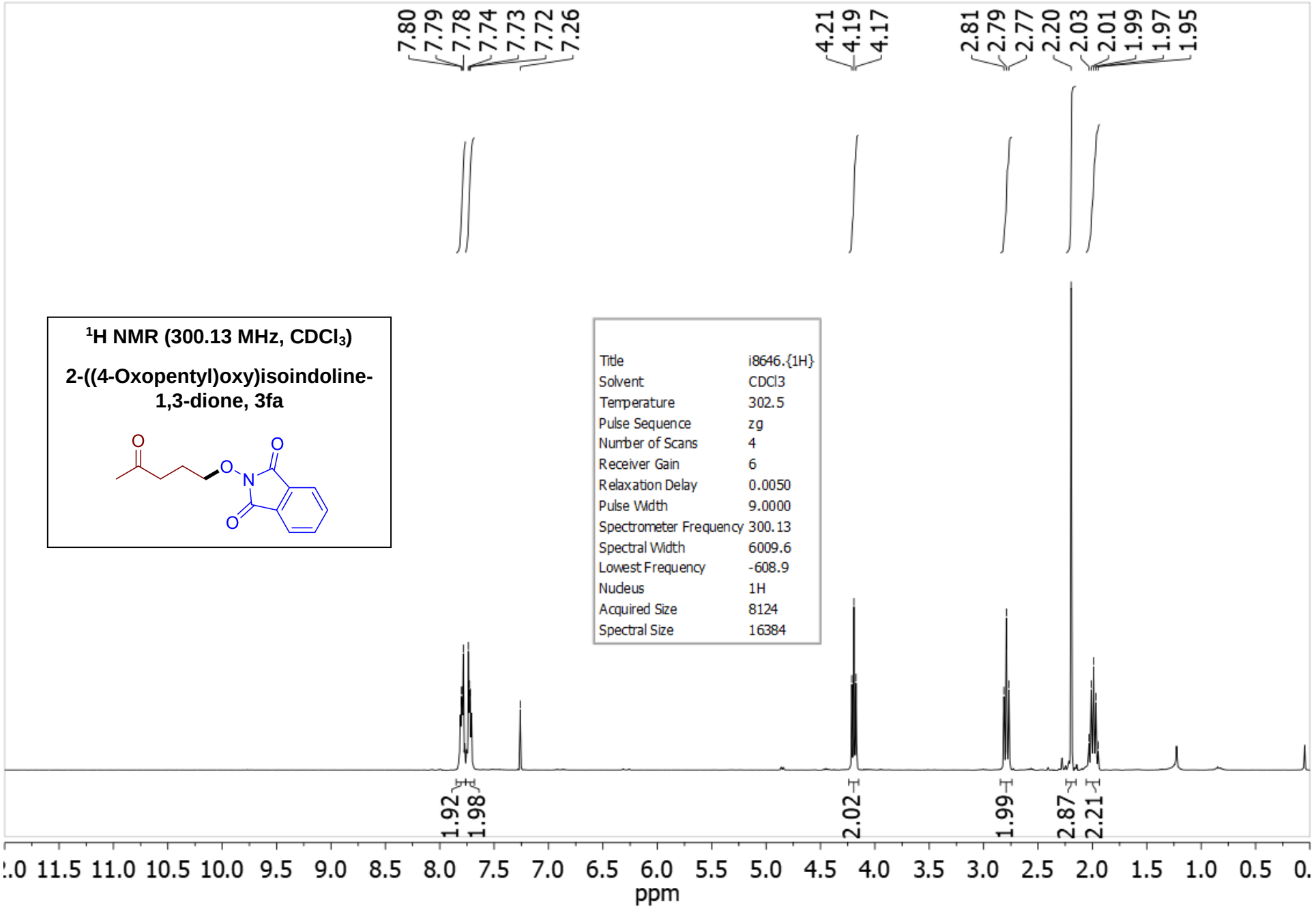

201.00
160.11
158.74
156.91
135.84
133.91
133.62
130.48
130.01
129.67
128.20
127.89
123.90
120.84
111.71
77.58
77.16
76.74
55.63
48.23
40.87
22.19
13C NMR (75.47 MHz, CDCl3)
3-(4-(2-methoxyphenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3da'
OMe
O
O
O
N
O
1 Solvent CDCl3
2 Temperature 302.2
3 Pulse Sequence zgpg30
4 Number of Scans 820
5 Receiver Gain 3250.0
6 Relaxation Delay 1.0000
7 Pulse Width 13.0000
8 Acquisition Time 0.9002
9 Spectrometer Frequency 75.48
10 Spectral Width 18115.9
11 Lowest Frequency -743.7
12 Nucleus 13C
13 Acquired Size 16308
14 Spectral Size 32768
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

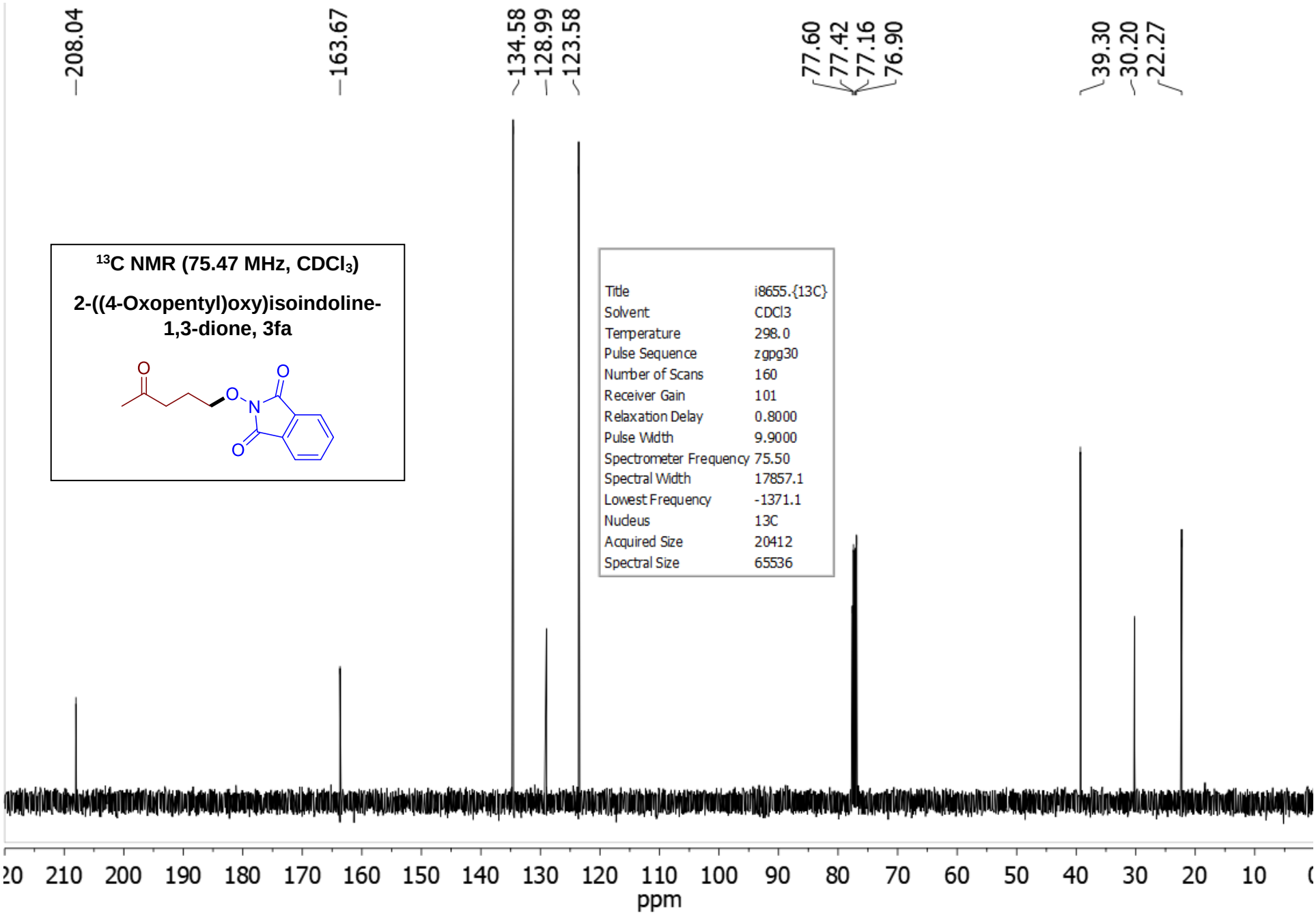

7.91
7.88
7.84
7.83
7.82
7.81
7.76
7.75
7.74
7.73
7.63
7.60
7.26
4.35
4.34
4.32
4.30
3.37
3.34
3.32
2.23
2.21
2.19
2.17
2.15
1H NMR (300.13 MHz, CDCl3)
2-(4-(4-Bromophenyl)-4-oxobutoxy)isoindoline-1,3-dione, 3ea
Br
O
O
N
O
O
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
1.89
2.20
2.11
1.89
2.00
1.99
2.04
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
ppm

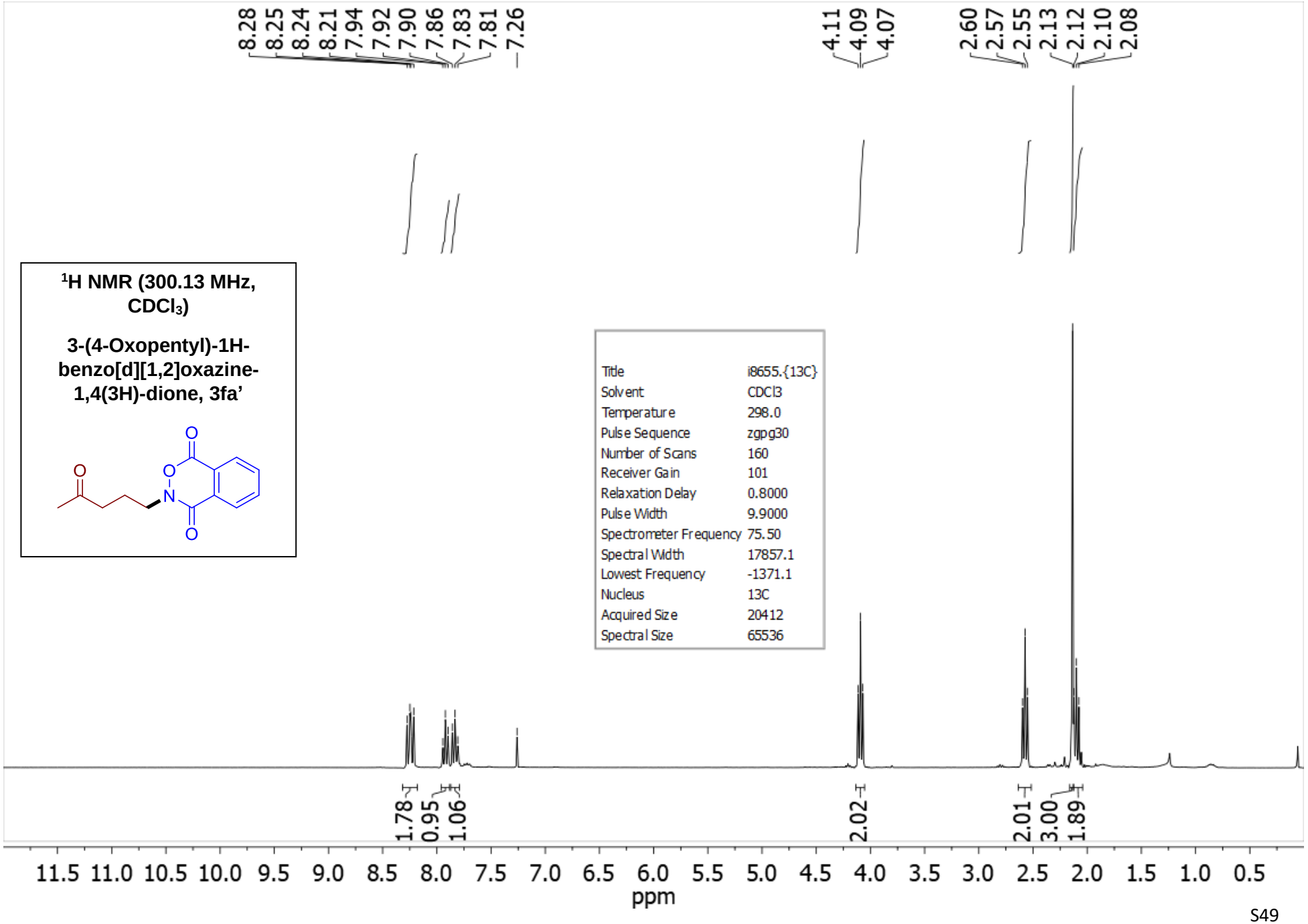

198.50
163.79
135.75
134.66
132.05
129.78
129.02
128.39
123.68
77.78
77.58
77.16
76.74
34.60
22.67
13C NMR (75.47 MHz, CDCl3)
2-(4-(4-Bromophenyl)-4-oxobutoxy)isoindoline-1,3-dione, 3ea
Br
O
O
O
N
O
1 Solvent CDCl3
2 Temperature 298.0
3 Pulse Sequence zgpg30
4 Number of Scans 180
5 Receiver Gain 101.0
6 Relaxation Delay 0.8000
7 Pulse Width 9.9000
8 Acquisition Time 1.1431
9 Spectrometer Frequency 75.50
10 Spectral Width 17857.1
11 Lowest Frequency -1370.0
12 Nucleus 13C
13 Acquired Size 20412
14 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

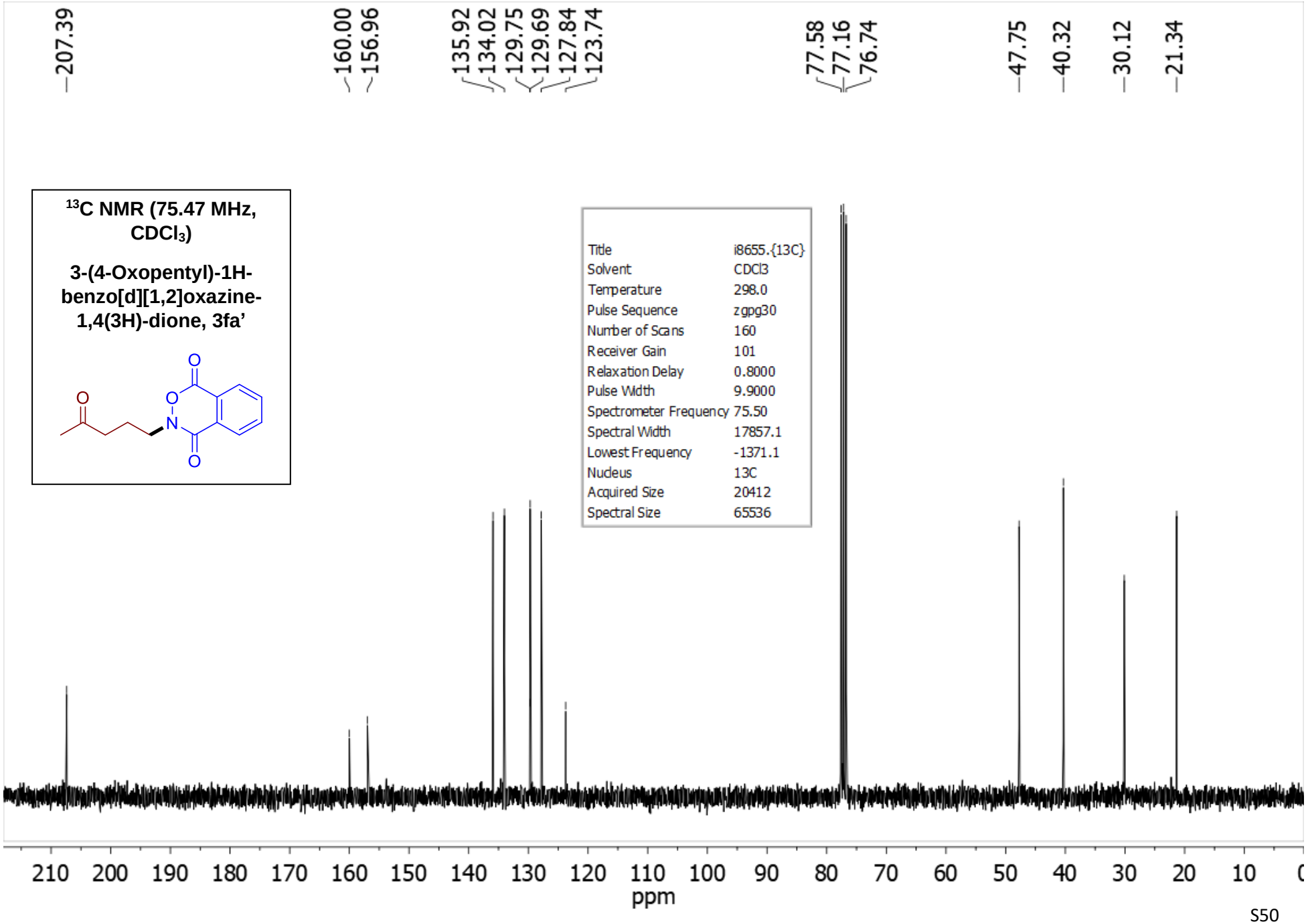

8.25
8.23
7.95
7.94
7.92
7.92
7.90
7.89
7.86
7.86
7.84
7.79
7.76
7.58
7.55
7.26
4.23
4.20
4.18
3.11
3.09
3.06
2.34
2.32
2.30
2.28
2.25
1H NMR (300.13 MHz, CDCl3)
3-(4-(4-Bromophenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ea'
Br
O
O
N
O
O
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
1.98
1.25
1.28
2.13
2.01
2.00
1.98
2.05
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
ppm

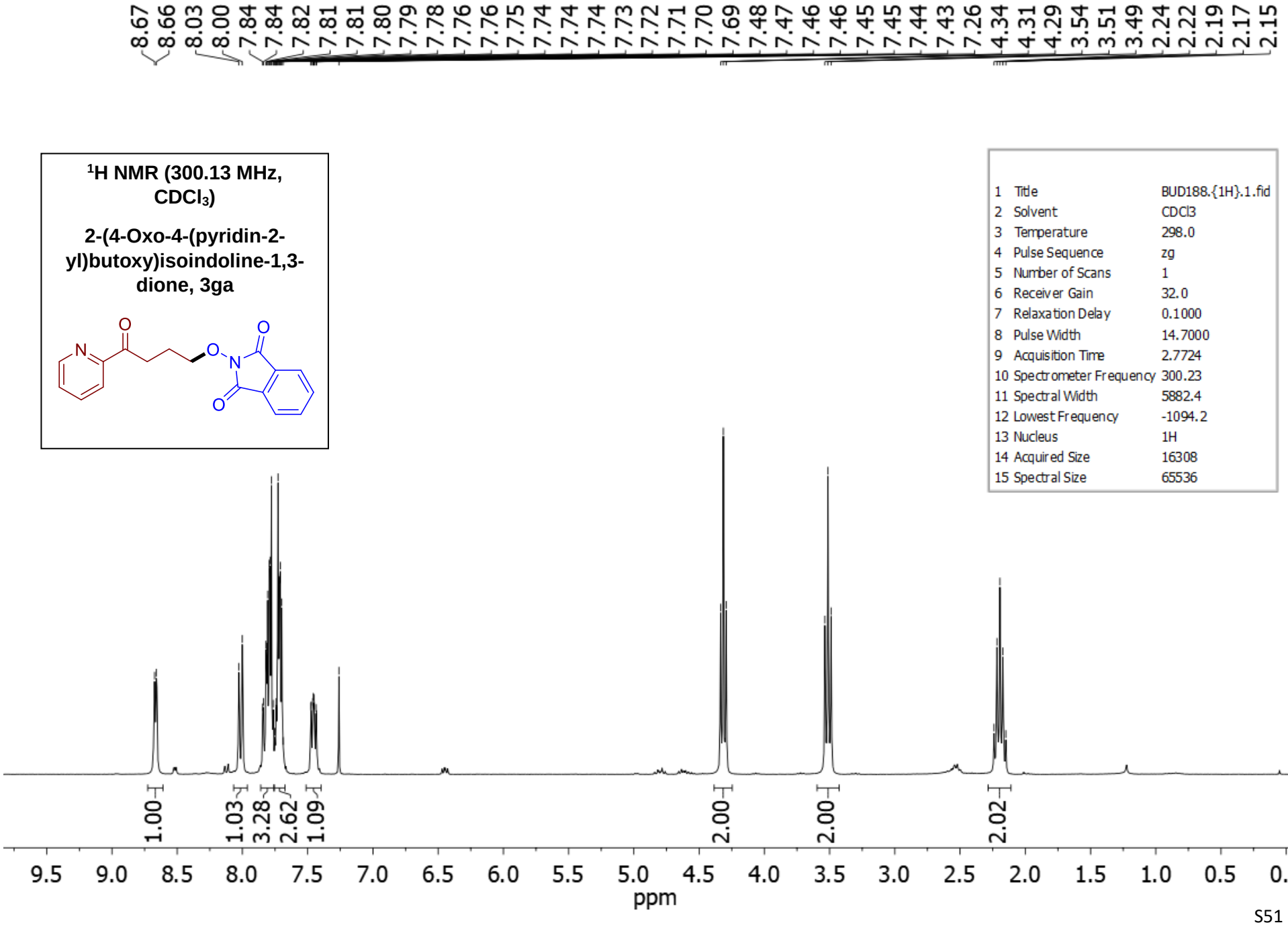

197.72
160.00
157.06
135.92
135.51
134.04
132.02
129.76
129.71
129.65
128.43
127.89
123.78
77.58
77.16
76.74
47.89
35.43
21.77
1H NMR (300.13 MHz, CDCl3)
3-(4-(4-Bromophenyl)-4-oxobutyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ea'
Br
O
O
N
O
O
1 Solvent CDCl3
2 Temperature 298.0
3 Pulse Sequence zgpg30
4 Number of Scans 500
5 Receiver Gain 101.0
6 Relaxation Delay 0.8000
7 Pulse Width 9.9000
8 Acquisition Time 1.1431
9 Spectrometer Frequency 75.50
10 Spectral Width 17857.1
11 Lowest Frequency -1370.1
12 Nucleus 13C
13 Acquired Size 20412
14 Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

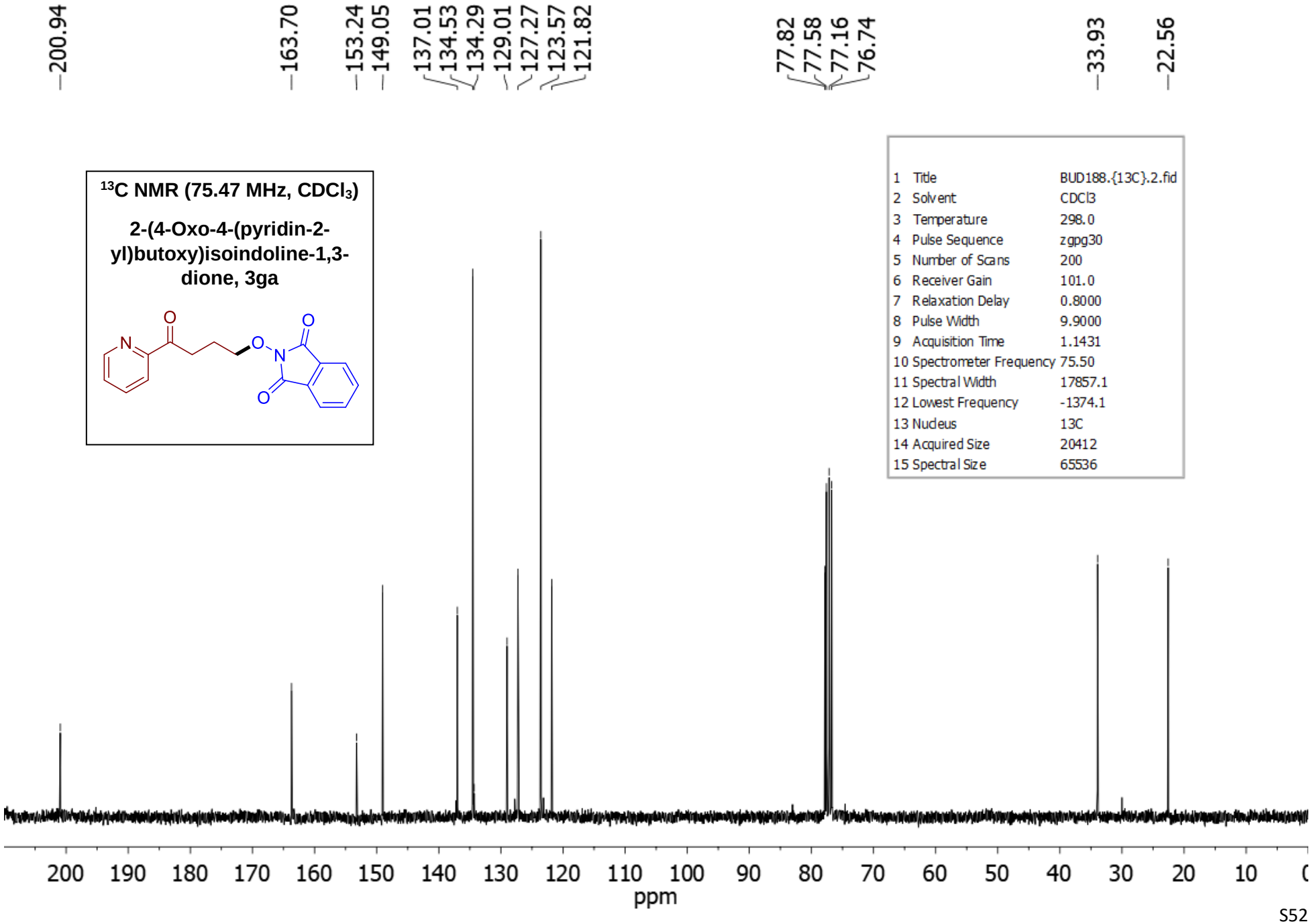

7.80
7.79
7.78
7.74
7.73
7.72
7.26
4.21
4.19
4.17
2.81
2.79
2.77
2.20
2.03
2.01
1.99
1.97
1.95
^{1}H NMR (300.13 MHz, $CDCl_3$)
2-((4-Oxopentyl)oxy)isoindoline-1,3-dione, 3fa
Title i8646.{1H}
Solvent CDCl3
Temperature 302.5
Pulse Sequence zg
Number of Scans 4
Receiver Gain 6
Relaxation Delay 0.0050
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -608.9
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
1.92
1.98
2.02
1.99
2.87
2.21
ppm

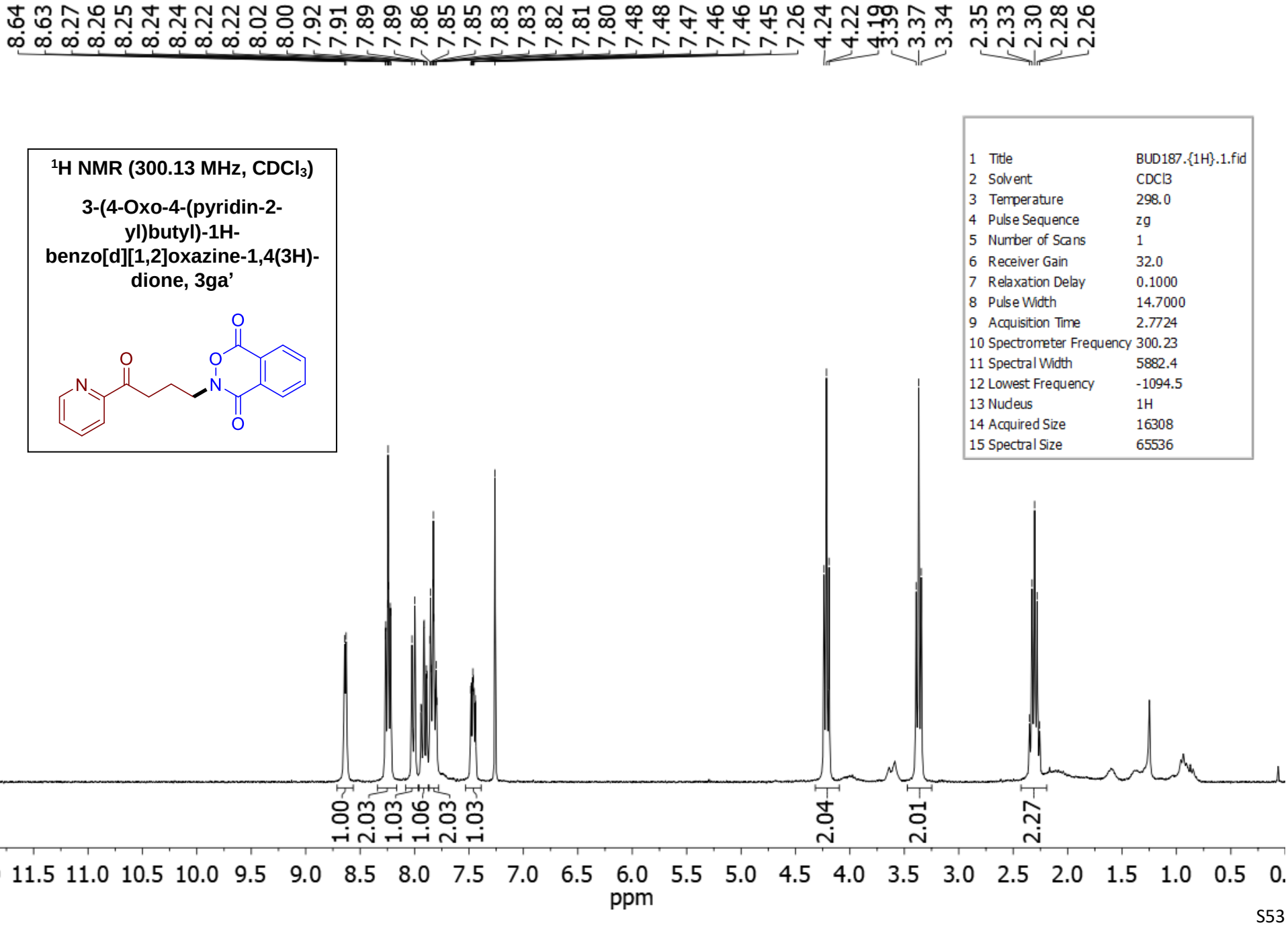

208.04
163.67
134.58
128.99
123.58
77.60
77.42
77.16
76.90
39.30
30.20
22.27
13C NMR (75.47 MHz, CDCl3)
2-((4-Oxopentyl)oxy)isoindoline-1,3-dione, 3fa
Title i8655.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 160
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1371.1
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
ppm

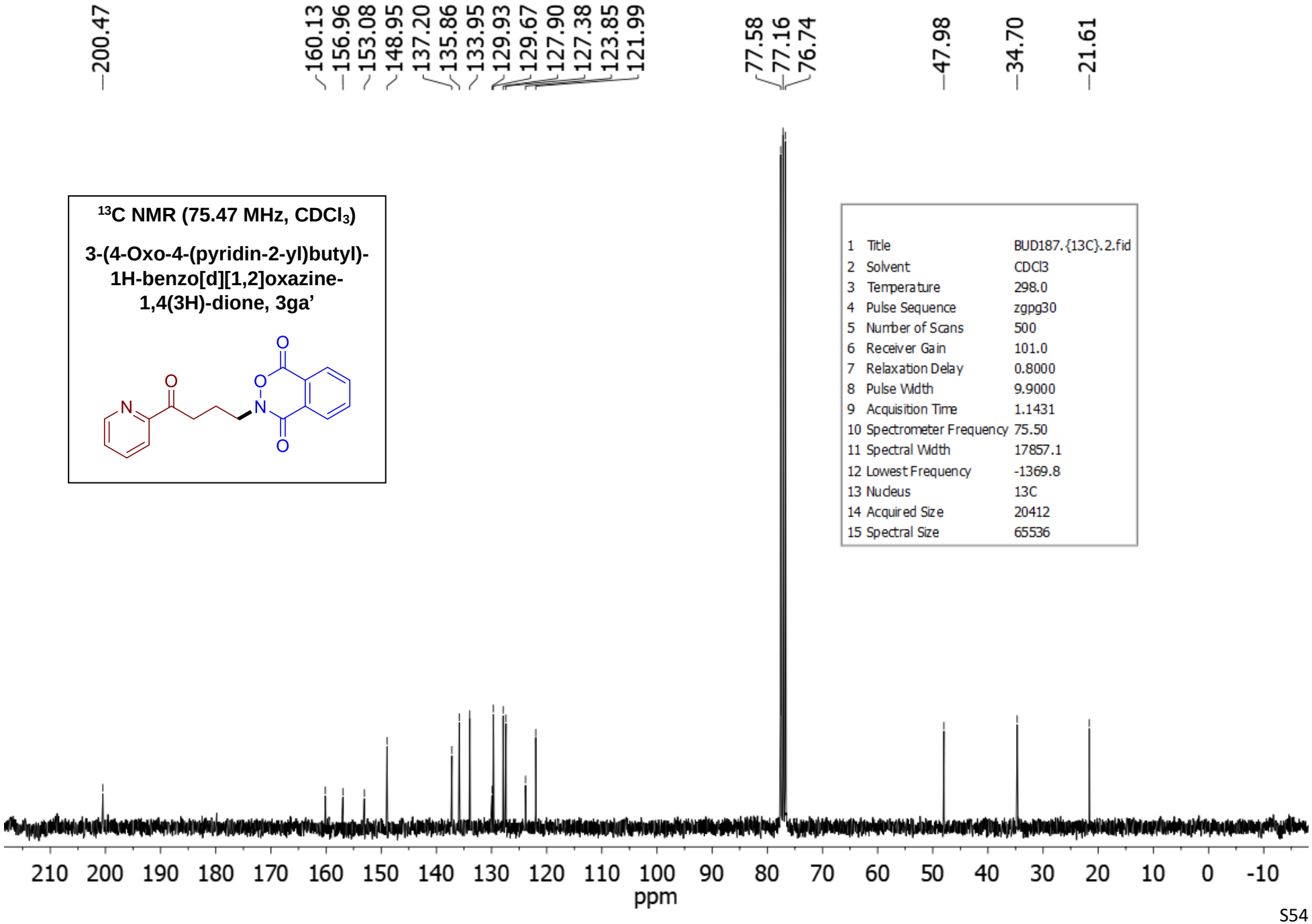

8.28
8.25
8.24
8.21
7.94
7.92
7.90
7.86
7.83
7.81
7.26
4.11
4.09
4.07
2.60
2.57
2.55
2.13
2.12
2.10
2.08
1H NMR (300.13 MHz, CDCl3)
3-(4-Oxopentyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3fa'
Title i8655.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 160
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1371.1
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
1.78
0.95
1.06
2.02
2.01
3.00
1.89
11.5 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
ppm

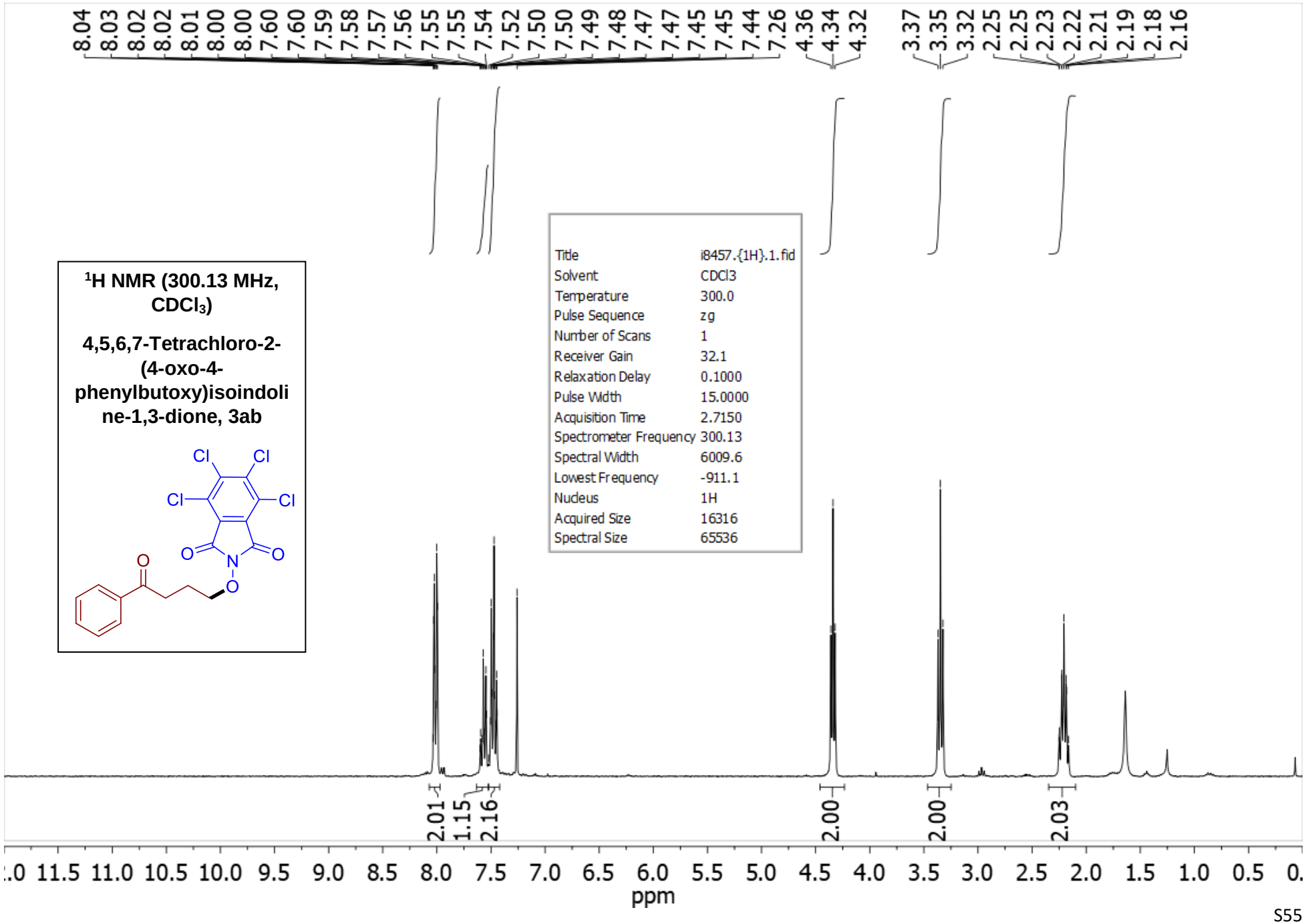

207.39
160.00
156.96
135.92
134.02
129.75
129.69
127.84
123.74
77.58
77.16
76.74
47.75
40.32
30.12
21.34
13C NMR (75.47 MHz, CDCl3)
3-(4-Oxopentyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3fa'
Title i8655.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 160
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1371.1
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

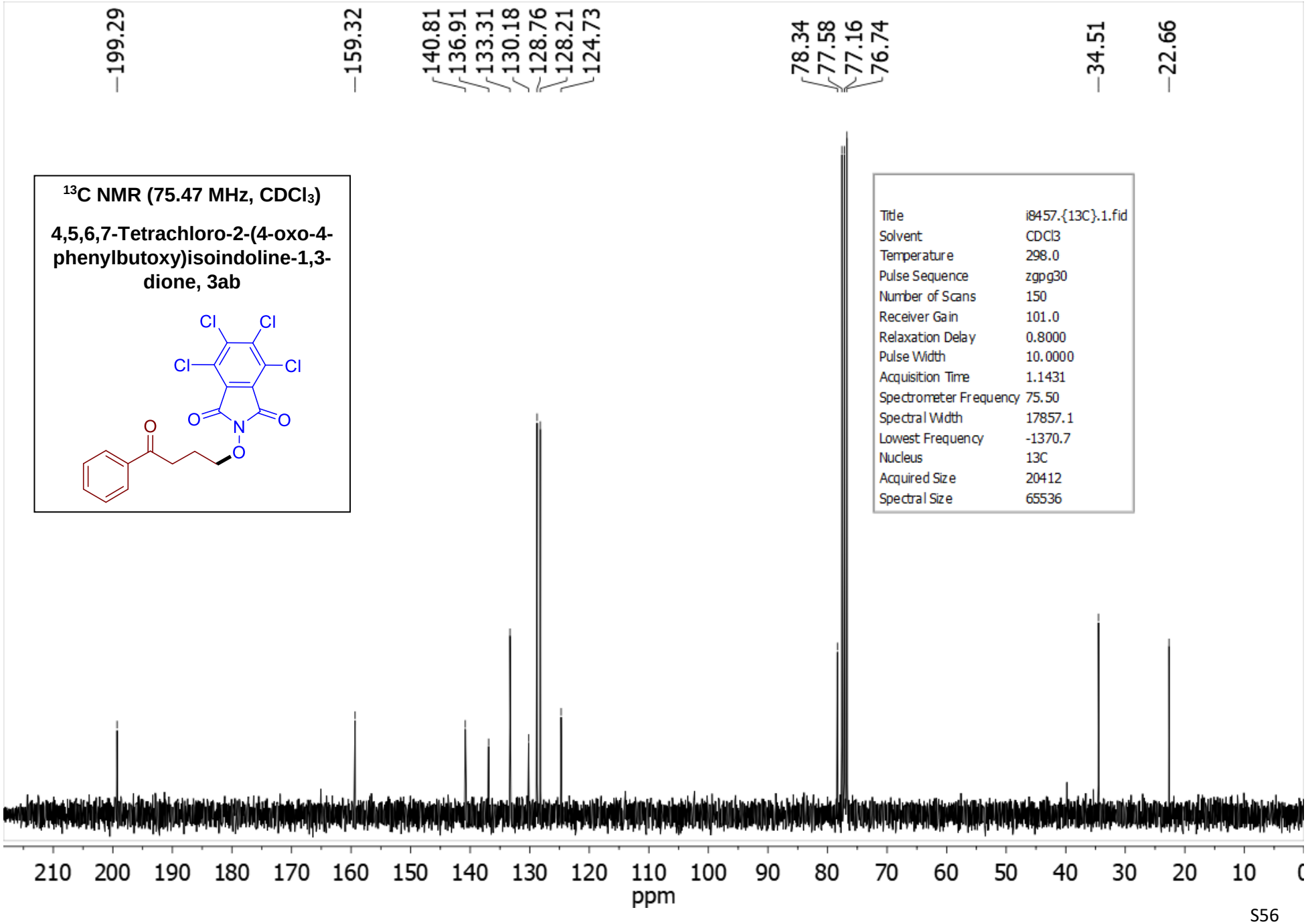

8.67 8.66 8.03 8.00 7.84 7.84 7.82 7.81 7.81 7.80 7.79 7.78 7.76 7.76 7.75 7.74 7.74 7.74 7.73 7.72 7.71 7.70 7.69 7.48 7.47 7.46 7.46 7.45 7.45 7.44 7.43 7.26 4.34 4.31 4.29 3.54 3.51 3.49 2.24 2.22 2.19 2.17 2.15
^{1}H NMR (300.13 MHz, $CDCl_3$)
2-(4-Oxo-4-(pyridin-2-yl)butoxy)isoindoline-1,3-dione, 3ga
1 Title BUD188.{1H}.1.fid
2 Solvent CDCl3
3 Temperature 298.0
4 Pulse Sequence zg
5 Number of Scans 1
6 Receiver Gain 32.0
7 Relaxation Delay 0.1000
8 Pulse Width 14.7000
9 Acquisition Time 2.7724
10 Spectrometer Frequency 300.23
11 Spectral Width 5882.4
12 Lowest Frequency -1094.2
13 Nucleus 1H
14 Acquired Size 16308
15 Spectral Size 65536
1.00 1.03 3.28 2.62 1.09 2.00 2.00 2.02
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
ppm

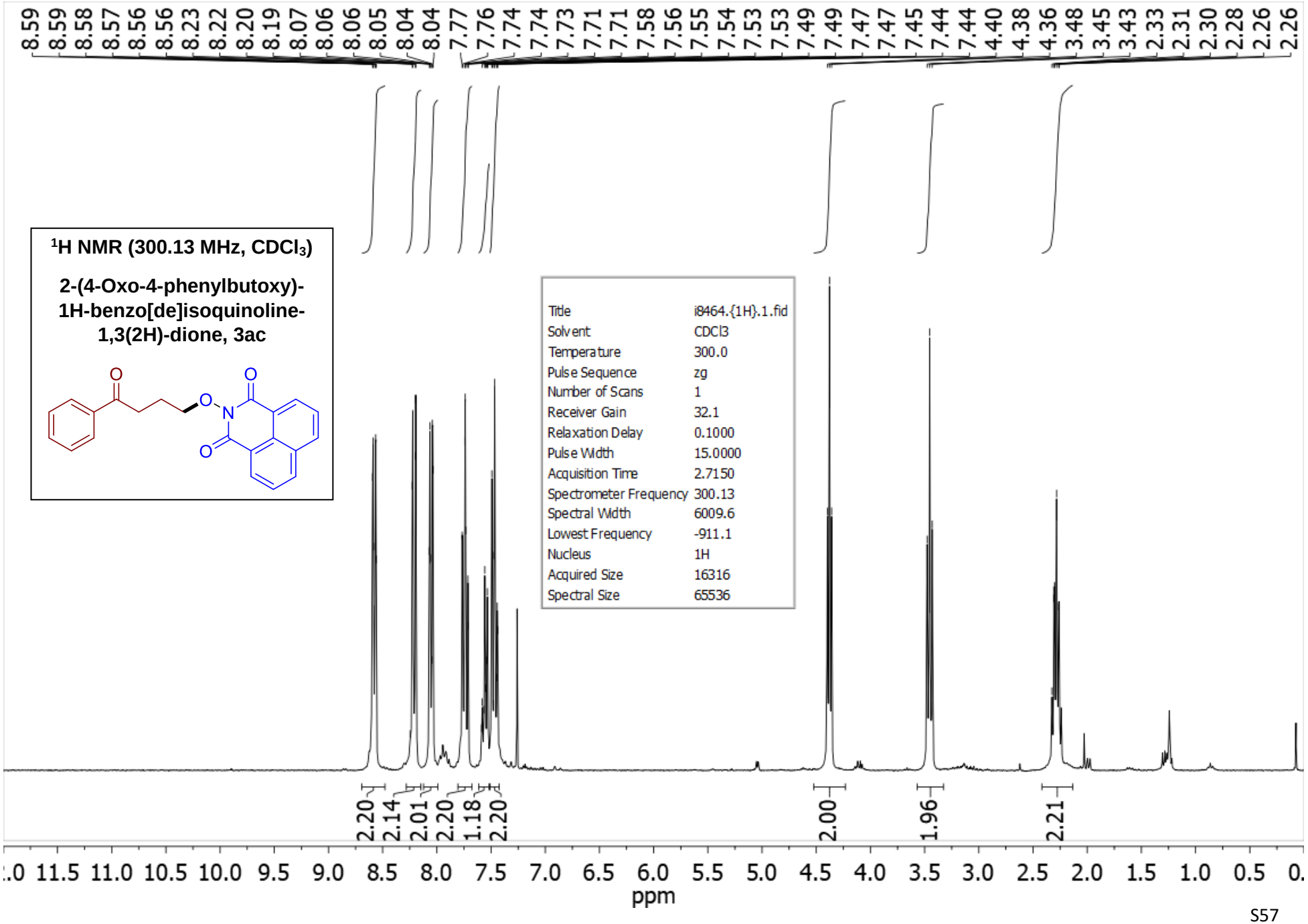

200.94
163.70
153.24
149.05
137.01
134.53
134.29
129.01
127.27
123.57
121.82
77.82
77.58
77.16
76.74
33.93
22.56
13C NMR (75.47 MHz, CDCl3)
2-(4-Oxo-4-(pyridin-2-yl)butoxy)isoindoline-1,3-dione, 3ga
1 Title BUD188.{13C}.2.fid
2 Solvent CDCl3
3 Temperature 298.0
4 Pulse Sequence zgpg30
5 Number of Scans 200
6 Receiver Gain 101.0
7 Relaxation Delay 0.8000
8 Pulse Width 9.9000
9 Acquisition Time 1.1431
10 Spectrometer Frequency 75.50
11 Spectral Width 17857.1
12 Lowest Frequency -1374.1
13 Nucleus 13C
14 Acquired Size 20412
15 Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

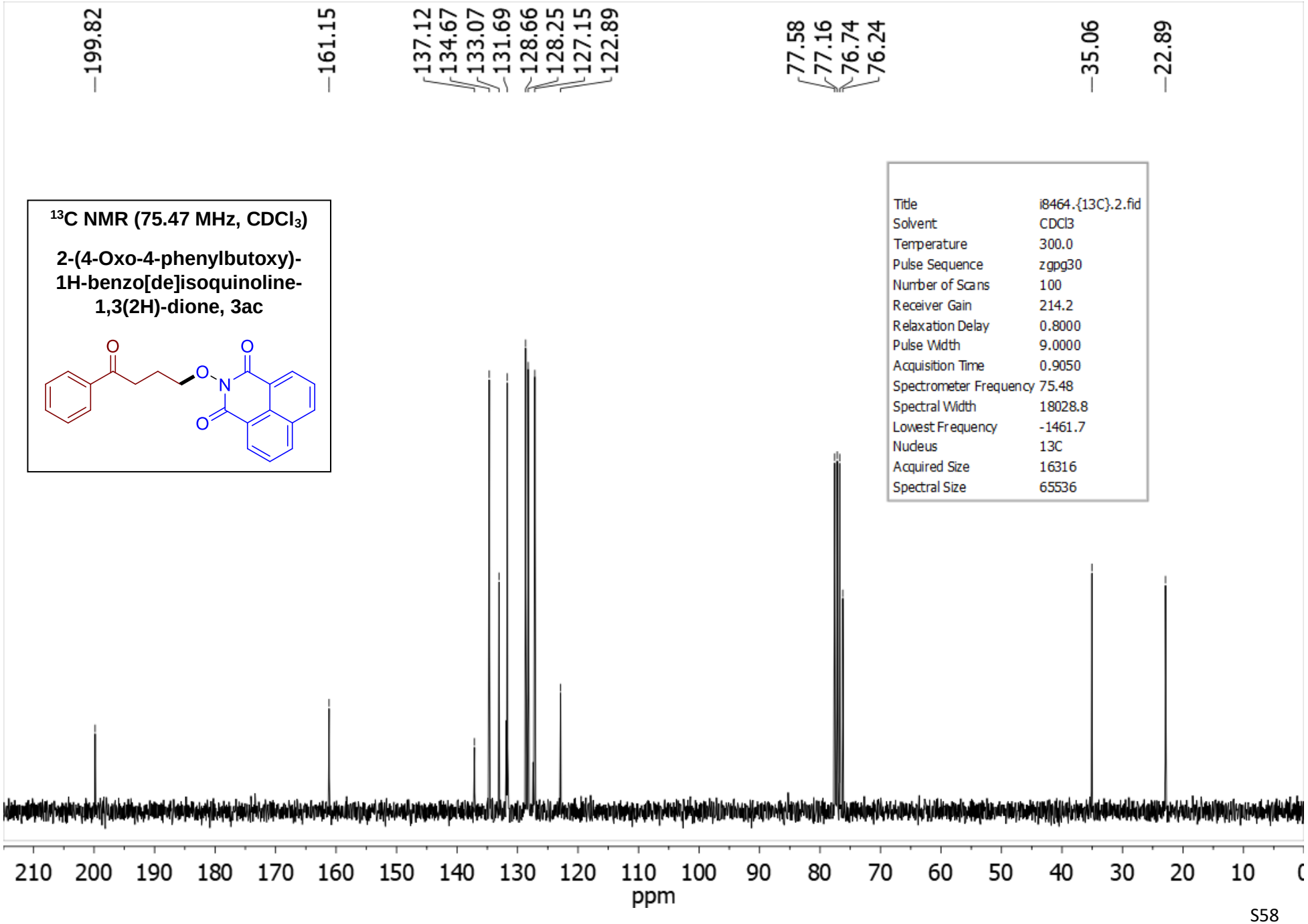

8.64 8.63 8.27 8.26 8.25 8.24 8.24 8.22 8.22 8.02 8.00 7.92 7.91 7.89 7.89 7.86 7.85 7.85 7.83 7.83 7.82 7.81 7.80 7.48 7.48 7.47 7.46 7.46 7.45 7.26 4.24 4.22 4.19 3.39 3.37 3.34 2.35 2.33 2.30 2.28 2.26
^{1}H NMR (300.13 MHz, CDCl$_3$)
3-(4-Oxo-4-(pyridin-2-yl)butyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ga'
1 Title BUD187.{1H}.1.fid
2 Solvent CDCl3
3 Temperature 298.0
4 Pulse Sequence zg
5 Number of Scans 1
6 Receiver Gain 32.0
7 Relaxation Delay 0.1000
8 Pulse Width 14.7000
9 Acquisition Time 2.7724
10 Spectrometer Frequency 300.23
11 Spectral Width 5882.4
12 Lowest Frequency -1094.5
13 Nucleus 1H
14 Acquired Size 16308
15 Spectral Size 65536
1.00 2.03 1.03 1.06 2.03 1.03 2.04 2.01 2.27
ppm


200.47
160.13
156.96
153.08
148.95
137.20
135.86
133.95
129.93
129.67
127.90
127.38
123.85
121.99
77.58
77.16
76.74
47.98
34.70
21.61
^{13}C NMR (75.47 MHz, CDCl$_3$)
3-(4-Oxo-4-(pyridin-2-yl)butyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ga'
1 Title BUD187.{13C}.2.fid
2 Solvent CDCl3
3 Temperature 298.0
4 Pulse Sequence zgpg30
5 Number of Scans 500
6 Receiver Gain 101.0
7 Relaxation Delay 0.8000
8 Pulse Width 9.9000
9 Acquisition Time 1.1431
10 Spectrometer Frequency 75.50
11 Spectral Width 17857.1
12 Lowest Frequency -1369.8
13 Nucleus 13C
14 Acquired Size 20412
15 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm


8.04 8.03 8.02 8.02 8.01 8.00 8.00 7.60 7.60 7.59 7.58 7.57 7.56 7.55 7.55 7.54 7.52 7.50 7.50 7.49 7.48 7.47 7.47 7.45 7.45 7.44 7.26 4.36 4.34 4.32 3.37 3.35 3.32 2.25 2.25 2.23 2.22 2.21 2.19 2.18 2.16
¹H NMR (300.13 MHz, CDCl₃)
4,5,6,7-Tetrachloro-2-(4-oxo-4-phenylbutoxy)isoindoline-1,3-dione, 3ab
Cl Cl Cl Cl O O N O O
Title i8457.{1H}.1.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.1
Relaxation Delay 0.1000
Pulse Width 15.0000
Acquisition Time 2.7150
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -911.1
Nucleus 1H
Acquired Size 16316
Spectral Size 65536
2.01 1.15 2.16 2.00 2.00 2.03
.0 11.5 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.
ppm


199.29
159.32
140.81
136.91
133.31
130.18
128.76
128.21
124.73
78.34
77.58
77.16
76.74
34.51
22.66
13C NMR (75.47 MHz, CDCl3)
4,5,6,7-Tetrachloro-2-(4-oxo-4-phenylbutoxy)isoindoline-1,3-dione, 3ab
Cl
Cl
Cl
Cl
O
O
N
O
O
Title i8457.{13C}.1.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 150
Receiver Gain 101.0
Relaxation Delay 0.8000
Pulse Width 10.0000
Acquisition Time 1.1431
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1370.7
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

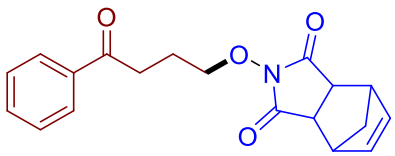

8.59 8.59 8.58 8.57 8.56 8.56 8.23 8.22 8.20 8.19 8.07 8.06 8.06 8.05 8.04 8.04
7.77 7.76 7.74 7.74 7.73 7.71 7.71 7.58 7.56 7.55 7.54 7.53 7.53 7.49 7.49 7.47 7.47 7.45 7.44 7.44
4.40 4.38 4.36 3.48 3.45 3.43 2.33 2.31 2.30 2.28 2.26 2.26
^{1}H NMR (300.13 MHz, $CDCl_3$)
2-(4-Oxo-4-phenylbutoxy)-1H-benzo[de]isoquinoline-1,3(2H)-dione, 3ac
Title i8464.{1H}.1.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.1
Relaxation Delay 0.1000
Pulse Width 15.0000
Acquisition Time 2.7150
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -911.1
Nucleus 1H
Acquired Size 16316
Spectral Size 65536
2.20 2.14 2.01 2.20 1.18 2.20 2.00 1.96 2.21
ppm

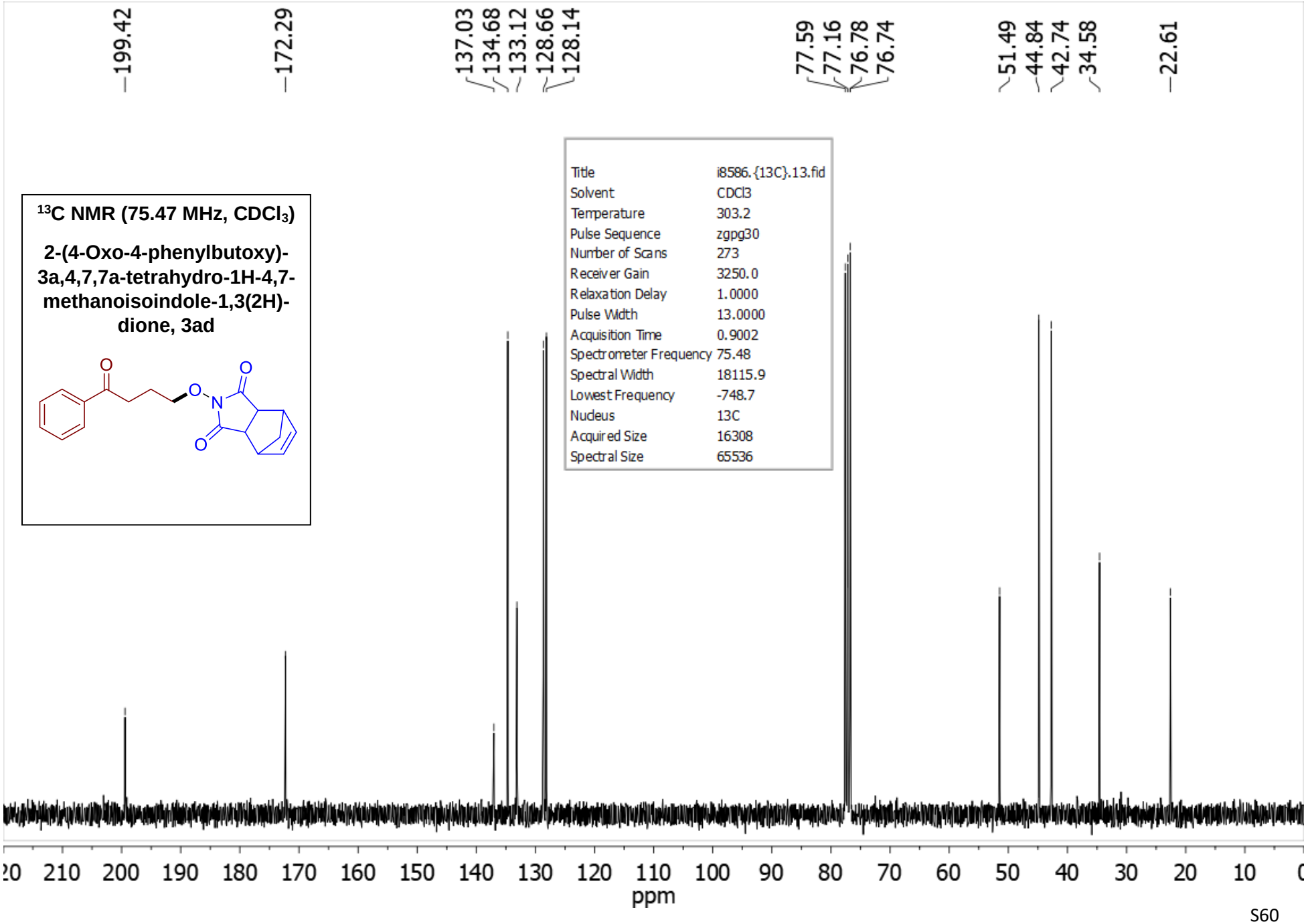

199.82
161.15
137.12
134.67
133.07
131.69
128.66
128.25
127.15
122.89
77.58
77.16
76.74
76.24
35.06
22.89
13C NMR (75.47 MHz, CDCl3)
2-(4-Oxo-4-phenylbutoxy)-1H-benzo[de]isoquinoline-1,3(2H)-dione, 3ac
Title i8464.{13C}.2.fid
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 100
Receiver Gain 214.2
Relaxation Delay 0.8000
Pulse Width 9.0000
Acquisition Time 0.9050
Spectrometer Frequency 75.48
Spectral Width 18028.8
Lowest Frequency -1461.7
Nucleus 13C
Acquired Size 16316
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

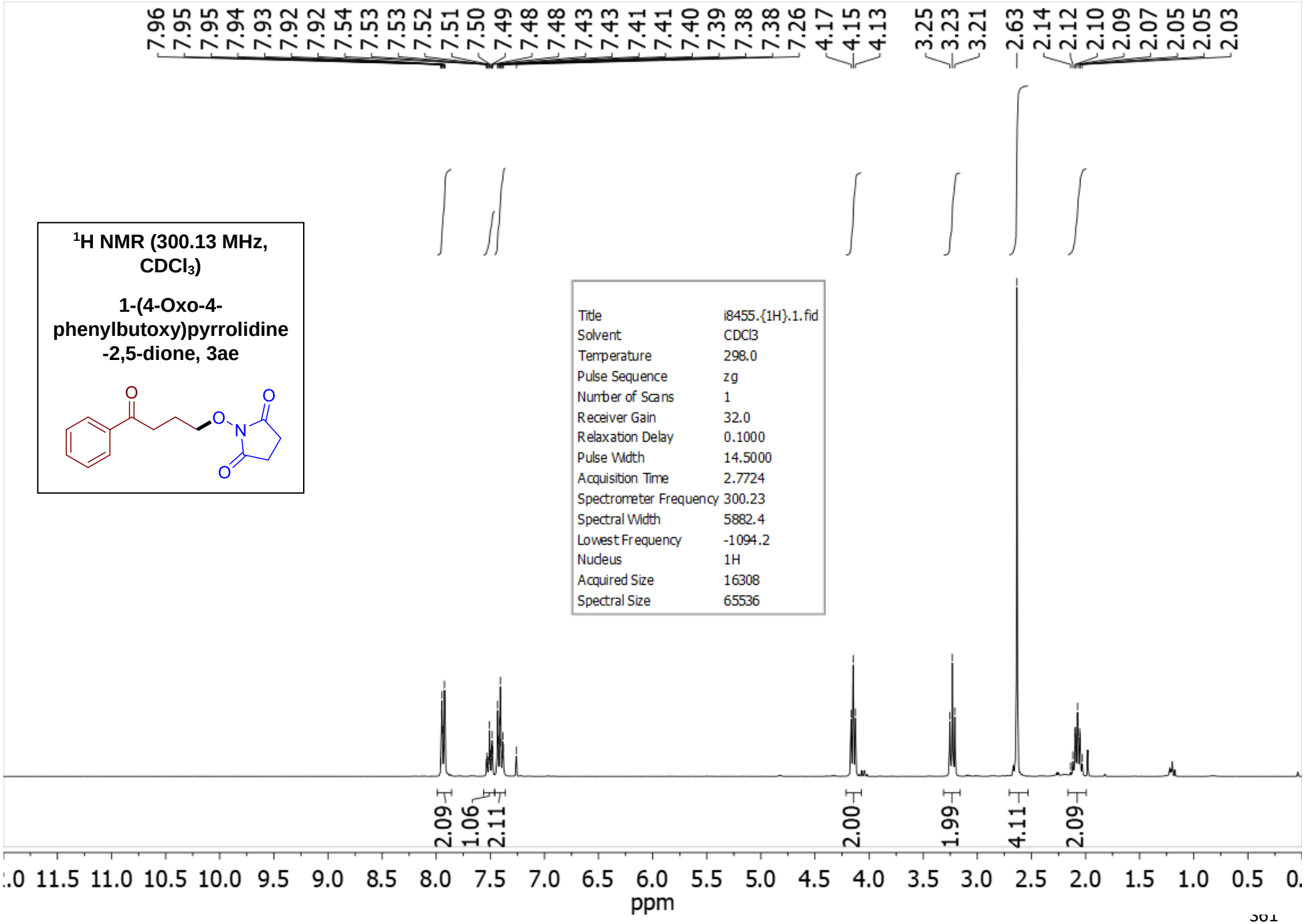
Parameter	Value
Title	i8586.{1H}.1.fid
Solvent	CDCl3
Temperature	303.2
Pulse Sequence	zg
Number of Scans	4
Receiver Gain	6.3
Relaxation Delay	1.0000
Pulse Width	9.0000
Acquisition Time	1.3518
Spectrometer Frequency	300.13
Spectral Width	6009.6
Lowest Frequency	-610.2
Nucleus	1H
Acquired Size	8124
Spectral Size	65536

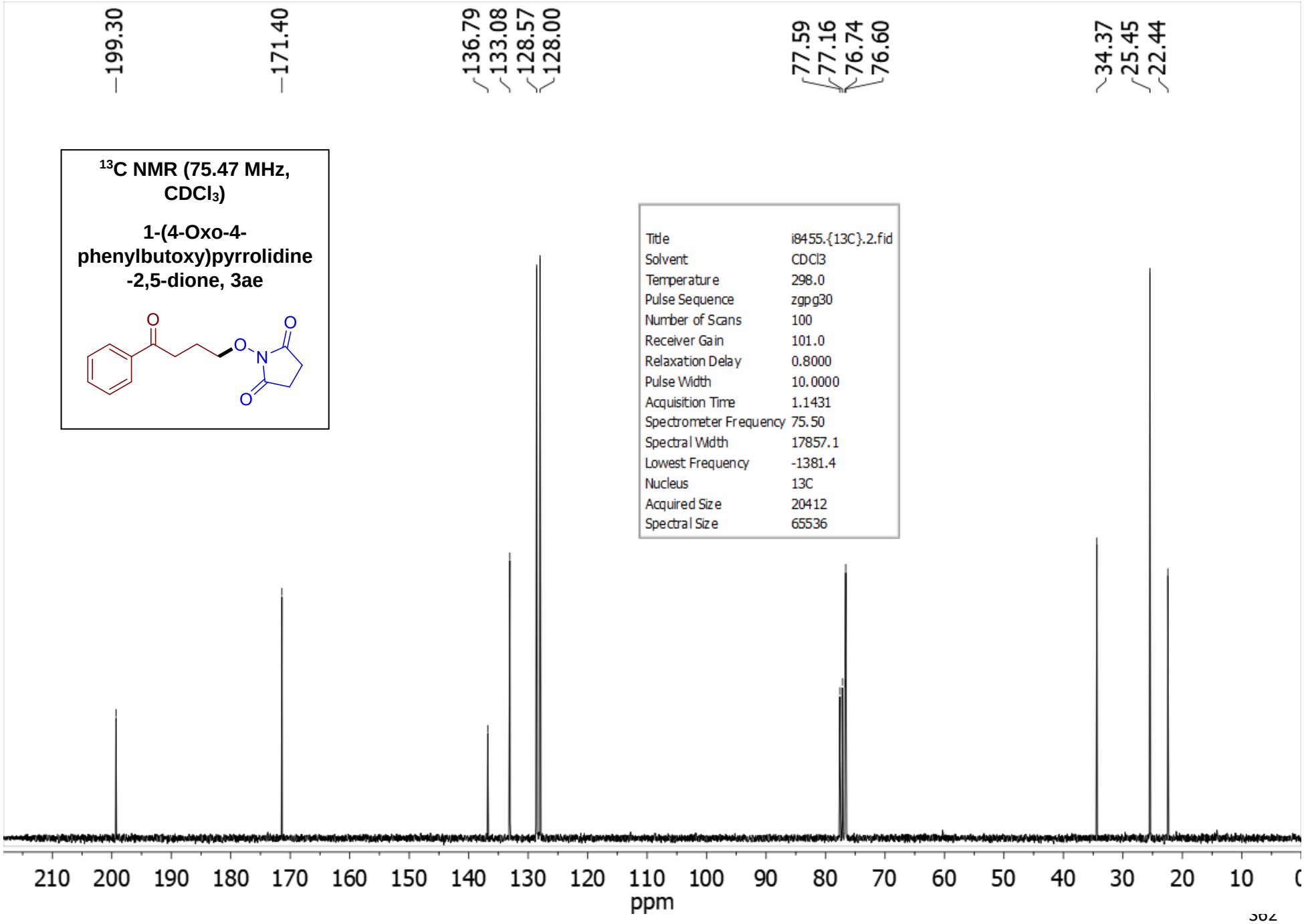
^{1}H NMR (300.13 MHz, $CDCl_3$)

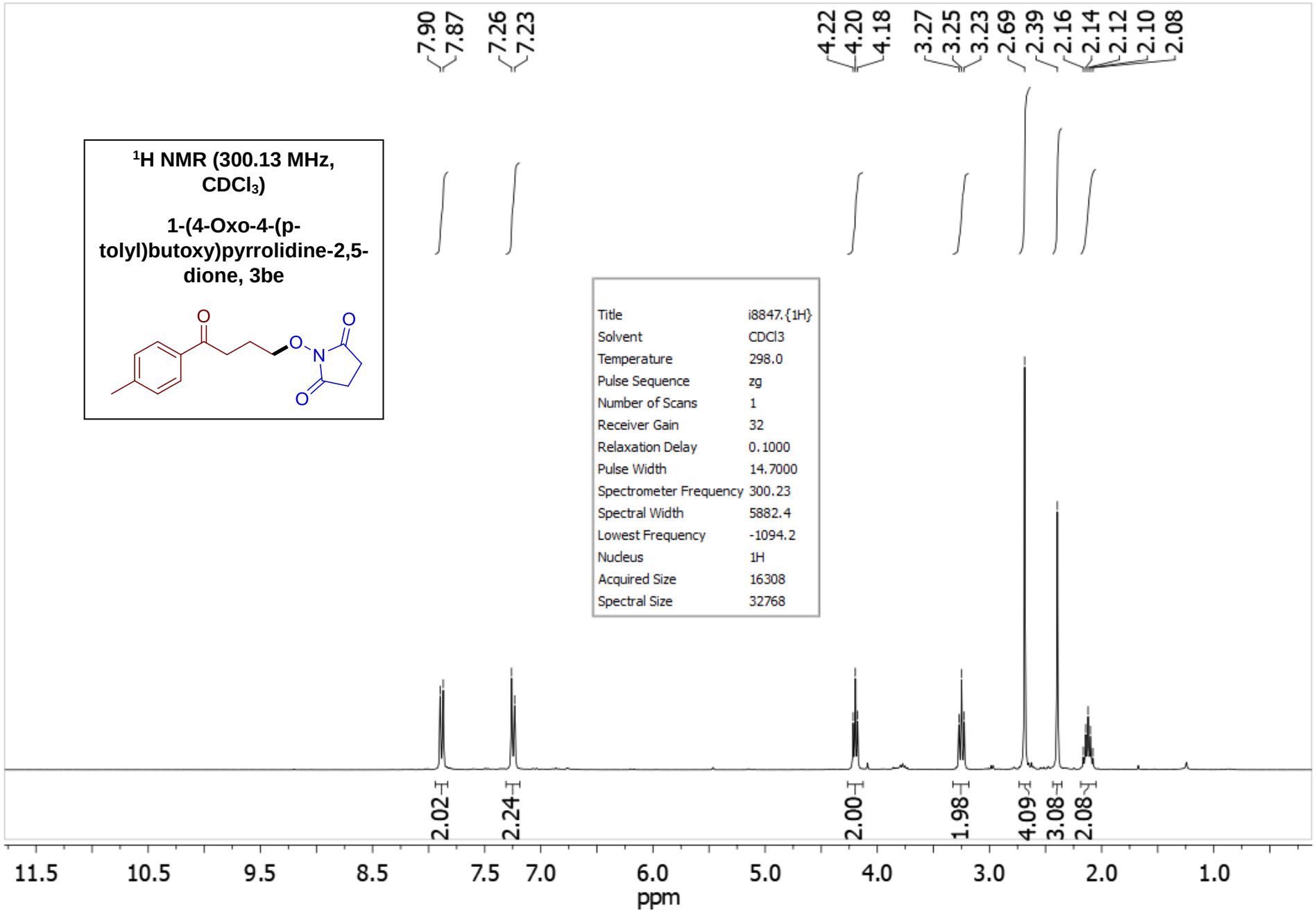
2-(4-Oxo-4-phenylbutoxy)-3a,4,7,7a-tetrahydro-1H-4,7-methanoisoindole-1,3(2H)-dione, 3ad

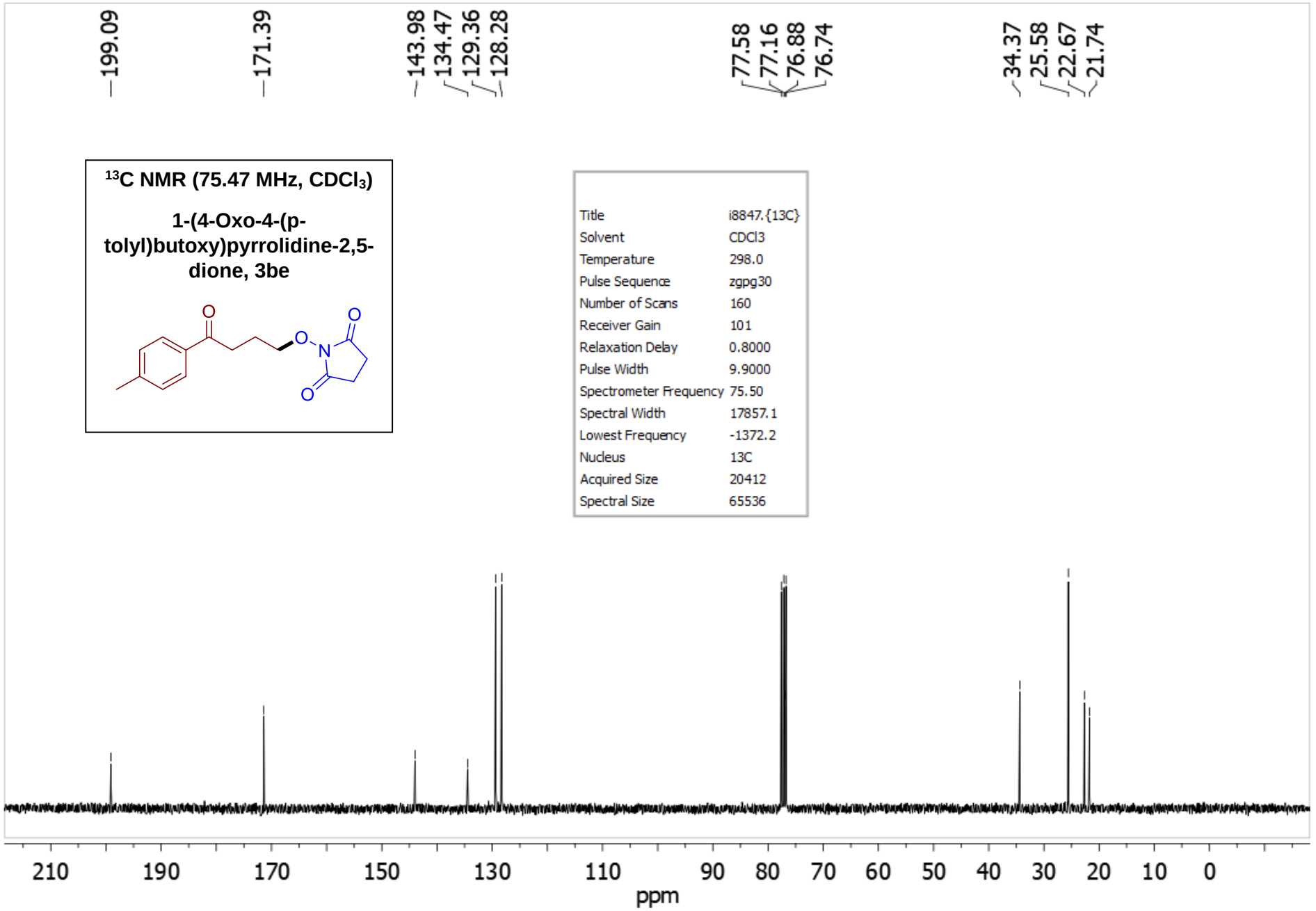



199.42
172.29
137.03
134.68
133.12
128.66
128.14
77.59
77.16
76.78
76.74
51.49
44.84
42.74
34.58
22.61
13C NMR (75.47 MHz, CDCl3)
2-(4-Oxo-4-phenylbutoxy)-3a,4,7,7a-tetrahydro-1H-4,7-methanoisoindole-1,3(2H)-dione, 3ad
Title i8586.{13C}.13.fid
Solvent CDCl3
Temperature 303.2
Pulse Sequence zgpg30
Number of Scans 273
Receiver Gain 3250.0
Relaxation Delay 1.0000
Pulse Width 13.0000
Acquisition Time 0.9002
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -748.7
Nucleus 13C
Acquired Size 16308
Spectral Size 65536
ppm


7.96 7.95 7.95 7.94 7.93 7.92 7.92 7.54 7.53 7.53 7.52 7.51 7.50 7.49 7.48 7.48 7.43 7.43 7.41 7.41 7.40 7.39 7.38 7.38 7.26 4.17 4.15 4.13 3.25 3.23 3.21 2.63 2.14 2.12 2.10 2.09 2.07 2.05 2.05 2.03
¹H NMR (300.13 MHz, CDCl₃)
1-(4-Oxo-4-phenylbutoxy)pyrrolidine-2,5-dione, 3ae
O
O
O
N
O
Title i8455.{1H}.1.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.0
Relaxation Delay 0.1000
Pulse Width 14.5000
Acquisition Time 2.7724
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.2
Nucleus 1H
Acquired Size 16308
Spectral Size 65536
2.09 1.06 2.11 2.00 1.99 4.11 2.09
11.5 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
ppm

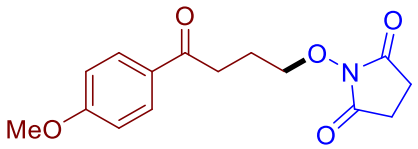

199.30
171.40
136.79
133.08
128.57
128.00
77.59
77.16
76.74
76.60
34.37
25.45
22.44
13C NMR (75.47 MHz, CDCl3)
1-(4-Oxo-4-phenylbutoxy)pyrrolidine-2,5-dione, 3ae
Title i8455.{13C}.2.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 100
Receiver Gain 101.0
Relaxation Delay 0.8000
Pulse Width 10.0000
Acquisition Time 1.1431
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1381.4
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


7.90
7.87
7.26
7.23
4.22
4.20
4.18
3.27
3.25
3.23
2.69
2.39
2.16
2.14
2.12
2.10
2.08
¹H NMR (300.13 MHz, CDCl₃)
1-(4-Oxo-4-(p-tolyl)butoxy)pyrrolidine-2,5-dione, 3be
O
O
O
N
O
Title i8847.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.2
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
2.02
2.24
2.00
1.98
4.09
3.08
2.08
11.5
10.5
9.5
8.5
7.5
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm

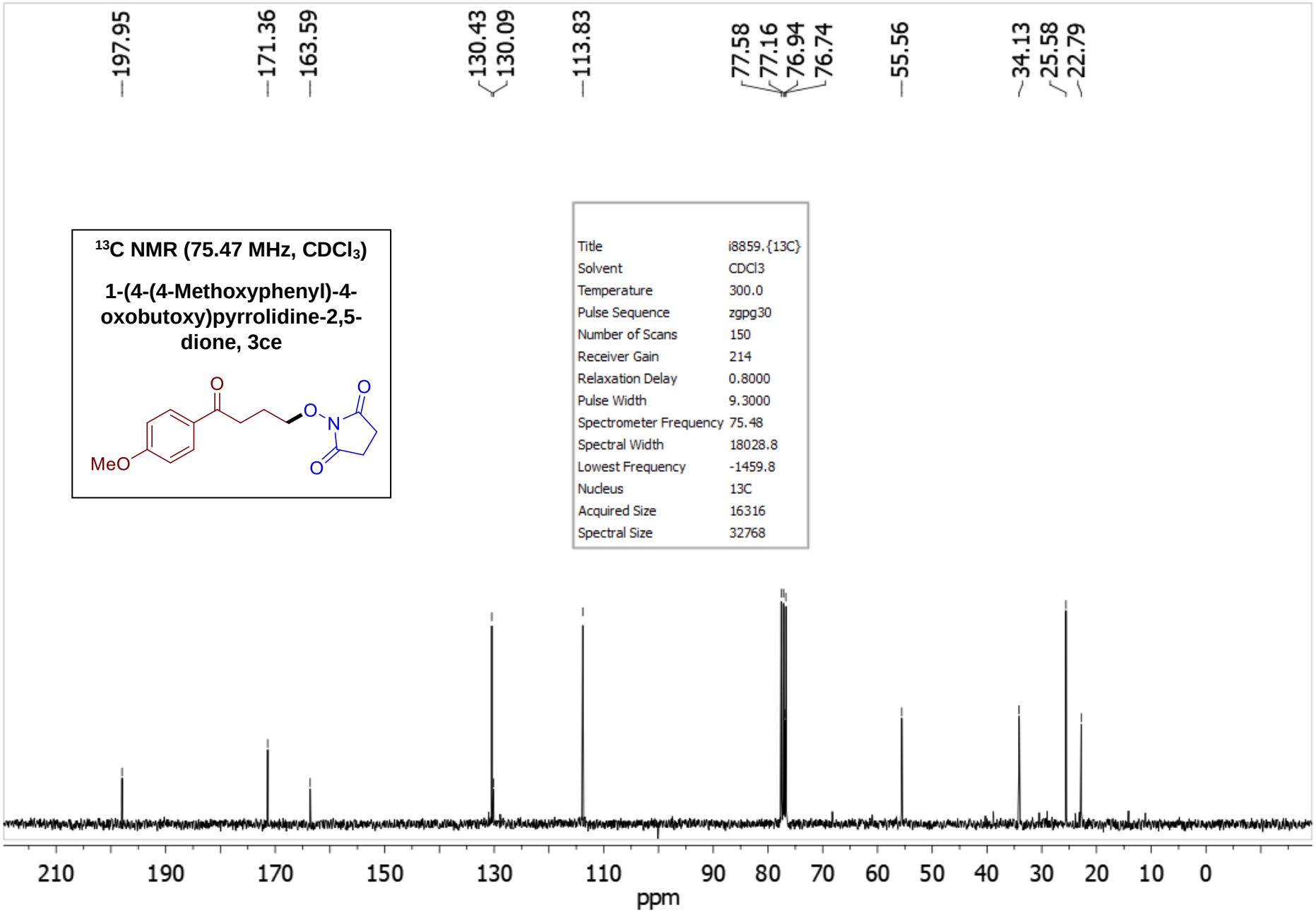

199.09
171.39
143.98
134.47
129.36
128.28
77.58
77.16
76.88
76.74
34.37
25.58
22.67
21.74
^{13}C NMR (75.47 MHz, $CDCl_3$)
1-(4-Oxo-4-(p-tolyl)butoxy)pyrrolidine-2,5-dione, 3be
Title i8847.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 160
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1372.2
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
ppm

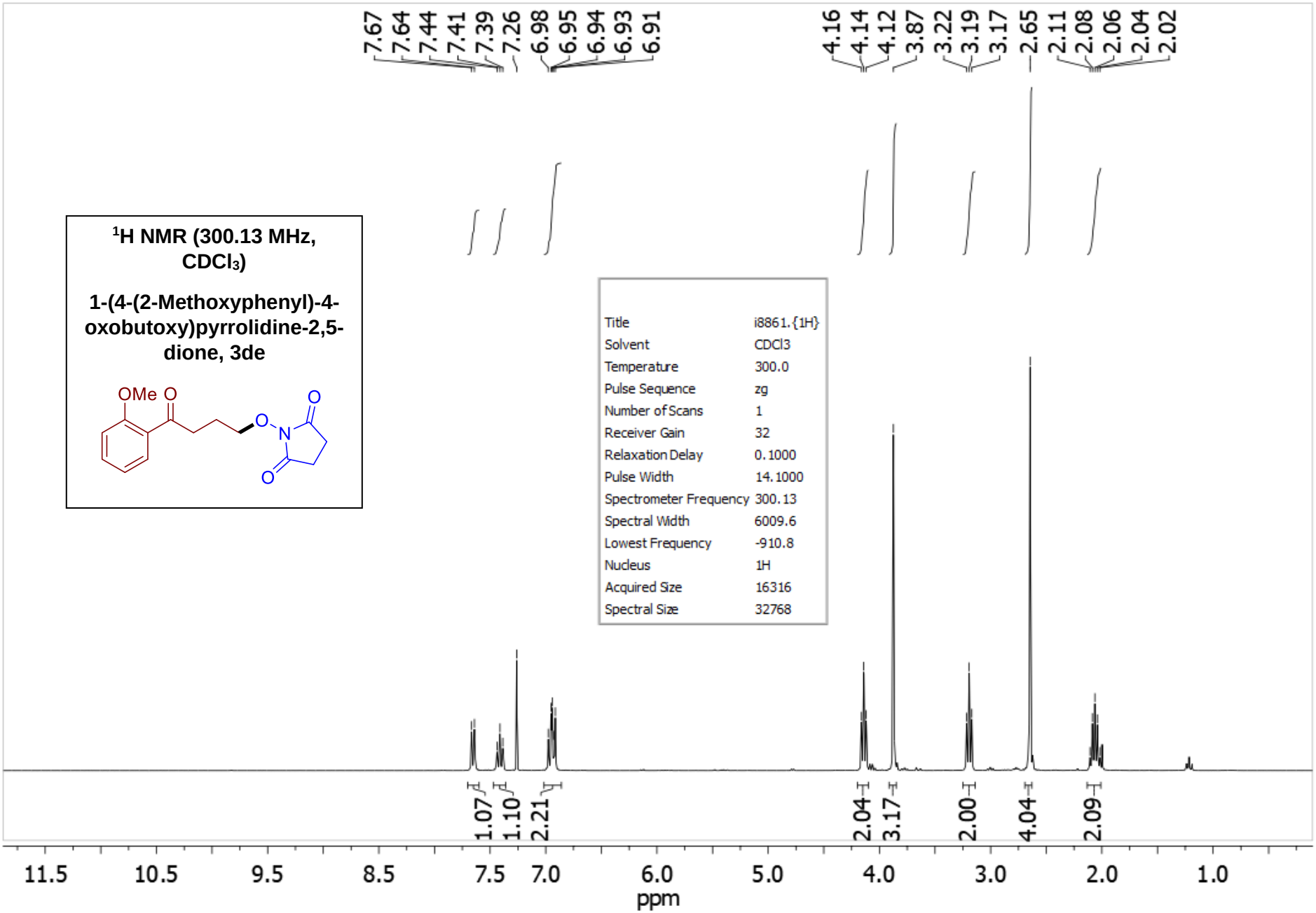
^{1}H NMR (300.13 MHz, $CDCl_3$)

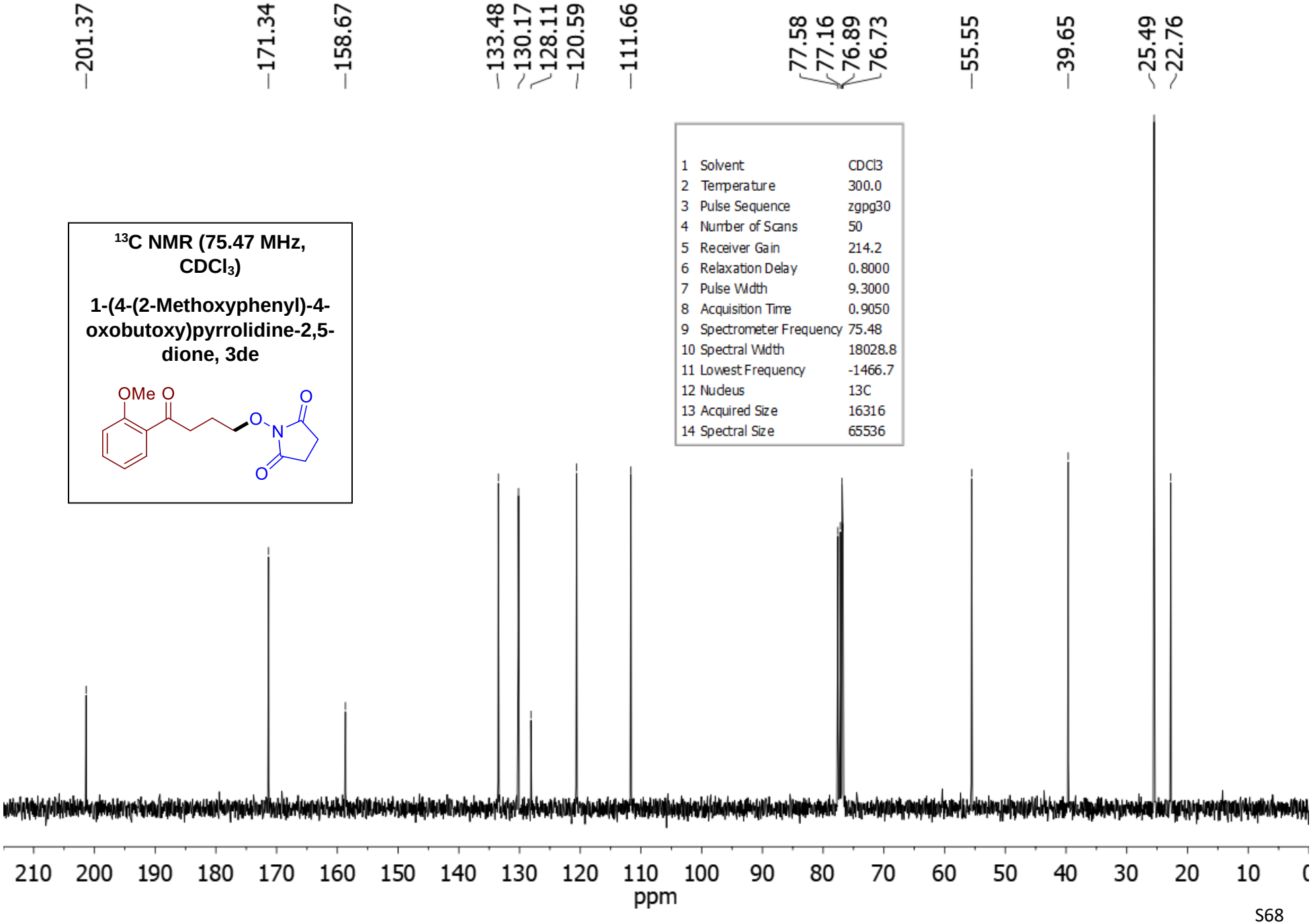
1-(4-(4-Methoxyphenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, 3ce

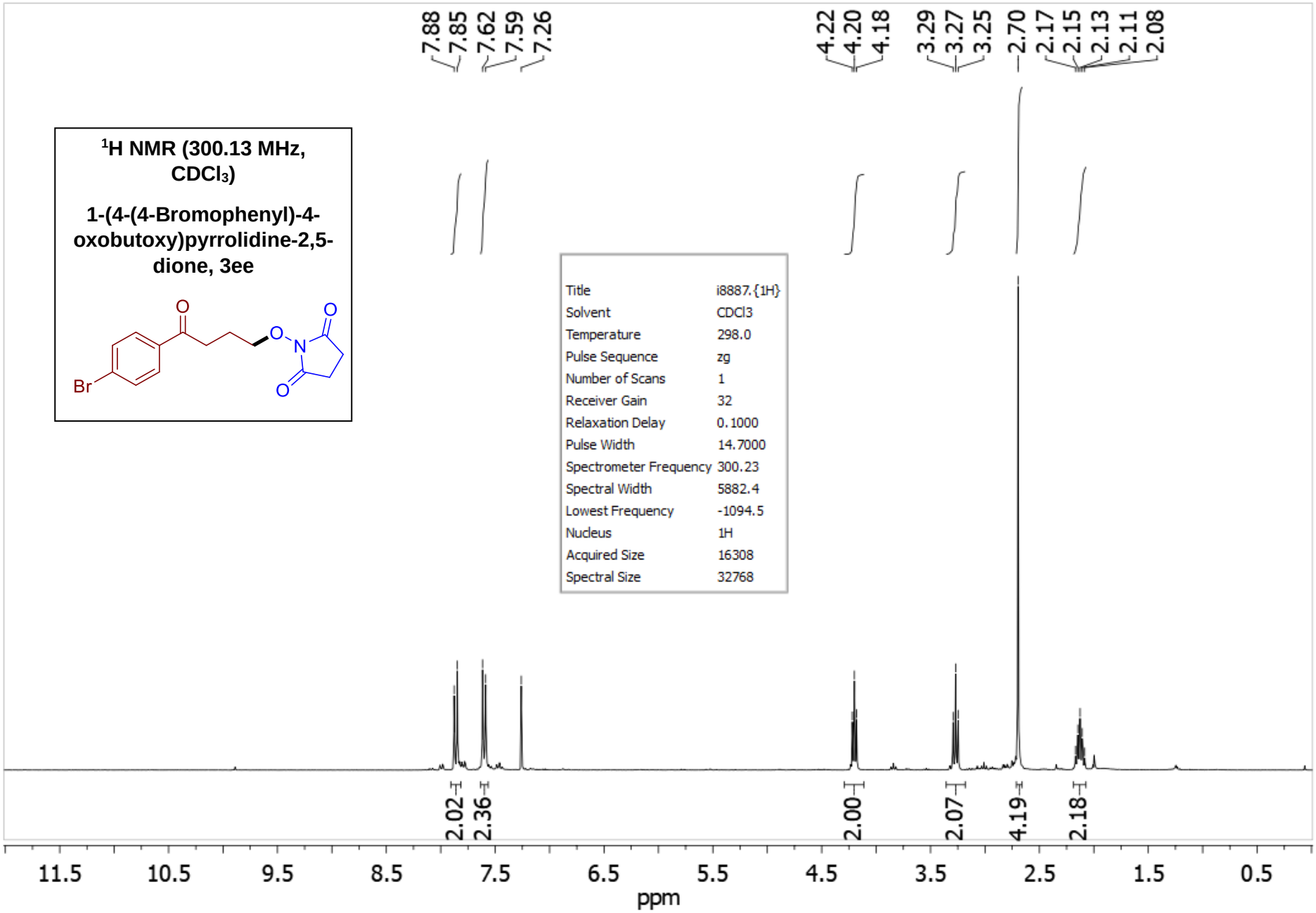


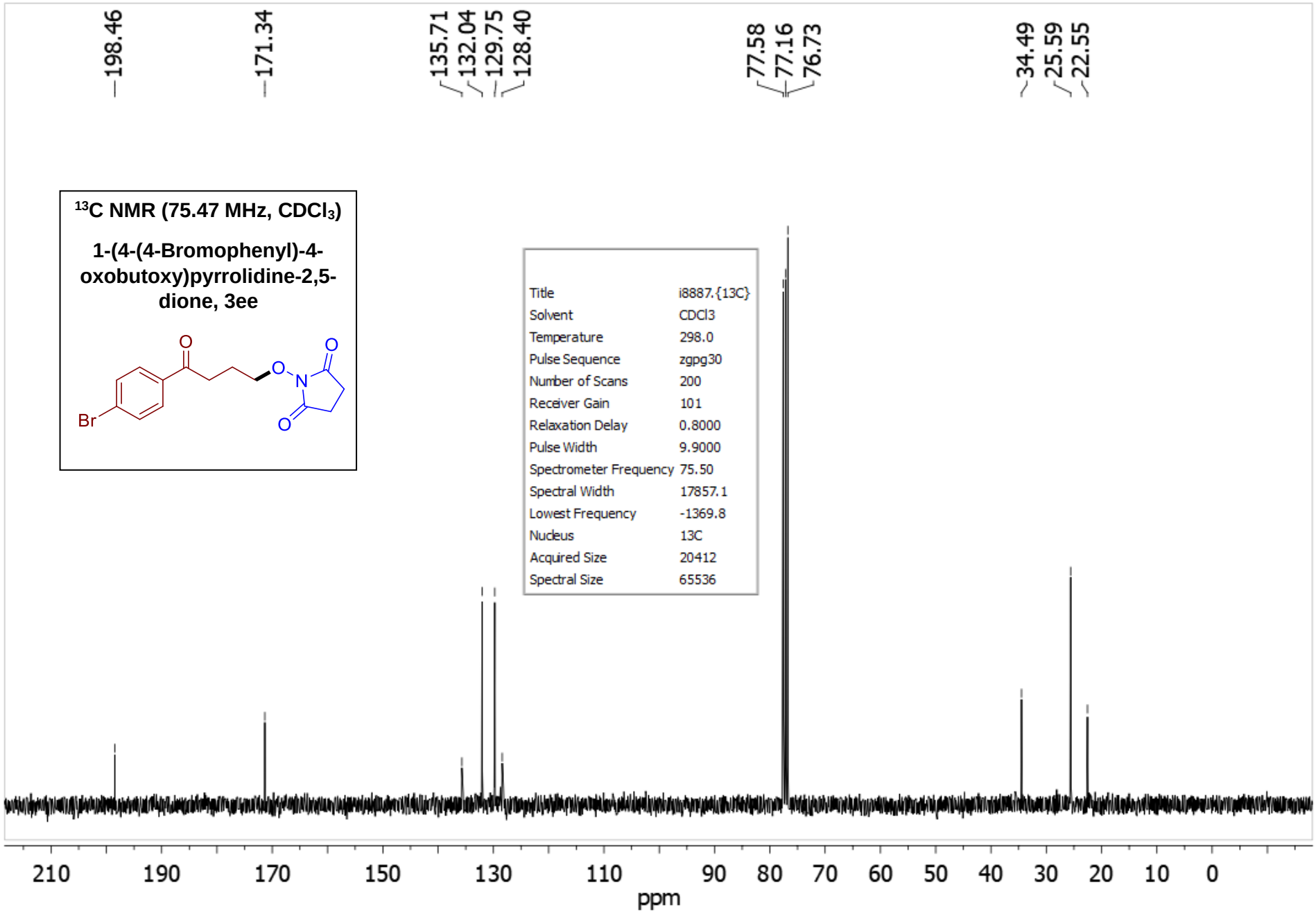
1	Solvent	CDCl3
2	Temperature	300.0
3	Pulse Sequence	zg
4	Number of Scans	1
5	Receiver Gain	32.1
6	Relaxation Delay	0.1000
7	Pulse Width	14.1000
8	Acquisition Time	2.7150
9	Spectrometer Frequency	300.13
10	Spectral Width	6009.6
11	Lowest Frequency	-911.1
12	Nucleus	1H
13	Acquired Size	16316
14	Spectral Size	65536

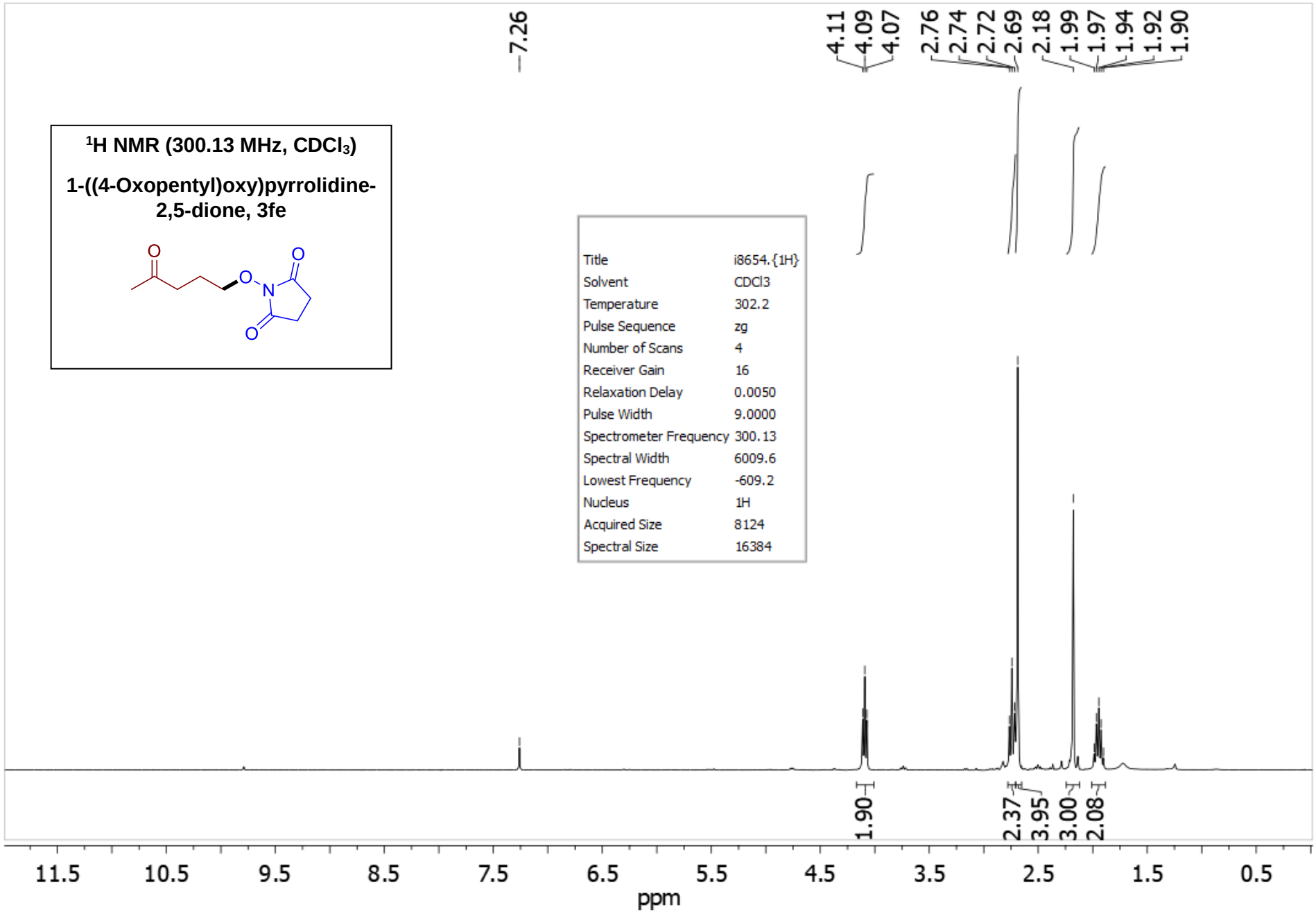

197.95
171.36
163.59
130.43
130.09
113.83
77.58
77.16
76.94
76.74
55.56
34.13
25.58
22.79
^{13}C NMR (75.47 MHz, CDCl$_3$)
1-(4-(4-Methoxyphenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, 3ce
MeO
O
O
N
O
O
Title i8859.{13C}
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Number of Scans 150
Receiver Gain 214
Relaxation Delay 0.8000
Pulse Width 9.3000
Spectrometer Frequency 75.48
Spectral Width 18028.8
Lowest Frequency -1459.8
Nucleus 13C
Acquired Size 16316
Spectral Size 32768
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
ppm

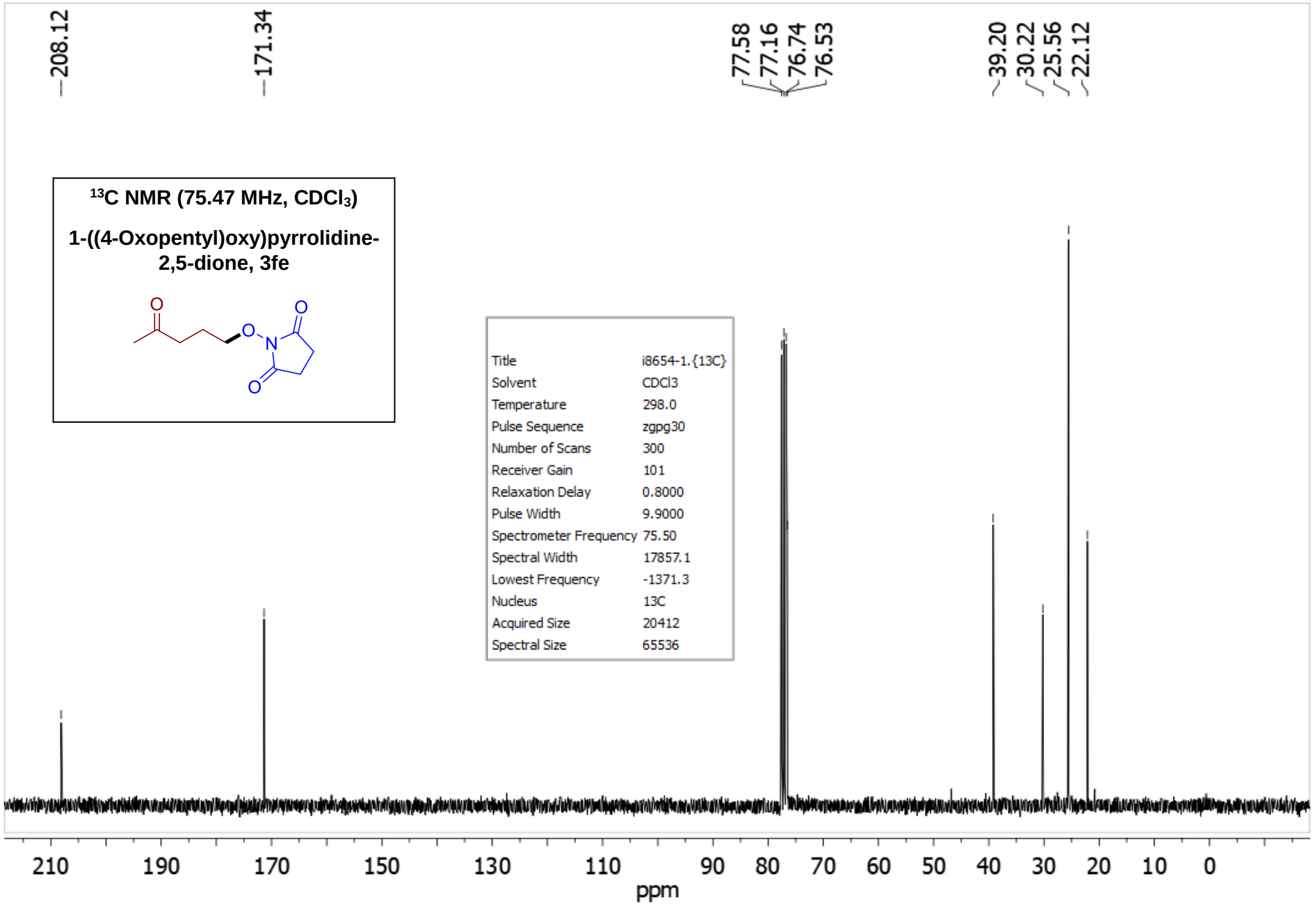

7.67
7.64
7.44
7.41
7.39
7.26
6.98
6.95
6.94
6.93
6.91
4.16
4.14
4.12
3.87
3.22
3.19
3.17
2.65
2.11
2.08
2.06
2.04
2.02
1H NMR (300.13 MHz, CDCl3)
1-(4-(2-Methoxyphenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, 3de
OMe
O
O
O
N
O
Title i8861.{1H}
Solvent CDCl3
Temperature 300.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.1000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -910.8
Nucleus 1H
Acquired Size 16316
Spectral Size 32768
1.07
1.10
2.21
2.04
3.17
2.00
4.04
2.09
11.5
10.5
9.5
8.5
7.5
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm

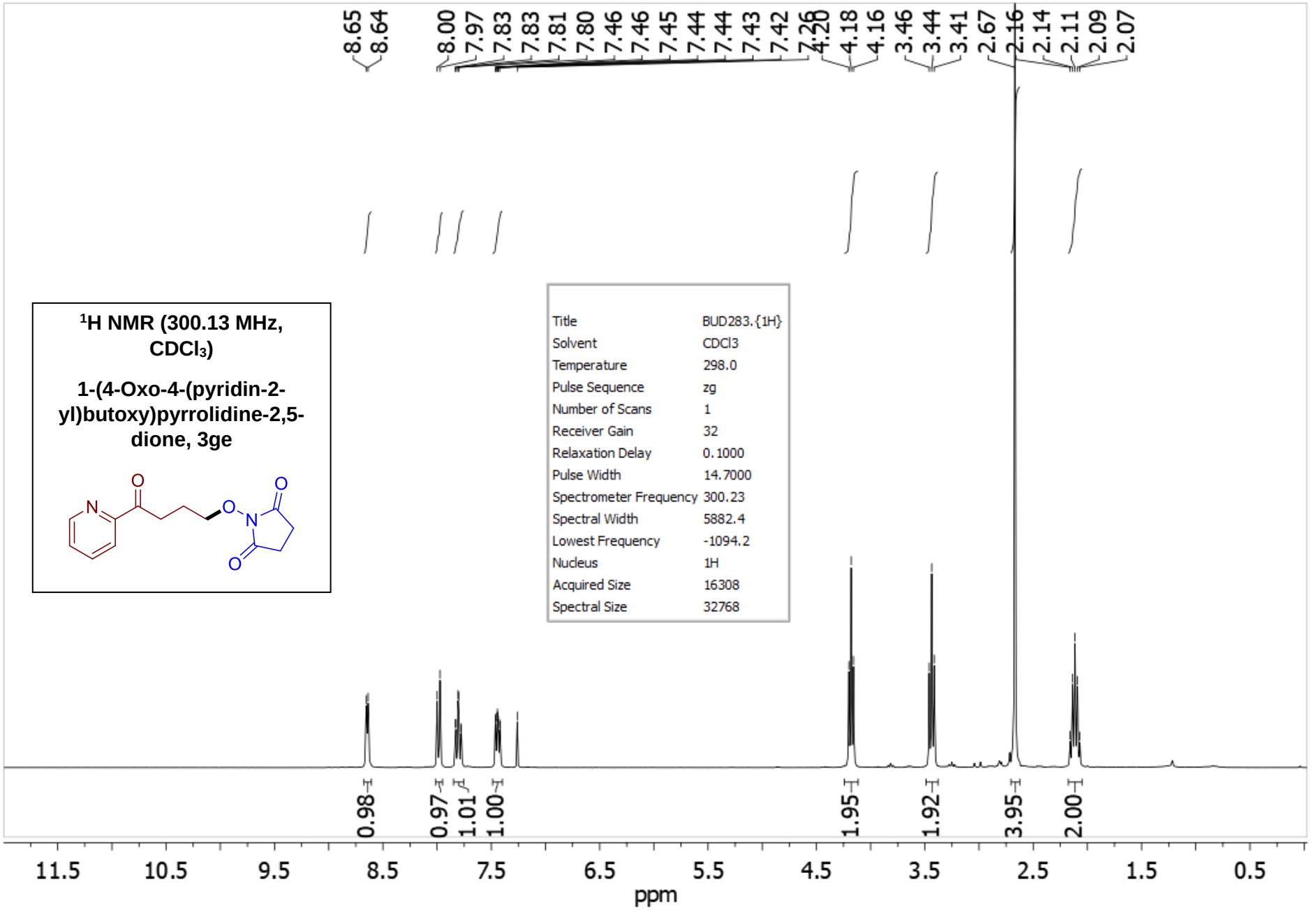

201.37
171.34
158.67
133.48
130.17
128.11
120.59
111.66
77.58
77.16
76.89
76.73
55.55
39.65
25.49
22.76
^{13}C NMR (75.47 MHz, $CDCl_3$)
1-(4-(2-Methoxyphenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, 3de
OMe O
O
O
N
O
1 Solvent CDCl3
2 Temperature 300.0
3 Pulse Sequence zgpg30
4 Number of Scans 50
5 Receiver Gain 214.2
6 Relaxation Delay 0.8000
7 Pulse Width 9.3000
8 Acquisition Time 0.9050
9 Spectrometer Frequency 75.48
10 Spectral Width 18028.8
11 Lowest Frequency -1466.7
12 Nucleus 13C
13 Acquired Size 16316
14 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


^{1}H NMR (300.13 MHz, $CDCl_3$)
1-(4-(4-Bromophenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, 3ee
Br
O
O
N
O
O
Title i8887.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
7.88
7.85
7.62
7.59
7.26
4.22
4.20
4.18
3.29
3.27
3.25
2.70
2.17
2.15
2.13
2.11
2.08
2.02
2.36
2.00
2.07
4.19
2.18
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
ppm


198.46
171.34
135.71
132.04
129.75
128.40
77.58
77.16
76.73
34.49
25.59
22.55
13C NMR (75.47 MHz, CDCl3)
1-(4-(4-Bromophenyl)-4-oxobutoxy)pyrrolidine-2,5-dione, 3ee
Br
O
O
N
O
O
Title i8887.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 200
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1369.8
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
ppm


^{1}H NMR (300.13 MHz, $CDCl_3$)
1-((4-Oxopentyl)oxy)pyrrolidine-2,5-dione, 3fe
Title i8654.{1H}
Solvent CDCl3
Temperature 302.2
Pulse Sequence zg
Number of Scans 4
Receiver Gain 16
Relaxation Delay 0.0050
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.2
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
7.26
4.11
4.09
4.07
2.76
2.74
2.72
2.69
2.18
1.99
1.97
1.94
1.92
1.90
1.90
2.37
3.95
3.00
2.08
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
ppm

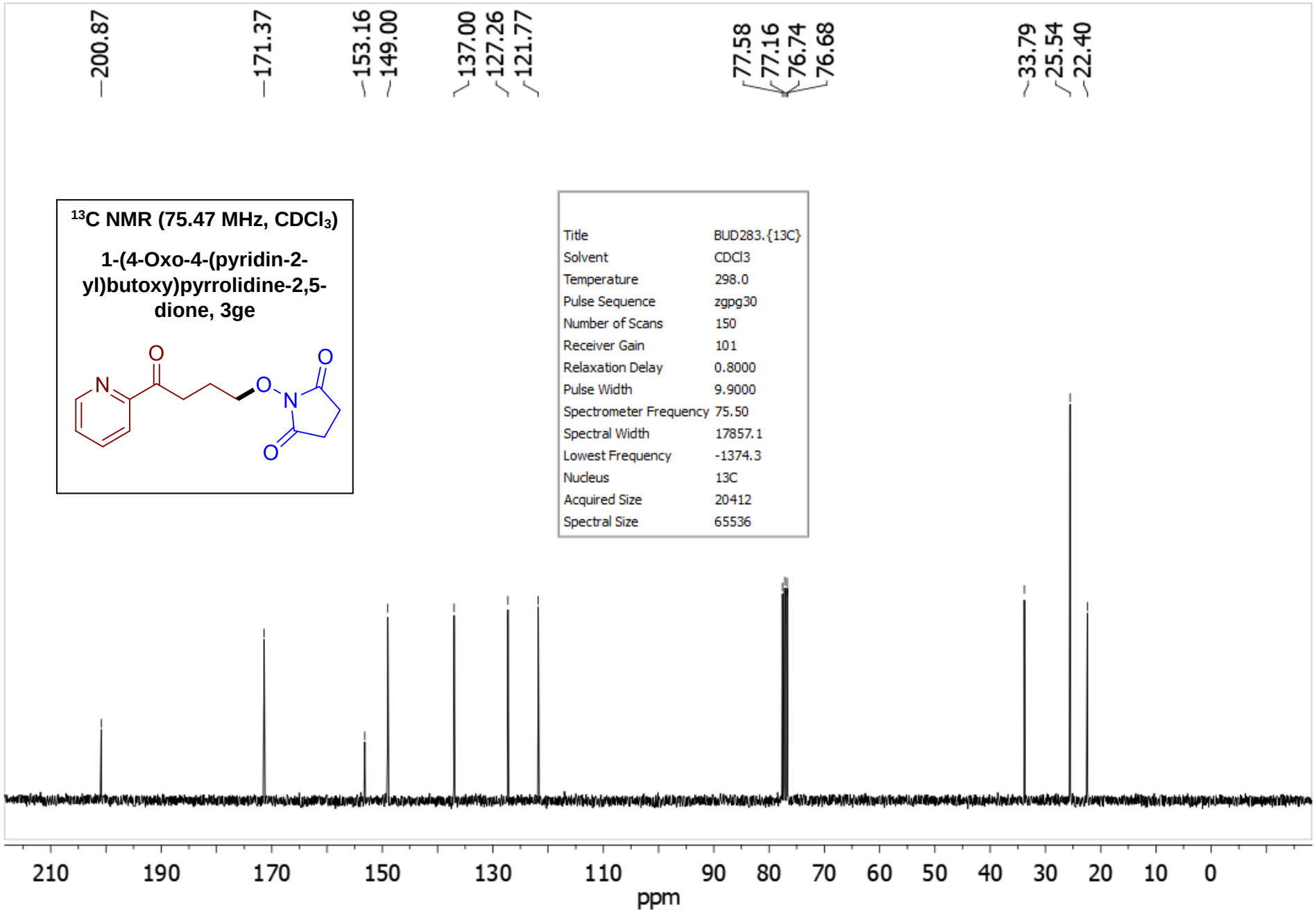

208.12
171.34
77.58
77.16
76.74
76.53
39.20
30.22
25.56
22.12
^{13}C NMR (75.47 MHz, $CDCl_3$)
1-((4-Oxopentyl)oxy)pyrrolidine-2,5-dione, 3fe
Title i8654-1.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 300
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1371.3
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
ppm

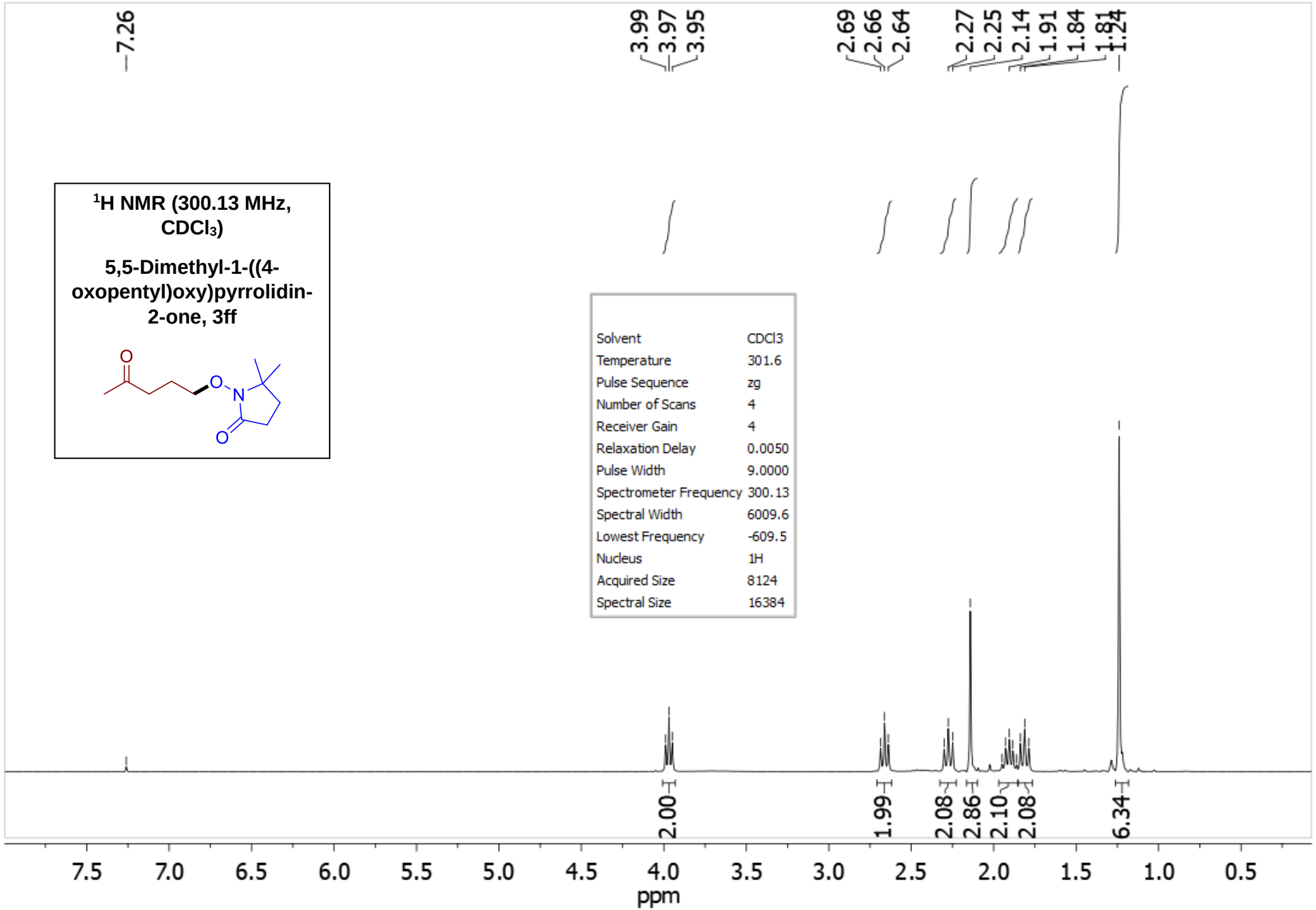


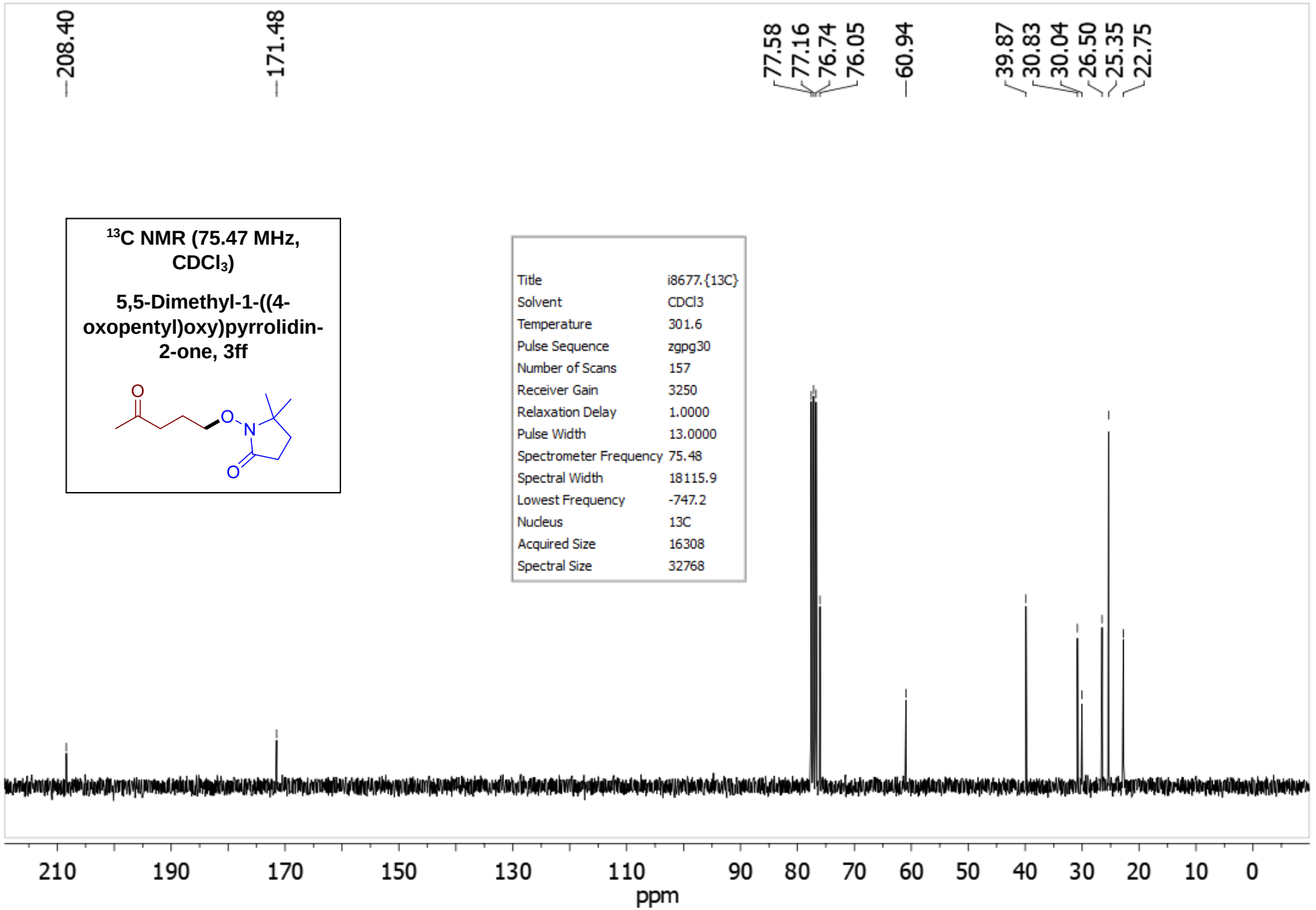
^{1}H NMR (300.13 MHz, $CDCl_3$)

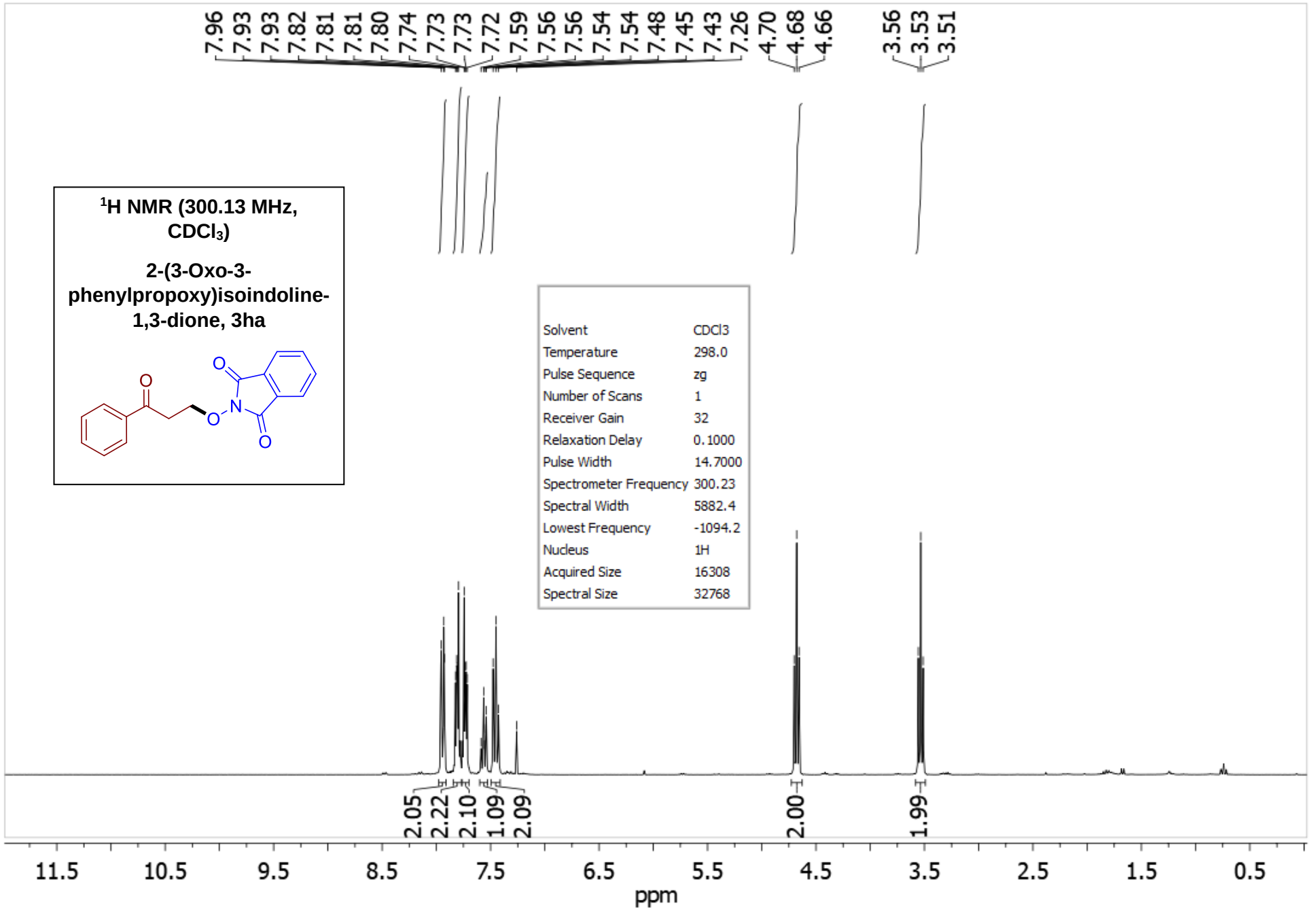
1-(4-Oxo-4-(pyridin-2-yl)butoxy)pyrrolidine-2,5-dione, 3ge

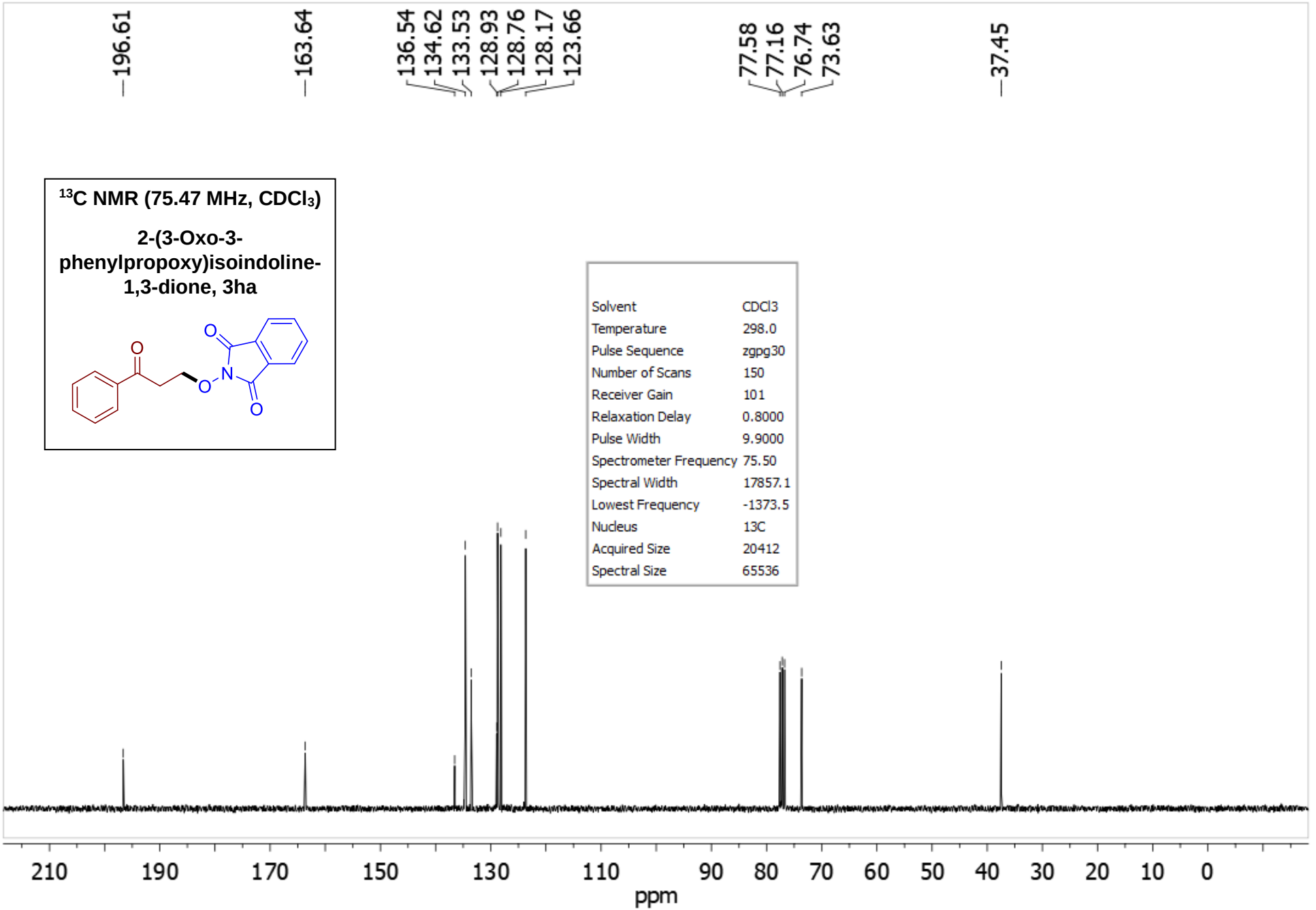
Title	BUD283.{1H}
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg
Number of Scans	1
Receiver Gain	32
Relaxation Delay	0.1000
Pulse Width	14.7000
Spectrometer Frequency	300.23
Spectral Width	5882.4
Lowest Frequency	-1094.2
Nucleus	1H
Acquired Size	16308
Spectral Size	32768

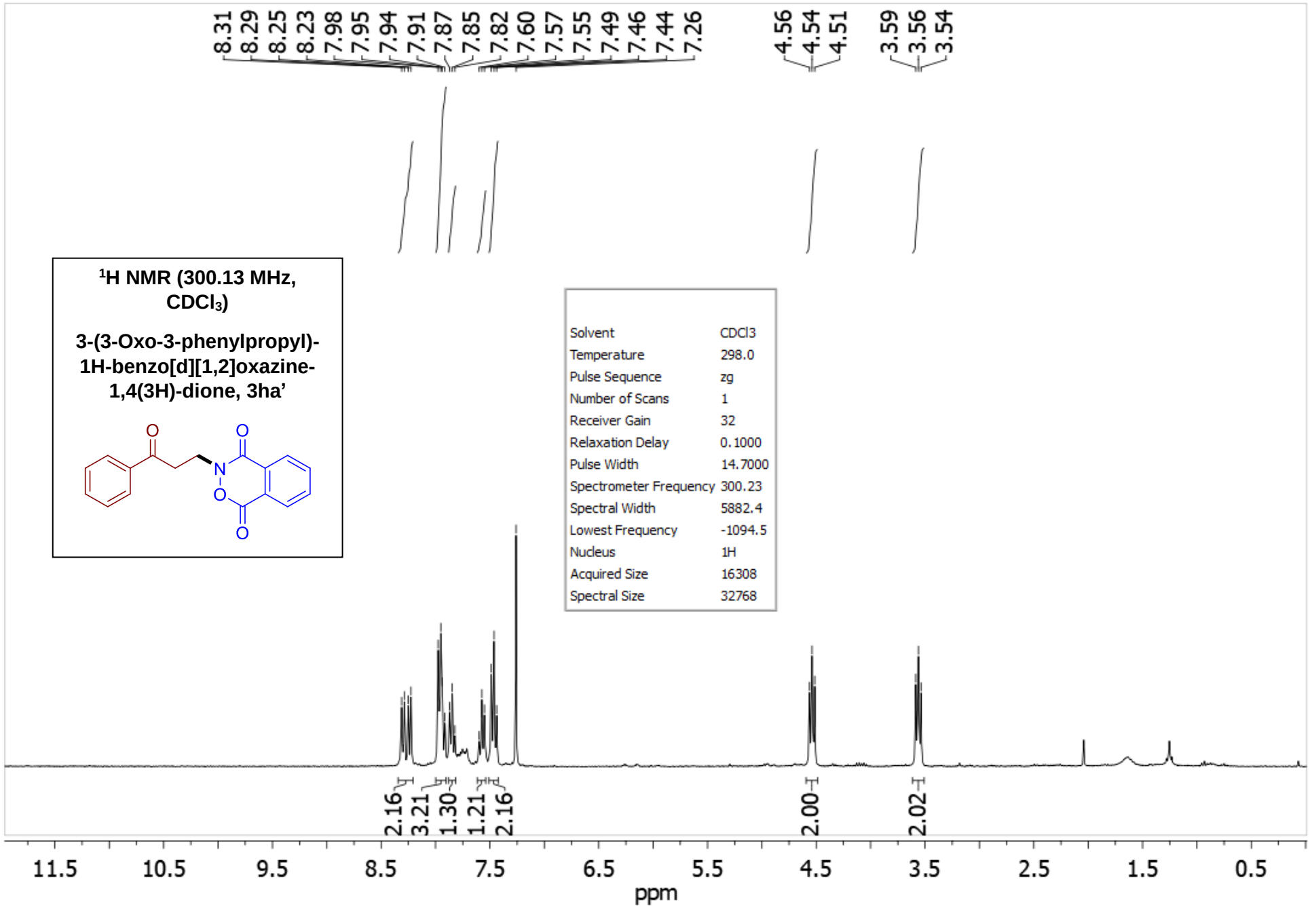

200.87
171.37
153.16
149.00
137.00
127.26
121.77
77.58
77.16
76.74
76.68
33.79
25.54
22.40
13C NMR (75.47 MHz, CDCl3)
1-(4-Oxo-4-(pyridin-2-yl)butoxy)pyrrolidine-2,5-dione, 3ge
Title BUD283.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 150
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1374.3
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
ppm

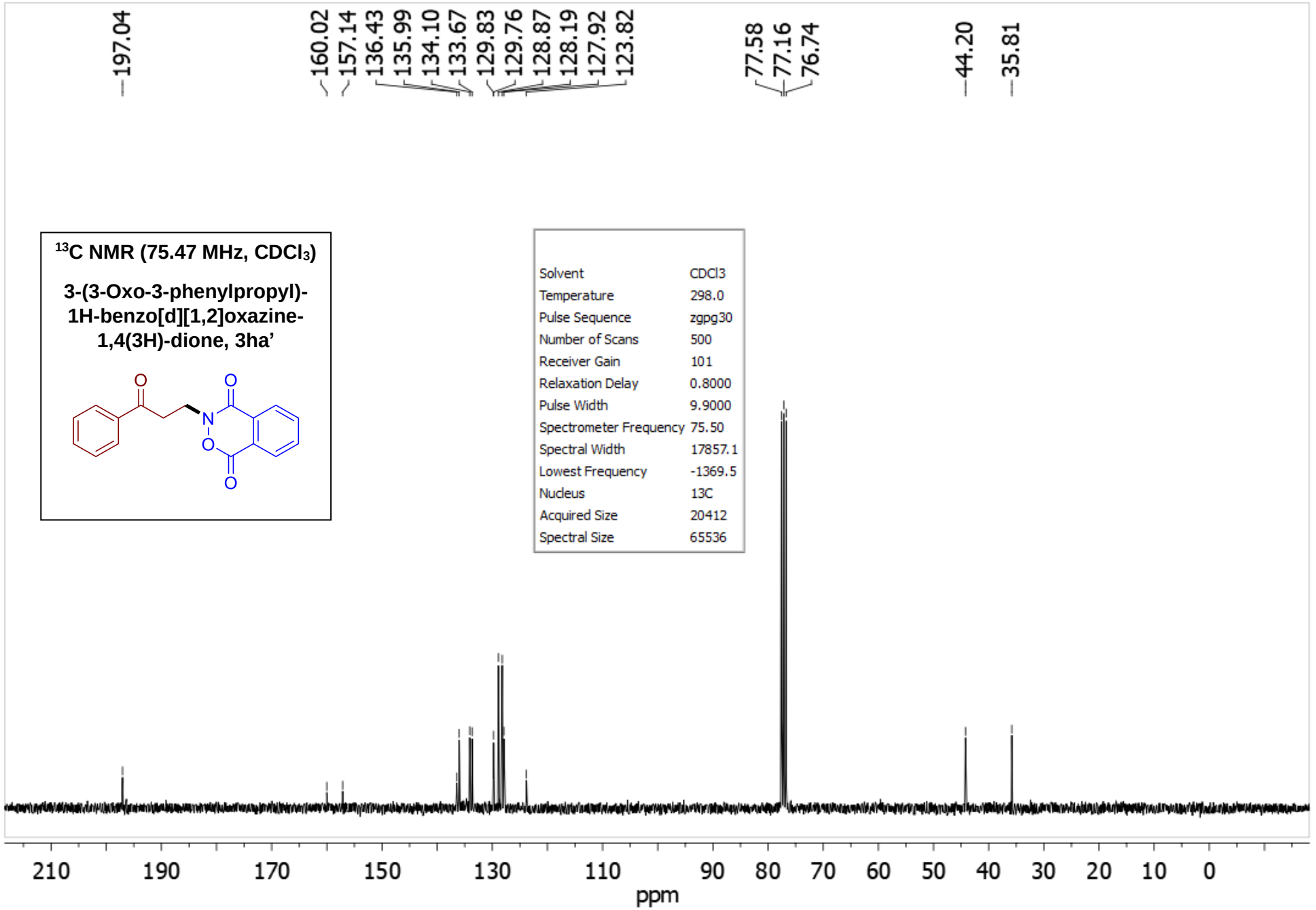

7.26
3.99
3.97
3.95
2.69
2.66
2.64
2.27
2.25
2.14
1.91
1.84
1.81
1.24
^{1}H NMR (300.13 MHz, $CDCl_3$)
5,5-Dimethyl-1-((4-oxopentyl)oxy)pyrrolidin-2-one, 3ff
Solvent CDCl3
Temperature 301.6
Pulse Sequence zg
Number of Scans 4
Receiver Gain 4
Relaxation Delay 0.0050
Pulse Width 9.0000
Spectrometer Frequency 300.13
Spectral Width 6009.6
Lowest Frequency -609.5
Nucleus 1H
Acquired Size 8124
Spectral Size 16384
2.00
1.99
2.08
2.86
2.10
2.08
6.34
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
ppm

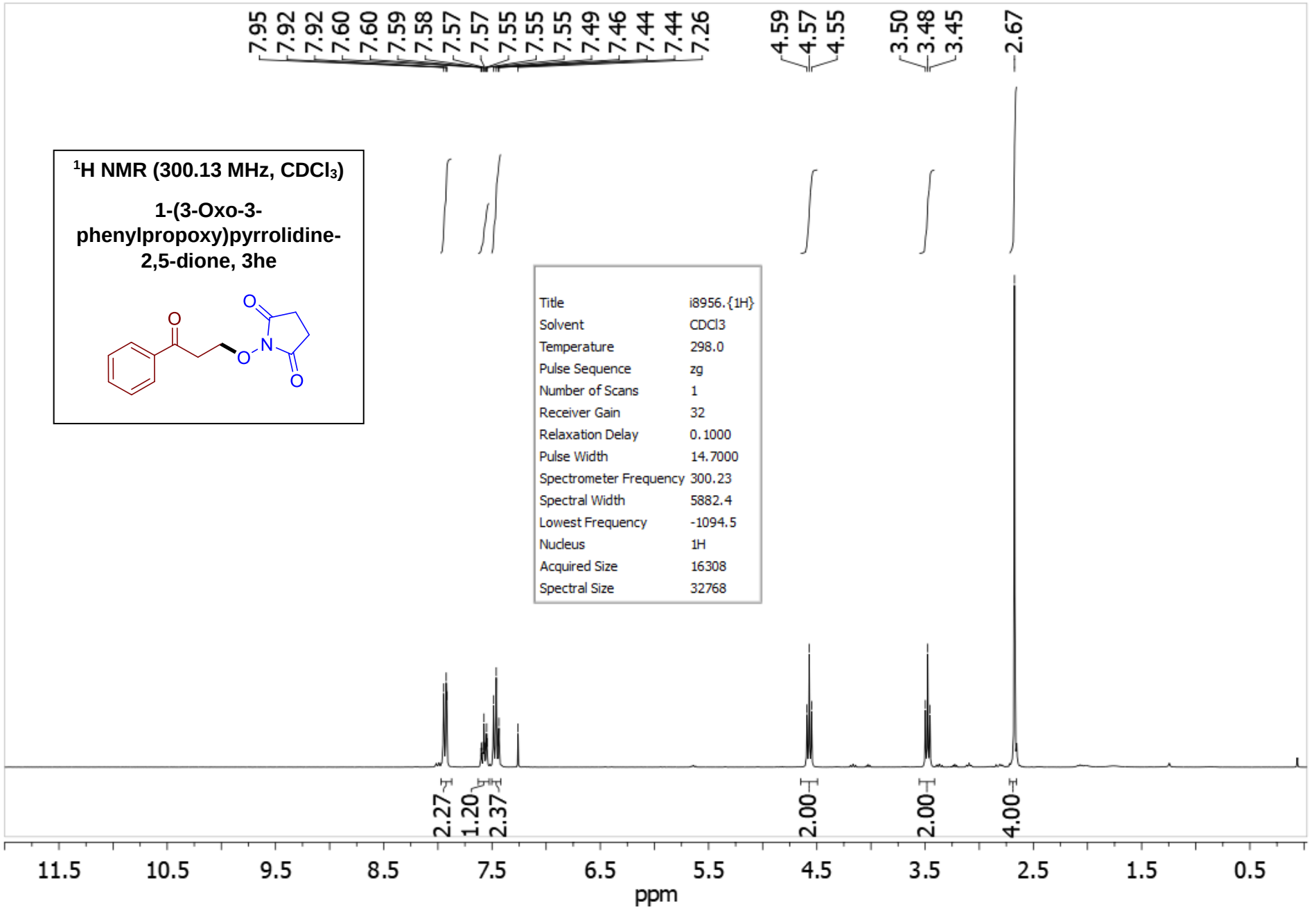

208.40
171.48
77.58
77.16
76.74
76.05
60.94
39.87
30.83
30.04
26.50
25.35
22.75
^{13}C NMR (75.47 MHz, $CDCl_3$)
5,5-Dimethyl-1-((4-oxopentyl)oxy)pyrrolidin-2-one, 3ff
Title i8677.{13C}
Solvent CDCl3
Temperature 301.6
Pulse Sequence zgpg30
Number of Scans 157
Receiver Gain 3250
Relaxation Delay 1.0000
Pulse Width 13.0000
Spectrometer Frequency 75.48
Spectral Width 18115.9
Lowest Frequency -747.2
Nucleus 13C
Acquired Size 16308
Spectral Size 32768
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
ppm

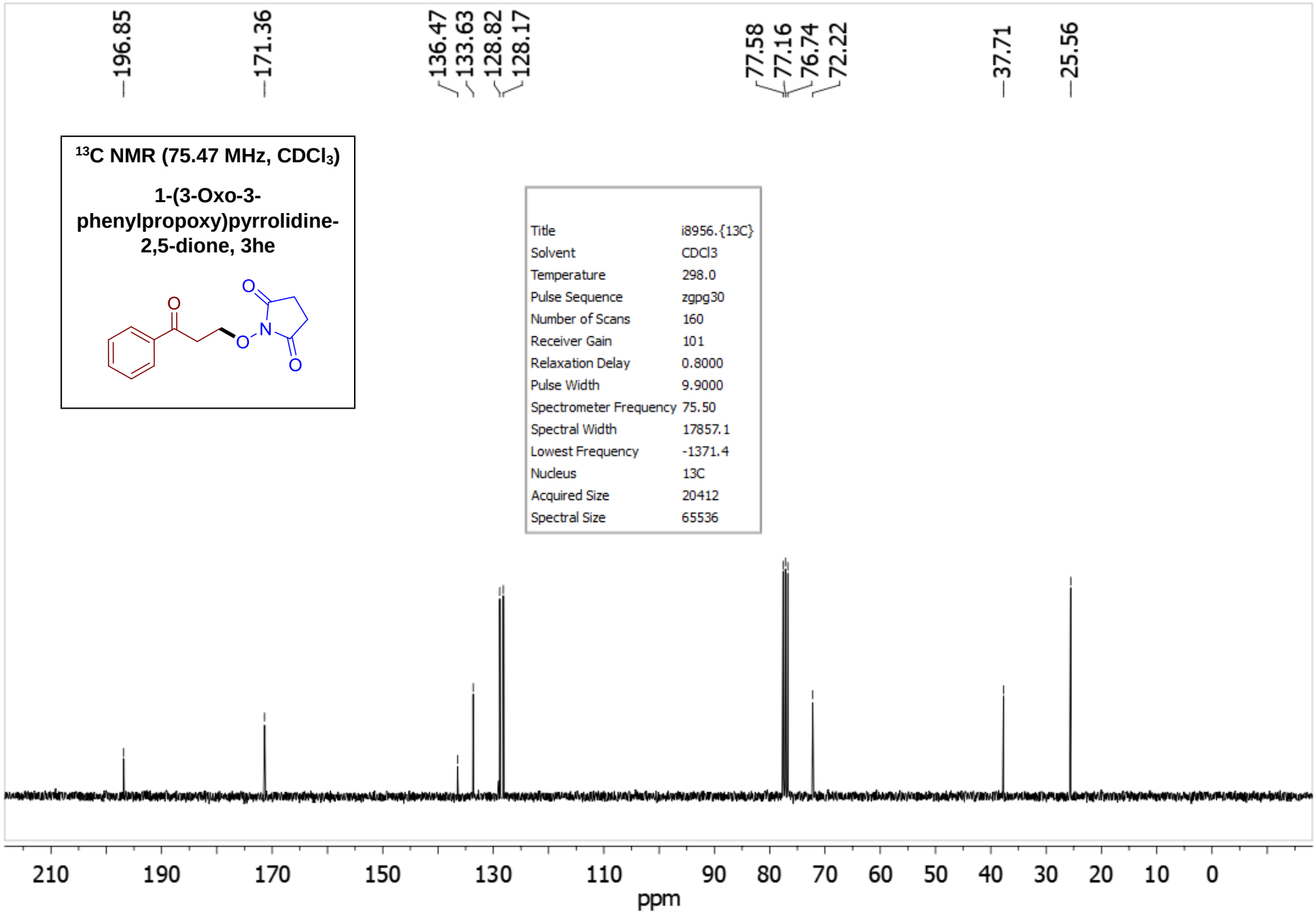

7.96
7.93
7.93
7.82
7.81
7.81
7.80
7.74
7.73
7.73
7.72
7.59
7.56
7.56
7.54
7.54
7.48
7.45
7.43
7.26
4.70
4.68
4.66
3.56
3.53
3.51
^{1}H NMR (300.13 MHz, CDCl$_3$)
2-(3-Oxo-3-phenylpropoxy)isoindoline-1,3-dione, 3ha
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.2
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
2.05
2.22
2.10
1.09
2.09
2.00
1.99
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
ppm

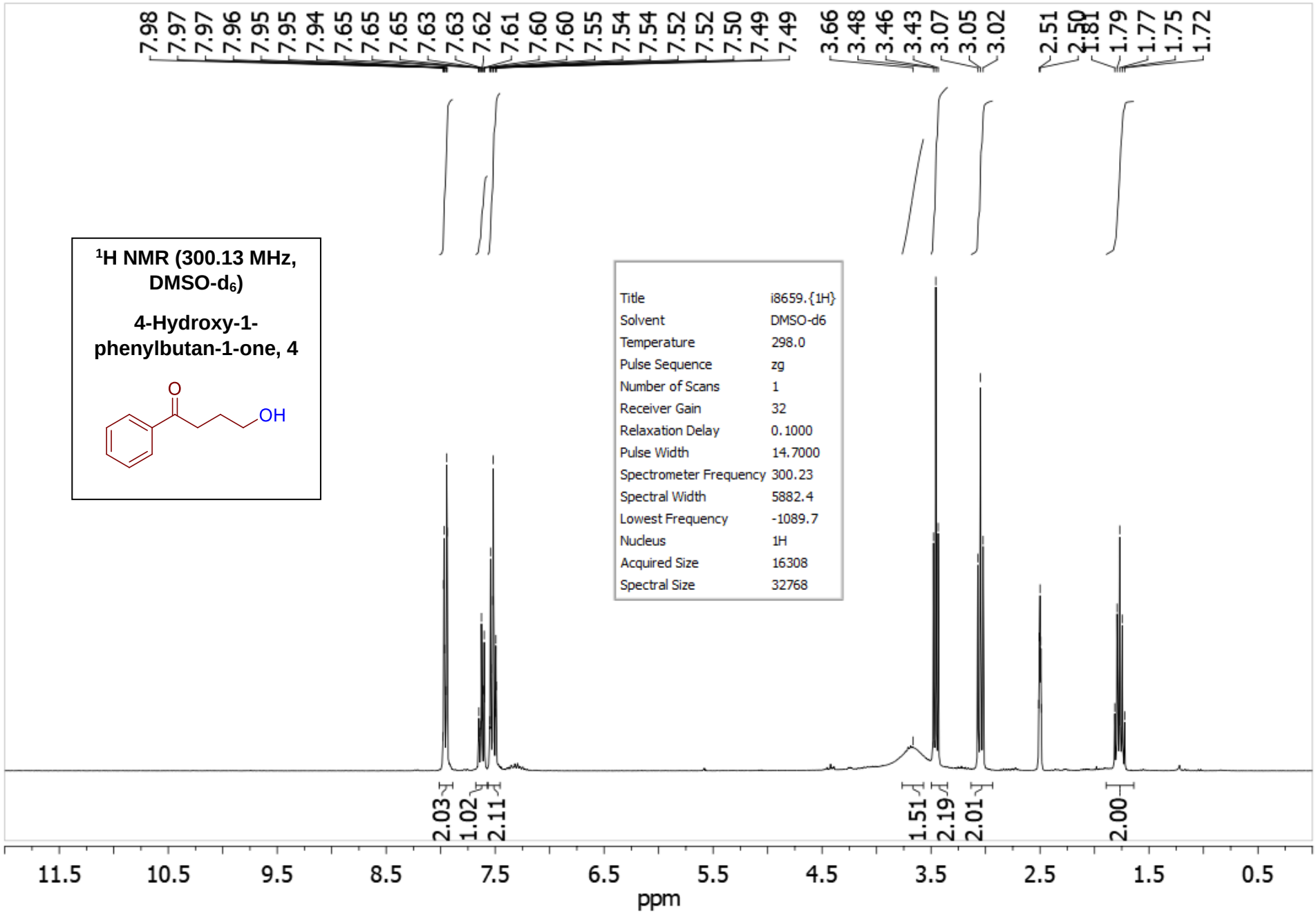

196.61
163.64
136.54
134.62
133.53
128.93
128.76
128.17
123.66
77.58
77.16
76.74
73.63
37.45
13C NMR (75.47 MHz, CDCl3)
2-(3-Oxo-3-phenylpropoxy)isoindoline-1,3-dione, 3ha
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 150
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1373.5
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
ppm

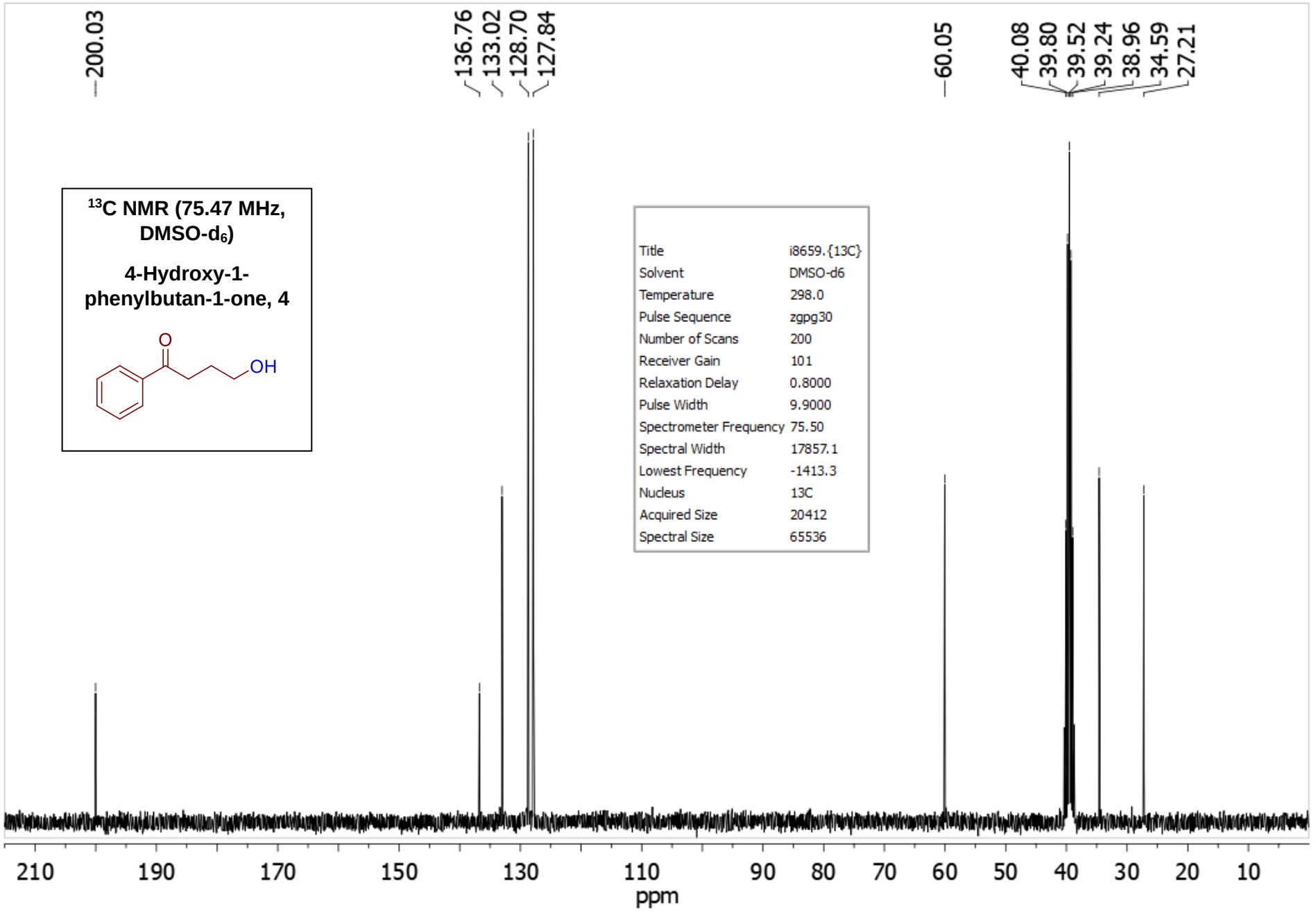

8.31
8.29
8.25
8.23
7.98
7.95
7.94
7.91
7.87
7.85
7.82
7.60
7.57
7.55
7.49
7.46
7.44
7.26
4.56
4.54
4.51
3.59
3.56
3.54
^{1}H NMR (300.13 MHz, $CDCl_3$)
3-(3-Oxo-3-phenylpropyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ha'
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
2.16
3.21
1.30
1.21
2.16
2.00
2.02
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
ppm

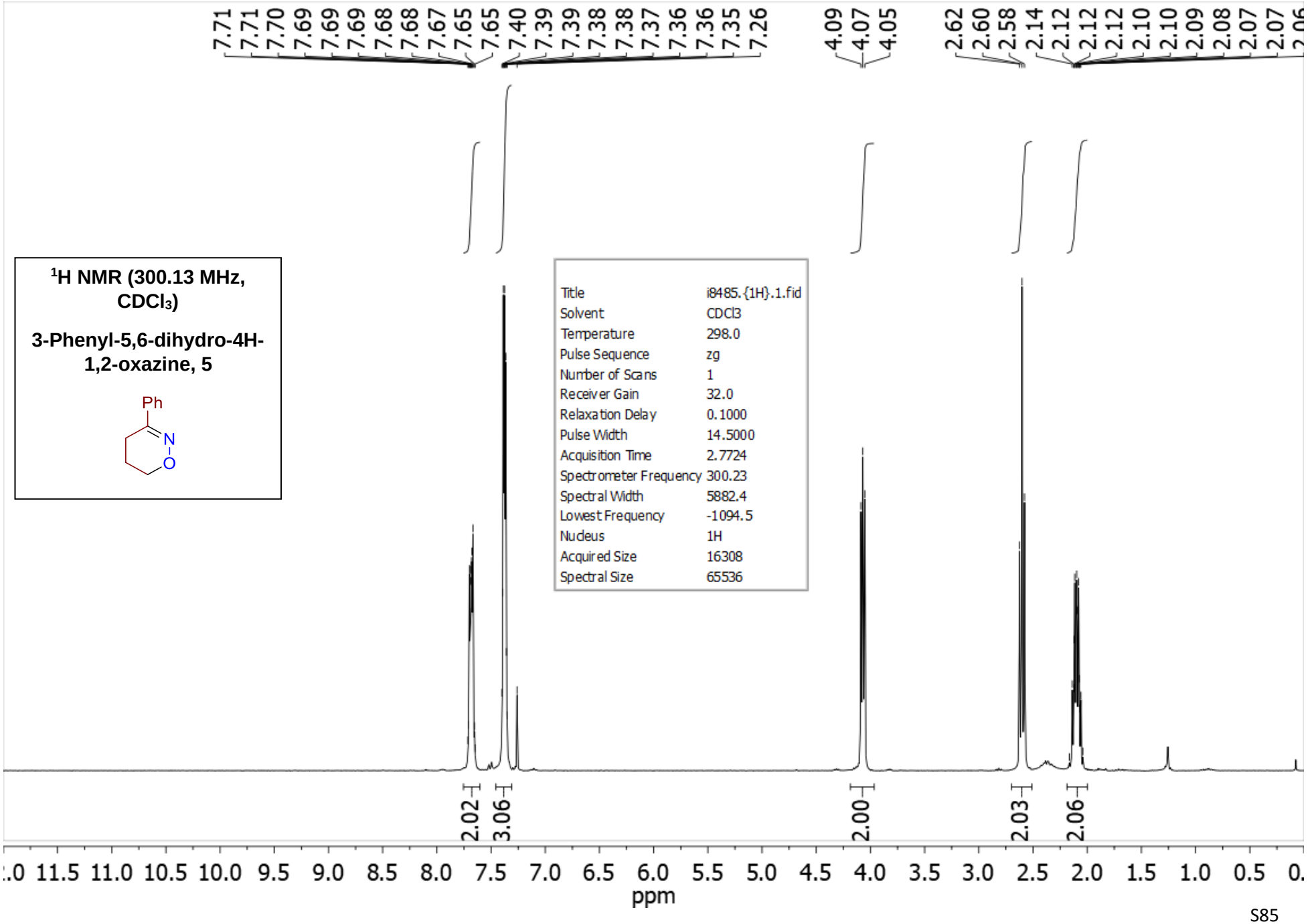

197.04
160.02
157.14
136.43
135.99
134.10
133.67
129.83
129.76
128.87
128.19
127.92
123.82
77.58
77.16
76.74
44.20
35.81
13C NMR (75.47 MHz, CDCl3)
3-(3-Oxo-3-phenylpropyl)-1H-benzo[d][1,2]oxazine-1,4(3H)-dione, 3ha'
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 500
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1369.5
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
ppm

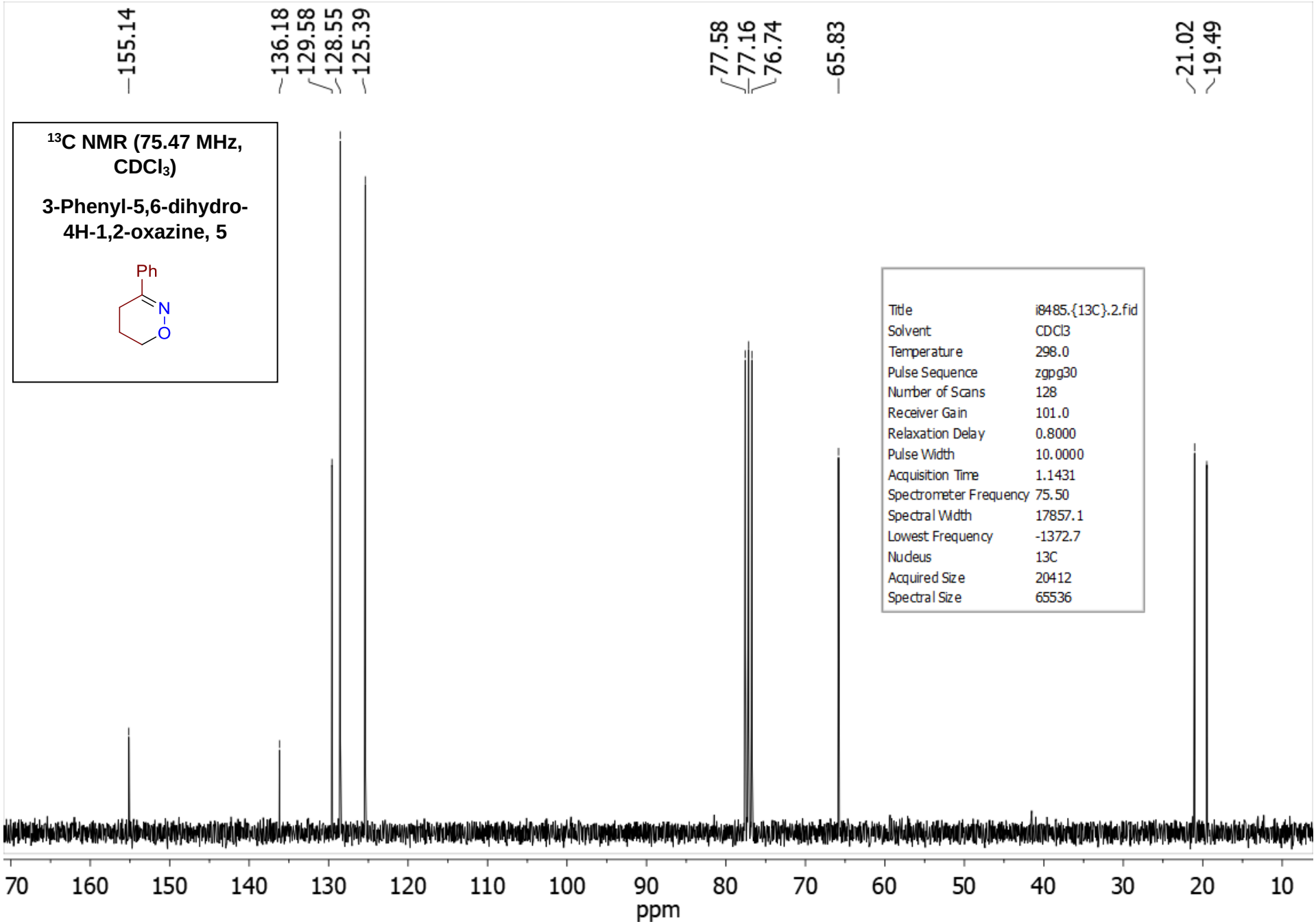

7.95
7.92
7.92
7.60
7.60
7.59
7.58
7.57
7.57
7.55
7.55
7.55
7.49
7.46
7.44
7.44
7.26
4.59
4.57
4.55
3.50
3.48
3.45
2.67
1H NMR (300.13 MHz, CDCl3)
1-(3-Oxo-3-phenylpropoxy)pyrrolidine-2,5-dione, 3he
Title i8956.{1H}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
2.27
1.20
2.37
2.00
2.00
4.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
ppm

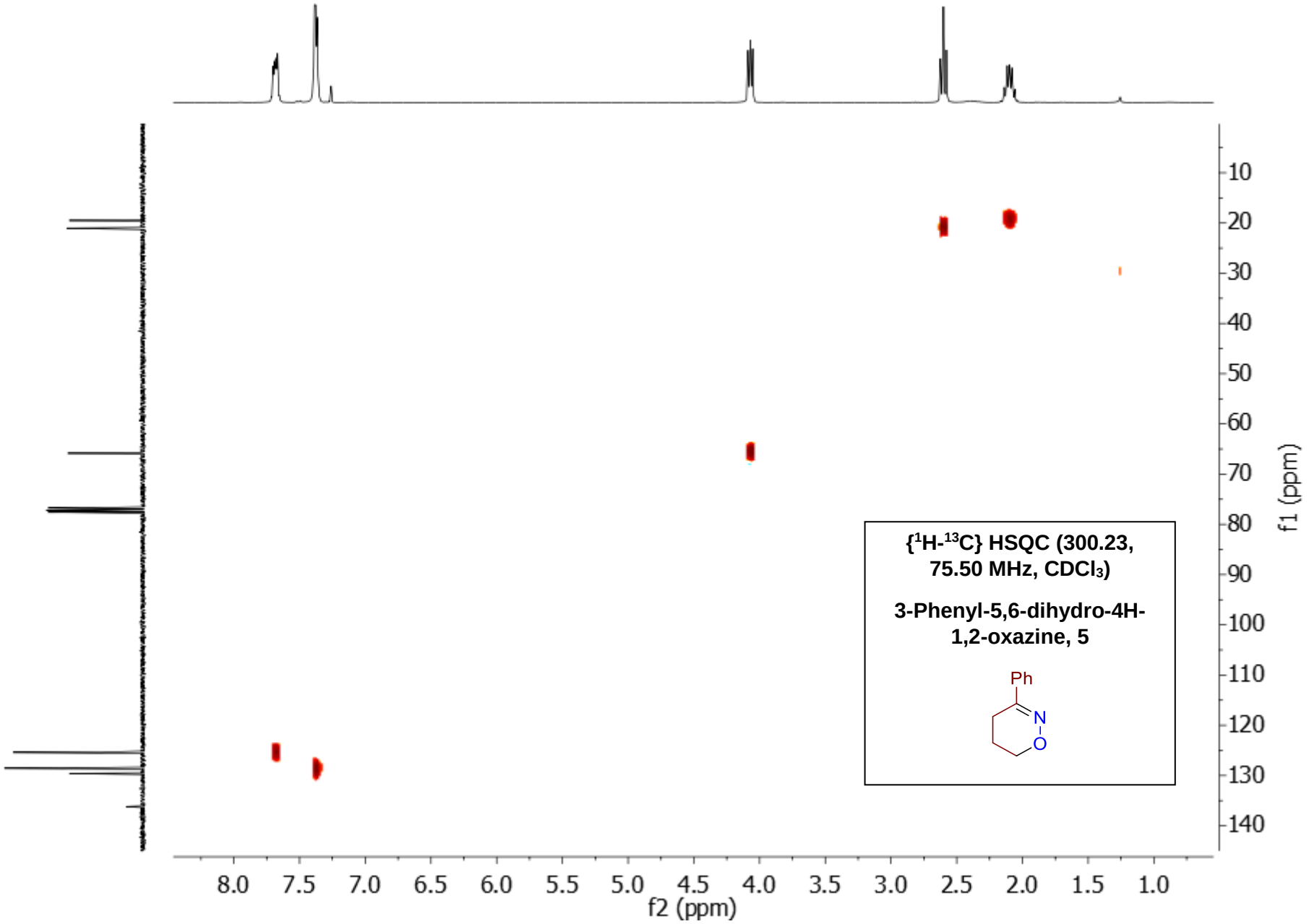

196.85
171.36
136.47
133.63
128.82
128.17
77.58
77.16
76.74
72.22
37.71
25.56
13C NMR (75.47 MHz, CDCl3)
1-(3-Oxo-3-phenylpropoxy)pyrrolidine-2,5-dione, 3he
Title i8956.{13C}
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 160
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1371.4
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
ppm

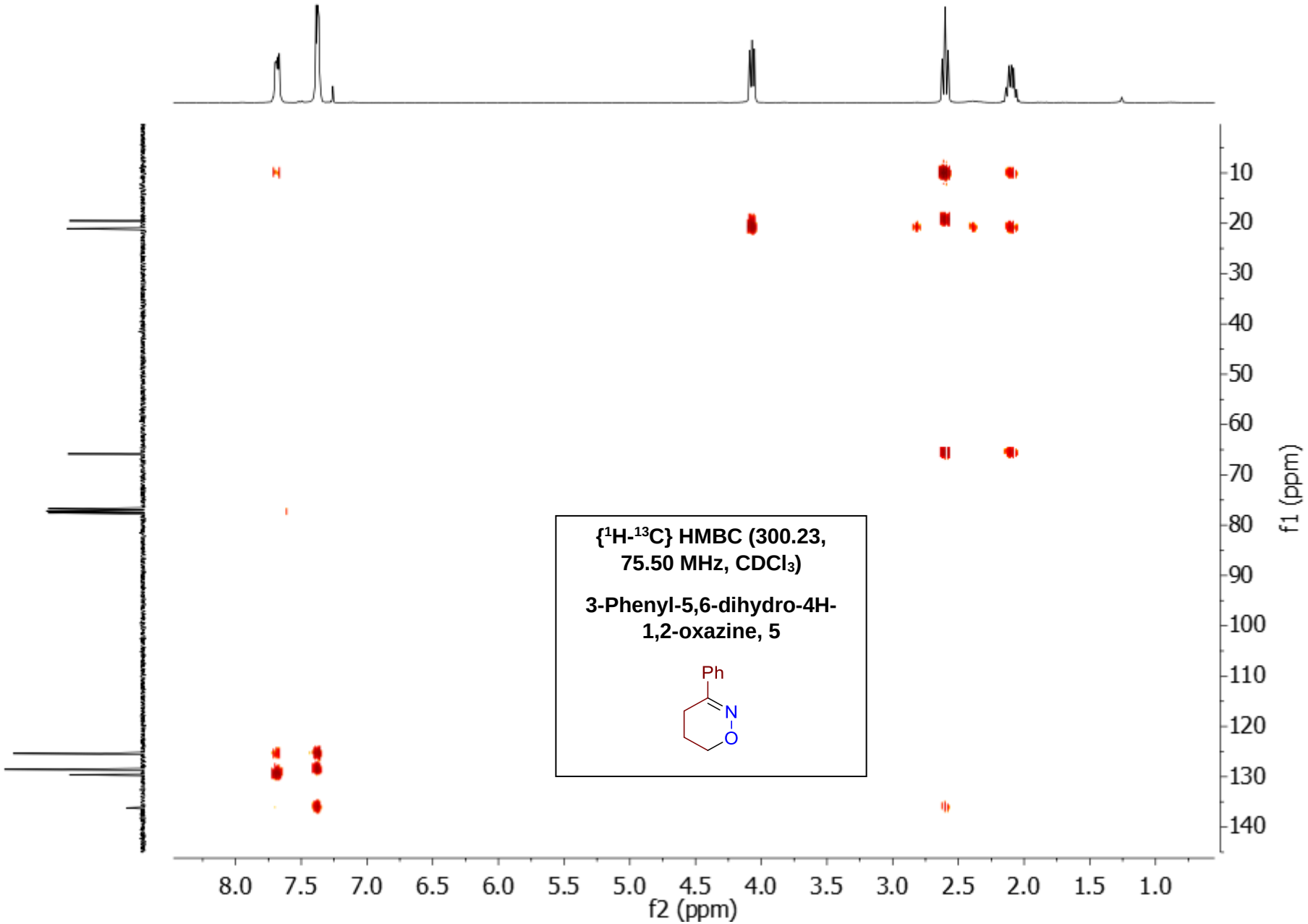

7.98 7.97 7.97 7.96 7.95 7.95 7.94 7.65 7.65 7.65 7.63 7.63 7.62 7.61 7.60 7.60 7.55 7.54 7.54 7.52 7.52 7.50 7.49 7.49
3.66 3.48 3.46 3.43 3.07 3.05 3.02
2.51 2.50 1.81 1.79 1.77 1.75 1.72
^{1}H NMR (300.13 MHz, DMSO-d$_6$)
4-Hydroxy-1-phenylbutan-1-one, 4
O
OH
Title i8659.{1H}
Solvent DMSO-d6
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32
Relaxation Delay 0.1000
Pulse Width 14.7000
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1089.7
Nucleus 1H
Acquired Size 16308
Spectral Size 32768
2.03 1.02 2.11 1.51 2.19 2.01 2.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
ppm


200.03
136.76
133.02
128.70
127.84
60.05
40.08
39.80
39.52
39.24
38.96
34.59
27.21
^{13}C NMR (75.47 MHz, DMSO-d$_6$)
4-Hydroxy-1-phenylbutan-1-one, 4
O
OH
Title i8659.{13C}
Solvent DMSO-d6
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 200
Receiver Gain 101
Relaxation Delay 0.8000
Pulse Width 9.9000
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1413.3
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
ppm


7.71 7.71 7.70 7.69 7.69 7.69 7.68 7.68 7.67 7.65 7.65 7.40 7.39 7.39 7.38 7.38 7.37 7.36 7.36 7.35 7.26
4.09 4.07 4.05
2.62 2.60 2.58 2.14 2.12 2.12 2.12 2.10 2.10 2.09 2.08 2.07 2.07
¹H NMR (300.13 MHz, CDCl₃)
3-Phenyl-5,6-dihydro-4H-1,2-oxazine, 5
Ph
N
O
Title i8485.{1H}.1.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg
Number of Scans 1
Receiver Gain 32.0
Relaxation Delay 0.1000
Pulse Width 14.5000
Acquisition Time 2.7724
Spectrometer Frequency 300.23
Spectral Width 5882.4
Lowest Frequency -1094.5
Nucleus 1H
Acquired Size 16308
Spectral Size 65536
2.02
3.06
2.00
2.03
2.06
11.5 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
ppm

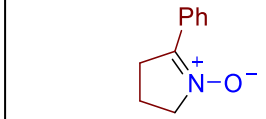

155.14
136.18
129.58
128.55
125.39
77.58
77.16
76.74
65.83
21.02
19.49
^{13}C NMR (75.47 MHz, $CDCl_3$)
3-Phenyl-5,6-dihydro-4H-1,2-oxazine, 5
Ph
N
O
Title i8485.{13C}.2.fid
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Number of Scans 128
Receiver Gain 101.0
Relaxation Delay 0.8000
Pulse Width 10.0000
Acquisition Time 1.1431
Spectrometer Frequency 75.50
Spectral Width 17857.1
Lowest Frequency -1372.7
Nucleus 13C
Acquired Size 20412
Spectral Size 65536
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


{^{1}H-^{13}C} HSQC (300.23, 75.50 MHz, $CDCl_3$)
3-Phenyl-5,6-dihydro-4H-1,2-oxazine, 5
Ph
N
O
f2 (ppm)
f1 (ppm)
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
10
20
30
40
50
60
70
80
90
100
110
120
130
140


{^{1}H-^{13}C} HMBC (300.23, 75.50 MHz, $CDCl_3$)
3-Phenyl-5,6-dihydro-4H-1,2-oxazine, 5
Ph
N
O
f2 (ppm)
f1 (ppm)

^{1}H NMR (300.13 MHz, $CDCl_3$)

5-Phenyl-3,4-dihydro-2H-pyrrole 1-oxide, 6



^{13}C NMR (75.47 MHz, $CDCl_3$)

5-Phenyl-3,4-dihydro-2H-pyrrole 1-oxide, 6