

Rhodium(III)-Catalyzed Redox-Neutral 1,1-Cyclization of *N*-Methoxy Benzamides with Maleimides via C-H/N-H/N-O Activation: Detailed Mechanistic Investigation

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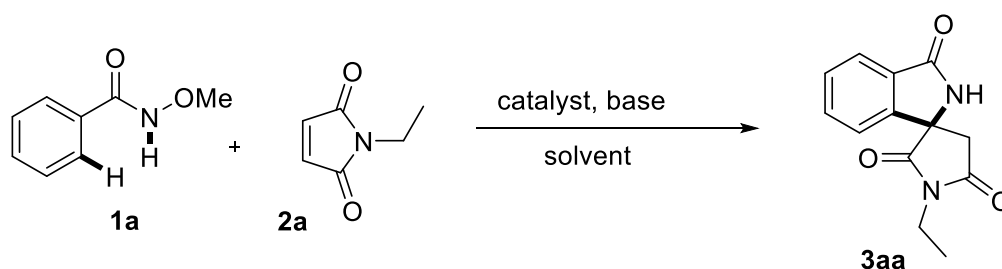
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Supporting Information (SI)

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Table S1. Optimization of Spiroisoindolinone.



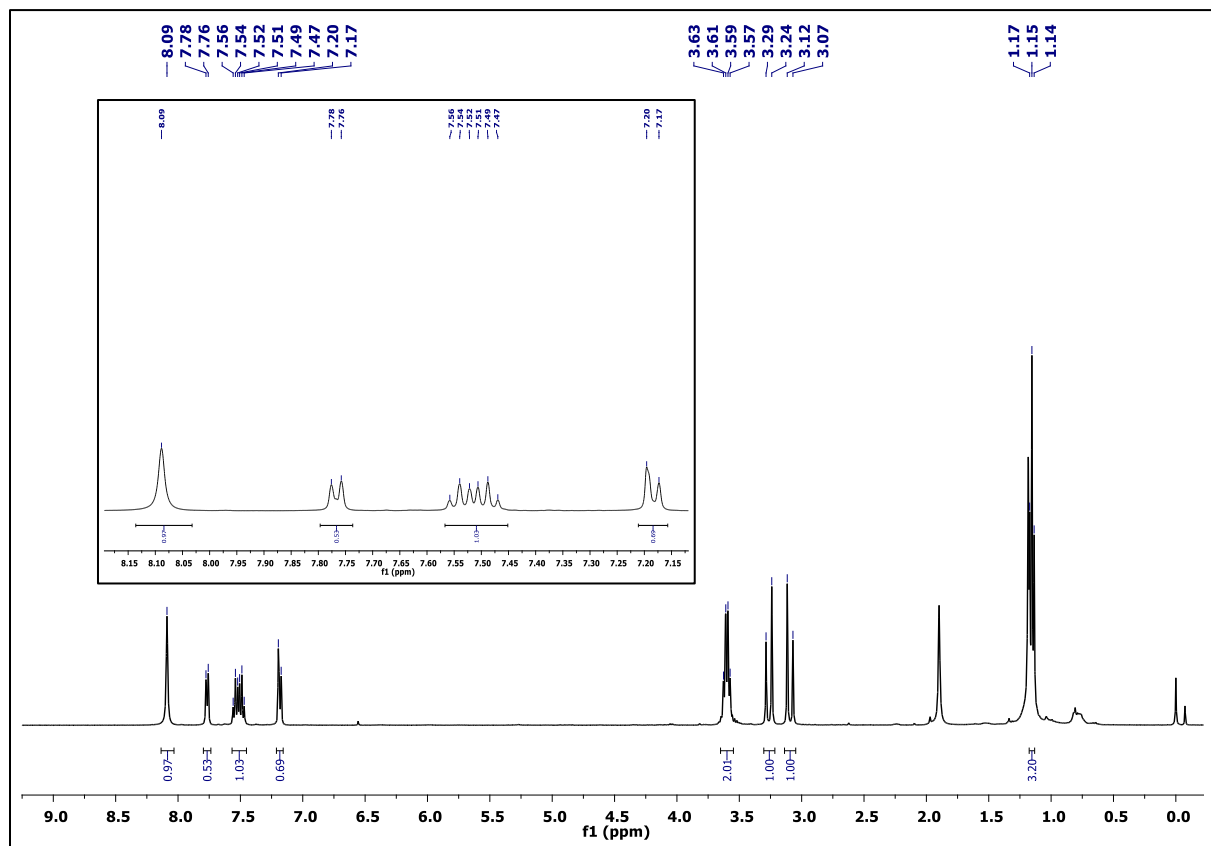
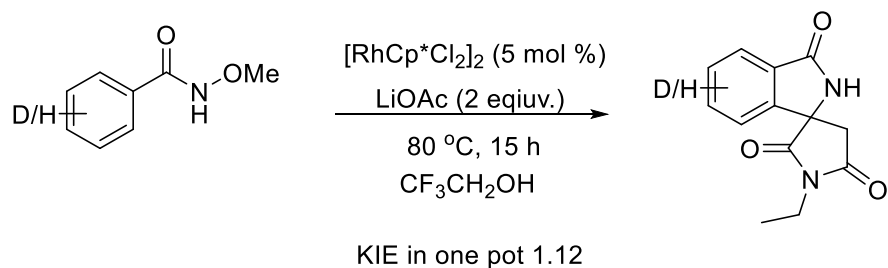
entry	catalyst	solvent	base	yield (%) ^b
1	[RhCp*Cl ₂] ₂	TFE	Cu(OAc) ₂ .H ₂ O (30 mol%)	55
2 ^c	Cp*Co(CO)I ₂	TFE	Cu(OAc) ₂ .H ₂ O (30 mol%)	NR
3 ^d	[RuCl ₂ (<i>p</i> -cymene)] ₂	TFE	Cu(OAc) ₂ .H ₂ O (30 mol%)	NR
4	[RhCp*Cl ₂] ₂	TFE	LiOAc (2 equiv.)	85
5	[RhCp*Cl ₂] ₂	TFE	NaOAc (2 equiv.)	76
6	[RhCp*Cl ₂] ₂	TFE	KOAc (2 equiv.)	65
7	[RhCp*Cl ₂] ₂	TFE	CsOAc (2 equiv.)	68
8	[RhCp*Cl ₂] ₂	TFE	AgOAc (2 equiv.)	45
9	[RhCp*Cl ₂] ₂	TFE	K ₂ CO ₃ (2 equiv)	10
10	[RhCp*Cl ₂] ₂	TFE	K ₃ PO ₄ (2 equiv.)	5
11	[RhCp*Cl ₂] ₂	TFE	Na ₂ HPO ₄ (2 equiv.)	NR
12	[RhCp*Cl ₂] ₂	TFE	Et ₃ N (2 equiv.)	NR
13	[RhCp*Cl ₂] ₂	THF	LiOAc (2 equiv.)	25
14	[RhCp*Cl ₂] ₂	HFIP	LiOAc (2 equiv.)	30
15	[RhCp*Cl ₂] ₂	chlorobenzene	LiOAc (2 equiv.)	15
16	[RhCp*Cl ₂] ₂	CH ₃ CN	LiOAc (2 equiv.)	28
17	[RhCp*Cl ₂] ₂	toluene	LiOAc (2 equiv.)	NR
18	[RhCp*Cl ₂] ₂	ClCH ₂ CH ₂ Cl	LiOAc (2 equiv.)	NR
19	[RhCp*Cl ₂] ₂	MeOH	LiOAc (2 equiv.)	NR

^aReaction conditions: **1a** (75 mg), **2a** (2.0 equiv.), catalyst (5 mol %), base (quantity noted), solvent (3 mL) under N₂ at 80 °C for 15 h in pressure tube. ^bIsolated yield of **3aa**. ^c5 mol % of Co(III) catalyst was used. ^d5 mol % of Ru(II) catalyst was used.

Spectra of Mechanistic Studies

KIE studies

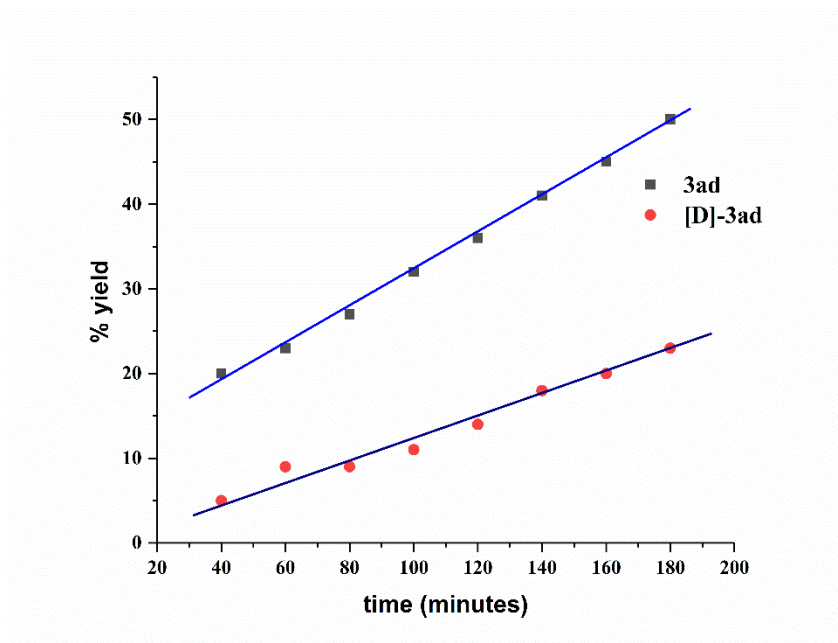
For competition reaction



For parallel reaction

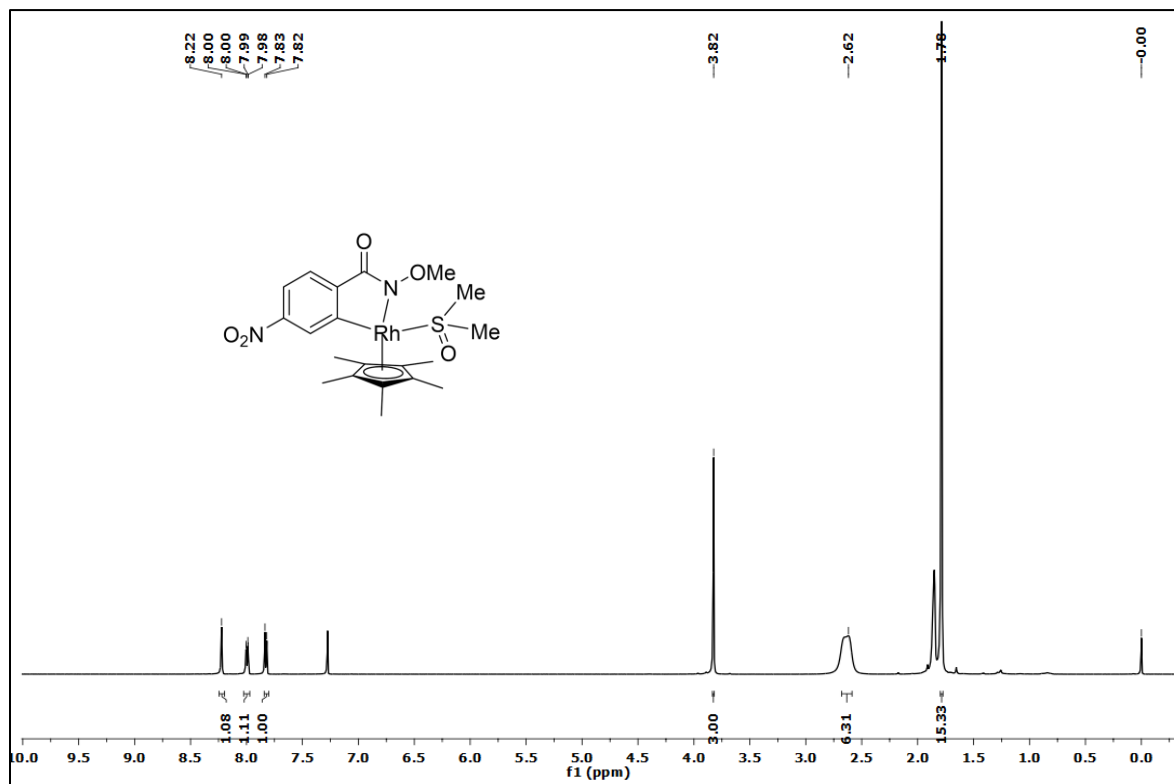
Table S2:

Time (min)	40	60	80	100	120	140	160	180
3ad (%)	20	23	27	32	36	41	45	56
[D]-3ad (%)	5	9	9	11	14	18	20	23



Intermediate Isolation

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **5i**.



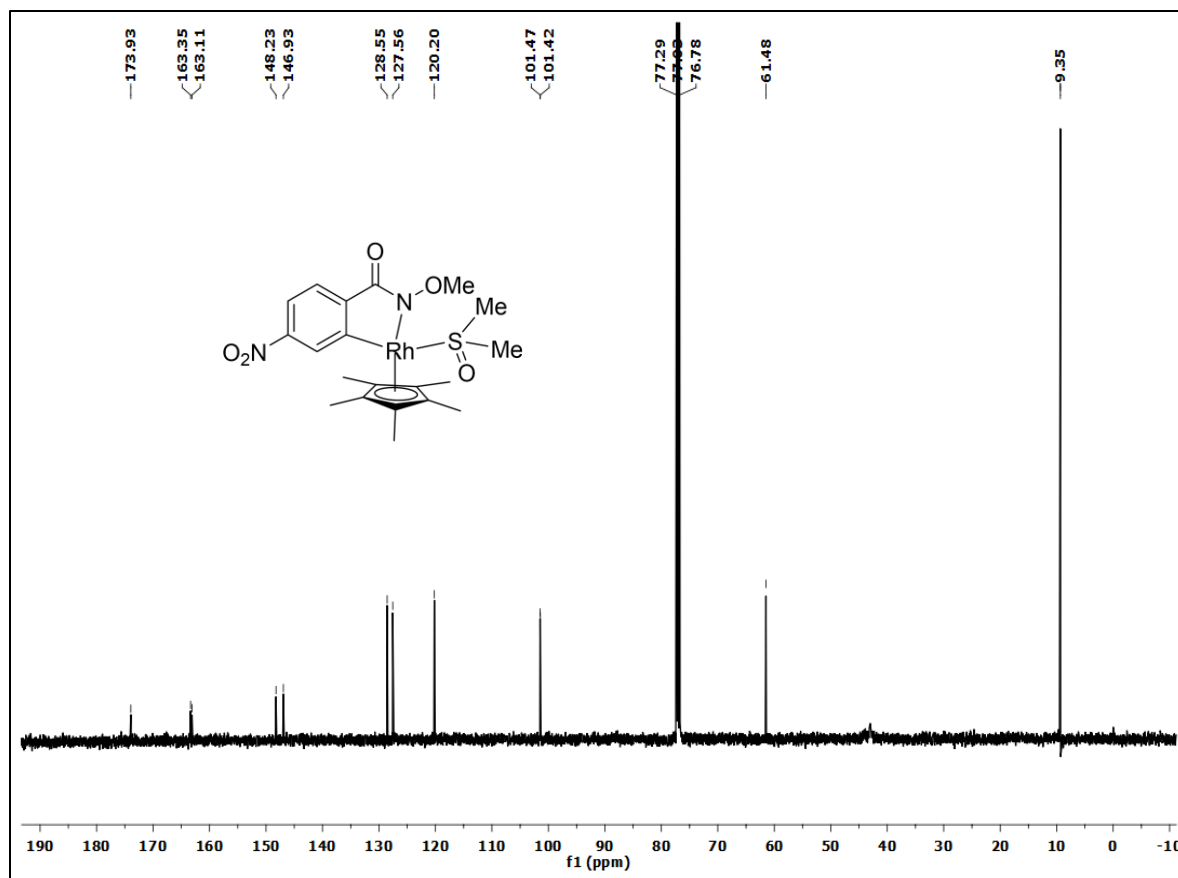
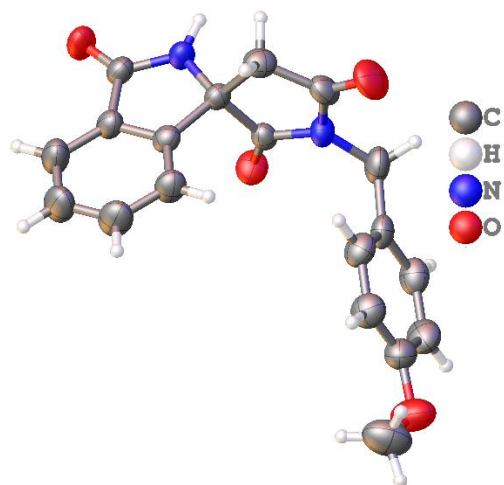


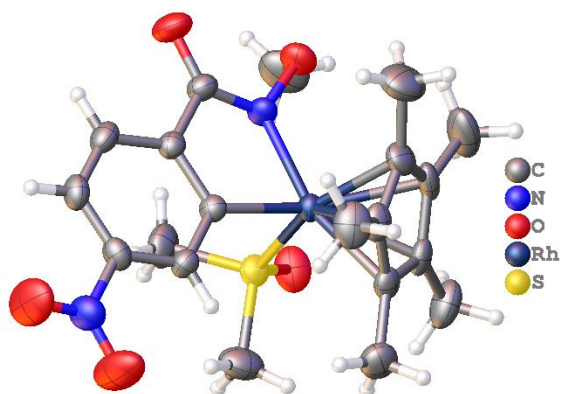
Table S2. X-Ray Analysis of Compound 3ah and 5i.

	3ah	5i
empirical formula	C ₁₉ H ₁₆ N ₂ O ₄	C ₂₀ H ₂₉ N ₂ O ₆ RhS
formula wt	336.35	528.43
temp (K)	296.15	296.15
Cryst. syst.	monoclinic	monoclinic
space group	P2 ₁ /c	P2 ₁ /c
<i>a</i> (Å)	17.3441(7)	8.4313(3)
<i>b</i> (Å)	5.5569(3)	16.3170(7)
<i>c</i> (Å)	18.2798(8)	17.1584(8)
α (deg)	90	90.00
β (deg)	107.5267(18)	101.057(2)
γ (deg)	90	90.00
<i>V</i> (Å ³)	1680.01(14)	2316.72(17)
<i>Z</i>	4	4
ρ_{calcd} (Mg m ⁻³)	1.3297	1.5149
μ (mm ⁻¹)	0.095	0.864
<i>F</i> (000)	704.4	1084.5
Cryst size (mm)	0.25 × 0.22 × 0.1	0.15 × 0.15 × 0.1
θ range (deg)	4.58 to 50	4.84 to 55.5
no. of collected/unique rflns	10164/2971 [R _{int} = 0.0315]	42975/5436 [R _{int} = 0.0525]
no.of. data /restraints/ params	2971/0/232	5436/3/285
<i>R</i> 1, <i>wR</i> 2 (<i>I</i> > 2 σ (<i>I</i>))	0.0398, 0.0876	0.0359, 0.0706
<i>R</i> 1, <i>wR</i> 2 (all data)	0.0676, 0.1022	0.0780, 0.0942
GOF	1.057	1.137
$\Delta\rho_{\text{max}}/\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.24/-0.20	1.56/-1.16

ORTEP Diagram (50% probability ellipsoids) of Compounds 3ah (CCDC No. 1873224) and 5i (CCDC. 1881004).



3ah



Rhodacycle 5i

Cartesian coordinates of the computed structures:

Active catalyst (Hartree/Particle)
Zero-point correction = 0.327148
Thermal correction to Energy= 0.350337
Thermal correction to Gibbs Free Energy= 0.275544
Lowest Frequency = 20.3211 cm⁻¹
SCF (M06) Energy = -956.0432961

Rh	0.03878100	0.16699000	-0.10741300
O	-1.30911100	1.52482000	0.99123500
O	-0.75954800	1.95121700	-1.08239400
C	-1.45943700	2.21806600	0.06129400
C	-2.55903800	-1.40944600	0.23578900
C	-2.47846600	3.31089000	0.11149500
H	-2.17338700	4.08766900	0.81894600
H	-3.42771700	2.88705100	0.46212600
H	-2.63988200	3.73635200	0.88353000
O	-1.61789200	-0.76764100	0.88598100
C	1.97470000	0.47481000	0.84446900
C	1.39330100	-0.78744300	1.27477100
C	1.24262400	-1.63150300	0.12878700
C	2.14897500	0.40833800	-0.56663400
C	1.65472700	-0.87748300	-1.02555200
C	1.04612800	-1.09729000	2.68769800
H	0.35300200	-0.34674800	3.09249500
H	0.56955100	-2.07806400	2.78990400
H	1.94771700	-1.09230600	3.31689700
C	2.27707200	1.61462700	1.75228900
H	1.41323500	1.84375800	2.38979600
H	3.13036500	1.38696300	2.40715700
H	2.51814700	2.52327900	1.18983300
C	2.63129700	1.48684200	-1.46810400
H	1.91969200	1.65166600	-2.28722100
H	2.74820300	2.43800300	-0.93856300
H	3.60080700	1.21779700	-1.91005600
C	1.61584600	-1.37159000	-2.42767300
H	1.74983400	-0.55475800	-3.14540600
H	2.40650000	-2.11473400	-2.60783200
H	0.64856200	-1.84419500	-2.64147100
C	0.70393800	-3.01597400	0.06875500
H	1.48276400	-3.71176000	-0.27375000
H	0.34728000	-3.36666600	1.04306500
H	-0.13359100	-3.07793000	-0.63870500
O	-3.45856900	-1.98928700	-0.81888000
C	-2.47623800	-1.41901100	1.27998200
H	-2.43572500	-0.39648700	1.67372700
H	-3.34173000	-1.94730300	1.69022400
H	-1.56039200	-1.93201800	1.60790900

Int1

Zero-point correction= 0.423844
Thermal correction to Energy= 0.452849

Thermal correction to Gibbs Free Energy= 0.365646

Lowest Frequency = 42.8089 cm⁻¹

SCF (M06) Energy = -1471.1427698

Rh	-0.80502900	-0.04335900	0.12392300
N	0.43130200	1.47479500	-0.64316800
C	-0.15116200	-2.09086400	-0.09694000
C	-1.43965600	-2.09733900	0.58525200
C	-2.39178500	-1.50070100	-0.27388200
C	-1.70399600	-1.10136600	-1.49655500
C	-0.34218600	-1.54568600	-1.40849000
O	-2.04437600	1.62519000	0.86484400
O	-0.50075900	0.78443700	2.17436000
C	-1.38276900	1.66463600	1.94352600
C	-1.61286300	2.77682300	2.92006500
H	-1.30206600	2.48105800	3.92642700
H	-1.01071700	3.64253200	2.61475100
H	-2.66388500	3.08219100	2.91629200
O	-0.36577600	2.04860800	-1.65482200
C	1.68898900	1.21210100	-1.13810700
C	2.62156600	0.52654100	-0.18207400
C	2.47534700	0.55812900	1.20692600
C	3.71034300	-0.15055100	-0.73943400
C	3.39591200	-0.09788200	2.01966300
H	1.63886500	1.09231000	1.65183700
C	4.62070100	-0.81588000	0.07279700
H	3.82925000	-0.12438000	-1.82187400
C	4.46351800	-0.79223800	1.45713900
H	3.27931700	-0.05922000	3.10202200
H	5.46293400	-1.34333500	-0.37333500
H	5.18112500	-1.30427300	2.09707600
O	2.07524800	1.52074600	-2.26232100
C	0.66146900	-1.42543200	-2.49867300
H	0.74044800	-0.39887900	-2.88271600
H	1.66127800	-1.72344500	-2.16391500
H	0.37505000	-2.07773300	-3.33611600
C	-2.31514700	-0.43077200	-2.67349800
H	-1.64078000	0.34187900	-3.06161600
H	-2.52053500	-1.15407000	-3.47663700
H	-3.25897000	0.05897600	-2.40795700
C	-3.82378600	-1.22361700	0.01228000
H	-4.07905600	-0.18570500	-0.23605200
H	-4.47364600	-1.88096200	-0.58285200
H	-4.06244400	-1.37680700	1.07039900
C	-1.64415500	-2.59184300	1.97276000
H	-2.62838600	-2.30952600	2.36172800
H	-1.56244900	-3.68742500	2.01672800
H	-0.88918500	-2.17245500	2.65040100
C	1.09539600	-2.66056500	0.47703600
H	1.25556100	-2.29739400	1.50085000
H	1.03581300	-3.75853400	0.51461400
H	1.97978400	-2.38182100	-0.10595600
C	-0.43523400	3.44092500	-1.45420300

H	0.55416700	3.90586600	-1.58011000
H	-1.11668700	3.82499700	-2.22174000
H	-0.83529500	3.67539100	-0.45665900

TS1

Zero-point correction= 0.419571
Thermal correction to Energy= 0.446727
Thermal correction to Gibbs Free Energy= 0.365255
Lowest Frequency = -1557.1725 cm⁻¹
SCF (M06) Energy = -1242.1350789

Rh	0.41201800	-0.17631400	-0.12315600
C	-2.23198700	0.86069600	0.38048200
C	-1.59223200	0.50622200	-0.82273100
C	-3.59828500	0.67143700	0.55593200
C	-2.37230400	-0.05040100	-1.84660800
C	-4.35170300	0.12180700	-0.47636400
C	-3.74127300	-0.23844100	-1.67969100
H	-4.04051200	0.94210300	1.51407600
H	-1.90243500	-0.29926200	-2.80068000
H	-5.42285800	-0.02859300	-0.34685600
H	-4.34053400	-0.65305900	-2.48977200
C	0.35303200	-2.32028900	-0.76665900
C	1.70297900	-1.91002400	-0.65391100
C	1.94453500	-1.48761100	0.71683100
C	0.73476700	-1.68441200	1.45375900
C	-0.27547600	-2.12912400	0.53132200
C	-0.31170600	-2.87849900	-1.97664700
C	2.72273000	-1.84896200	-1.73541400
C	3.24589000	-1.00408100	1.25262200
C	0.54336900	-1.40978200	2.90160100
C	-1.67787100	-2.49017900	0.87776400
H	-0.17571600	-3.96871500	-2.03011800
H	0.09542200	-2.44554800	-2.89872000
H	-1.38973900	-2.67974900	-1.96802900
H	3.58674400	-2.48443900	-1.49504700
H	3.08566400	-0.81964300	-1.86101200
H	2.31678600	-2.18255700	-2.69664300
H	3.82671200	-0.49558900	0.47303500
H	3.85702700	-1.83338100	1.63920700
H	3.09428000	-0.28903400	2.07040000
H	1.19219000	-0.59350600	3.23494500
H	0.77492300	-2.30589500	3.49513800
H	-0.48478600	-1.10497200	3.12941600
H	-1.75026800	-3.55228200	1.15407200
H	-2.35988700	-2.31086700	0.03721700
H	-2.04702100	-1.89573100	1.72202200
O	1.69935300	1.23757900	-1.15700700
C	1.16163800	2.17507400	-1.81131300
O	-0.07830900	2.31384300	-1.99056900
H	-0.71006200	1.33932400	-1.33928200
C	2.07536100	3.22227100	-2.38957700
H	1.61056800	3.71080000	-3.25039600

H	2.25367000	3.98405800	-1.61913900
H	3.04145800	2.78809100	-2.66324500
O	-1.87648200	1.62070600	2.62632600
C	-1.40527000	1.34471400	1.53306500
N	-0.08252900	1.40982800	1.15202400
O	0.75862800	1.63652400	2.23052900
C	1.73102900	2.59212600	1.86244100
H	1.25338100	3.53311900	1.55260400
H	2.33862200	2.76350700	2.75782500
H	2.36439700	2.22270200	1.04117900

Int2

Zero-point correction= 0.423764

Thermal correction to Energy= 0.452289

Thermal correction to Gibbs Free Energy= 0.366531

Lowest Frequency = -9.9967 cm⁻¹

SCF (M06) Energy = -1242.151082

Rh	0.47323800	0.11146500	0.05648200
C	1.81368100	0.40265700	-1.55681200
C	1.72049500	1.67830400	-0.87215200
C	2.18687200	1.48098100	0.44892000
C	2.72758700	0.12424300	0.54120200
C	2.55103600	-0.51535200	-0.68996700
C	1.48203400	0.18480700	-2.99225600
C	1.24788500	2.94418100	-1.49667300
C	2.23380900	2.47181500	1.55926500
C	3.31898700	-0.45796700	1.77624800
C	2.93696100	-1.91916200	-1.01263100
H	2.30247400	0.52092500	-3.64483100
H	0.57805300	0.73938300	-3.27368800
H	1.29284500	-0.87364100	-3.20505300
H	0.30592400	2.80661100	-2.04162300
H	1.99718400	3.31562900	-2.21126300
H	1.08777600	3.73260400	-0.75181500
H	1.55336900	3.31265100	1.37992300
H	3.24630900	2.88150700	1.69446700
H	1.93543400	2.00584400	2.50726200
H	2.61453200	-0.39423200	2.61649100
H	4.23359400	0.07764600	2.07060500
H	3.57133000	-1.51520900	1.63759800
H	3.96266900	-2.13031800	-0.68332000
H	2.89242000	-2.10758300	-2.09199400
H	2.26238200	-2.63518500	-0.52054300
C	-1.93695400	-1.45088600	-0.85725400
O	-2.69372900	-2.35782400	-1.19559900
N	-0.65798900	-1.55667000	-0.40886000
O	-0.11257200	-2.82835800	-0.31918700
C	-0.03474400	-3.47123200	-1.58143700
H	-1.03338000	-3.74053500	-1.94171200
H	0.45803700	-2.81808400	-2.31982100
H	0.57509300	-4.36830700	-1.42230300
O	-0.07334900	-0.24344600	2.28003200

C	-1.14359100	-0.45878800	2.83693500
O	-2.32351100	-0.22424600	2.30216400
C	-1.23839200	-1.03396000	4.21272500
H	-2.01750500	-0.52621300	4.78987500
H	-1.52452900	-2.08978500	4.13041500
H	-0.27252900	-0.96532600	4.71778600
C	-2.31925400	-0.00590600	-0.83970900
C	-3.61453500	0.38563300	-1.16750700
C	-1.36110000	0.91780000	-0.39776100
C	-3.97763000	1.72251700	-1.04771400
H	-4.31383500	-0.38216200	-1.49901900
C	-1.74705000	2.25333400	-0.25919500
C	-3.04637700	2.65057600	-0.58494100
H	-4.98845800	2.04142300	-1.29738900
H	-1.04156400	2.99872900	0.11396500
H	-3.33379400	3.69578900	-0.46923900
H	-2.20665200	0.10802900	1.38056900

Int3

Zero-point correction= 0.360782
Thermal correction to Energy= 0.383996
Thermal correction to Gibbs Free Energy= 0.310160
Lowest Frequency = 35.8020 cm⁻¹
SCF (M06) Energy = -1013.1761529

Rh	-0.30054300	-0.03970000	0.02217300
C	-2.04560700	-0.55462700	-1.17556200
C	-1.60563900	-1.76180500	-0.51334600
C	-1.67121900	-1.51698500	0.87973100
C	-2.24075500	-0.17909500	1.07295500
C	-2.52613600	0.38306300	-0.18845100
C	-2.08253300	-0.36982700	-2.64935100
C	-1.17047200	-3.00489500	-1.20952000
C	-1.31154100	-2.44716700	1.98373500
C	-2.45845300	0.48159400	2.38632800
C	-3.08064300	1.74730900	-0.42549900
H	-3.03241000	-0.74238300	-3.06265300
H	-1.26881300	-0.91950300	-3.13687900
H	-1.98597700	0.68588400	-2.92835400
H	-0.41259000	-2.79554300	-1.97592200
H	-2.01942600	-3.49817100	-1.70497300
H	-0.73670800	-3.72786200	-0.50880700
H	-0.66832500	-3.26196200	1.63350400
H	-2.21109100	-2.89530400	2.43169400
H	-0.76816300	-1.92621600	2.78176400
H	-1.74060700	0.12805500	3.13574600
H	-3.46921900	0.27507800	2.76947400
H	-2.34386700	1.56922400	2.30105500
H	-4.09189100	1.84664900	-0.00685300
H	-3.14554300	1.97609100	-1.49574400
H	-2.44384200	2.51333300	0.04064200
C	2.08353400	1.67464100	0.21228100
O	2.75793100	2.68090400	0.33212200

N	0.69097000	1.63895100	0.17679500
O	0.05808400	2.85283100	0.39372300
C	0.05682000	3.62632200	-0.79243900
H	1.07916800	3.89408800	-1.08649300
H	-0.43917600	3.07609500	-1.61019300
H	-0.51257100	4.53285200	-0.55962100
C	2.60134800	0.28654800	0.06616700
C	3.96513300	0.03332800	0.05010600
C	1.64933400	-0.73425500	-0.04447400
C	4.41010700	-1.28149500	-0.07303000
H	4.65831000	0.86985500	0.13898200
C	2.11005000	-2.04240600	-0.16562000
C	3.48289000	-2.31292000	-0.17861200
H	5.47660800	-1.50139100	-0.08427700
H	1.41017900	-2.87594800	-0.25419100
H	3.82816100	-3.34289900	-0.27239800

Int4

Zero-point correction= 0.461029
Thermal correction to Energy= 0.491345
Thermal correction to Gibbs Free Energy= 0.403694
Lowest Frequency = 28.3577 cm⁻¹
SCF (M06) Energy = -1411.7115048

Rh	-0.04591500	-0.18886000	0.04671700
C	2.65995200	0.67310100	-0.58417400
C	1.44402300	1.24561800	-0.22195600
C	3.82293900	1.43768500	-0.61971800
C	1.35600300	2.60895400	0.02377600
C	3.75297200	2.79487800	-0.32744400
C	2.52177000	3.37832400	-0.02820800
C	-1.34320900	-0.49096100	-1.69212700
C	-0.76806900	0.79323400	-1.74579100
H	4.76081500	0.94741500	-0.88079400
H	0.39685900	3.08564600	0.22957200
H	4.65263700	3.40771800	-0.35139700
H	2.46218800	4.44964300	0.16289700
C	0.65455400	-0.27768400	2.16950200
C	-0.55152400	0.51343700	2.16215200
C	-1.61434900	-0.33683600	1.74777600
C	-1.08409300	-1.66046800	1.50433700
C	0.30571100	-1.62623300	1.79899500
C	1.98965100	0.15555900	2.66717800
C	-0.69846100	1.92425300	2.61557000
C	-3.05743000	0.01707000	1.78258400
C	-1.87939400	-2.85258900	1.09764600
C	1.24751000	-2.77675300	1.74659400
H	2.07917600	-0.05281800	3.74343200
H	2.15774100	1.22805700	2.51314600
H	2.80434400	-0.37385700	2.15846500
H	0.25631400	2.46046300	2.58703200
H	-1.07500200	1.96552400	3.64848100
H	-1.40543100	2.48031800	1.98483200

H	-3.22077900	1.08256000	1.58308200
H	-3.45651000	-0.18871200	2.78747700
H	-3.65079400	-0.57015100	1.07307700
H	-2.67650500	-2.58403300	0.39170900
H	-2.35032800	-3.33066200	1.96966100
H	-1.24410400	-3.60136100	0.61021600
H	1.24181700	-3.31274700	2.70706500
H	2.27640500	-2.45478100	1.54884300
H	0.97969000	-3.48060800	0.95253700
C	-2.79055800	-0.32438300	-1.38253000
C	-1.82867000	1.78070500	-1.39399300
O	-1.75538300	2.98335000	-1.26258400
O	-3.65212300	-1.17646000	-1.28631900
N	-3.00720700	1.04518500	-1.22416300
C	-4.28768900	1.65575000	-0.96602700
H	-5.01777900	0.85558600	-0.81287700
H	-4.24034200	2.29854100	-0.07920300
H	-4.59511900	2.27257600	-1.81871200
H	0.08322600	1.09235600	-2.34868500
H	-1.00458900	-1.38912300	-2.19909500
C	2.65381600	-0.77200100	-0.93266900
O	3.64459800	-1.47751800	-1.05993000
N	1.34852000	-1.14958300	-1.16739800
O	1.15583900	-2.52394400	-1.30832900
C	1.45310900	-2.92348700	-2.63493100
H	1.15660700	-3.97542700	-2.70487800
H	0.88428900	-2.32654900	-3.36433100
H	2.52732300	-2.82255000	-2.83483900

TS2

Zero-point correction= 0.462233

Thermal correction to Energy= 0.491100

Thermal correction to Gibbs Free Energy= 0.406823

Lowest Frequency = -270.4208 cm⁻¹

SCF (M06) Energy = -1411.6856788

Rh	0.02055400	-0.45436500	0.00453300
N	1.52109000	-0.60943300	-1.50349200
C	0.05175500	-0.46233400	2.30816600
C	-1.23129300	-0.90195700	1.83214200
C	-1.03311600	-2.13002300	1.10335900
C	0.37024000	-2.38634000	1.05721500
C	1.04759500	-1.33322500	1.78648000
O	1.97542200	-1.85592700	-1.91354600
C	2.57578200	0.25485600	-1.32655400
C	2.12232500	1.46446400	-0.57691200
C	0.79783000	1.56916800	-0.11721600
C	3.07111100	2.40632300	-0.19532400
C	0.45409500	2.61618200	0.73621100
C	2.71693800	3.46090900	0.63960100
H	4.09115800	2.26137100	-0.54964800
C	1.41055200	3.55554100	1.11250400
H	-0.56360400	2.71790300	1.10961500

H	3.45901700	4.20194400	0.93152500
H	1.12451400	4.37164300	1.77465400
O	3.73014200	0.09368700	-1.69243000
C	-1.23971600	-0.07165000	-1.66345000
C	-0.65556600	1.23352400	-1.44699600
H	-0.96403600	-0.70212600	-2.50356600
C	-2.11479200	-2.99794500	0.56602100
H	-2.85613700	-2.42590800	-0.00758200
H	-1.71493200	-3.77448700	-0.09654600
H	-2.64349800	-3.50184100	1.38894100
C	-2.55481700	-0.30723700	2.16962400
H	-3.29295500	-0.50728800	1.38099600
H	-2.95532600	-0.72497400	3.10566300
H	-2.48589300	0.78145600	2.29989200
C	0.31143000	0.67176600	3.23396200
H	-0.50284100	1.40551100	3.23578100
H	0.41264100	0.29098100	4.26118500
H	1.23934900	1.20048500	2.98362500
C	2.51880600	-1.22824800	2.00076400
H	2.84593300	-0.17939100	1.99726500
H	2.82299400	-1.67080100	2.96102900
H	3.07379400	-1.74134000	1.20523100
C	1.05363700	-3.57264500	0.47989600
H	1.80857600	-3.26873900	-0.25763200
H	1.56321900	-4.13757400	1.27347800
H	0.34848700	-4.25084800	-0.01364600
C	1.05144000	-2.45317100	-2.78557900
H	0.10053500	-2.67880600	-2.27116500
H	0.85219200	-1.80909700	-3.65521300
H	1.51110600	-3.39012500	-3.11793200
C	-2.66509100	-0.00317100	-1.28635900
C	-1.80756500	2.13047100	-1.02729800
N	-2.91227100	1.31200700	-0.86127200
H	0.00923900	1.64385800	-2.20618300
C	-4.20526800	1.81160600	-0.46108900
H	-4.56089800	2.56653700	-1.17164100
H	-4.89661500	0.96423700	-0.44509600
H	-4.14973100	2.27147300	0.53256500
O	-1.82406800	3.33178900	-0.89069300
O	-3.52410100	-0.86290500	-1.33223400

Int5

Zero-point correction= 0.461649
Thermal correction to Energy= 0.491086
Thermal correction to Gibbs Free Energy= 0.405507
Lowest Frequency = 36.9741 cm⁻¹
SCF (M06) Energy = -1411.7209081

Rh	0.90329600	-0.34888900	-0.19689700
N	0.67985800	1.37182100	-1.30289300
C	1.45691900	-0.14002700	1.83214400
C	1.18845700	-1.55680500	1.62467100
C	2.10545300	-2.00441800	0.65414800

C	3.02143700	-0.89184600	0.33800500
C	2.66178300	0.22535800	1.10696000
O	1.91329500	1.65839400	-1.91346000
C	0.02638100	2.51668900	-0.92929400
C	-1.11340000	2.29652600	0.03233700
C	-2.02886100	1.22670400	0.01671200
C	-1.19883700	3.26356000	1.03678200
C	-2.94934500	1.13225900	1.06424900
C	-2.12415200	3.15830400	2.06693800
H	-0.51378500	4.10824700	0.98044700
C	-2.99265500	2.07456800	2.08772700
H	-3.68577800	0.32955100	1.06759700
H	-2.17099700	3.92088700	2.84260800
H	-3.72913200	1.97035800	2.88309600
O	0.36503100	3.64733900	-1.25530500
C	-0.92625100	-0.85504000	-1.02106800
C	-2.02996200	0.20684900	-1.11244400
H	-0.46893700	-1.02991000	-2.01717100
C	2.19522100	-3.37235400	0.07859100
H	1.19936900	-3.82308400	-0.00232000
H	2.63682300	-3.35226300	-0.92546000
H	2.82856800	-4.01983800	0.70343000
C	0.13443500	-2.34410100	2.31704300
H	-0.17229600	-3.20872800	1.71951000
H	0.49461400	-2.69730100	3.29436700
H	-0.76351100	-1.73617900	2.49372600
C	0.72168500	0.75033600	2.76247400
H	-0.33000200	0.45697900	2.85965300
H	1.17968400	0.71544600	3.76319100
H	0.74120100	1.79001600	2.41551900
C	3.25800100	1.58964400	1.09875600
H	2.48640600	2.36124600	0.97402400
H	3.78750900	1.79372500	2.04036100
H	3.96258200	1.71803200	0.27160900
C	4.09221600	-0.97712400	-0.68866500
H	4.53200100	0.00326900	-0.89796600
H	4.89345100	-1.65881400	-0.36832000
H	3.69114900	-1.36769600	-1.63472300
C	1.78930200	1.49115300	-3.30575200
H	1.47836800	0.46158100	-3.55602400
H	1.06708800	2.20520200	-3.72705900
H	2.78170300	1.68449800	-3.72855700
C	-1.60051600	-2.12192100	-0.63319800
C	-3.31304900	-0.61297800	-1.07838700
N	-2.98009700	-1.89329500	-0.65442200
H	-1.98429300	0.74825200	-2.06718000
C	-3.97411100	-2.91997900	-0.44830500
H	-4.58972500	-2.68747800	0.42895500
H	-4.63106900	-2.98361800	-1.32239400
H	-3.45115700	-3.86784200	-0.29566100
O	-4.44343300	-0.25514500	-1.31658800
O	-1.11206800	-3.21263300	-0.39417500

Int5'

Zero-point correction= 0.452239
Thermal correction to Energy= 0.481952
Thermal correction to Gibbs Free Energy= 0.394826
Lowest Frequency = 27.1973 cm⁻¹
SCF (M06) Energy = -1410.894912

Rh	-0.52542500	-0.47094100	-0.00536500
N	0.93021200	-1.68559400	-0.47143300
C	-1.85935400	-0.27073900	1.73405900
C	-2.49668000	0.45621300	0.68001200
C	-2.74679100	-0.45231600	-0.39225100
C	-2.34831800	-1.78390300	0.03891000
C	-1.79647200	-1.67321500	1.34361400
C	2.22534400	-1.41992100	-0.98447100
C	2.94078400	-0.26578000	-0.36469200
C	2.34827800	0.91305800	0.13932500
C	4.30475600	-0.47532900	-0.19447700
C	3.14637800	1.80929300	0.86194200
C	5.09349800	0.44042500	0.50115100
H	4.73874900	-1.38449700	-0.60491200
C	4.50594600	1.56994800	1.04707500
H	2.70646100	2.71543800	1.26704000
H	6.15887000	0.25765100	0.62090200
H	5.10160200	2.28415000	1.61091700
O	2.76399100	-2.17742600	-1.76306400
C	-3.40306600	-0.14520300	-1.68540600
H	-3.07641800	0.81582500	-2.10144300
H	-3.20167400	-0.92220300	-2.43078000
H	-4.49359800	-0.09273100	-1.54508000
C	-2.95044700	1.86767700	0.75264400
H	-3.04638200	2.31966800	-0.24071400
H	-3.94509800	1.89973900	1.22097700
H	-2.28522600	2.48345600	1.36891900
C	-1.41211300	0.29811700	3.02910900
H	-0.97436300	1.29639800	2.90062200
H	-2.26588600	0.39635400	3.71639700
H	-0.66585100	-0.33735600	3.51746100
C	-1.26672900	-2.78192000	2.17685300
H	-0.42272900	-2.45602500	2.79590800
H	-2.04603500	-3.15937400	2.85431200
H	-0.92579500	-3.61735200	1.55602600
C	-2.51675700	-3.01146100	-0.77581600
H	-2.20537900	-3.90885200	-0.23369500
H	-3.57131900	-3.13025900	-1.06071300
H	-1.92394300	-2.96422400	-1.69939200
C	0.33949800	2.55334300	0.37968500
C	0.99347500	1.32266700	-0.23254500
C	0.31442700	1.07834300	-1.42276100
C	-0.65004300	2.19450500	-1.65968600
O	-1.41965200	2.34129900	-2.57955900
O	0.48367900	3.00712500	1.49207400

N	-0.50090000	3.07617800	-0.58885000
C	-1.17658500	4.35438900	-0.47683700
H	-0.49333500	5.16573800	-0.74964700
H	-2.02592100	4.35881700	-1.16572100
H	-1.51474500	4.50987300	0.55154200
H	0.66845200	0.50054600	-2.27406200
O	0.49170400	-2.96759000	-0.71780400
C	1.30270000	-3.98611100	-0.12010700
H	0.67862700	-4.88505300	-0.13325800
H	2.21449000	-4.15575100	-0.69871600
H	1.54725000	-3.71144500	0.91536600

Int6

Zero-point correction= 0.527451
Thermal correction to Energy= 0.562895
Thermal correction to Gibbs Free Energy= 0.461584
Lowest Frequency = 21.6366 cm⁻¹
SCF (M06) Energy = -1640.6770216

Rh	-0.93377500	-0.33033800	-0.19573800
N	0.77531200	-1.59093500	-0.39037200
C	-2.37312700	-0.91823600	1.42440300
C	-2.63218600	0.45142600	0.94881100
C	-3.02750800	0.38958200	-0.40499500
C	-2.85539300	-0.99997900	-0.81106700
C	-2.58453500	-1.81048900	0.36335000
C	0.96611300	-1.69253900	0.98200800
C	1.60666000	-0.49129100	1.65440700
C	1.79659600	0.83882300	1.19486200
C	2.14757100	-0.85358100	2.90235800
C	2.61053100	1.67431700	1.97784200
C	2.90225300	0.00942500	3.67248800
H	1.96784800	-1.87319400	3.23268200
C	3.15637300	1.28666800	3.18852200
H	2.80674100	2.68148300	1.61943000
H	3.30961500	-0.32173300	4.62617100
H	3.77556600	1.98433700	3.74986300
O	0.70907500	-2.70637900	1.63095700
C	-3.58253000	1.47194300	-1.25871500
H	-3.59210200	2.43199100	-0.72911200
H	-3.00577700	1.61452800	-2.18217600
H	-4.62060900	1.23575300	-1.53411500
C	-2.53837700	1.65169500	1.81999200
H	-2.62179700	2.58405400	1.25038600
H	-3.33537300	1.64158200	2.57839900
H	-1.57998200	1.68083600	2.35609700
C	-1.94177700	-1.28197200	2.79852400
H	-1.45023900	-0.44181900	3.30373800
H	-2.80931900	-1.57885500	3.40673100
H	-1.23041500	-2.11812300	2.77595800
C	-2.43634100	-3.28956300	0.43187200
H	-2.50708900	-3.74797200	-0.55999000
H	-1.45914700	-3.56174800	0.85307900

H	-3.22703500	-3.71929400	1.06361500
C	-3.04593100	-1.50327200	-2.19237100
H	-2.38032100	-2.35116200	-2.39394200
H	-4.08343200	-1.83914400	-2.34405100
H	-2.83118700	-0.71583500	-2.92527500
H	2.17720200	-1.20725100	-1.55264400
C	0.47378100	2.84873500	0.33884300
C	1.26055500	1.57561000	-0.02885600
C	0.38325100	0.98777300	-1.13775500
C	-0.39042400	2.10962900	-1.68254400
O	-1.00242000	2.18862000	-2.73463500
O	0.53322700	3.53284900	1.33726600
N	-0.35373800	3.14080200	-0.73149100
C	-1.14011100	4.34590100	-0.80828100
H	-1.69642300	4.31613000	-1.75024900
H	-1.83396700	4.41263700	0.04094000
H	-0.49438700	5.23088700	-0.78525800
H	2.17241700	1.94712900	-0.53477300
O	3.77634700	0.49765200	-1.29753500
C	3.76614000	-0.33223900	-2.18092500
O	2.82463400	-1.26766200	-2.31153200
H	0.90068200	0.42484600	-1.91591000
O	0.20454500	-2.78850200	-0.90895600
C	1.17613400	-3.80669200	-1.05715500
H	0.65219300	-4.63301200	-1.55054000
H	2.00837800	-3.47830400	-1.69528900
H	1.55428200	-4.14535600	-0.08398900
C	4.80009800	-0.43864400	-3.26359200
H	5.55756200	0.33749700	-3.13361700
H	5.27020700	-1.42844500	-3.23545900
H	4.32461100	-0.33711900	-4.24614900

TS3

Zero-point correction= 0.524818
Thermal correction to Energy= 0.559352
Thermal correction to Gibbs Free Energy= 0.461115
Lowest Frequency = -33.3022 cm⁻¹
SCF (M06) Energy = -1640.6593912

Rh	-0.97991500	-0.31531600	-0.17266700
N	0.72051100	-1.60126300	-0.49411500
C	-2.39445900	-1.00345600	1.46688600
C	-2.58961500	0.41084900	1.10664300
C	-3.04807600	0.48148500	-0.23209800
C	-2.94726800	-0.86878500	-0.75769400
C	-2.65848600	-1.78799900	0.33997200
C	0.98749000	-1.75806100	0.89202900
C	1.72596000	-0.62788900	1.53368200
C	1.90774500	0.70376300	1.07969400
C	2.37799700	-1.05545300	2.70741900
C	2.83241300	1.48630700	1.79082100
C	3.23767800	-0.23815200	3.41118500
H	2.19851200	-2.07898300	3.02706900

C	3.48385100	1.04301900	2.92731400
H	3.03512700	2.49134500	1.43161400
H	3.73405300	-0.60408900	4.30774100
H	4.18689900	1.70201400	3.43343700
O	0.65870800	-2.76976000	1.48644900
C	-3.60662200	1.64876000	-0.96193400
H	-3.51877600	2.57148200	-0.37655100
H	-3.10162000	1.82385500	-1.92065600
H	-4.67507000	1.48188200	-1.16109700
C	-2.39135500	1.53592600	2.05756100
H	-2.44987900	2.51053000	1.55970700
H	-3.15109300	1.50770400	2.85277900
H	-1.40737300	1.47944000	2.54432100
C	-1.95075900	-1.47314200	2.80414600
H	-1.18756500	-0.80646300	3.22695500
H	-2.79712600	-1.48938500	3.50683100
H	-1.51674400	-2.47688200	2.75425100
C	-2.54164900	-3.26901200	0.25075900
H	-2.56865600	-3.61095500	-0.78864000
H	-1.59268000	-3.61346500	0.68141100
H	-3.36856900	-3.75244400	0.78960400
C	-3.22559300	-1.24112600	-2.16515000
H	-2.64332000	-2.11816200	-2.47130100
H	-4.29268000	-1.47809100	-2.29802900
H	-2.97460300	-0.41247900	-2.83853400
H	1.55249700	-1.19810100	-1.12136800
C	0.57236200	2.77181700	0.43677100
C	1.26443900	1.49674400	-0.05132000
C	0.29487600	1.00402800	-1.13394900
C	-0.46150900	2.19325700	-1.55810900
O	-1.13523600	2.35579600	-2.56079400
O	0.73094300	3.39697100	1.46328100
N	-0.31912900	3.15754000	-0.55317200
C	-1.02662900	4.41320000	-0.52479900
H	-1.63026500	4.47079300	-1.43555800
H	-1.67156300	4.47657100	0.36220900
H	-0.32164300	5.25103100	-0.48949700
H	2.15456000	1.80319800	-0.64634200
O	3.64177700	0.86186600	-1.56344900
C	3.54193500	-0.19177800	-2.20476000
O	2.58158400	-1.04264900	-2.14861200
H	0.77253000	0.47728800	-1.96735200
O	0.21664900	-2.75707800	-1.09924600
C	1.26247900	-3.69965300	-1.35338000
H	0.78111200	-4.49938400	-1.92353400
H	2.05690500	-3.22906200	-1.94496600
H	1.65476300	-4.10361700	-0.41137000
C	4.64341600	-0.57251800	-3.18199800
H	5.40415200	0.21134100	-3.24230700
H	5.11139600	-1.51283100	-2.86379800
H	4.21406600	-0.75275500	-4.17518100

Int7OAc

Zero-point correction= 0.526015
Thermal correction to Energy= 0.561357
Thermal correction to Gibbs Free Energy= 0.460933
Lowest Frequency = 26.1809 cm⁻¹
SCF (M06) Energy = -1640.6595592

Rh	-0.99371200	-0.28764600	-0.18418000
N	0.67586300	-1.59740800	-0.58355900
C	-2.45254600	-1.06344600	1.38815900
C	-2.59716800	0.37725700	1.13379200
C	-3.03669600	0.56785700	-0.20230700
C	-2.96443000	-0.73648200	-0.83181700
C	-2.70944600	-1.74757300	0.19709000
C	0.91727500	-1.85572800	0.79372700
C	1.66253400	-0.77952700	1.51265500
C	1.87834600	0.57034800	1.13036700
C	2.28606900	-1.28287900	2.67158800
C	2.81128700	1.29254600	1.89244800
C	3.15271800	-0.52232900	3.42857700
H	2.08021300	-2.31793700	2.93360800
C	3.43529800	0.77531300	3.01380700
H	3.04381700	2.30907800	1.58803300
H	3.62746100	-0.94503900	4.31179000
H	4.14623400	1.39022400	3.56261900
O	0.56063800	-2.89818300	1.31190000
C	-3.55085400	1.80917800	-0.83641400
H	-3.42441000	2.67801800	-0.17947600
H	-3.04302800	2.03771700	-1.78240800
H	-4.62599500	1.70289700	-1.04075200
C	-2.36457600	1.42055700	2.16636500
H	-2.44401500	2.43116200	1.75199600
H	-3.09264000	1.32423300	2.98530800
H	-1.36120900	1.32763200	2.60727800
C	-2.04437100	-1.64893400	2.69097400
H	-1.26894500	-1.04094500	3.17563600
H	-2.90112900	-1.69629000	3.37943400
H	-1.63826500	-2.65788700	2.56754200
C	-2.61797100	-3.21902100	-0.00693800
H	-2.64116600	-3.48017900	-1.06977800
H	-1.67934600	-3.61393800	0.40508300
H	-3.45846500	-3.72700400	0.48649600
C	-3.23319200	-0.98779200	-2.26772900
H	-2.67472600	-1.85759500	-2.63290000
H	-4.30493700	-1.17633300	-2.43534500
H	-2.94073300	-0.11737900	-2.86862800
H	1.51605700	-1.15498300	-1.12806000
C	0.62671400	2.71100800	0.55838400
C	1.27729100	1.43448800	0.02675100
C	0.31094200	1.03027100	-1.09493100
C	-0.40131300	2.26185300	-1.47141800
O	-1.06824900	2.48336400	-2.46765900
O	0.78157800	3.27907100	1.61847200

N	-0.22769600	3.17912400	-0.43046900
C	-0.88408700	4.46073400	-0.35679100
H	-1.50286200	4.56438700	-1.25321100
H	-1.50642300	4.52572700	0.54496400
H	-0.14600300	5.26958700	-0.31787300
H	2.19198400	1.72472000	-0.55176900
O	3.66336600	1.05310600	-1.55082500
C	3.61435400	-0.04295900	-2.13031400
O	2.67089700	-0.90656300	-2.07637500
H	0.78719300	0.53366500	-1.94719600
O	0.18660600	-2.69653700	-1.29065900
C	1.24401800	-3.61084700	-1.60013700
H	0.79019000	-4.34264500	-2.27431400
H	2.06320700	-3.08101700	-2.10213900
H	1.59609300	-4.11372900	-0.69039300
C	4.78046400	-0.45132200	-3.01838000
H	5.53097000	0.34256000	-3.07572500
H	5.24311400	-1.36464400	-2.62300600
H	4.41498800	-0.69148900	-4.02437800

TS4

Zero-point correction= 0.523013
Thermal correction to Energy= 0.557552
Thermal correction to Gibbs Free Energy= 0.460877
Lowest Frequency = -926.5743 cm⁻¹
SCF (M06) Energy = -1640.6551869

Rh	-0.97377200	-0.18840400	-0.18987300
N	0.55033200	-1.57024900	-0.91515800
C	-2.46975100	-1.04427800	1.32937900
C	-2.57376000	0.40232200	1.20147400
C	-2.99449800	0.73030600	-0.12659000
C	-2.97739100	-0.50248200	-0.86962700
C	-2.72639200	-1.60188700	0.06866200
C	0.79752100	-2.15170500	0.36317100
C	1.59422000	-1.28190500	1.26627300
C	1.80504000	0.11626700	1.14356500
C	2.22529400	-2.00964400	2.28780600
C	2.74709900	0.67425300	2.02438500
C	3.10113000	-1.41268300	3.17336000
H	2.00885700	-3.07409400	2.34576200
C	3.37568900	-0.05836300	3.01880800
H	2.98563100	1.72897400	1.92593400
H	3.58268800	-1.99762100	3.95411200
H	4.09089100	0.43816100	3.67231800
O	0.40211400	-3.26759100	0.63923900
C	-3.43943600	2.05282000	-0.64176600
H	-3.29933900	2.84184600	0.10707700
H	-2.89382000	2.36001200	-1.54428100
H	-4.51034900	2.01882700	-0.88861500
C	-2.33453000	1.34574000	2.32629300
H	-2.56819500	2.38043200	2.05191500
H	-2.95393400	1.07375500	3.19275100

H	-1.28479900	1.32730400	2.65816900
C	-2.06468600	-1.76884400	2.56494100
H	-1.27749100	-1.22253900	3.10308600
H	-2.91061500	-1.89422700	3.25684300
H	-1.66713900	-2.76227400	2.32577100
C	-2.71268800	-3.05238100	-0.26567500
H	-2.90370900	-3.22320500	-1.33006200
H	-1.74639300	-3.51545500	-0.01959200
H	-3.49437900	-3.57275700	0.30540600
C	-3.29107900	-0.64009000	-2.31471900
H	-2.71103900	-1.45422700	-2.76644100
H	-4.35947000	-0.85297100	-2.47405300
H	-3.04192500	0.28452100	-2.85014800
H	1.39625100	-1.07132000	-1.30360300
C	0.67845500	2.38917100	0.90721200
C	1.20298600	1.16178900	0.21004700
C	0.34745300	1.09835700	-1.05946600
C	-0.24530900	2.43835000	-1.22048100
O	-0.84884300	2.88258100	-2.18241900
O	0.80707000	2.75032400	2.06176300
N	-0.05014000	3.12519500	-0.02580600
C	-0.61719800	4.41724100	0.26790300
H	-1.21348900	4.71941500	-0.59847600
H	-1.24656300	4.36612900	1.16590300
H	0.17155700	5.15643500	0.44802200
H	2.25164700	1.45119500	-0.39024800
O	3.46512600	1.49270600	-1.14691200
C	3.63373200	0.44877500	-1.84992400
O	2.84877800	-0.52542900	-1.94388200
H	0.81530400	0.71372600	-1.96762800
O	0.01575100	-2.43702100	-1.86194800
C	1.03940500	-3.27813400	-2.39699800
H	0.56252400	-3.81549000	-3.22096000
H	1.87452400	-2.67136100	-2.77190800
H	1.39169300	-3.99208200	-1.64189800
C	4.91035700	0.42289900	-2.66384300
H	5.76489000	0.68968800	-2.03222600
H	5.06696000	-0.55887800	-3.12007200
H	4.84767500	1.18174100	-3.45367600

Int-8AcOH

Zero-point correction= 0.529562
Thermal correction to Energy= 0.564870
Thermal correction to Gibbs Free Energy= 0.465626
Lowest Frequency = 21.7574 cm⁻¹
SCF (M06) Energy = -1640.7115894

Rh	-0.98025800	-0.34173900	-0.13766500
N	0.82509400	-1.57098300	-0.38753800
C	-2.48077600	-1.12389800	1.39999200
C	-2.90127400	0.15168100	0.94139000
C	-3.15592400	0.05722700	-0.49011100

C	-2.91659800	-1.28703300	-0.90040700
C	-2.43868200	-1.99287600	0.25390100
C	1.17815600	-1.60325400	0.99661400
C	1.92230400	-0.38226100	1.42715700
C	1.58800600	0.92837500	1.02895600
C	3.02524900	-0.61816600	2.24991900
C	2.41124900	1.96989100	1.48410300
C	3.83083700	0.42850800	2.67830600
H	3.23437200	-1.64290000	2.55200300
C	3.51872100	1.72715600	2.29251100
H	2.14854900	2.99499900	1.22884100
H	4.68938400	0.23163300	3.31693300
H	4.13046200	2.56249400	2.62858500
O	0.98431200	-2.57713700	1.69500300
C	-3.72402000	1.12779100	-1.35740900
H	-3.69834200	2.10662300	-0.86462700
H	-3.17638600	1.23128900	-2.30411600
H	-4.77440500	0.90952400	-1.60045500
C	-3.16156300	1.32901600	1.81766100
H	-3.42013100	2.22393100	1.23966400
H	-4.00572300	1.11887500	2.49043500
H	-2.29442400	1.58893300	2.43890600
C	-2.14076900	-1.51241200	2.79782700
H	-1.91819300	-0.62927700	3.40969100
H	-2.96690000	-2.05515100	3.28351200
H	-1.25694800	-2.16550800	2.82719900
C	-2.09994500	-3.44095700	0.33646600
H	-1.95926500	-3.88773900	-0.65301700
H	-1.17953300	-3.60403800	0.91107700
H	-2.91485700	-3.98020900	0.84293300
C	-3.12172900	-1.84139400	-2.26830400
H	-2.39147100	-2.62883200	-2.49288900
H	-4.12642800	-2.27588800	-2.38992300
H	-3.00345700	-1.06243900	-3.03191500
H	1.53583000	-1.09485300	-0.96114000
C	-0.36340500	2.49801800	0.60644000
C	0.38011700	1.25984100	0.22880200
C	0.17787100	1.09442900	-1.20001200
C	-0.66642100	2.20480500	-1.67497900
O	-1.06556400	2.45069200	-2.79744500
O	-0.44761200	3.03853000	1.69462500
N	-0.97659400	2.98137000	-0.54634200
C	-1.81043300	4.15369200	-0.57224300
H	-2.21294800	4.24847200	-1.58575600
H	-2.63015600	4.06729500	0.15288600
H	-1.23205900	5.05089400	-0.31974100
H	3.59970900	1.13617100	-0.31803600
O	4.38783500	1.06205000	-0.89851400
C	4.23118600	0.02858900	-1.71890800
O	3.24693300	-0.68668200	-1.72052600
H	0.89644300	0.67811600	-1.90472700
O	0.51712700	-2.79943900	-0.96362300
C	1.68030200	-3.61185400	-1.09056900

H	1.35170900	-4.49016800	-1.65283100
H	2.46261400	-3.08323500	-1.65343200
H	2.05511700	-3.92203500	-0.10732900
C	5.39903400	-0.13566300	-2.63812900
H	6.33237300	-0.15674800	-2.06521200
H	5.28931600	-1.05115700	-3.22261400
H	5.45465900	0.72686600	-3.31281600

Int8

Zero-point correction= 0.463748
Thermal correction to Energy= 0.493694
Thermal correction to Gibbs Free Energy= 0.406608
Lowest Frequency = 30.2093 cm⁻¹
SCF (M06) Energy = -1411.7334178

Rh	-0.53037900	-0.38669300	0.01420300
N	1.24970700	-1.74426100	-0.36550300
C	-1.83545100	-0.31695000	1.86871900
C	-2.46391300	0.32108000	0.73136900
C	-2.78628500	-0.69340300	-0.25467400
C	-2.24310700	-1.90600500	0.20492400
C	-1.63280300	-1.66769200	1.51425900
C	2.38477900	-1.15610200	-1.04796900
C	2.97199500	-0.04216300	-0.27770800
C	2.21441600	1.03073900	0.24635600
C	4.34523400	-0.14637800	-0.03779100
C	2.88325100	1.91650200	1.10829500
C	4.98529800	0.75615700	0.79614600
H	4.89142700	-0.96504300	-0.50512800
C	4.23561000	1.77307800	1.38331300
H	2.32170600	2.73669800	1.54621700
H	6.05129000	0.66386800	0.99315500
H	4.71689200	2.48480700	2.05260600
O	2.79566000	-1.61692600	-2.08308600
C	-3.52903500	-0.43244300	-1.51843200
H	-3.07216900	0.38752800	-2.09301000
H	-3.54515100	-1.31633400	-2.16598800
H	-4.57264200	-0.15152300	-1.31111300
C	-3.03617800	1.69411400	0.74082200
H	-3.19432900	2.07373200	-0.27567000
H	-4.01768900	1.68115200	1.24015800
H	-2.40112700	2.40110400	1.28848200
C	-1.45871700	0.38376200	3.12907900
H	-0.94005300	1.33085600	2.92222600
H	-2.34860900	0.62197600	3.73179500
H	-0.79548400	-0.22823200	3.75219000
C	-1.00382600	-2.73251700	2.34747300
H	-0.30618700	-2.31556200	3.08531700
H	-1.76026600	-3.31036700	2.89968500
H	-0.45208600	-3.45413900	1.72893800
C	-2.34457300	-3.24120100	-0.44561200
H	-1.40798600	-3.80382000	-0.35803300
H	-3.14023000	-3.84348100	0.01935100

H	-2.56933900	-3.15371200	-1.51474300
C	0.13381700	2.54006800	0.21139300
C	0.82794700	1.27615600	-0.18445400
C	0.26621500	0.89599200	-1.46678100
C	-0.70482800	1.93160800	-1.86152200
O	-1.43423900	1.98847900	-2.83404600
O	0.20414600	3.17604600	1.25157000
N	-0.68895300	2.90432300	-0.84814100
C	-1.47822500	4.10950700	-0.88041400
H	-0.85997100	4.97264400	-1.15746700
H	-2.26203600	3.97790800	-1.63315800
H	-1.92016000	4.30318600	0.10215700
H	0.80430600	0.38812000	-2.26777900
O	0.80904000	-2.93328600	-0.93208500
C	1.69578600	-4.01216200	-0.67692400
H	2.66368100	-3.87114400	-1.17089300
H	1.83645400	-4.15320300	0.40851200
H	1.19649300	-4.89359600	-1.08961000
H	1.46373200	-1.88765700	0.63015100

TS5

Zero-point correction= 0.458318
Thermal correction to Energy= 0.488709
Thermal correction to Gibbs Free Energy= 0.400963
Lowest Frequency = -529.2045 cm⁻¹
SCF (M06) Energy = -1411.6694475

N	1.18514000	-1.37571200	-1.16395700
C	-2.66868700	-0.20672900	0.28024600
C	-2.07790800	-0.52286600	1.55526500
C	-1.55086700	-1.84084400	1.47191200
C	-1.74112100	-2.30556300	0.11303400
C	-2.48744000	-1.32923300	-0.60648500
Rh	-0.47969900	-0.46167500	-0.08499000
C	2.40960500	-0.84240700	-1.47140100
O	3.08473500	-1.32942400	-2.38008000
C	0.67711500	1.38810800	-0.15336900
C	0.00877400	1.14040100	-1.39709800
H	0.47370700	0.75630500	-2.30287800
C	2.89768200	0.23820300	-0.58268400
C	2.09180400	1.14870300	0.15145900
C	4.28732300	0.24532200	-0.40603800
C	2.72737600	1.93804100	1.13016500
C	4.89275600	1.05953300	0.53338500
H	4.87221300	-0.43794200	-1.01950500
C	4.09721400	1.89150300	1.32074100
H	2.12200300	2.61621500	1.72398400
H	5.97278700	1.03660800	0.66580800
H	4.55144900	2.52872900	2.07799700
O	1.35047400	-2.15178500	0.64410900
C	2.50842600	-2.89275400	0.49606500
H	2.43535100	-3.67144600	-0.28636100
H	2.66338000	-3.39700600	1.46705100

H	3.41250000	-2.28775700	0.31065000
C	-3.00863400	-1.39454800	-1.99963200
H	-2.92032600	-0.41779100	-2.49618300
H	-4.07122500	-1.68177200	-2.01747800
H	-2.45980900	-2.12535700	-2.60576200
C	-1.29455600	-3.63492100	-0.38690800
H	-1.36193800	-3.70035600	-1.47983900
H	-1.91327000	-4.44296000	0.02981800
H	-0.25419300	-3.82217200	-0.09074700
C	-0.79103900	-2.56672000	2.50590600
C	-2.10610400	0.36350500	2.75326500
H	-1.42853700	0.00131300	3.53421700
H	-3.11749900	0.41841600	3.18290000
H	-1.79200800	1.38957000	2.51352600
C	-3.57801900	0.93864100	0.01477300
H	-3.43567400	1.74666100	0.74088200
H	-4.62002400	0.59592600	0.10744300
H	-3.46075900	1.35088600	-0.99537200
H	1.03444200	-2.24318800	-1.68195700
C	-0.11289900	2.46797900	0.52511900
C	-1.09024100	2.11501200	-1.54251400
N	-1.09341900	2.88305000	-0.37459000
O	-1.88148000	2.24738400	-2.45701600
O	-0.01391800	2.93279400	1.64609700
C	-2.02283800	3.94425900	-0.08225900
H	-2.53970300	3.75889500	0.86785100
H	-1.49777000	4.90322200	-0.00099900
H	-2.74516700	3.99068200	-0.90273400
H	0.29101400	-2.51323500	2.24983200
H	-0.93752500	-2.14300800	3.50523400
H	-1.05384600	-3.63292900	2.53444600

Int9

Zero-point correction= 0.528483
Thermal correction to Energy= 0.564053
Thermal correction to Gibbs Free Energy= 0.463510
Lowest Frequency = 28.1788 cm⁻¹
SCF (M06) Energy = -1640.7208222

Rh	0.40992800	0.03052400	-0.42690200
N	-0.43267800	-1.89636800	0.32500300
C	0.71065000	0.82543500	-2.52919900
C	1.52331200	1.52846700	-1.55509900
C	2.54504600	0.62572200	-1.06136000
C	2.27761200	-0.63783000	-1.61222500
C	1.12969600	-0.52078900	-2.51456000
C	-1.62739400	-1.96710300	-0.46567700
C	-2.72579800	-1.07635000	-0.00741600
C	-2.56532200	0.24503400	0.45466600
C	-3.99818700	-1.65291800	-0.08906400
C	-3.72222600	0.93267900	0.84311300
C	-5.12480500	-0.95196800	0.30917300
H	-4.08162100	-2.66340900	-0.48458300

C	-4.97978800	0.34865100	0.78022400
H	-3.63013000	1.96489100	1.17518800
H	-6.10862600	-1.41177000	0.24105900
H	-5.85327900	0.92160500	1.08709400
O	-1.72126400	-2.76394800	-1.37285200
C	3.63218400	1.01263400	-0.11981000
H	3.24330600	1.61354600	0.71509100
H	4.12382600	0.13332000	0.31141200
H	4.40242300	1.61470200	-0.62594500
C	1.56268900	3.00606800	-1.38599800
H	1.92746000	3.29253400	-0.39126400
H	2.25228400	3.44464300	-2.12395500
H	0.57839300	3.46308400	-1.54486600
C	-0.38285800	1.44464600	-3.33065500
H	-1.03608700	2.07177700	-2.70688900
H	0.02306500	2.08224700	-4.13062100
H	-1.01417300	0.68218900	-3.80204300
C	0.59141700	-1.65145500	-3.32081400
H	-0.33913700	-1.37540700	-3.82989700
H	1.31525300	-1.96742100	-4.08745200
H	0.36304100	-2.52505900	-2.69506300
C	3.08416400	-1.87994300	-1.45590600
H	2.44439600	-2.76942500	-1.40339400
H	3.75340700	-2.01459300	-2.31945300
H	3.70784000	-1.85216700	-0.55442800
H	-0.55389500	-1.81805800	1.34555200
C	-1.28131200	2.42801500	0.21205800
C	-1.26326800	0.96085600	0.50374900
C	-0.20353100	0.76727800	1.47334300
C	0.38781000	2.08151100	1.77679800
O	1.32691700	2.35841000	2.50712500
O	-1.97046900	3.04698300	-0.57841700
N	-0.32033100	3.02691400	1.02970100
C	-0.07537700	4.44612800	1.08301600
H	0.93925200	4.60645000	1.46143400
H	-0.18604300	4.88422900	0.08611600
H	-0.78583200	4.93907200	1.75874900
H	-0.23184800	0.04307700	2.28744300
O	0.46772200	-2.94340700	0.08972800
H	1.90526000	-2.35964800	1.12827600
O	2.49880900	-1.90470500	1.77206000
C	1.76508700	-1.57327400	2.83360800
C	2.45918100	-0.62656300	3.74913300
H	2.20323200	0.39498700	3.41521200
H	2.08971200	-0.75191700	4.77027100
H	3.54614300	-0.73975000	3.70586900
O	0.61764600	-1.96407500	2.98899800
C	0.00198300	-4.17590100	0.65200000
H	-0.15077100	-4.05908200	1.73323600
H	-0.91041900	-4.50799900	0.14780200
H	0.80722100	-4.89228500	0.46597600

TS6

Zero-point correction= 0.524582
Thermal correction to Energy= 0.560123
Thermal correction to Gibbs Free Energy= 0.459641
Lowest Frequency = -214.8315 cm⁻¹
SCF (M06) Energy = -1640.6924724

Rh	0.27690500	-0.58956500	-0.12500000
N	-1.34318900	0.50829500	0.07982700
C	0.88011700	-1.70224800	-1.99229800
C	1.68135100	-2.17855500	-0.89697100
C	0.82376700	-2.83532000	0.05062500
C	-0.51155400	-2.73391900	-0.43446500
C	-0.48009500	-2.01441300	-1.68887100
C	-1.58368900	1.86803200	-0.25636800
C	-0.46562900	2.84005900	-0.26788800
C	0.90377300	2.53560000	-0.12378800
C	-0.86474500	4.16056900	-0.50956000
C	1.81798800	3.59037600	-0.25010200
C	0.05438400	5.18960100	-0.61381600
H	-1.92971200	4.34753400	-0.62294800
C	1.40668400	4.89446200	-0.49108400
H	2.88203600	3.38466000	-0.16844100
H	-0.27945200	6.20843700	-0.79893700
H	2.15415400	5.68065700	-0.58496800
O	-2.71896300	2.18689400	-0.55757500
C	1.28017800	-3.51524100	1.29540800
H	1.89931300	-2.85609000	1.92217600
H	0.43098500	-3.83945300	1.90820300
H	1.87929200	-4.40739400	1.05989500
C	3.16719300	-2.24604400	-0.90320700
H	3.57249200	-2.37690500	0.10667300
H	3.49335300	-3.11188500	-1.49962700
H	3.61998900	-1.35349200	-1.35254400
C	1.41274600	-1.04681200	-3.21888000
H	2.20608600	-0.32660200	-2.97695800
H	1.83986600	-1.79107500	-3.90838300
H	0.62795800	-0.50599500	-3.75995000
C	-1.66481200	-1.75696600	-2.55684900
H	-1.50288800	-0.89071200	-3.20986300
H	-1.86357000	-2.62589000	-3.20200400
H	-2.57443500	-1.56966500	-1.97237500
C	-1.73409900	-3.34331700	0.15850900
H	-2.60185800	-2.67619400	0.08260100
H	-1.98998300	-4.27244400	-0.37340900
H	-1.59160000	-3.59697300	1.21542900
C	2.88238900	0.90298300	-0.09519700
C	1.44355000	1.19961200	0.23235200
C	1.17929200	0.52317900	1.46592700
C	2.42623900	-0.12225500	1.92851100
O	2.62824900	-0.81269900	2.90798600
O	3.51573100	1.19118200	-1.09258000

N	3.40898800	0.19511300	0.98462000
C	4.78930300	-0.20236800	1.11119000
H	5.31026000	0.44382400	1.82834100
H	4.85335600	-1.23421100	1.47332800
H	5.26677600	-0.10914000	0.13147600
H	0.42841300	0.83974900	2.18730200
O	-2.06818000	0.68784700	1.88594700
H	-2.20930500	0.00056700	-0.16815000
C	-1.83651400	-0.51007200	2.50763900
H	-1.49584500	-0.35095300	3.54613900
H	-2.71723500	-1.18124300	2.50035500
H	-0.99731600	-1.05838200	2.00464600
O	-4.66954000	0.58798200	1.32710400
C	-4.82292500	-0.24105200	0.32093100
O	-3.90266300	-0.83773900	-0.22694100
C	-6.25182400	-0.37694700	-0.10710300
H	-6.53398500	0.51774700	-0.67588400
H	-6.37361000	-1.25587700	-0.74440900
H	-6.91414600	-0.43237500	0.76266100
H	-3.68617600	0.70495100	1.52406600

Int10

Zero-point correction= 0.524018

Thermal correction to Energy= 0.559761

Thermal correction to Gibbs Free Energy= 0.459561

Lowest Frequency = 21.7979 cm⁻¹

SCF (M06) Energy = -1640.7050598

Rh	0.31112900	-0.62964400	-0.33938900
N	-1.36804100	0.21302900	-0.72551500
C	1.33945100	-1.91978600	-1.77906300
C	2.08648700	-2.05771700	-0.55962400
C	1.20569500	-2.57730300	0.42647300
C	-0.07238200	-2.87532500	-0.20615200
C	0.00046100	-2.43128300	-1.55962700
C	-1.87423400	1.48880800	-0.59167400
C	-0.92931200	2.64810600	-0.63488300
C	0.46475100	2.58020100	-0.44477400
C	-1.51068400	3.85636700	-1.01284400
C	1.23030500	3.72540100	-0.70196700
C	-0.74371900	4.99253200	-1.23808300
H	-2.59006700	3.86640000	-1.14628200
C	0.63457600	4.91737100	-1.09925000
H	2.30905500	3.68940100	-0.58027900
H	-1.22098000	5.92359000	-1.53744400
H	1.25843300	5.78771800	-1.29423500
O	-3.08447500	1.67369800	-0.59132300
C	1.51787700	-2.92150500	1.83767900
H	0.70114000	-2.62268200	2.50671900
H	1.65009000	-4.00915500	1.93718900
H	2.42714100	-2.43184900	2.20088900
C	3.54908300	-1.82007600	-0.43734700
H	3.87335300	-1.82023000	0.60807100

H	4.09693200	-2.62596300	-0.94783500
H	3.85756100	-0.87264000	-0.89721200
C	1.87599900	-1.41556600	-3.07327400
H	2.96564200	-1.52336400	-3.12141200
H	1.43556100	-1.96036200	-3.91762200
H	1.64709200	-0.35036500	-3.21619100
C	-1.06624200	-2.55761700	-2.58869900
H	-0.99906800	-1.74884500	-3.32681600
H	-0.96700700	-3.51354700	-3.12437300
H	-2.06080600	-2.50345800	-2.12620700
C	-1.23778600	-3.46374200	0.47094100
H	-1.89115500	-3.98050900	-0.24050000
H	-0.92721200	-4.15664800	1.26269900
H	-1.87159100	-2.66392400	0.92868000
C	2.65801500	1.30468500	0.10382400
C	1.15043600	1.43666200	0.18987100
C	0.75554500	0.77875100	1.35739400
C	1.97948300	0.35691800	2.09204800
O	2.08189000	-0.17517000	3.17324100
O	3.39523300	1.60972500	-0.80957400
N	3.07024400	0.73324700	1.29957600
C	4.44454000	0.56587000	1.70705100
H	5.08155600	0.64888900	0.82195300
H	4.72782400	1.33926400	2.43087700
H	4.57680100	-0.41199200	2.18330400
H	-0.20612900	0.90596600	1.87079600
O	-2.08443200	0.95976600	2.27245700
H	-2.14660300	-0.46483900	-0.90823000
O	-3.18678600	-1.30164200	1.32612800
C	-3.91454700	-1.32369500	0.28941800
O	-3.51250900	-1.58755100	-0.87088000
C	-5.37322100	-0.94811900	0.46295500
H	-5.45875500	0.13190700	0.27961400
H	-6.00002900	-1.46072400	-0.27415900
H	-5.72147600	-1.15489000	1.48044100
H	-2.41442100	0.10037900	1.91196300
C	-3.22458800	1.71933400	2.57307400
H	-2.91432600	2.59713900	3.15327200
H	-3.73675700	2.06526600	1.65910200
H	-3.94535100	1.14385000	3.17609100

Int11

Zero-point correction= 0.418817

Thermal correction to Energy= 0.446632

Thermal correction to Gibbs Free Energy= 0.363142

Lowest Frequency = 32.1399 cm⁻¹

SCF (M06) Energy = - 1296.4882045

N	0.73439700	-1.93568500	-0.72067900
C	-1.92804300	-0.07576300	1.60563500
C	-2.57035800	0.38510100	0.42788500
C	-2.71964700	-0.73738600	-0.45982200
C	-2.26938900	-1.93512800	0.23213100

C	-1.77807700	-1.52598900	1.50667700
C	2.07658900	-1.88670200	-1.05471800
C	2.93671100	-0.82316100	-0.44028300
C	2.49994000	0.42358300	0.07027100
C	4.26115400	-1.20097500	-0.26276000
C	3.40537500	1.20513200	0.80689400
C	5.15880600	-0.39795100	0.44202200
H	4.57316000	-2.16039100	-0.66927000
C	4.72115200	0.79400500	0.99571600
H	3.08114100	2.15737200	1.21425700
H	6.18992000	-0.72060100	0.56703400
H	5.40034900	1.42140600	1.56827600
O	2.56791000	-2.78088500	-1.72390200
C	-3.29522000	-0.65947800	-1.82234900
H	-2.91311300	0.22072500	-2.35794000
H	-3.07538000	-1.55134400	-2.41786000
H	-4.38982500	-0.55732000	-1.76340700
C	-3.12425500	1.73912200	0.17500200
H	-2.98082200	2.06920600	-0.86040400
H	-4.20876400	1.71478500	0.35702600
H	-2.70326200	2.48942200	0.85133400
C	-1.52573500	0.73902300	2.78013200
H	-1.36991300	1.79213500	2.51901400
H	-2.30013500	0.69411900	3.55995400
H	-0.59146800	0.37280400	3.22280900
C	-1.20096200	-2.39363400	2.56137700
H	-0.36902400	-1.89996000	3.07695900
H	-1.96486300	-2.62190400	3.31960300
H	-0.83296900	-3.34294200	2.15825100
C	-2.35741100	-3.32314300	-0.29128200
H	-1.63720700	-3.99166600	0.19385500
H	-3.35873900	-3.73721100	-0.10856300
H	-2.18365000	-3.36267700	-1.37348400
H	0.38365400	-2.85580300	-0.99519300
C	0.68357700	2.28093600	0.39322900
C	1.22008100	1.02440500	-0.28657800
C	0.47547600	0.87184800	-1.44680700
C	-0.43247500	2.04355600	-1.60183300
O	-1.23255400	2.25730700	-2.48316000
O	0.94035100	2.71112200	1.49323500
N	-0.20244000	2.86448300	-0.49728900
C	-0.82051800	4.15572700	-0.27166200
H	-0.07541800	4.95174000	-0.37440900
H	-1.60275500	4.29243100	-1.02291900
H	-1.24336200	4.20481000	0.73778900
H	0.73820100	0.27841100	-2.31885000

TS5

Zero-point correction= 0.415386
 Thermal correction to Energy= 0.443620
 Thermal correction to Gibbs Free Energy= 0.357186
 Lowest Frequency = -385.7243 cm⁻¹
 SCF (M06) Energy = -1296.4630817

Rh	0.78976900	-0.25011700	0.02157900
N	-0.76170200	-0.20559700	-1.38568700
C	2.52556000	-1.12007900	-1.01198400
C	2.95063600	-0.04844900	-0.11571900
C	2.63517000	-0.41100200	1.23863200
C	1.93949100	-1.65649800	1.17849100
C	1.89613900	-2.11022400	-0.22133600
C	-1.73506500	-1.20115200	-1.40573600
C	-2.75631500	-1.00244600	-0.35676700
C	-2.64996700	0.14972700	0.42686200
C	-3.79332200	-1.90459800	-0.14923300
C	-3.56817700	0.38958500	1.44764600
C	-4.72546000	-1.65338600	0.84977100
H	-3.84971300	-2.78861600	-0.78215500
C	-4.61123600	-0.51146000	1.64227500
H	-3.48591700	1.28192000	2.06679000
H	-5.54424700	-2.34929800	1.01763000
H	-5.34408300	-0.31953500	2.42307000
O	-1.75141000	-2.10063400	-2.22830400
C	2.94877800	0.40906100	2.43960400
H	2.61950500	1.44875000	2.30596600
H	2.46405300	0.01349000	3.33851900
H	4.03144200	0.41776800	2.62615700
C	3.60357000	1.21698300	-0.51690100
H	3.24000100	2.05893400	0.08636400
H	4.68929100	1.13970700	-0.35082400
H	3.44873700	1.44437800	-1.57703000
C	2.67362600	-1.14488400	-2.48941900
H	2.56633500	-0.14541700	-2.92895200
H	3.66633100	-1.52072300	-2.77520800
H	1.92619800	-1.80132200	-2.95088600
C	1.25107900	-3.35124400	-0.72273500
H	0.48691200	-3.13257900	-1.48549800
H	1.99829100	-4.01054700	-1.18586600
H	0.76542200	-3.91233000	0.08174100
C	1.34234500	-2.39617300	2.31416100
H	0.36653800	-2.82072200	2.04497000
H	1.99212900	-3.23537300	2.60476800
H	1.20829000	-1.75631700	3.19250200
H	-0.32175100	-0.14893700	-2.30895400
C	-1.54338100	2.25282400	-0.75133400
C	-1.52158500	1.06047400	0.19721600
C	-0.45652700	1.24019500	1.09120400
C	0.23496100	2.50785700	0.71522200
O	1.21506900	3.01549300	1.21960200
O	-2.35752800	2.50038000	-1.59861800
N	-0.43647600	3.01839100	-0.39584600
C	-0.06456000	4.25518200	-1.05534000
H	-0.85609800	4.50335400	-1.76701800
H	0.03905600	5.05376700	-0.31465400
H	0.88699600	4.13771500	-1.58581900
H	-0.44969700	0.86397400	2.11513900

Int12

Zero-point correction= 0.419856
Thermal correction to Energy= 0.447276
Thermal correction to Gibbs Free Energy= 0.363909
Lowest Frequency = 27.7975 cm⁻¹
SCF (M06) Energy = -1296.5115964

Rh	-0.98470500	-0.05423400	-0.13394300
C	-2.53847000	-1.73116200	-0.36457600
C	-1.99023700	-1.55201800	0.98383300
C	-2.39733100	-0.25599500	1.49066600
C	-3.15489800	-0.52881100	-0.72285200
C	-3.02613500	0.41119200	0.40611900
C	-1.23667400	-2.59029300	1.72317100
H	-0.64146800	-3.21097700	1.04167400
H	-0.56813300	-2.15370400	2.47430800
H	-1.93534600	-3.25927300	2.24942800
C	-2.37897000	-2.96999700	-1.16976400
H	-1.32122100	-3.23895900	-1.29326600
H	-2.88183100	-3.81504500	-0.67913800
H	-2.80891100	-2.86117500	-2.17029200
C	-3.79522800	-0.17906500	-2.01452800
H	-3.40502700	0.76728600	-2.41248700
H	-3.64162700	-0.95237900	-2.77330400
H	-4.87830100	-0.04376300	-1.88125400
C	-3.52579700	1.80780600	0.43054900
H	-3.68658200	2.20339300	-0.57831500
H	-4.48673600	1.85990300	0.96388100
H	-2.82033000	2.46876900	0.95264900
C	-2.18075600	0.29326400	2.85543900
H	-3.09197700	0.18074200	3.45942700
H	-1.37229000	-0.22640400	3.38199600
H	-1.93020100	1.36028400	2.81890400
C	2.79247600	-0.20561600	0.17918800
C	2.66786400	-1.51568600	-0.27713400
C	3.58925900	-2.50376800	0.06206400
C	4.65085900	-2.13998200	0.87832400
C	4.77339600	-0.82425200	1.34205600
C	3.84238700	0.15730300	1.00770300
H	3.47350100	-3.51652800	-0.31956000
H	5.39893800	-2.87769100	1.15885300
H	5.61964400	-0.56143400	1.97366400
H	3.94949000	1.17747200	1.37520800
C	1.50299100	-1.64703400	-1.14616600
H	0.83341500	0.00251500	-2.18268100
O	1.05137800	-2.58989400	-1.73915000
N	0.88796000	-0.31241400	-1.20870300
C	1.62521200	0.61193300	-0.27654800
C	0.59419900	0.97334800	0.77606000
C	1.91488900	1.92951700	-1.00237500
C	0.36073000	2.43487200	0.66338000
H	0.75905100	0.62604700	1.80063600

O	-0.39083600	3.13157400	1.31041000
O	2.60394900	2.05609900	-1.98532500
N	1.17212600	2.91275600	-0.38601200
C	1.18503100	4.29322200	-0.83115700
H	0.90833100	4.34874800	-1.88927900
H	0.46790300	4.84658900	-0.22010100
H	2.18611300	4.71882800	-0.70869500

Product 3aa

Zero-point correction = 0.206631
 Thermal correction to Energy = 0.220400
 Thermal correction to Gibbs Free Energy = 0.165792
 Lowest Frequency = 27.7975 cm⁻¹
 SCF (M06) Energy = - 798.0104191

C	-0.80563000	0.46567300	-0.17811400
C	-2.03527700	-0.16628200	-0.06030200
C	-3.19850100	0.54380700	0.19168500
C	-3.09875200	1.92532400	0.32192600
C	-1.86190900	2.56440400	0.19754100
C	-0.69575100	1.84200600	-0.05340500
H	-4.14839500	0.01954600	0.28136700
H	-3.98900100	2.51841600	0.52225100
H	-1.80686000	3.64674500	0.30042800
H	0.26507100	2.34976800	-0.14590700
C	-1.85507400	-1.62460900	-0.24837100
O	-2.67453700	-2.51110000	-0.15727300
C	0.26674400	-0.57284700	-0.42726600
C	1.22696400	-0.22547400	-1.56796400
H	0.82811400	0.50264900	-2.28270900
H	1.50102000	-1.12476000	-2.13637100
N	-0.51400900	-1.77761300	-0.58153600
H	-0.09695400	-2.69587200	-0.48770100
C	1.18298700	-0.62291700	0.80897900
O	0.92203600	-1.09135700	1.88844300
C	2.47151300	0.30801100	-0.89221800
O	3.40988800	0.86965100	-1.40120700
N	2.36875400	0.00599300	0.46763600
C	3.42503800	0.24881800	1.42646700
H	4.22897900	0.77796900	0.90826900
H	3.04542700	0.85408400	2.25599900
H	3.79616600	-0.70024800	1.82820600

N-Methoxy Benzamide

Zero-point correction= 0.159856
 Thermal correction to Energy= 0.169907
 Thermal correction to Gibbs Free Energy= 0.123802
 Lowest Frequency = 62.0051 cm⁻¹
 SCF (M06) Energy = -515.0590564

C	-1.13040800	-1.16659000	0.14423100
C	-0.64532100	0.13655600	0.00527200
C	-1.54427600	1.19987300	-0.09584700

C	-2.91154400	0.96142400	-0.08612000
C	-3.39105900	-0.34023900	0.03922900
C	-2.50018300	-1.40250000	0.16083700
H	-0.43796300	-1.99677300	0.27929100
H	-1.14155300	2.20748500	-0.17999600
H	-3.60871200	1.79296500	-0.17261700
H	-4.46371700	-0.52663100	0.05140000
H	-2.87407900	-2.41794400	0.27953900
C	0.80795500	0.47142600	-0.02496400
H	1.28022000	-1.27827700	-1.01939900
O	1.24740100	1.56821200	0.25557100
C	3.73006200	-0.32880400	0.52025500
H	4.75284400	-0.12494000	0.18929400
H	3.41280600	0.44394500	1.23183000
H	3.68013700	-1.31953400	0.99406100
O	2.94109700	-0.28708100	-0.65579200
N	1.62866600	-0.60231700	-0.34700000

MeOH

Zero-point correction= 0.051508
Thermal correction to Energy= 0.054809
Thermal correction to Gibbs Free Energy= 0.028792
Lowest Frequency = 334.4452 cm⁻¹
SCF (M06) Energy = -115.641166

C	-0.04628900	0.65254200	0.00000000
H	0.43590700	1.08332700	0.89344200
H	0.43590700	1.08332700	-0.89344200
H	-1.09368200	0.97220700	0.00000000
O	-0.04628900	-0.75032400	0.00000000
H	0.86992100	-1.05151800	0.00000000

Acetic acid

Zero-point correction= 0.062337
Thermal correction to Energy= 0.066806
Thermal correction to Gibbs Free Energy= 0.035470
Lowest Frequency = 108.0503 cm⁻¹
SCF (M06) Energy = -115.641166

C	-1.38738700	-0.09771600	0.00001400
H	-1.67932100	-0.67914700	0.88211200
H	-1.67937700	-0.68112000	-0.88074600
H	-1.90452400	0.86389000	-0.00096800
C	0.09289800	0.12493400	-0.00018500
O	0.65509000	1.19169300	0.00004400
O	0.76047300	-1.04812900	0.00001100
H	1.70565000	-0.81544600	0.00019100

Acetate ion

Zero-point correction= 0.048439
Thermal correction to Energy= 0.052014
Thermal correction to Gibbs Free Energy= 0.022550
SCF (M06) Energy = -228.3723715

C	-0.21955000	0.00008100	-0.01287500
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O	-0.74446100	1.13533400	0.00285400
O	-0.74905400	-1.13297100	0.00285400
C	1.34416500	-0.00225600	-0.00493100
H	1.70127900	0.01272200	1.03728200
H	1.74869100	-0.91007000	-0.47563500
H	1.75046200	0.89149800	-0.50047000

Maleimide

Zero-point correction= 0.096399

Thermal correction to Energy= 0.102795

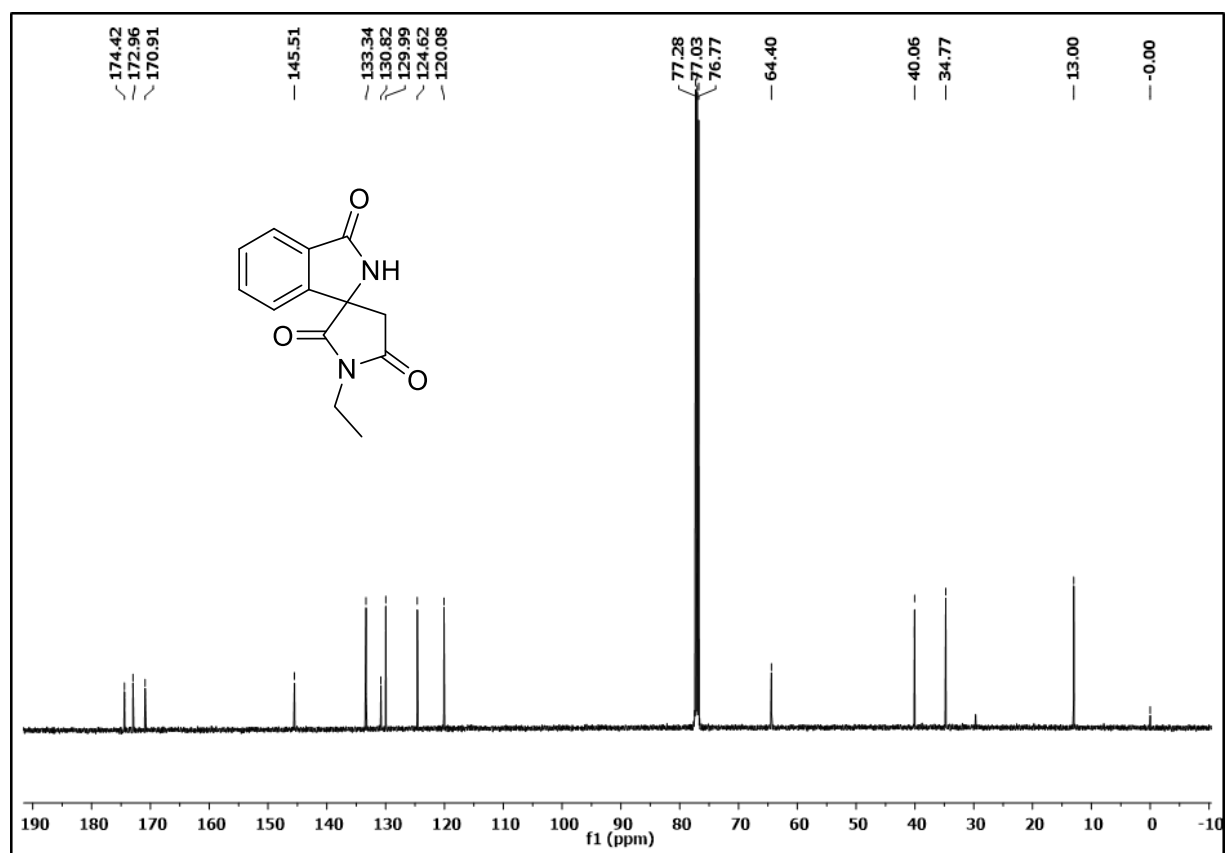
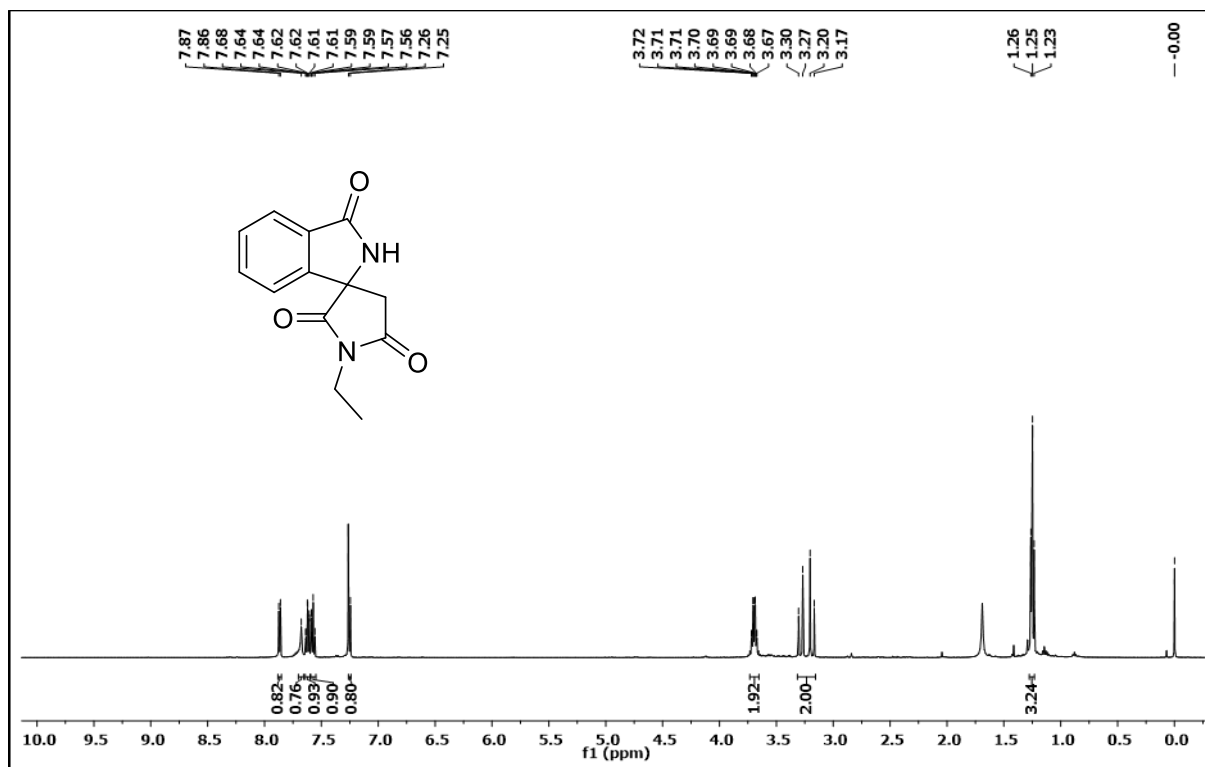
Thermal correction to Gibbs Free Energy= 0.065696

SCF (M06) Energy = -398.4946859

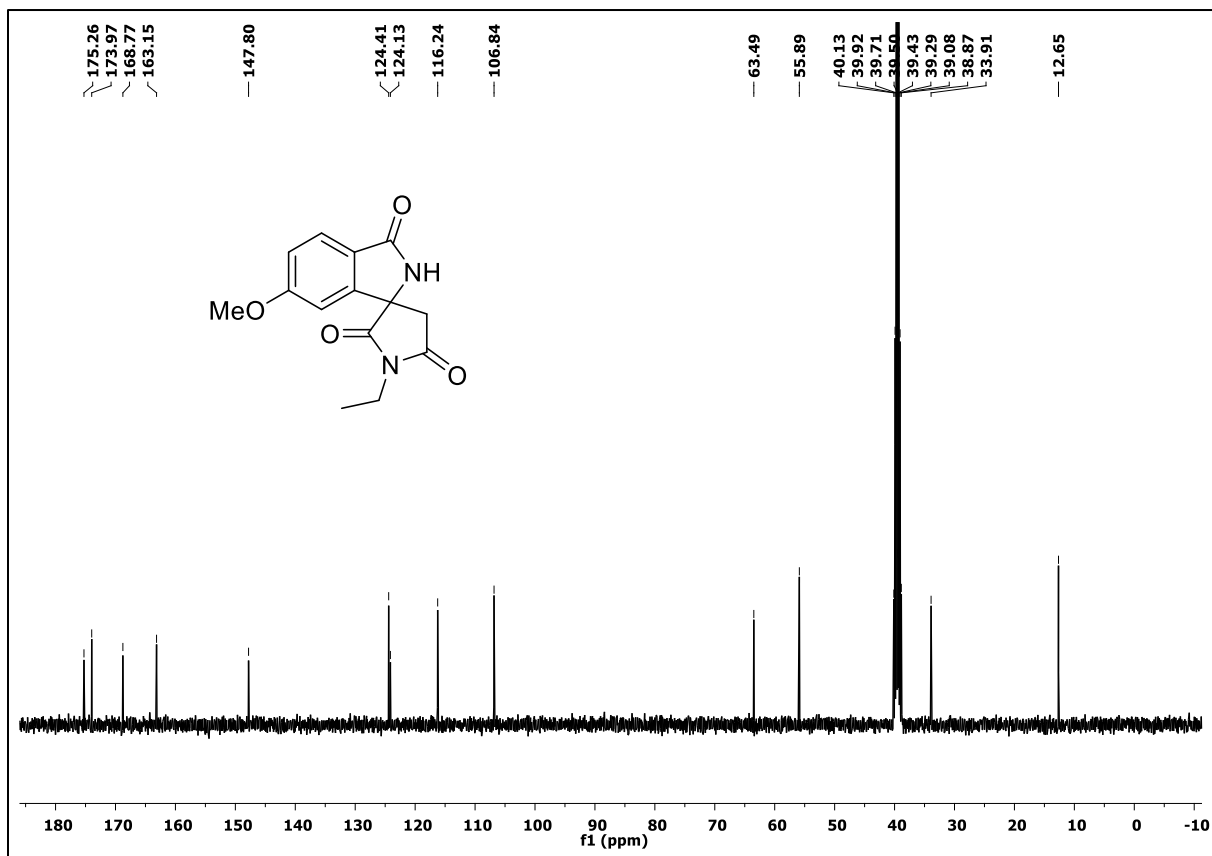
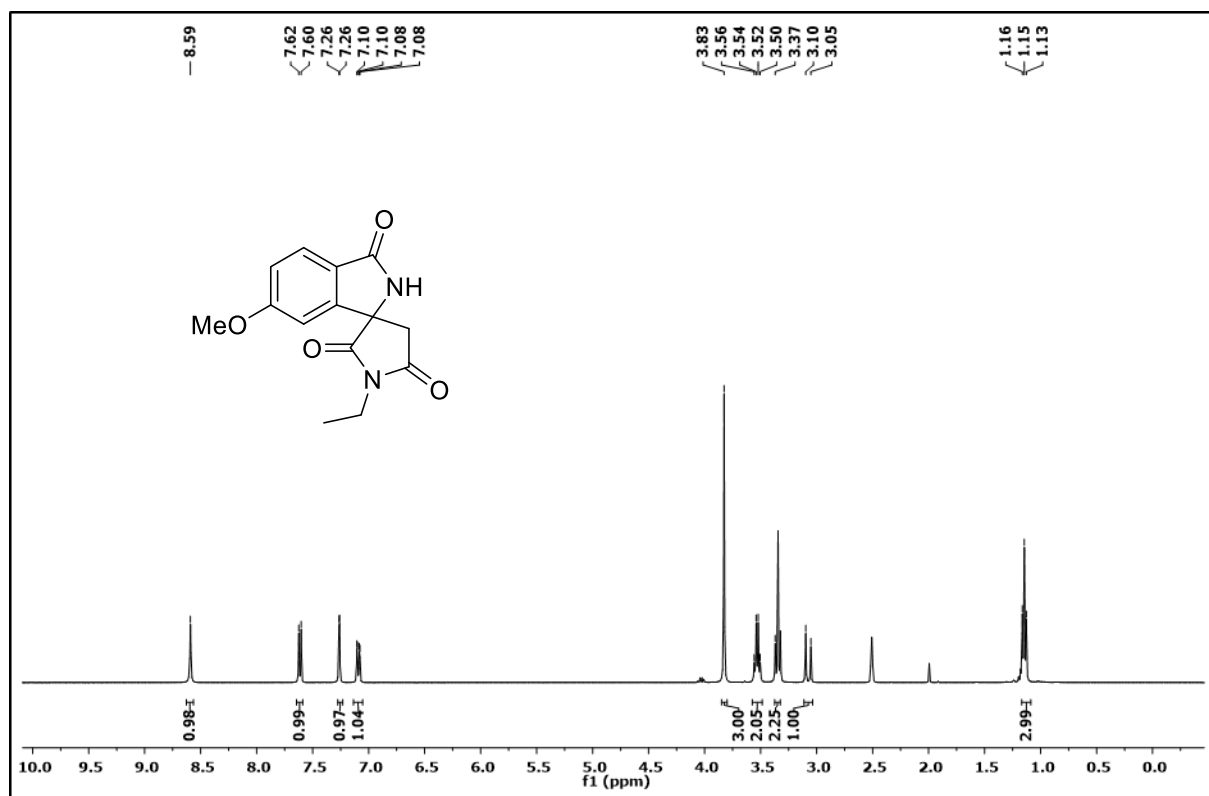
C	1.14715300	-0.20197000	0.00192900
C	0.66668900	-1.62063100	0.00286500
C	-0.66579300	-1.62099800	0.00285500
C	-1.14700000	-0.20258500	0.00186500
H	1.35723800	-2.45677200	0.00053000
H	-1.35588200	-2.45751800	0.00055200
O	-2.28429800	0.20442700	-0.00543800
O	2.28427100	0.20553900	-0.00546900
N	-0.00015800	0.58883000	0.00263500
C	-0.00070900	2.03205200	0.00298400
H	-0.89413100	2.38270400	-0.52213500
H	-0.00825000	2.43228200	1.02392200
H	0.90031200	2.38255900	-0.50905000

Characteristic spectra of all compounds

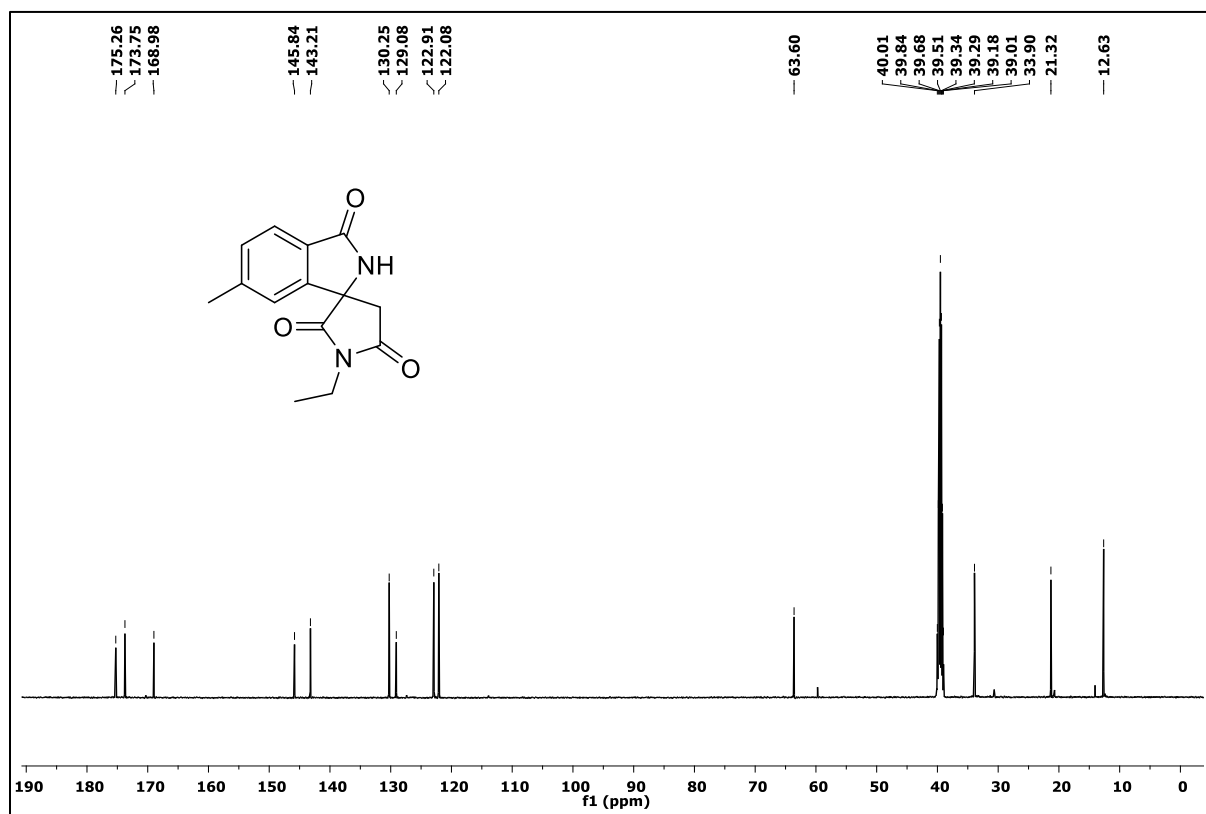
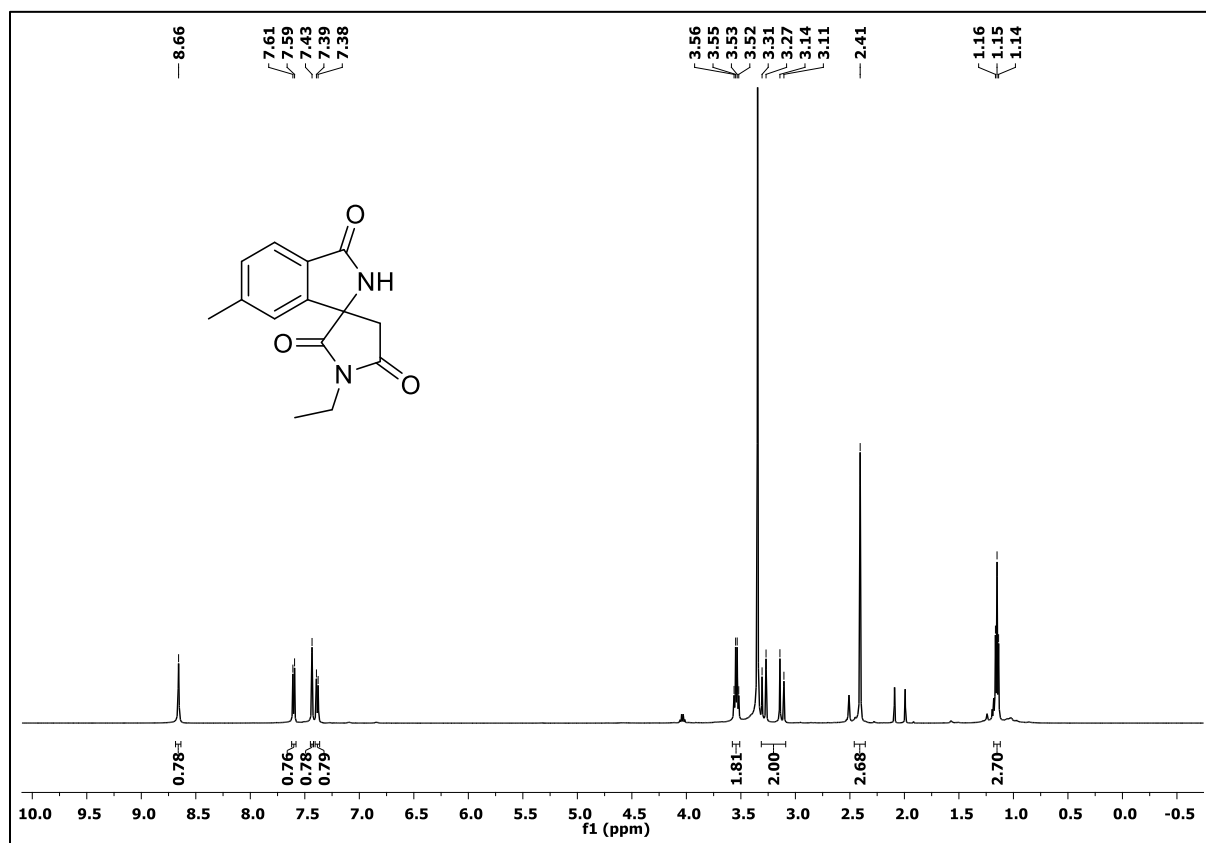
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3aa**.

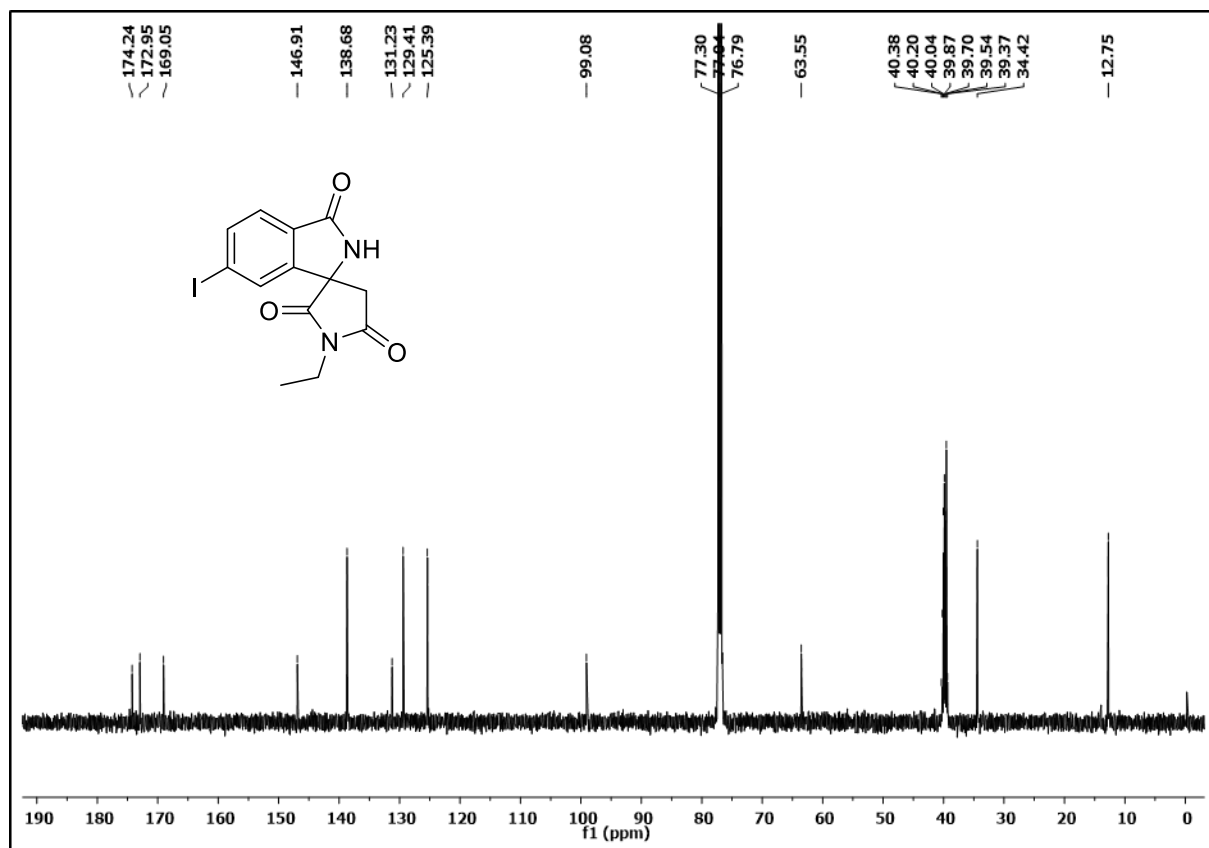
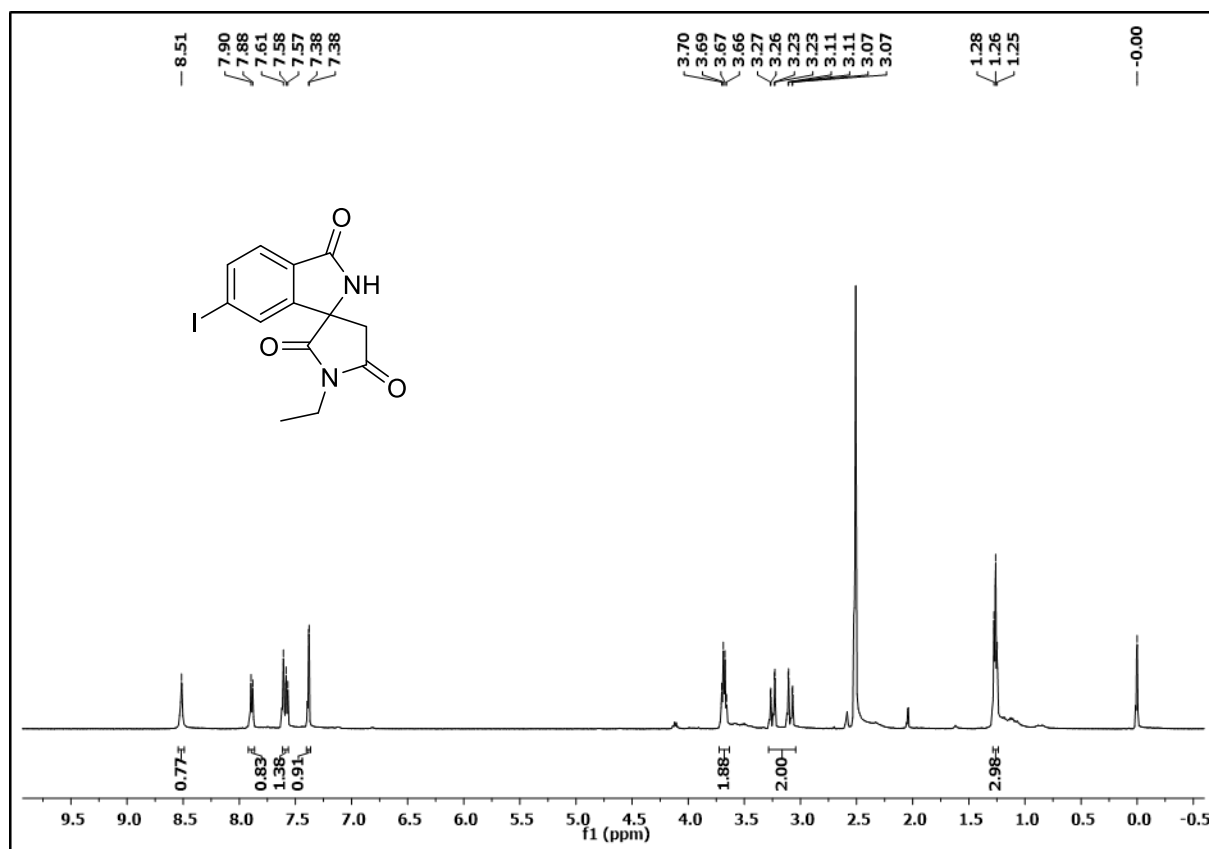


^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3ba**.

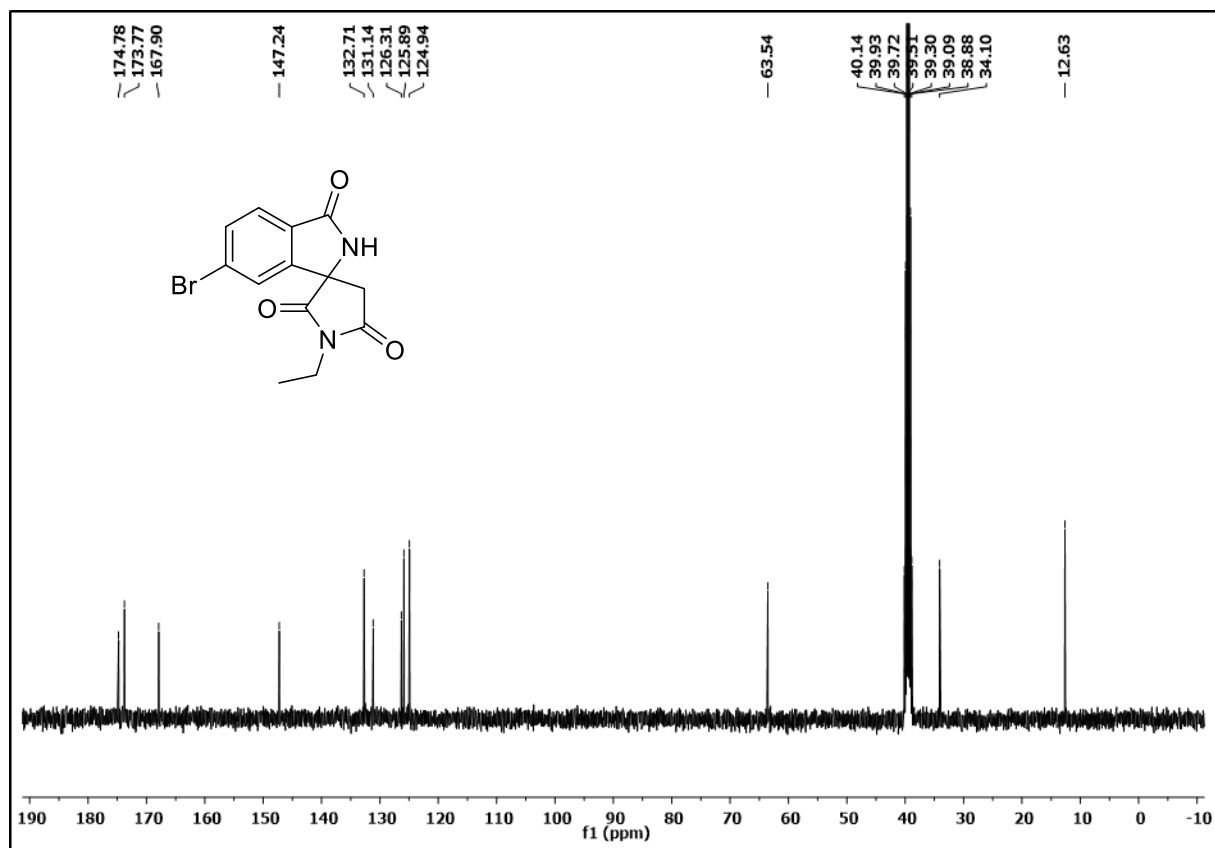
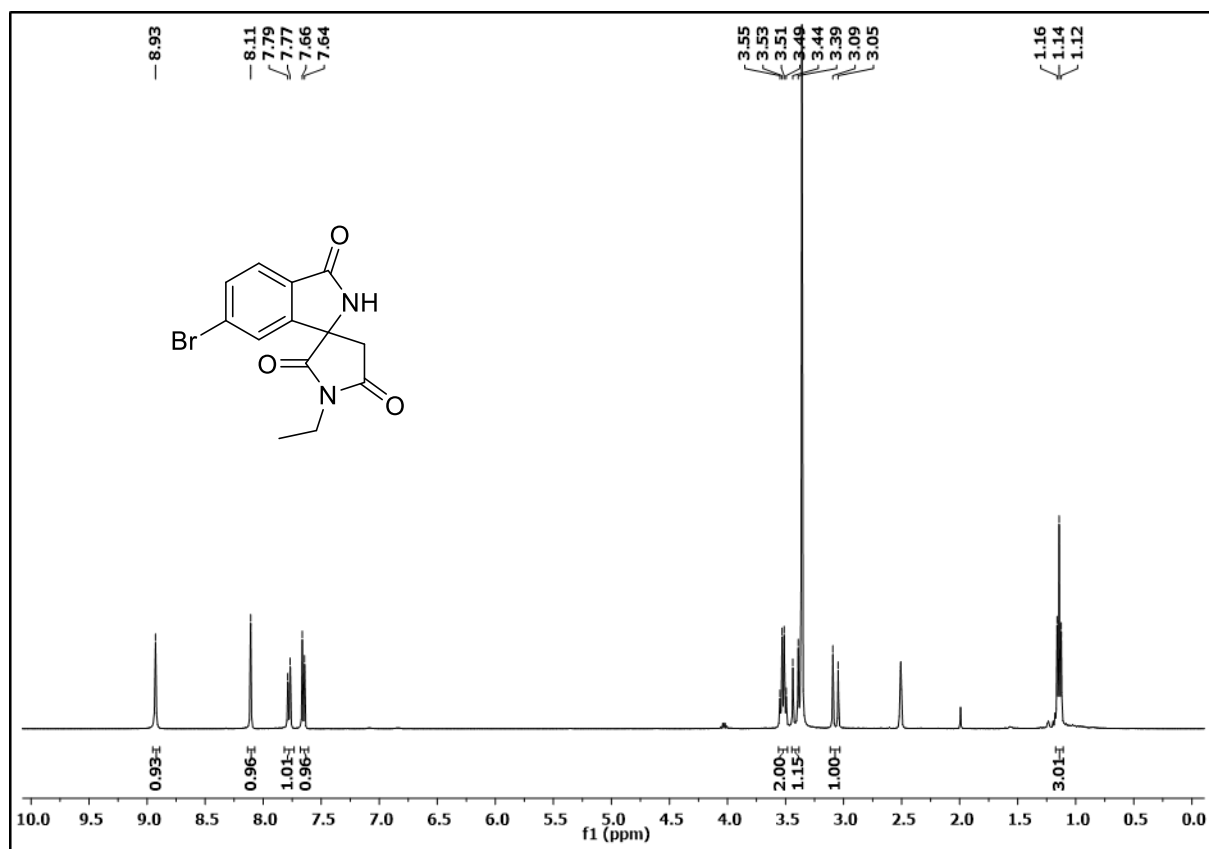


^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3ca**.

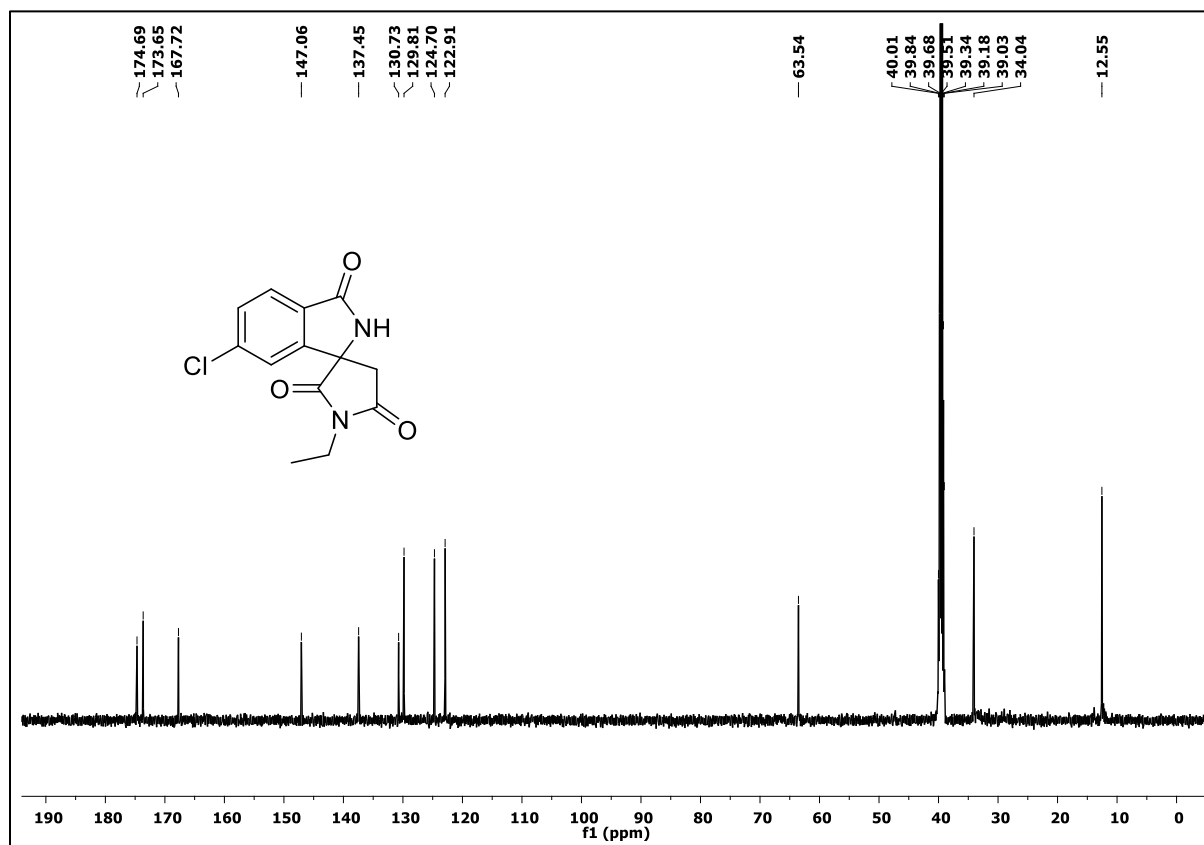
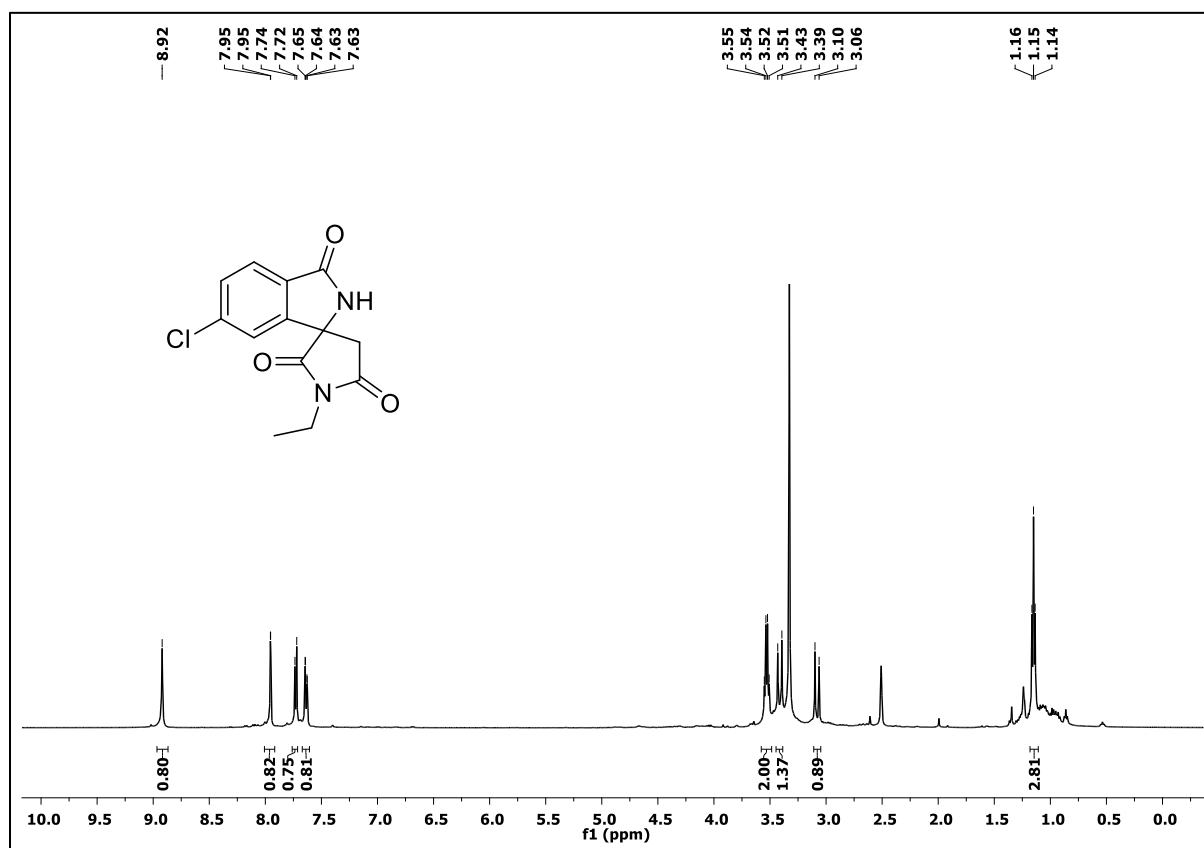


^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3da**.

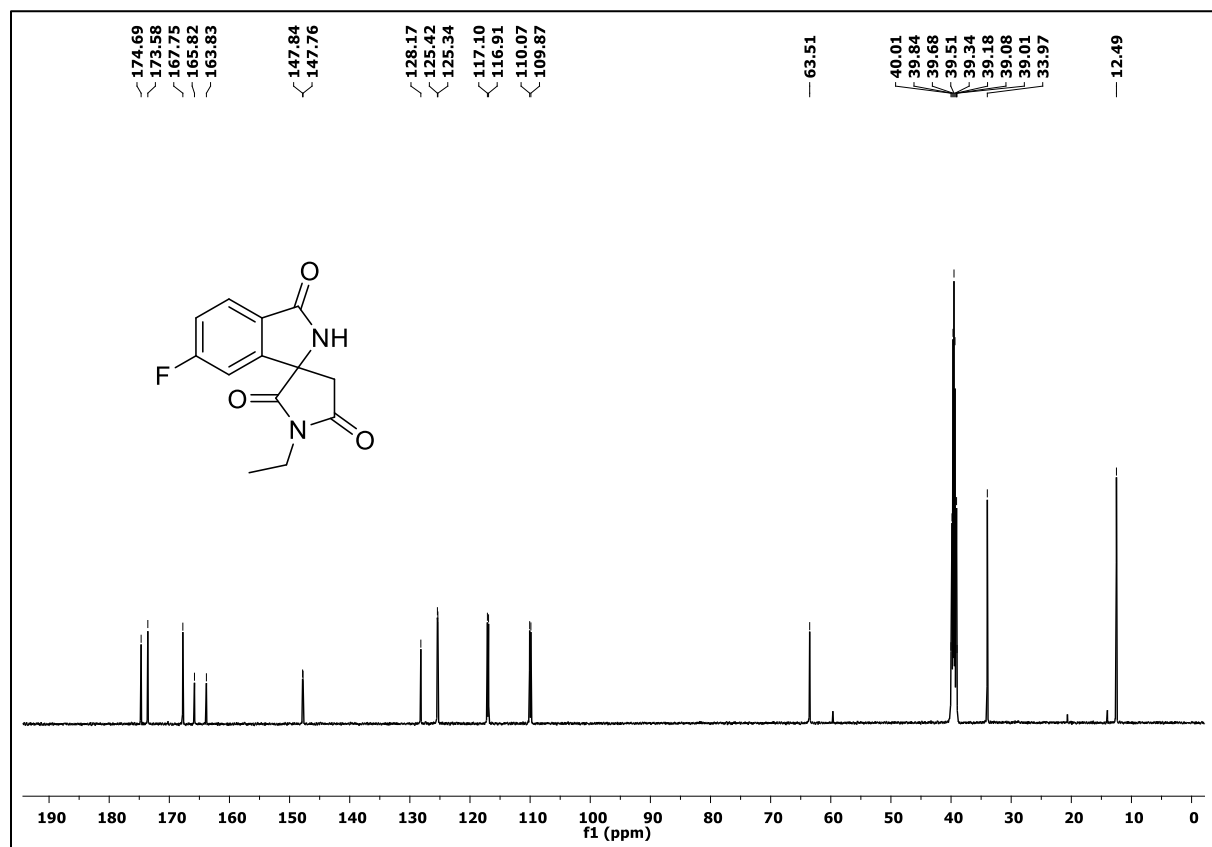
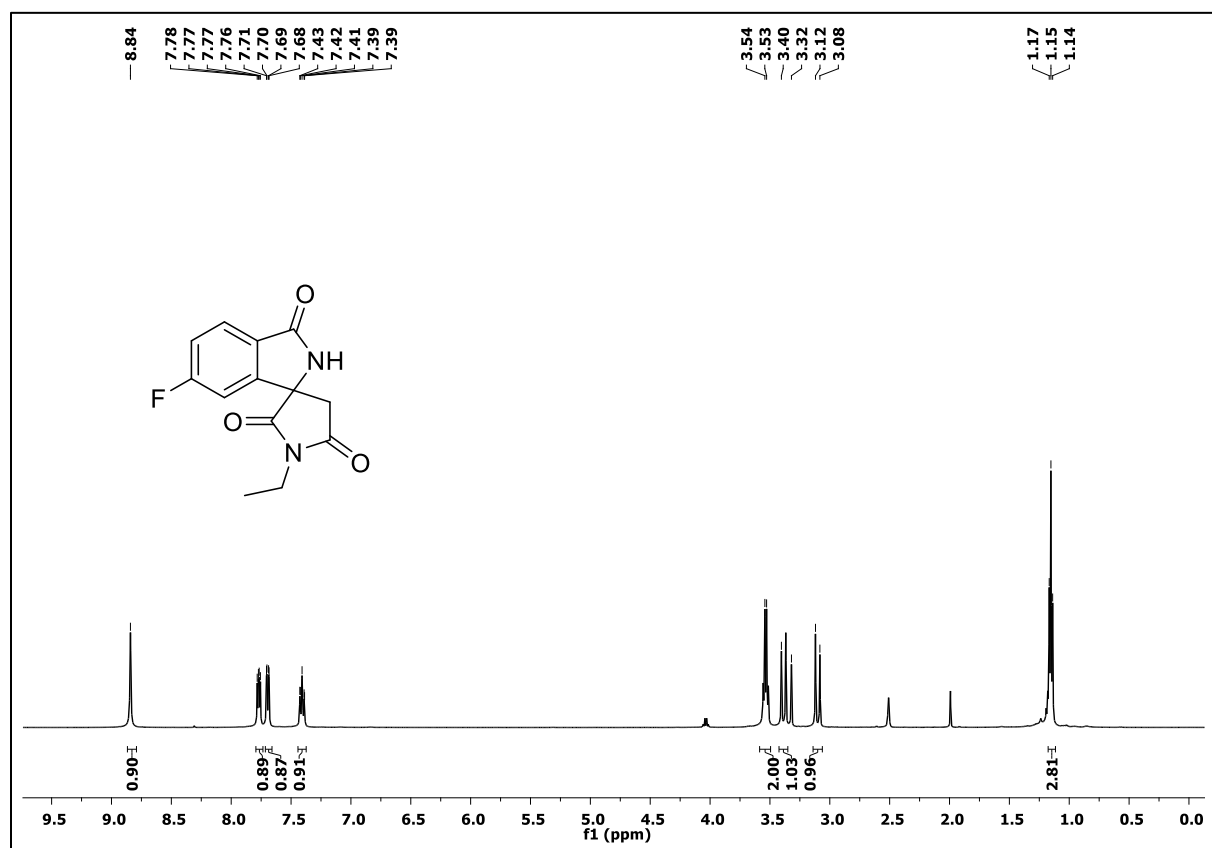
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3ea**.



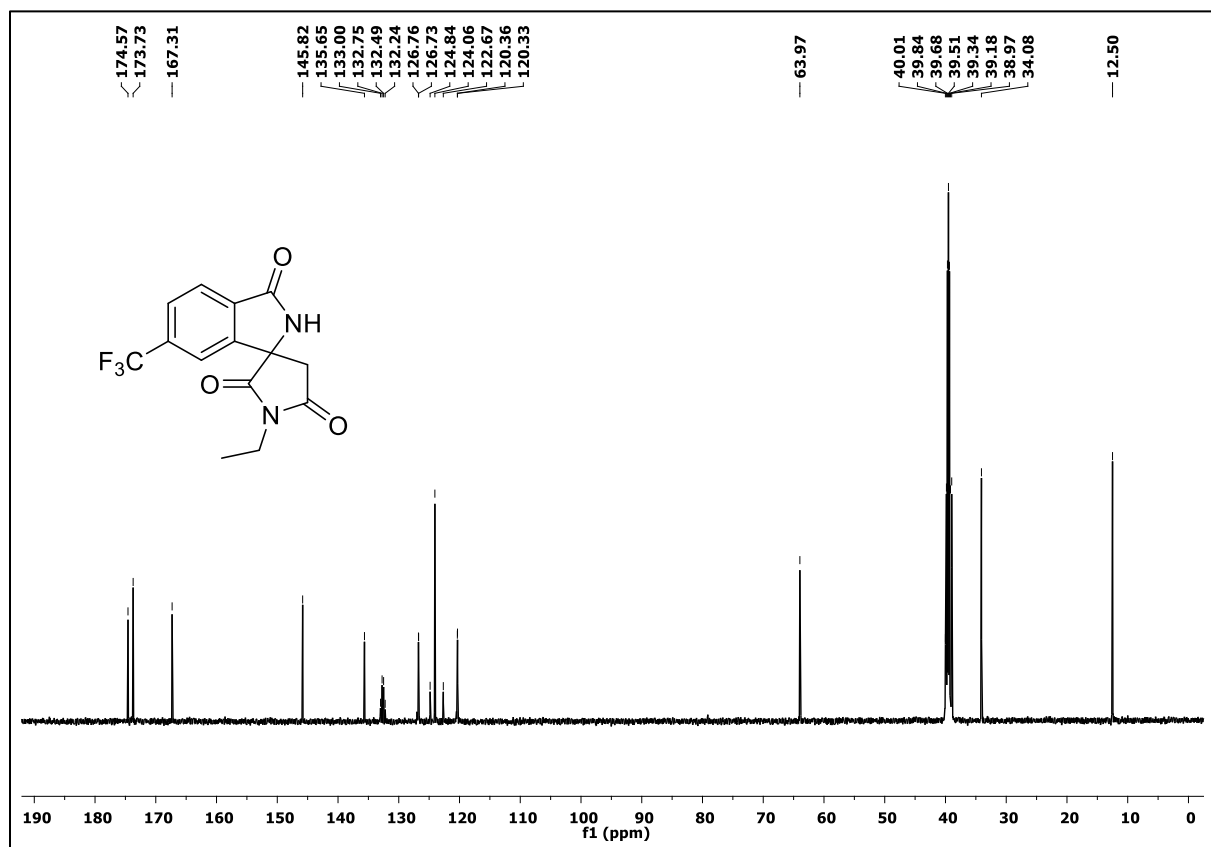
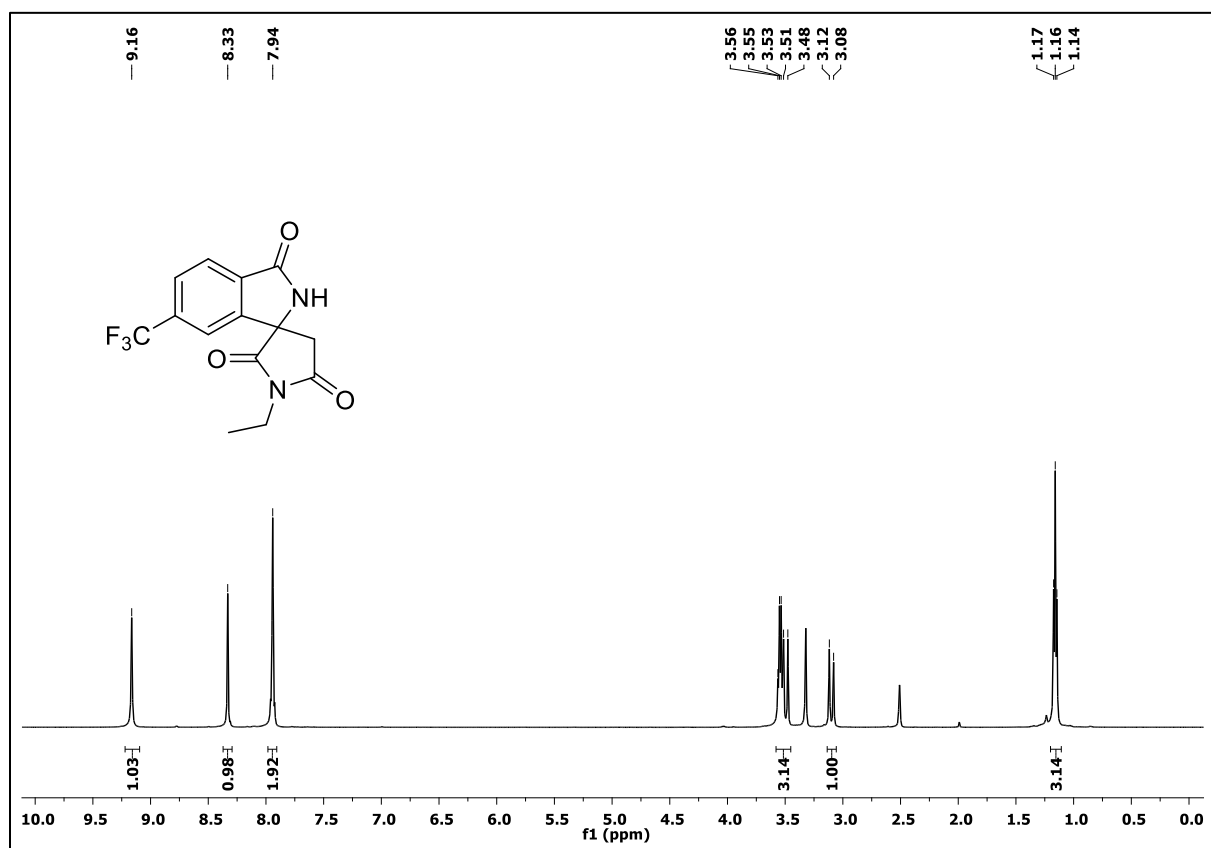
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3fa**.

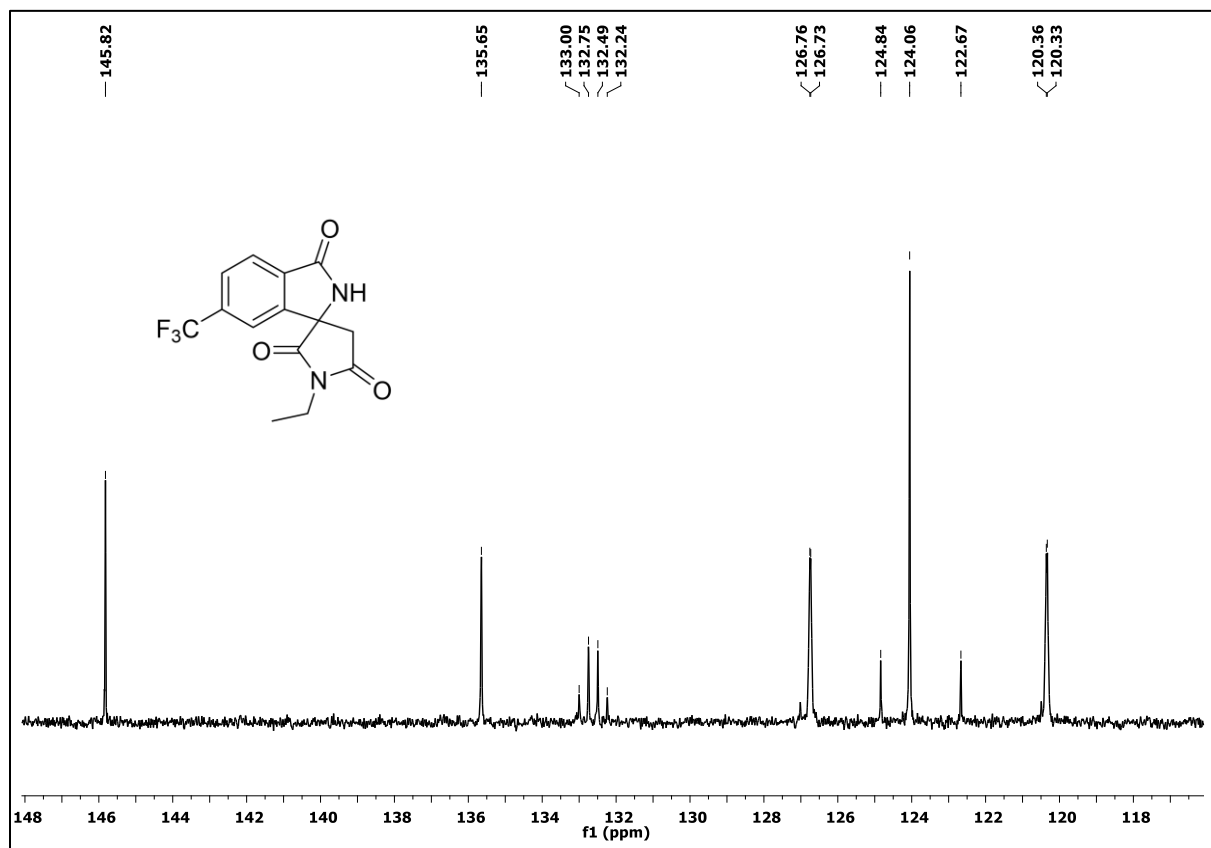


^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3ga**.

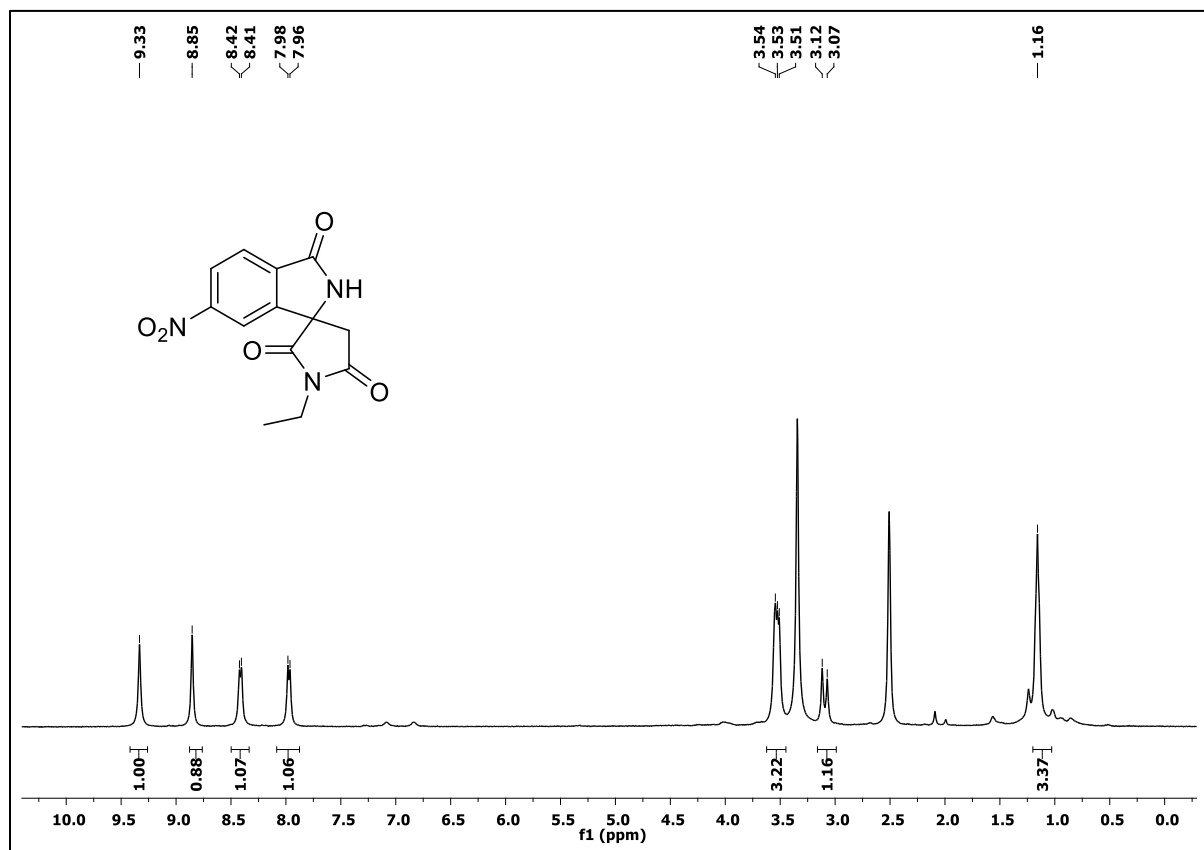


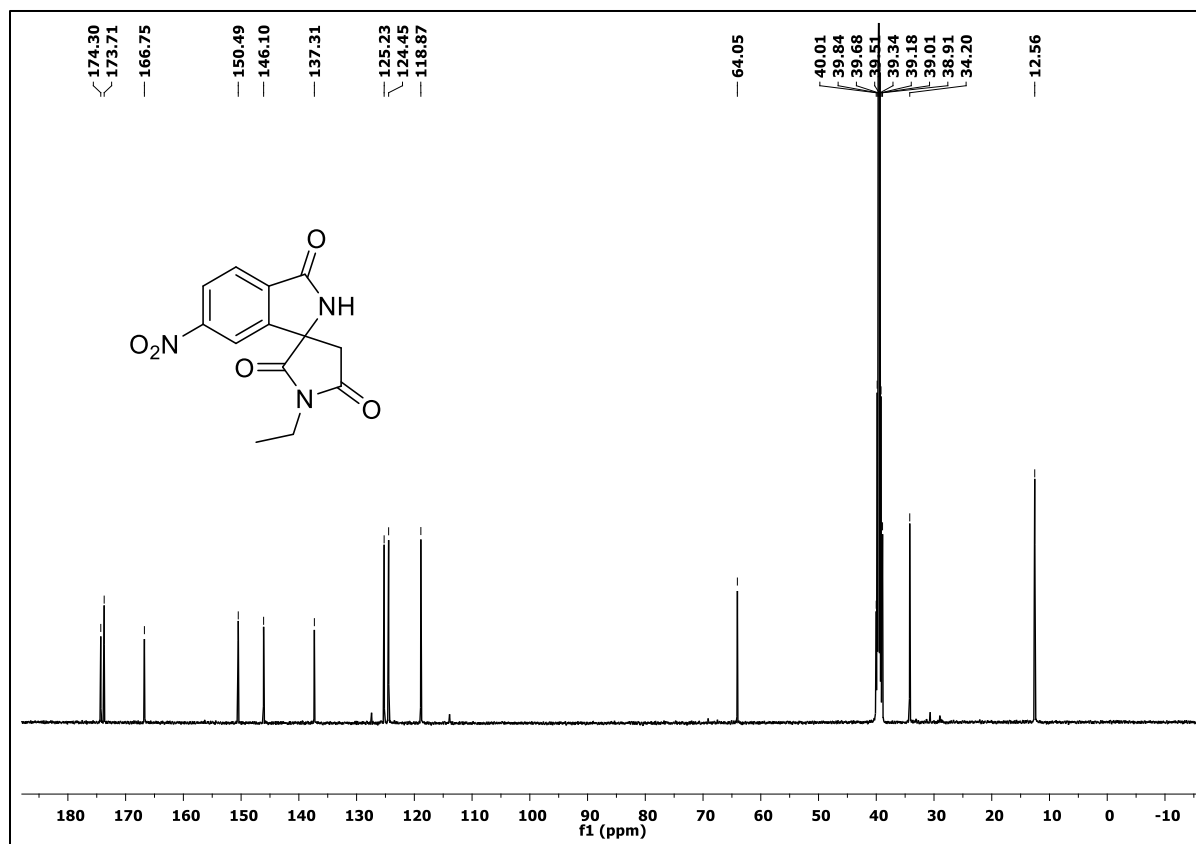
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3ha**.



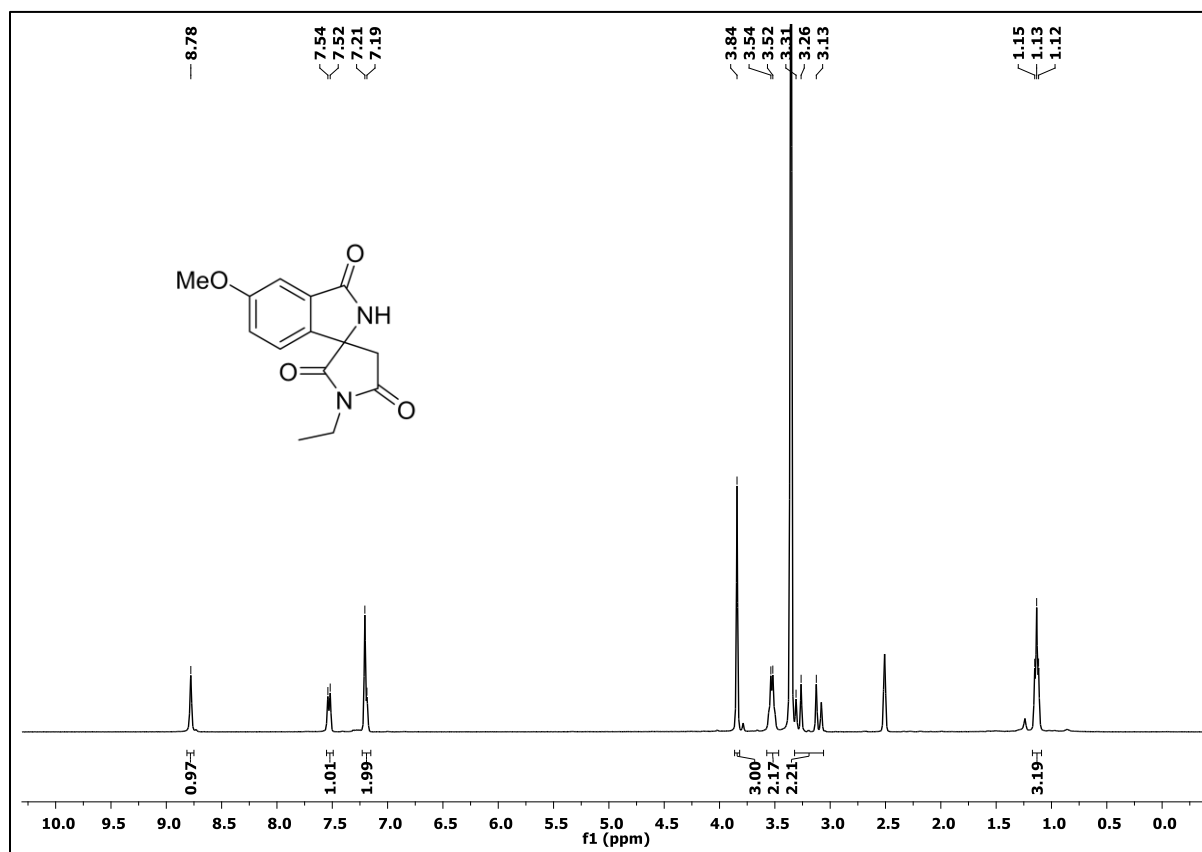


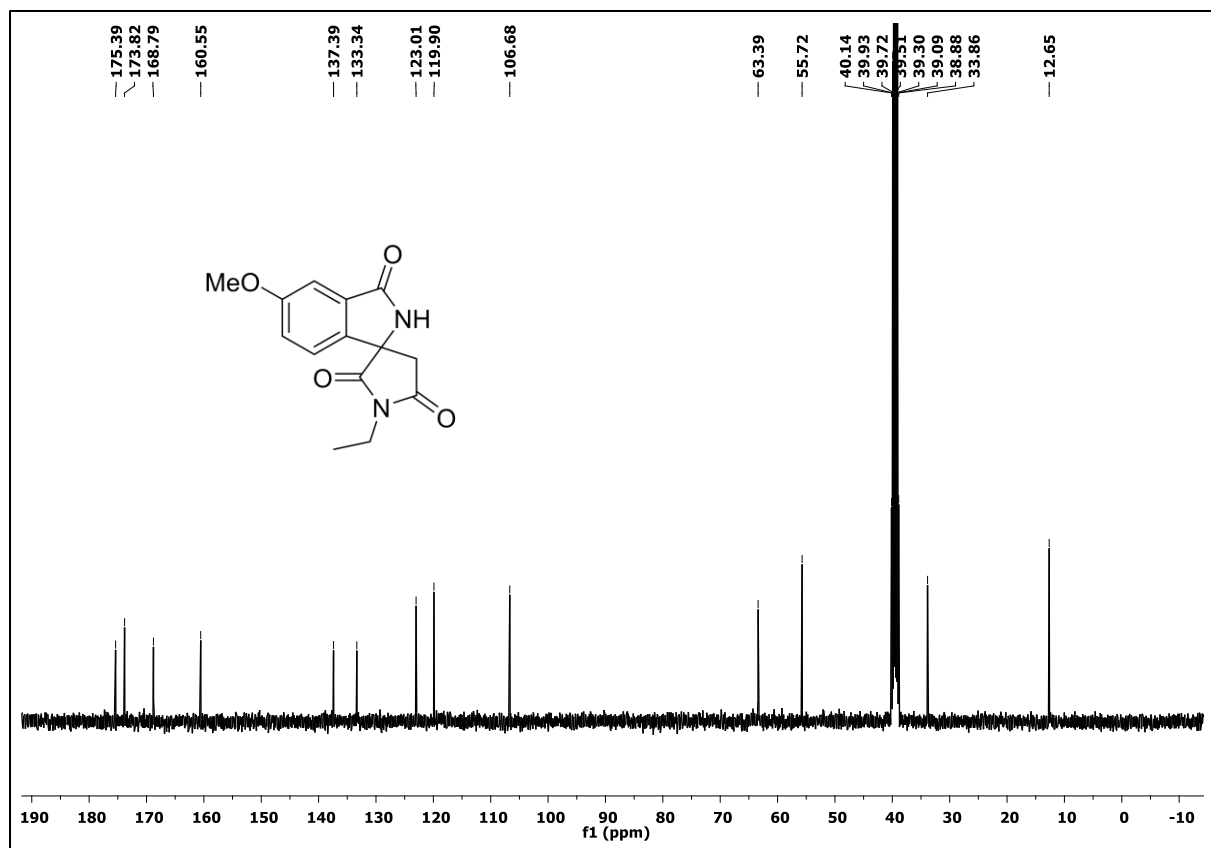
¹H and ¹³C{¹H} NMR Spectra of Compound 3ia.



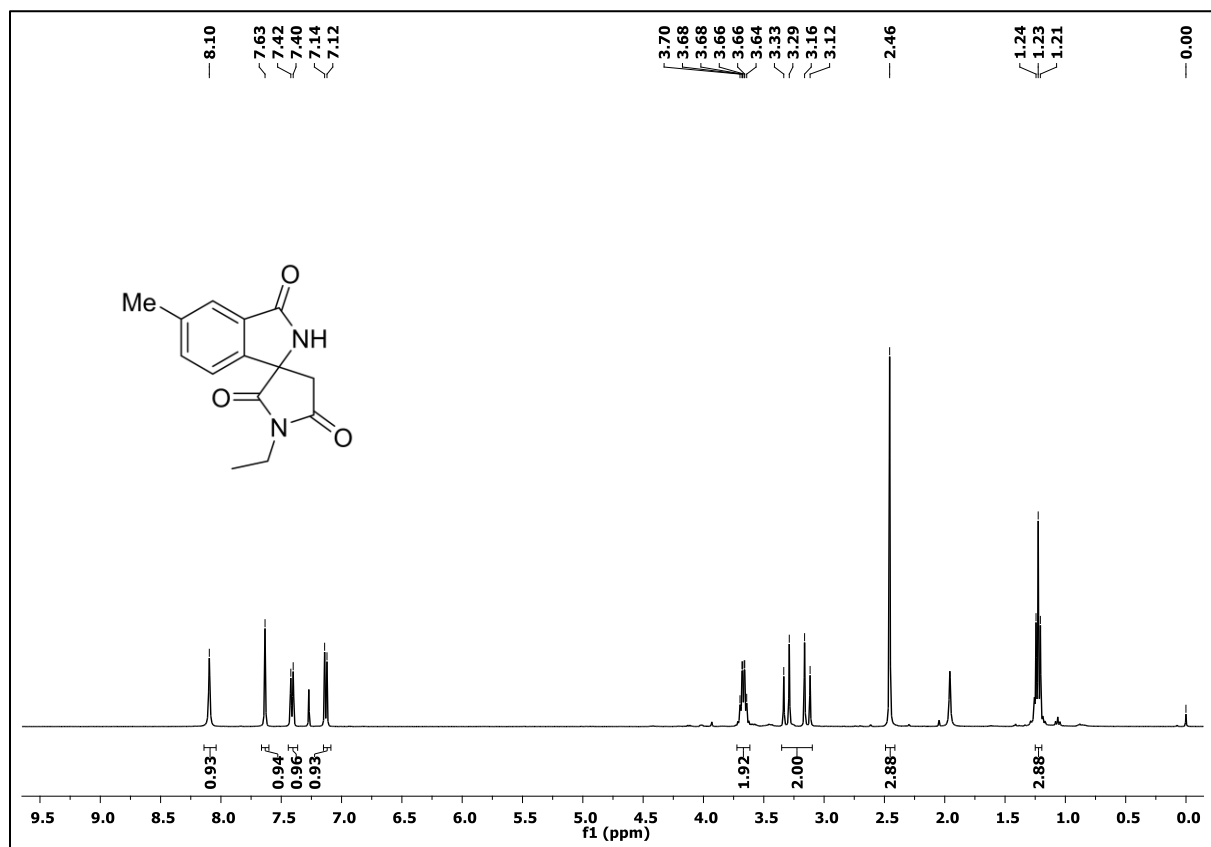


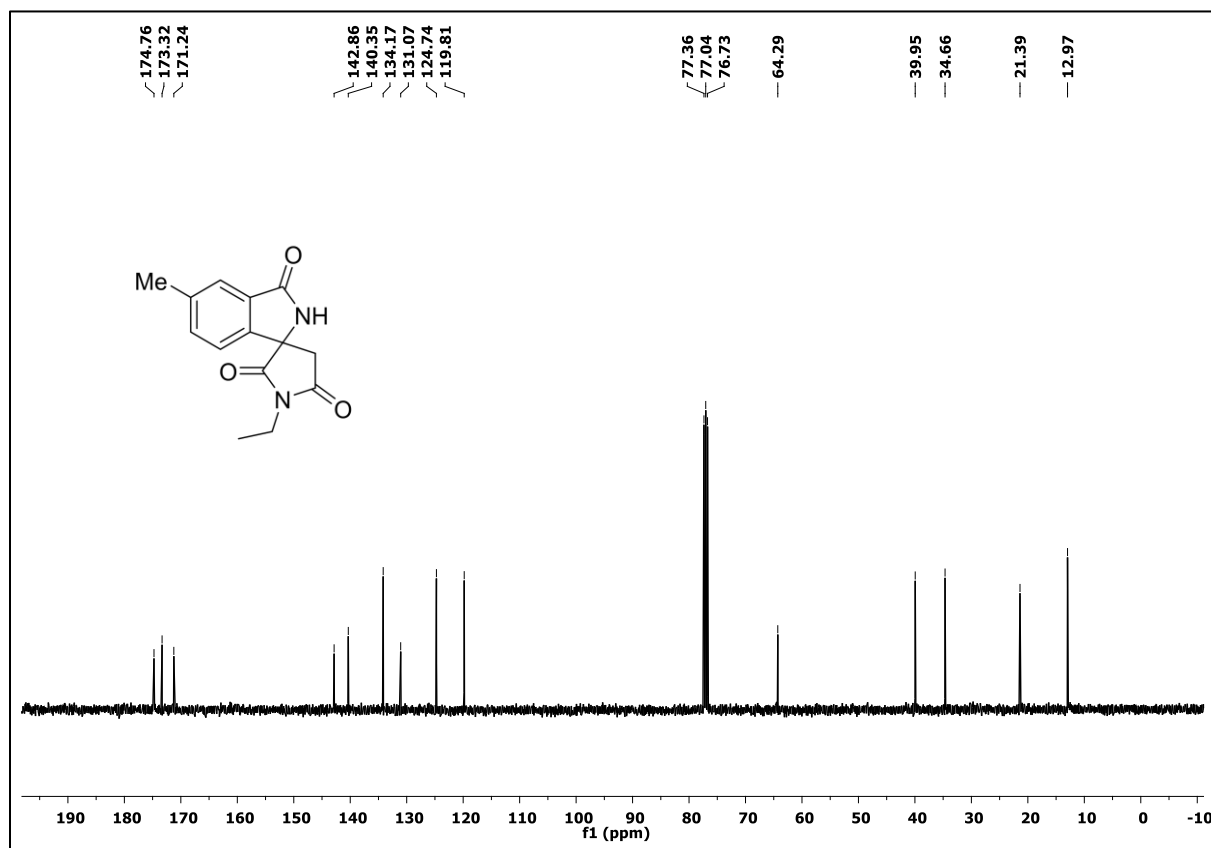
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3ja**.



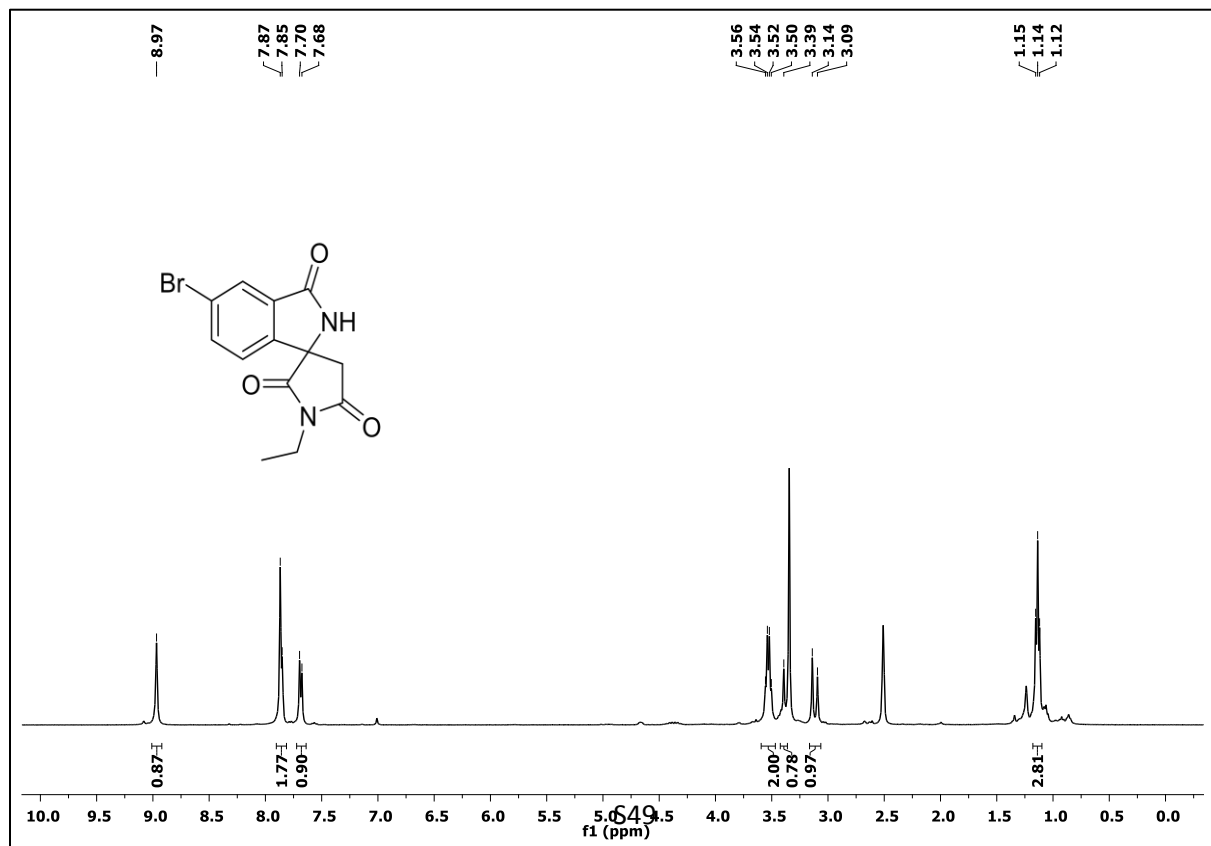


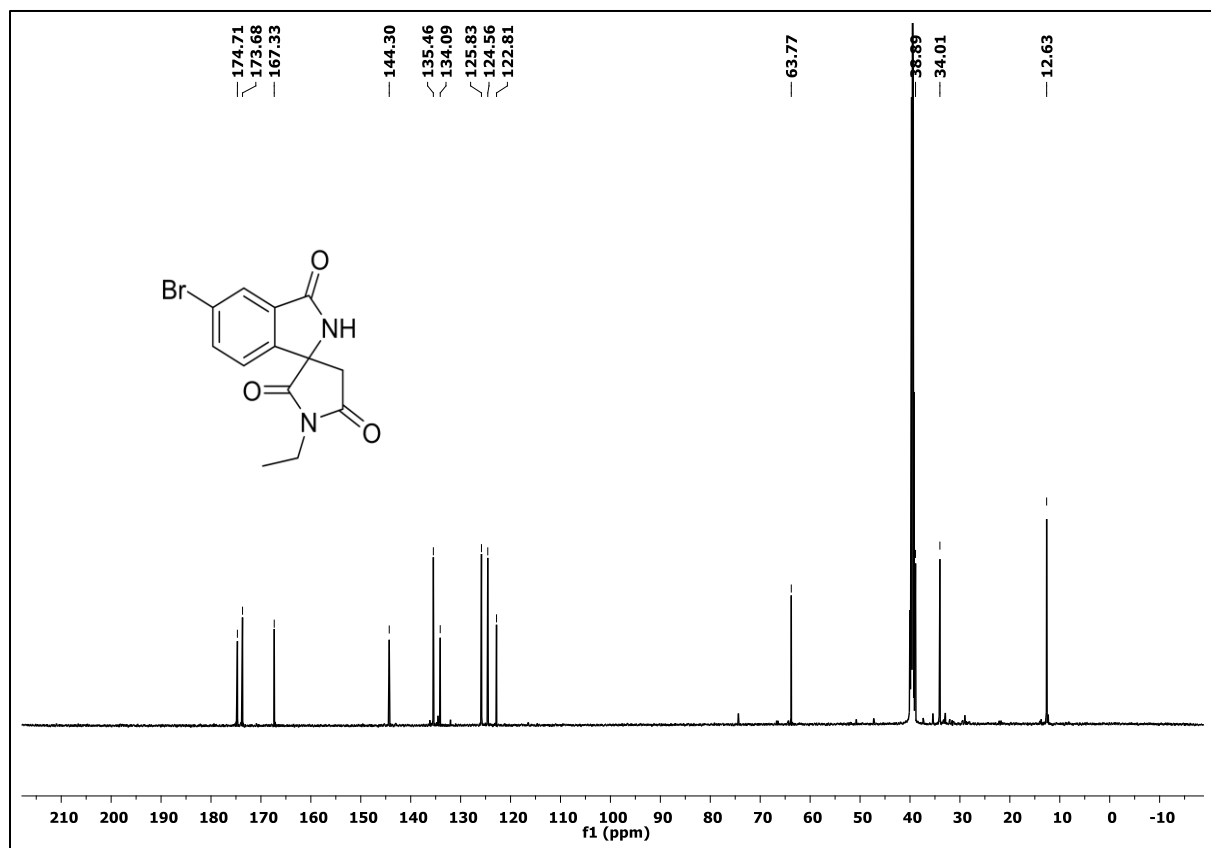
¹H and ¹³C{¹H} NMR Spectra of Compound **3ka**.



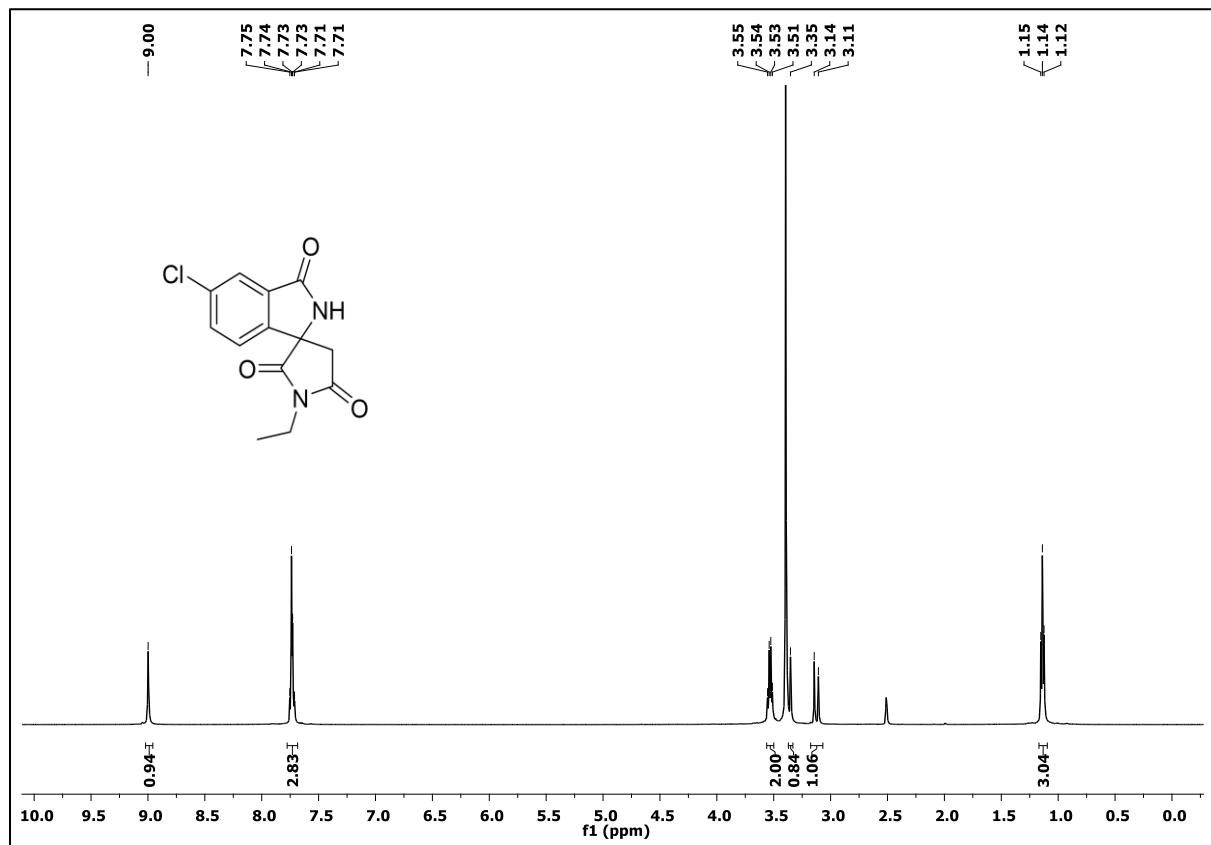


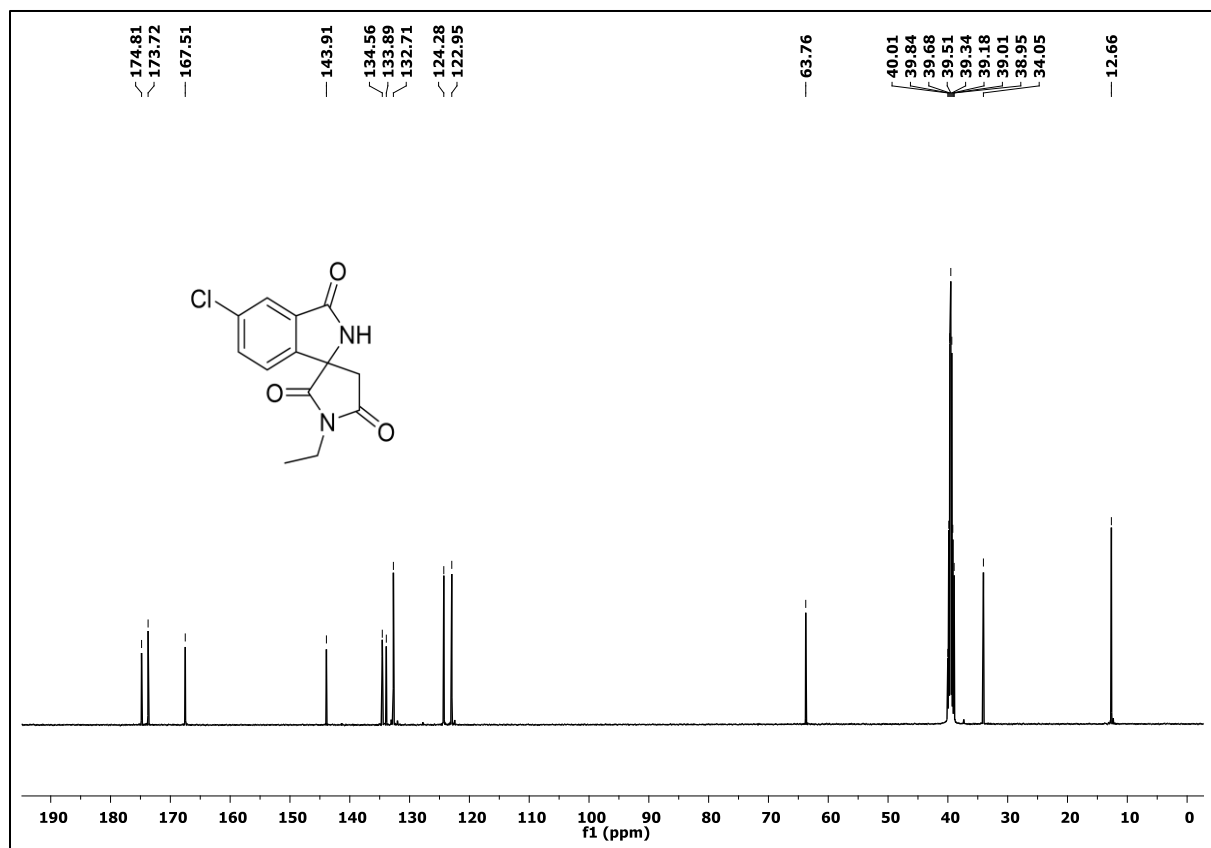
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound 3la.



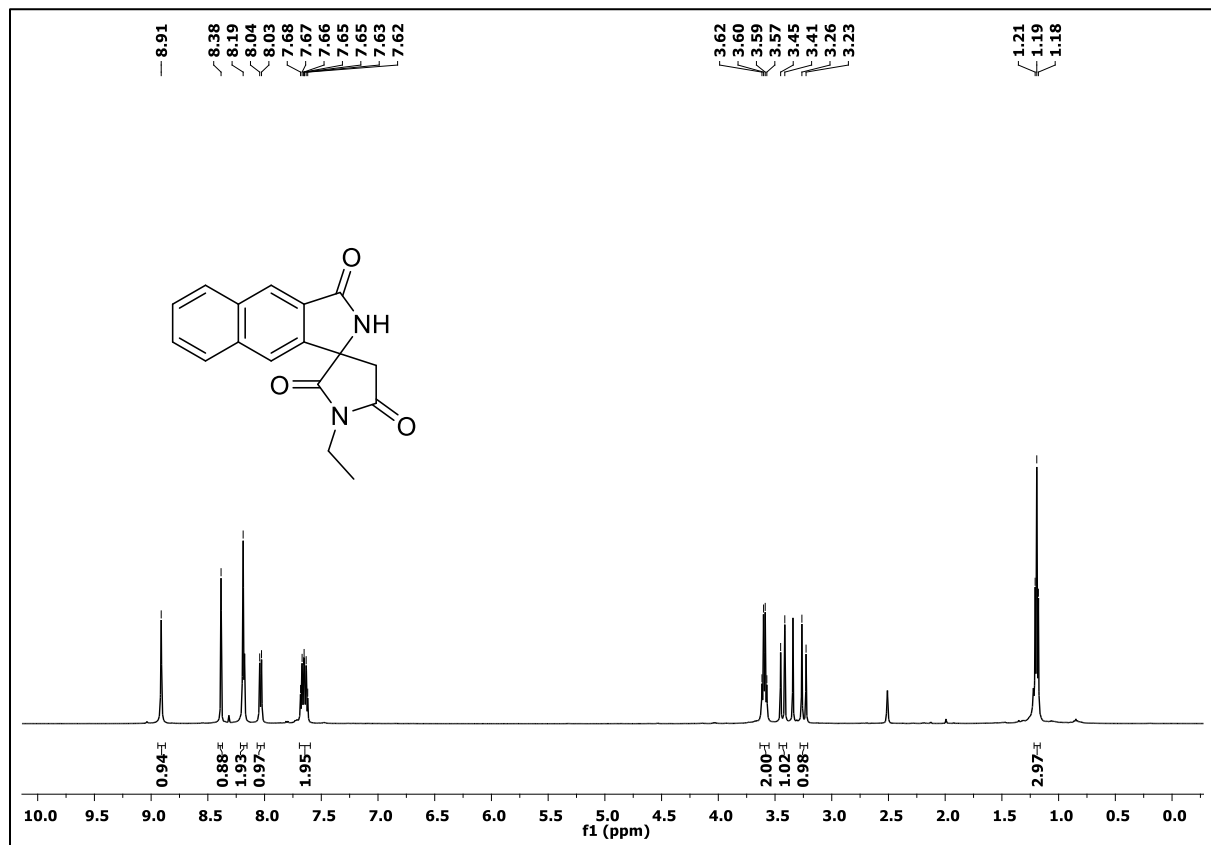


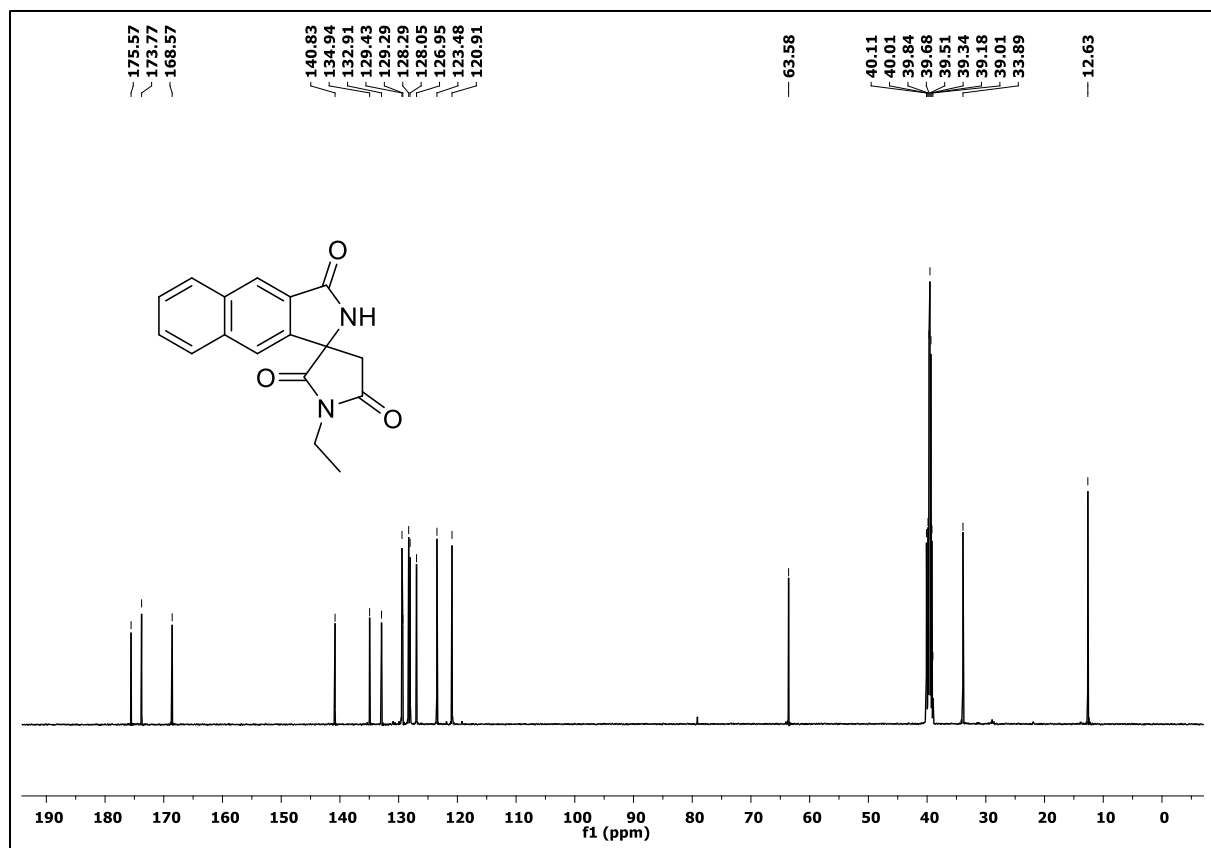
¹H and ¹³C{¹H} NMR Spectra of Compound **3ma**.



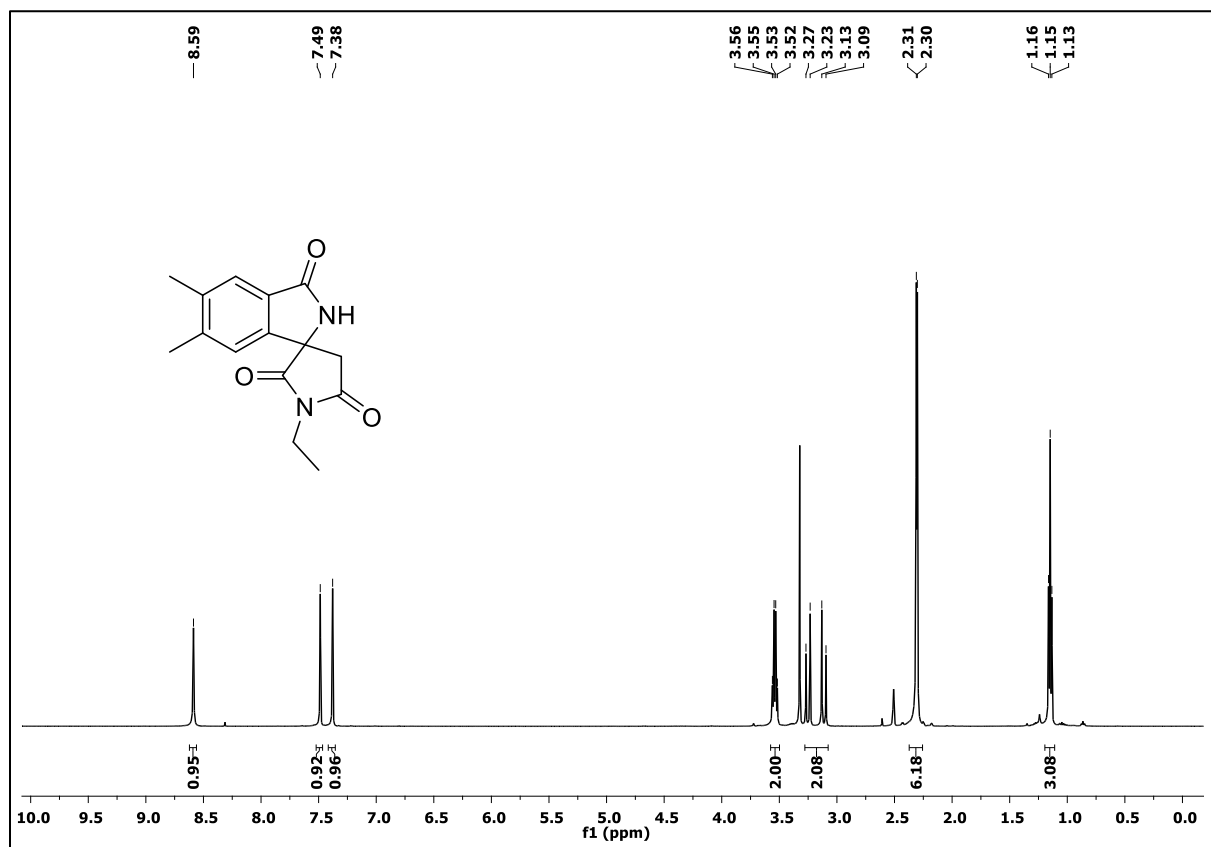


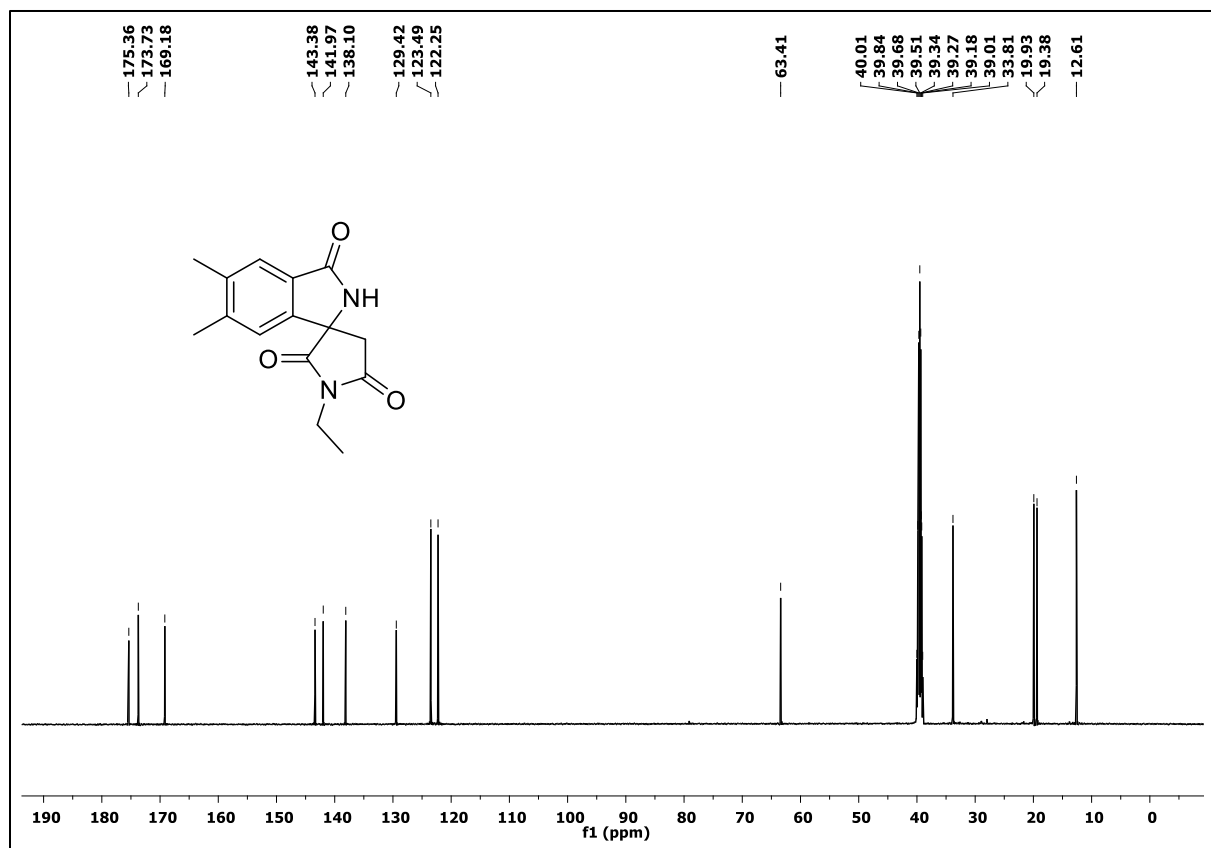
¹H and ¹³C{¹H} NMR Spectra of Compound **3na**.



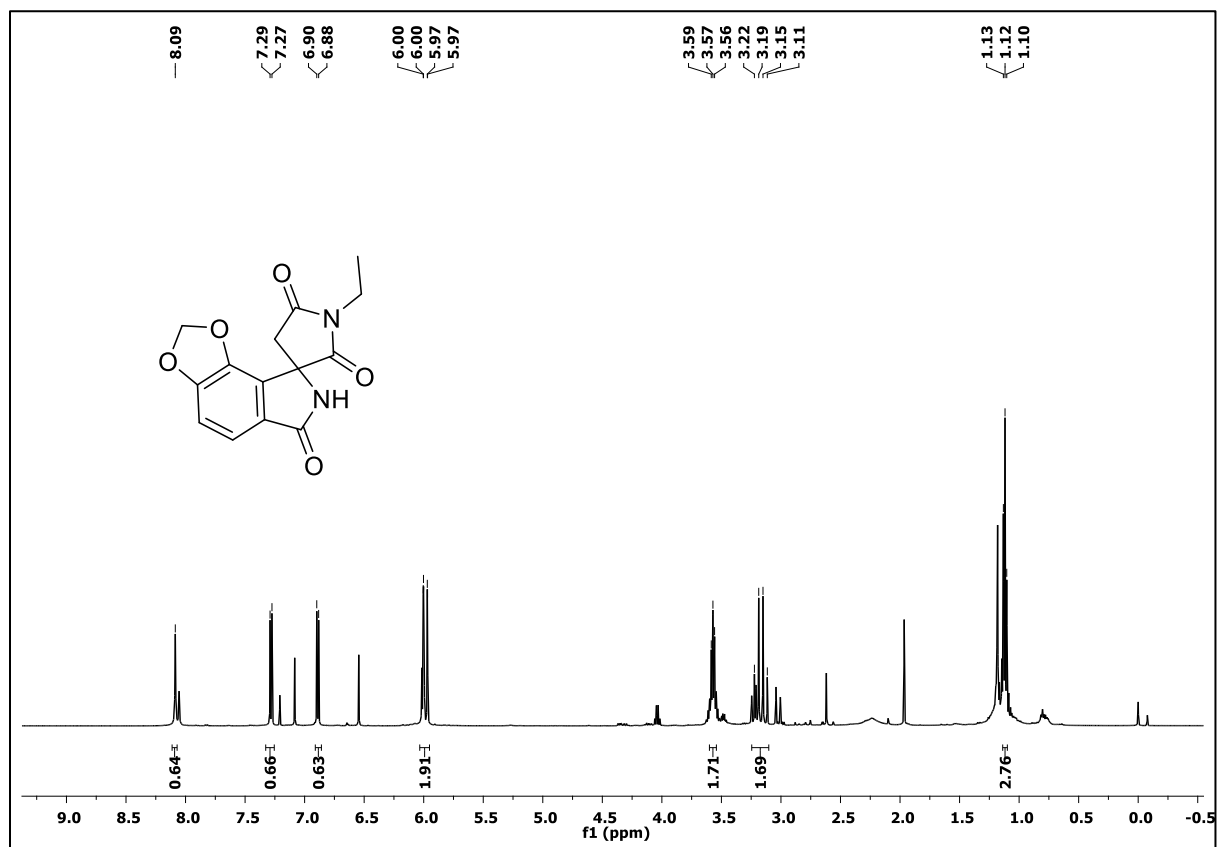


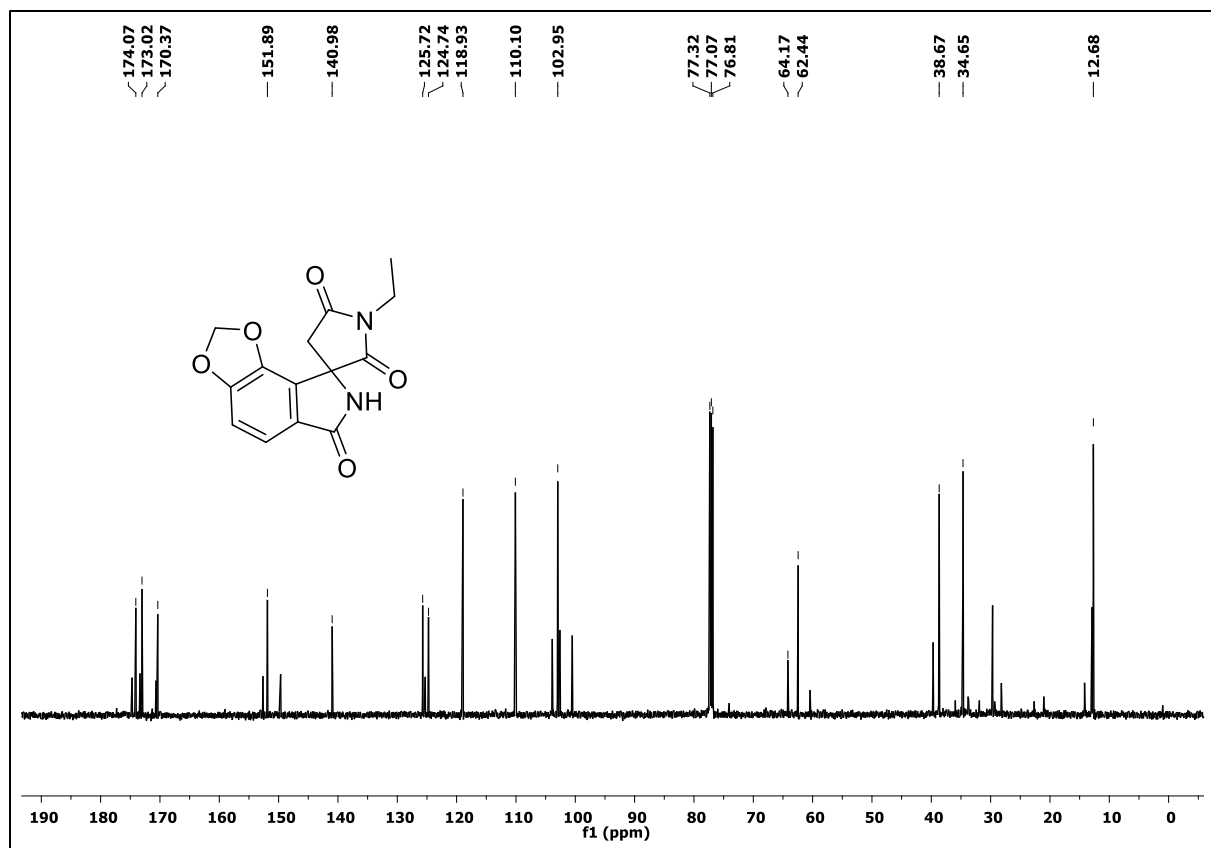
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **30a**.



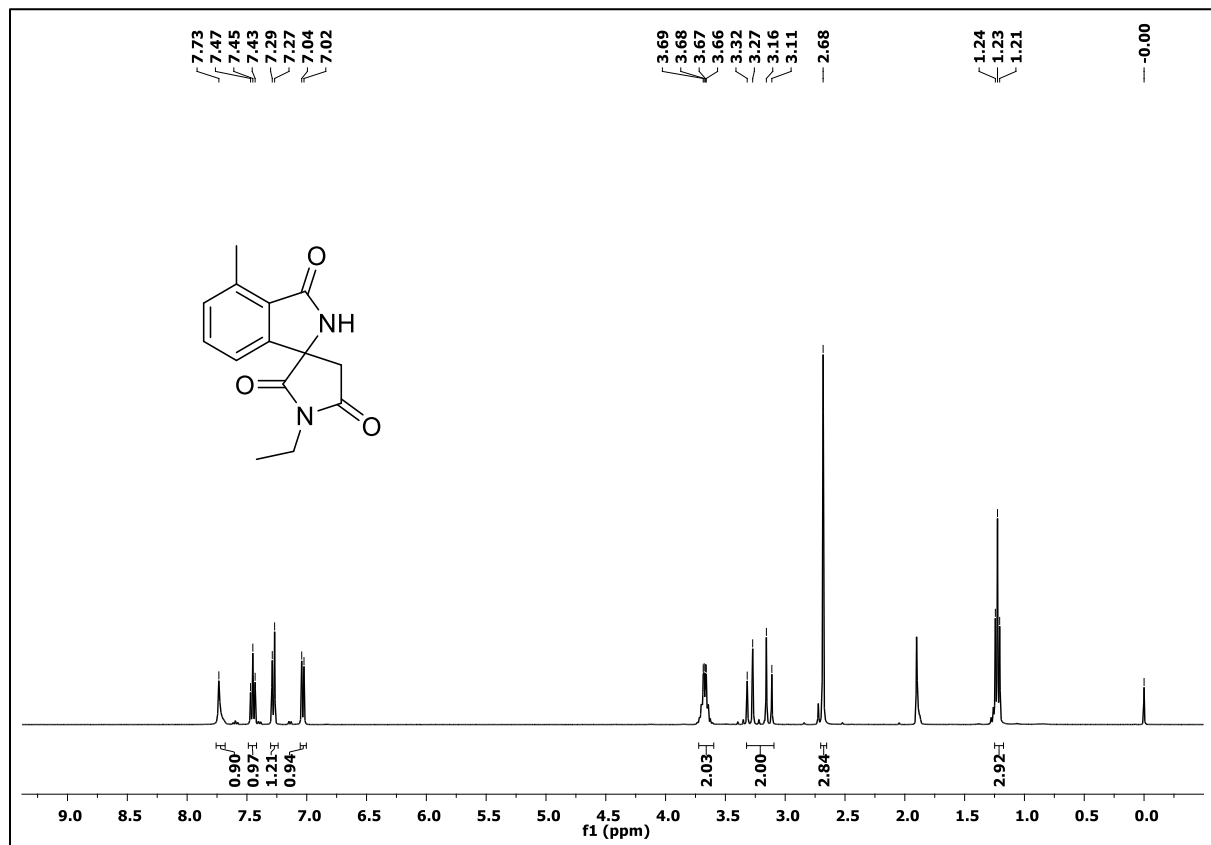


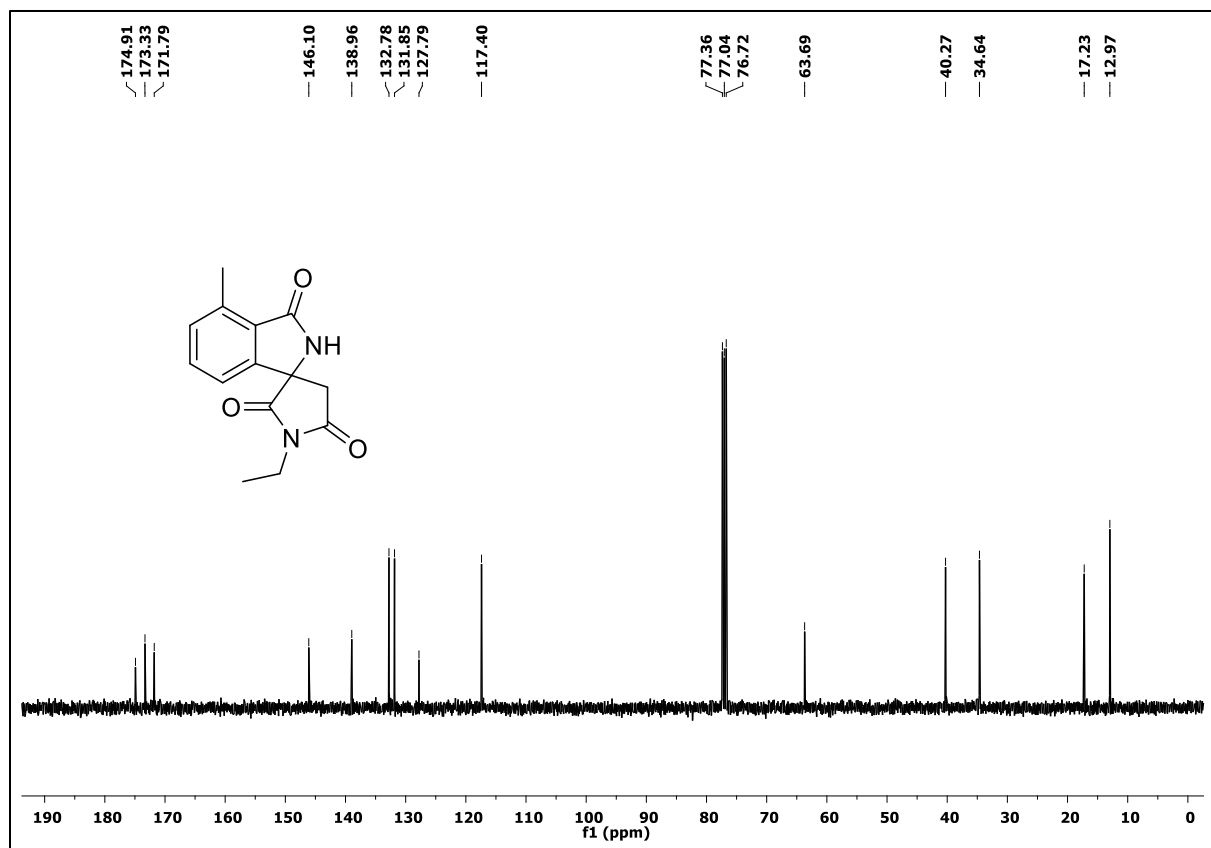
¹H and ¹³C{¹H} NMR Spectra of Compound **3pa**.



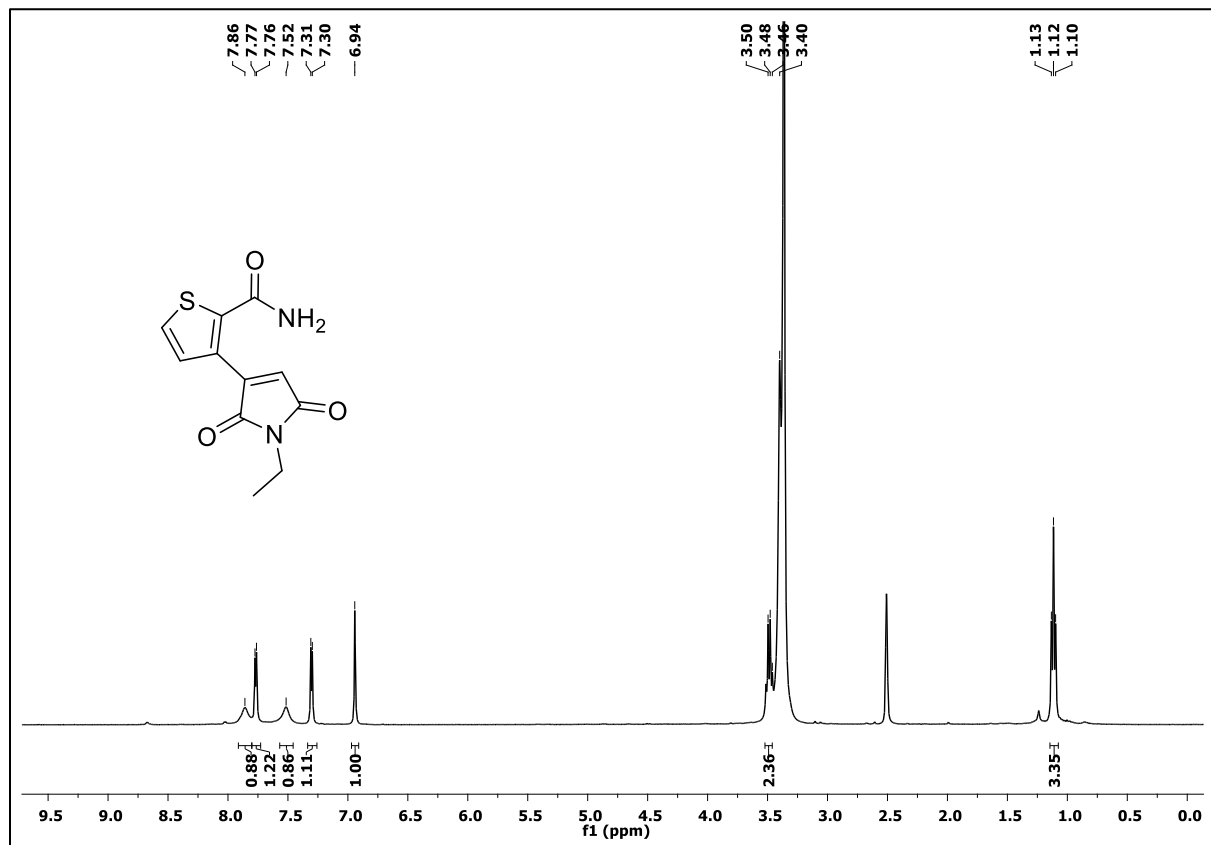


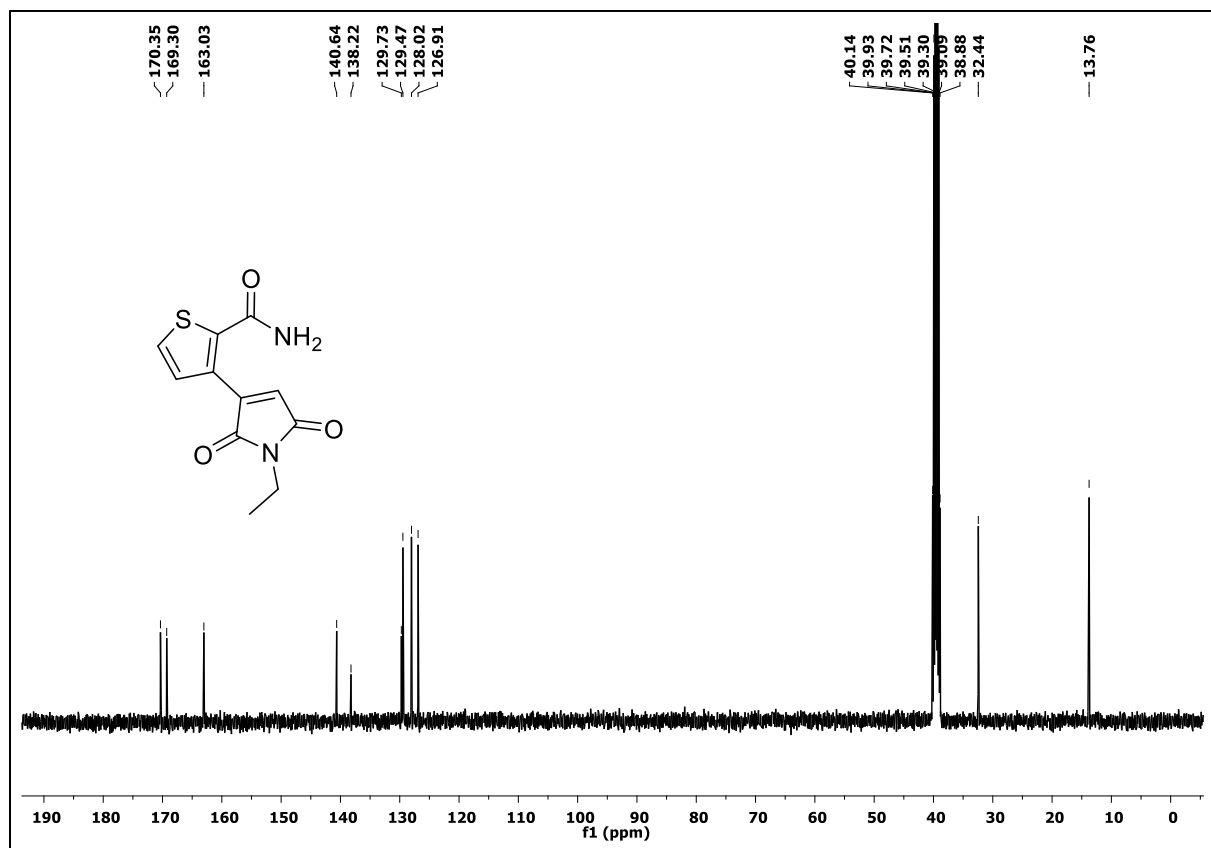
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3qa**.



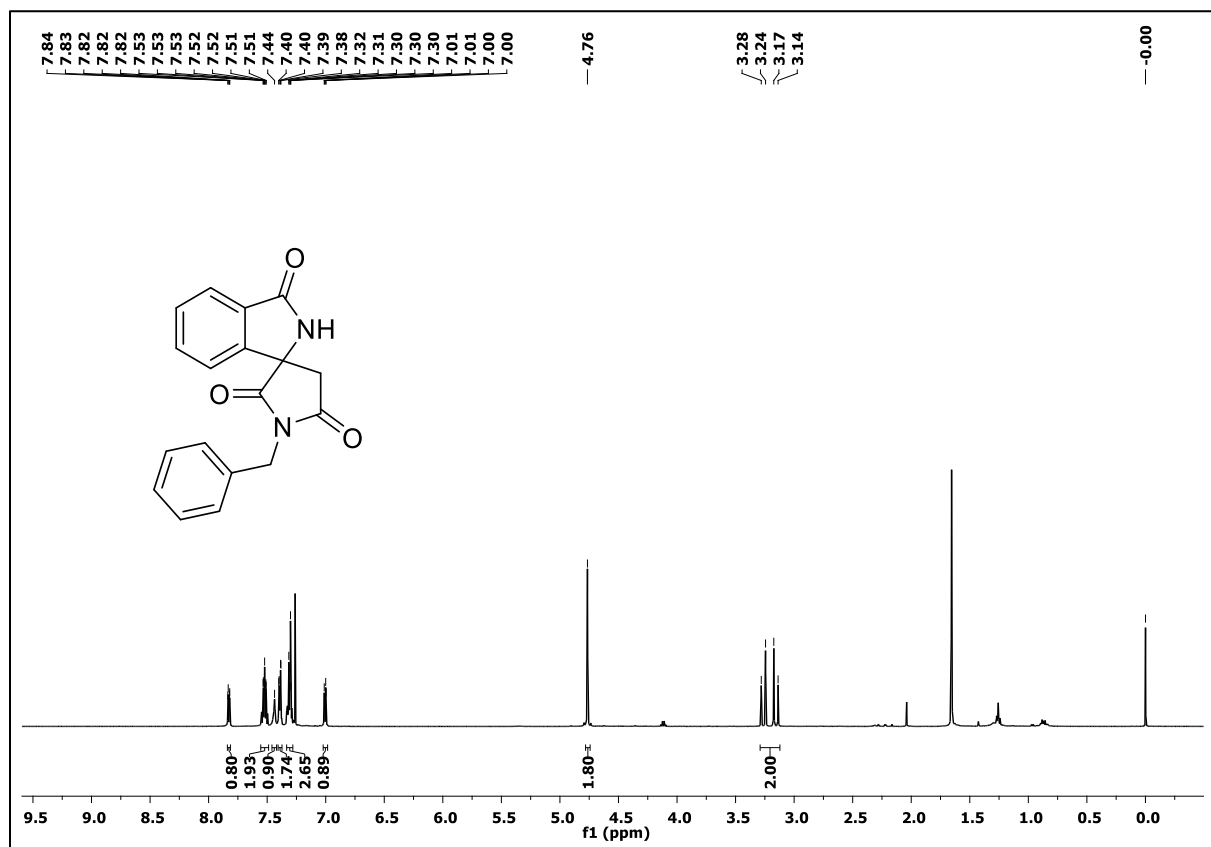


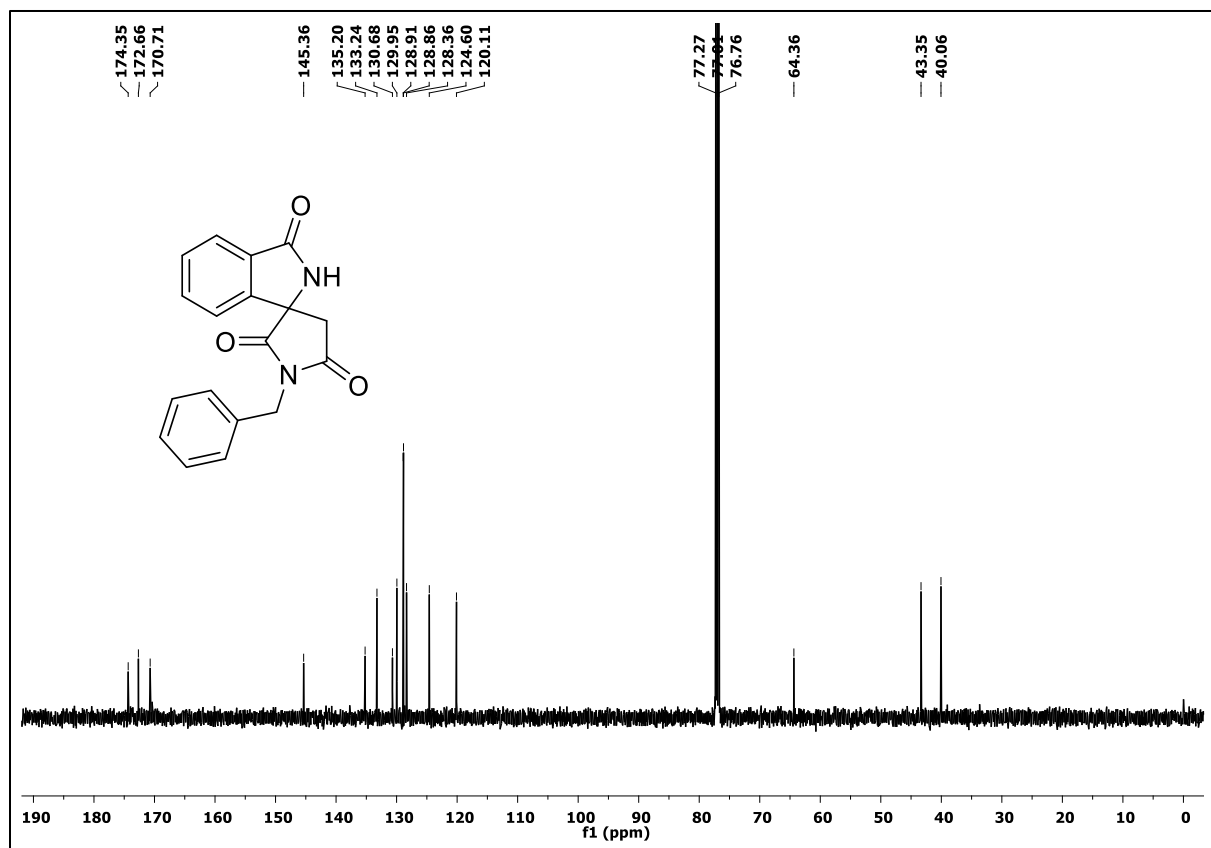
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound 3ra.



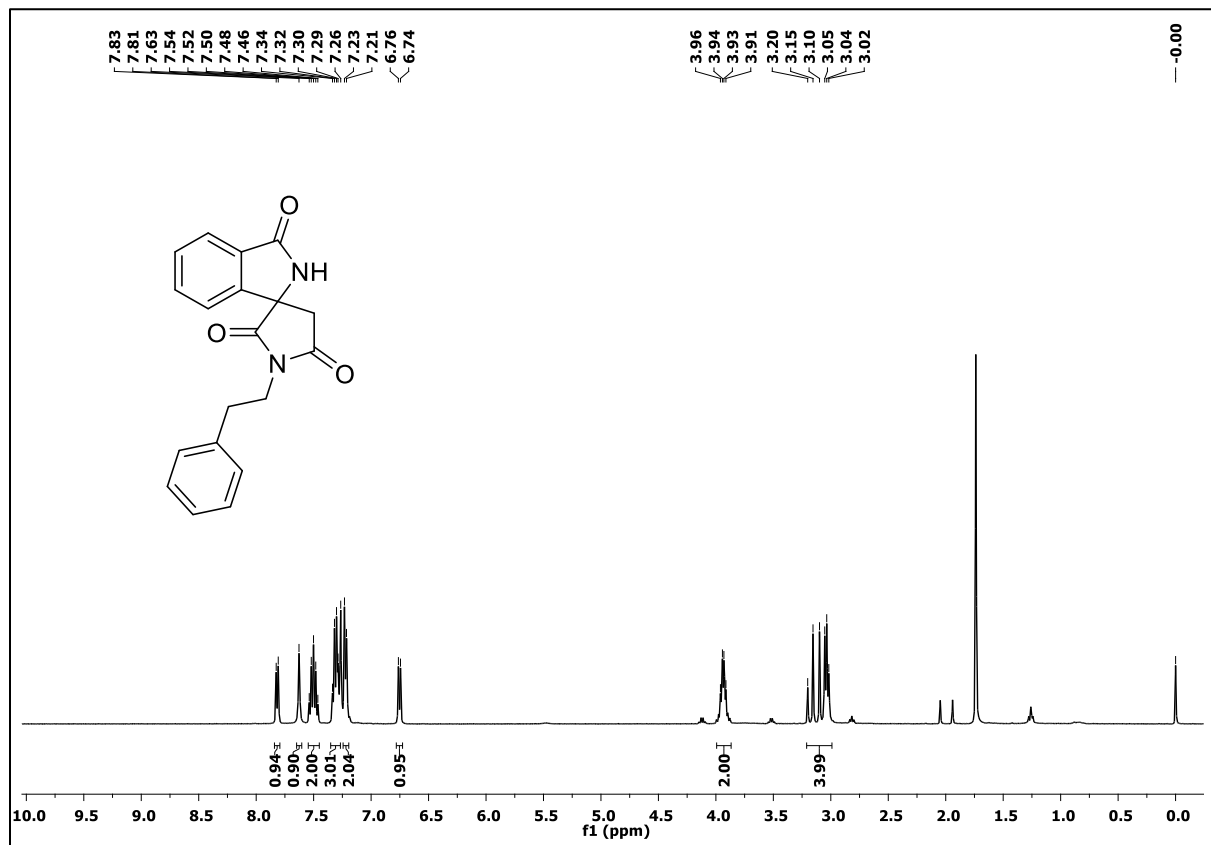


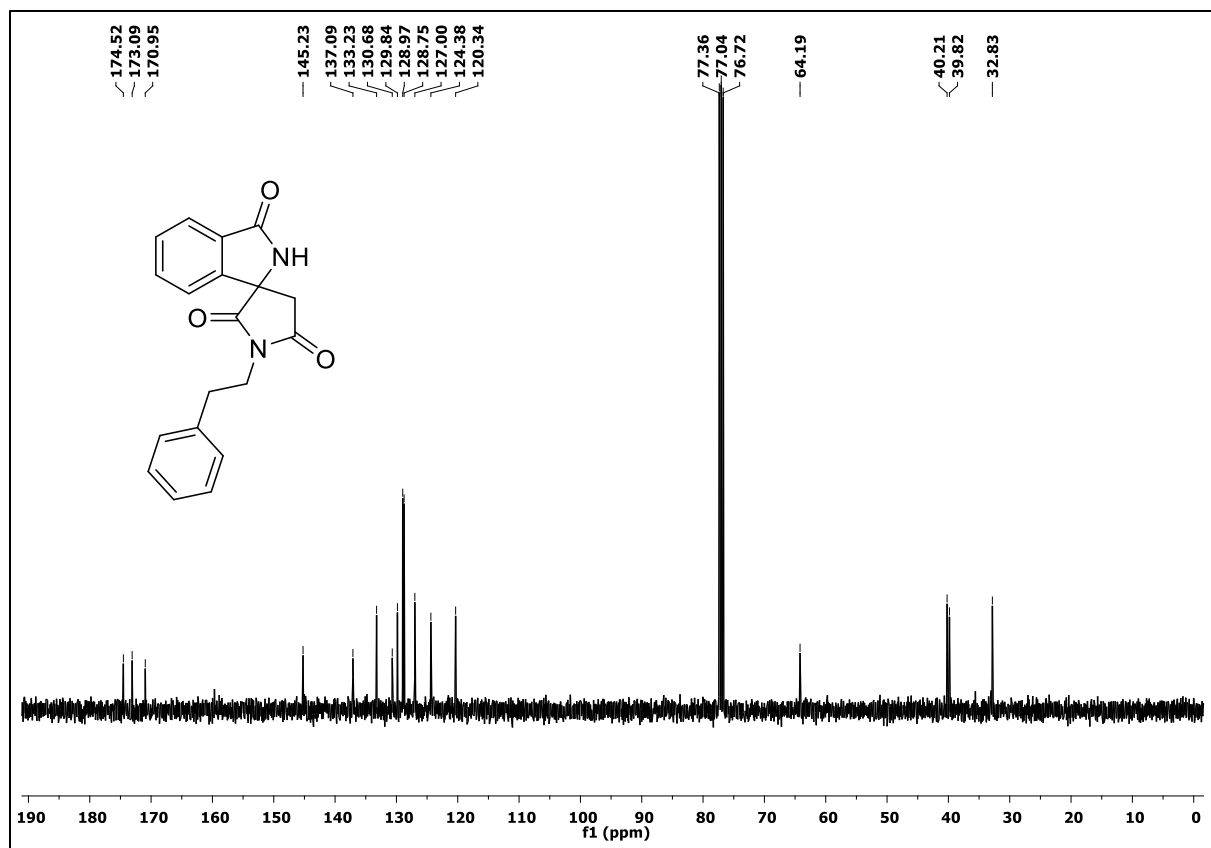
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of Compound **3ab**.



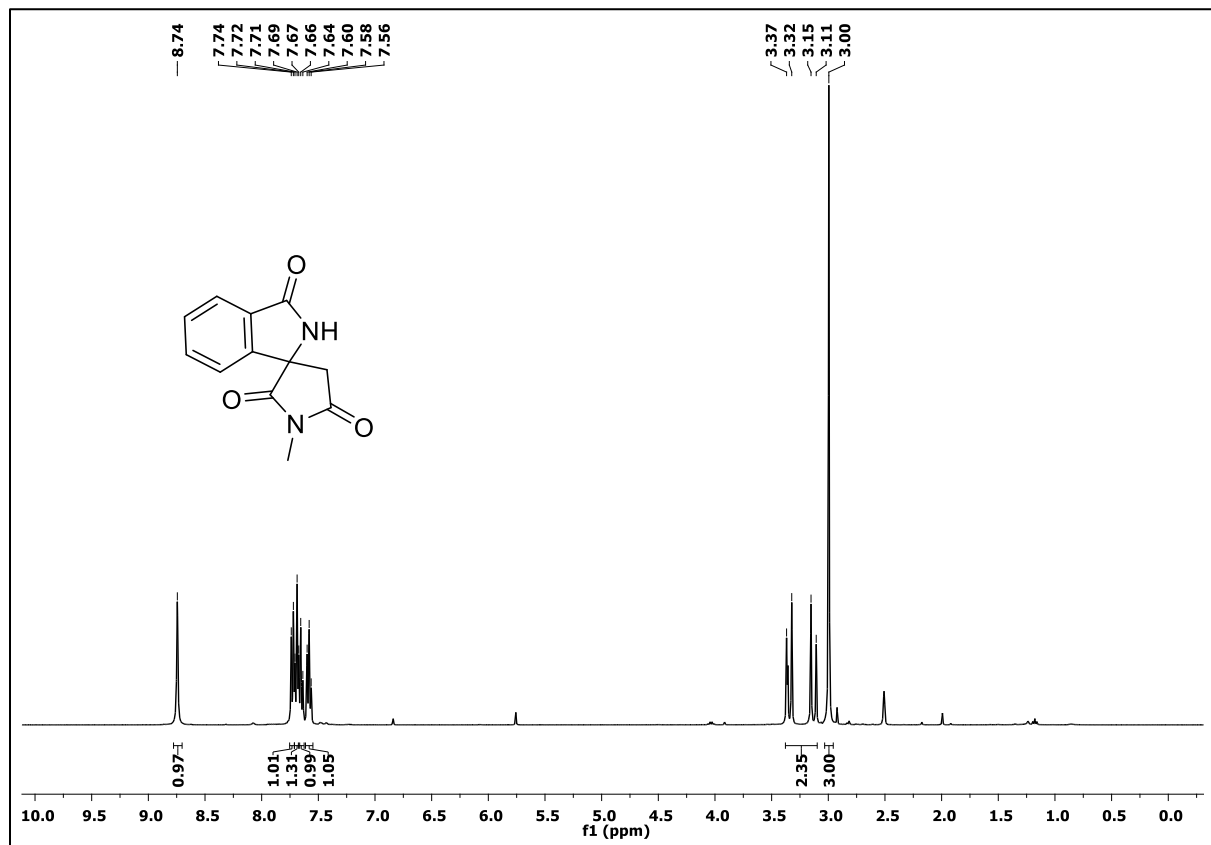


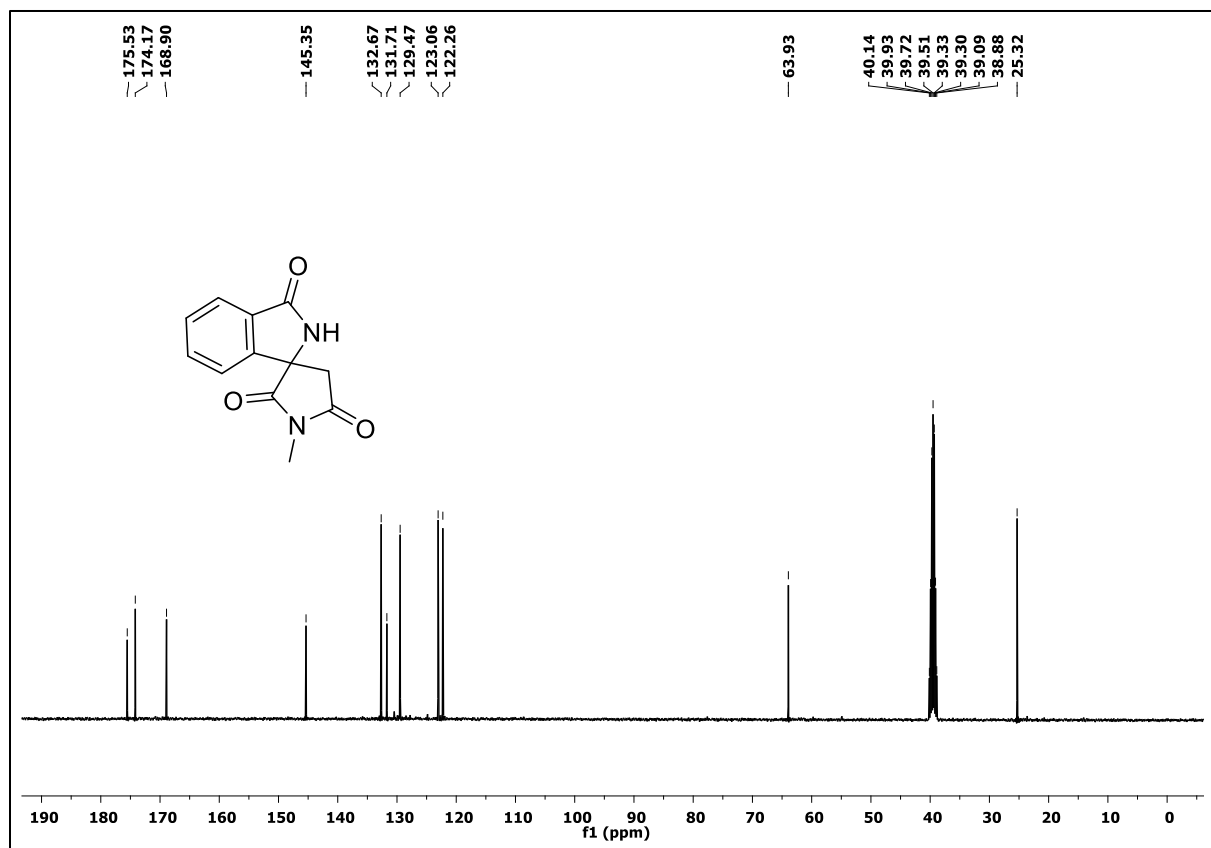
¹H and ¹³C{¹H} NMR Spectra of Compound 3ac.



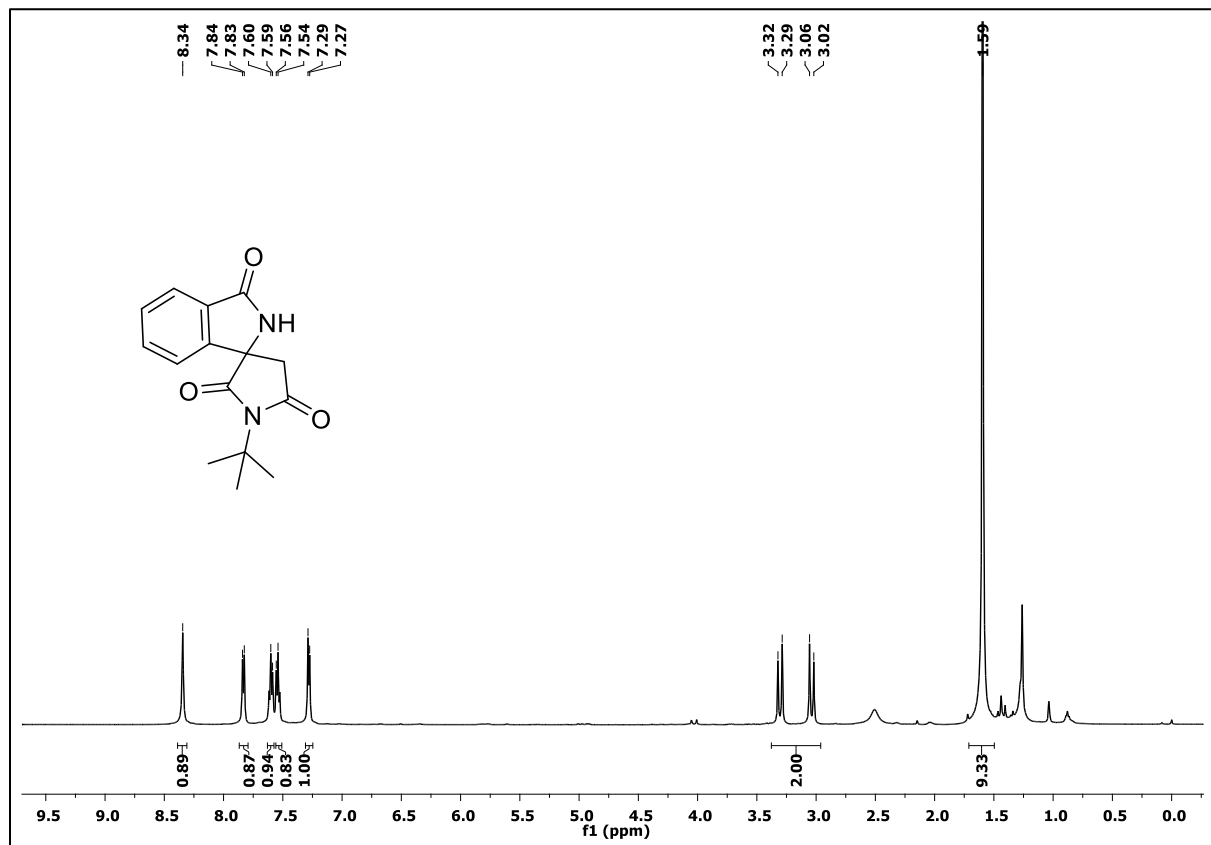


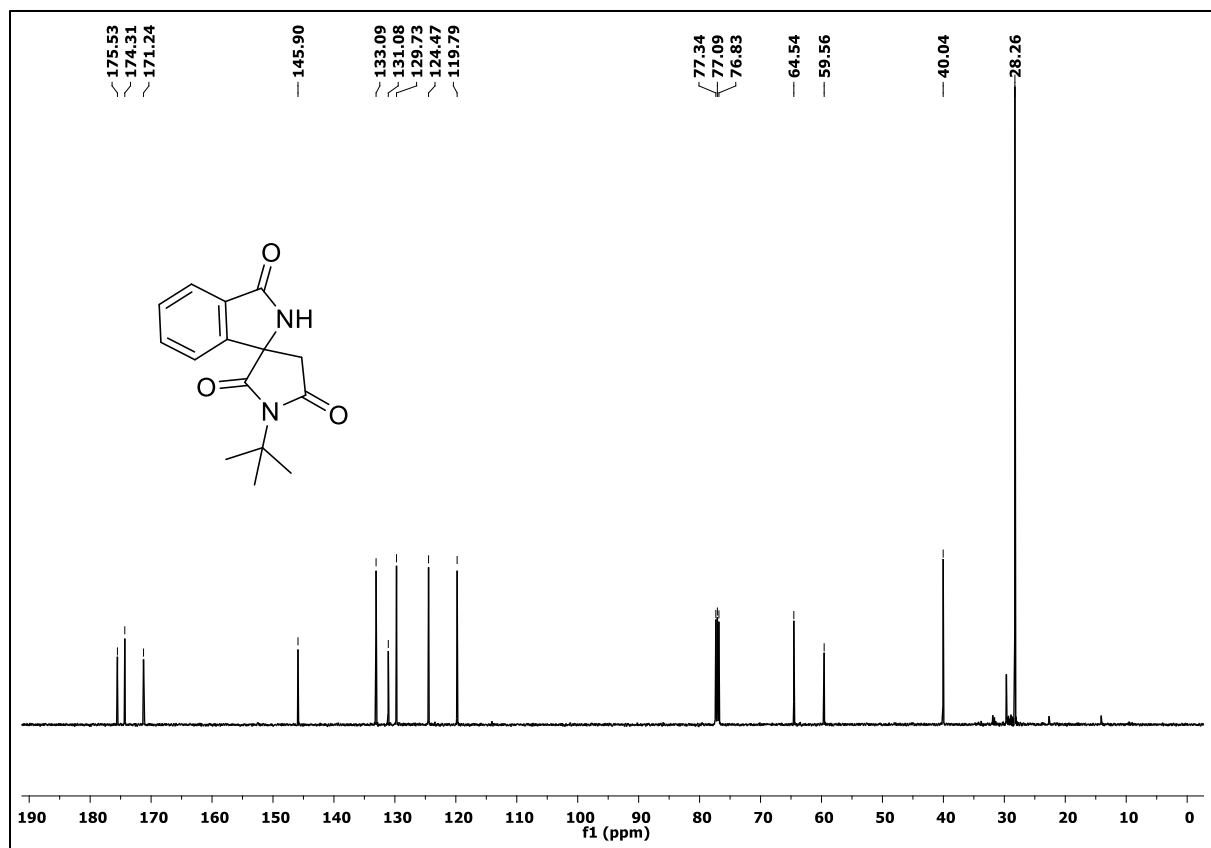
¹H and ¹³C{¹H} NMR Spectra of Compound **3ad**.



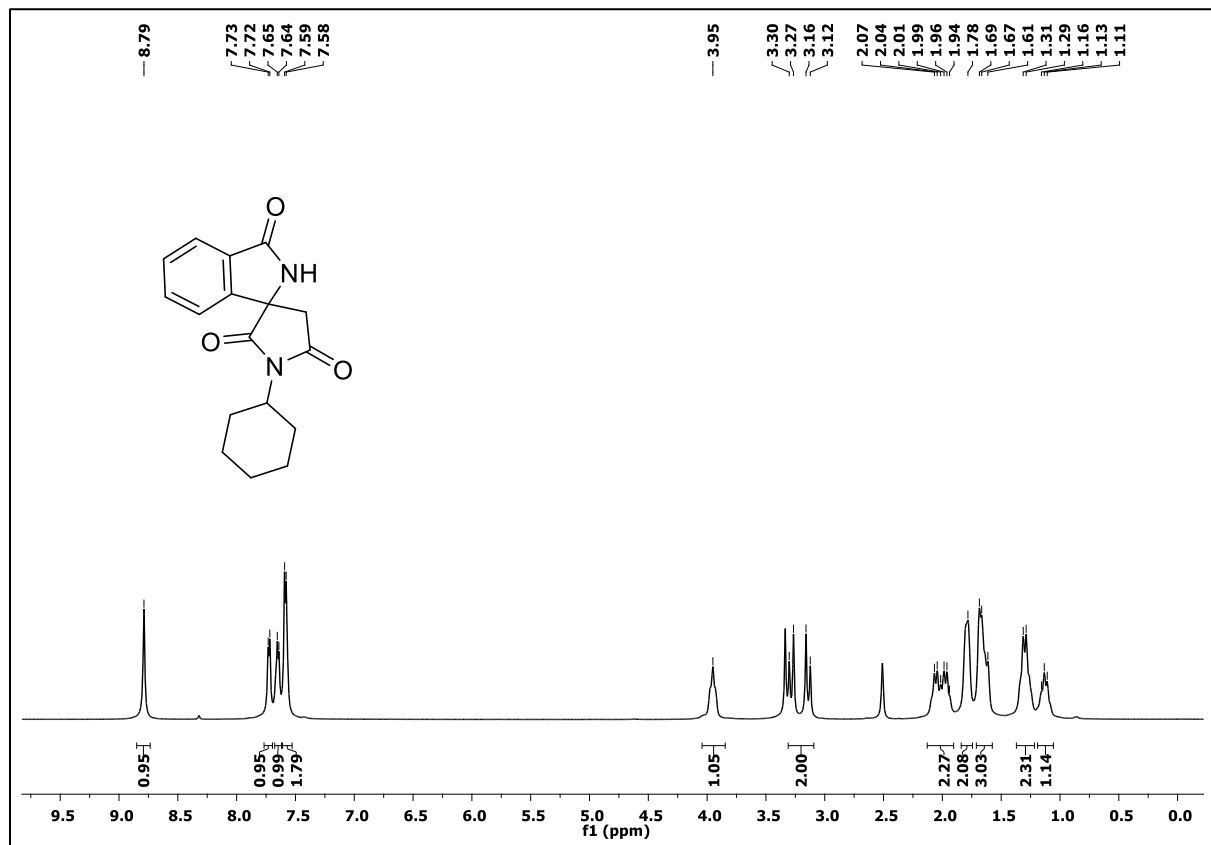


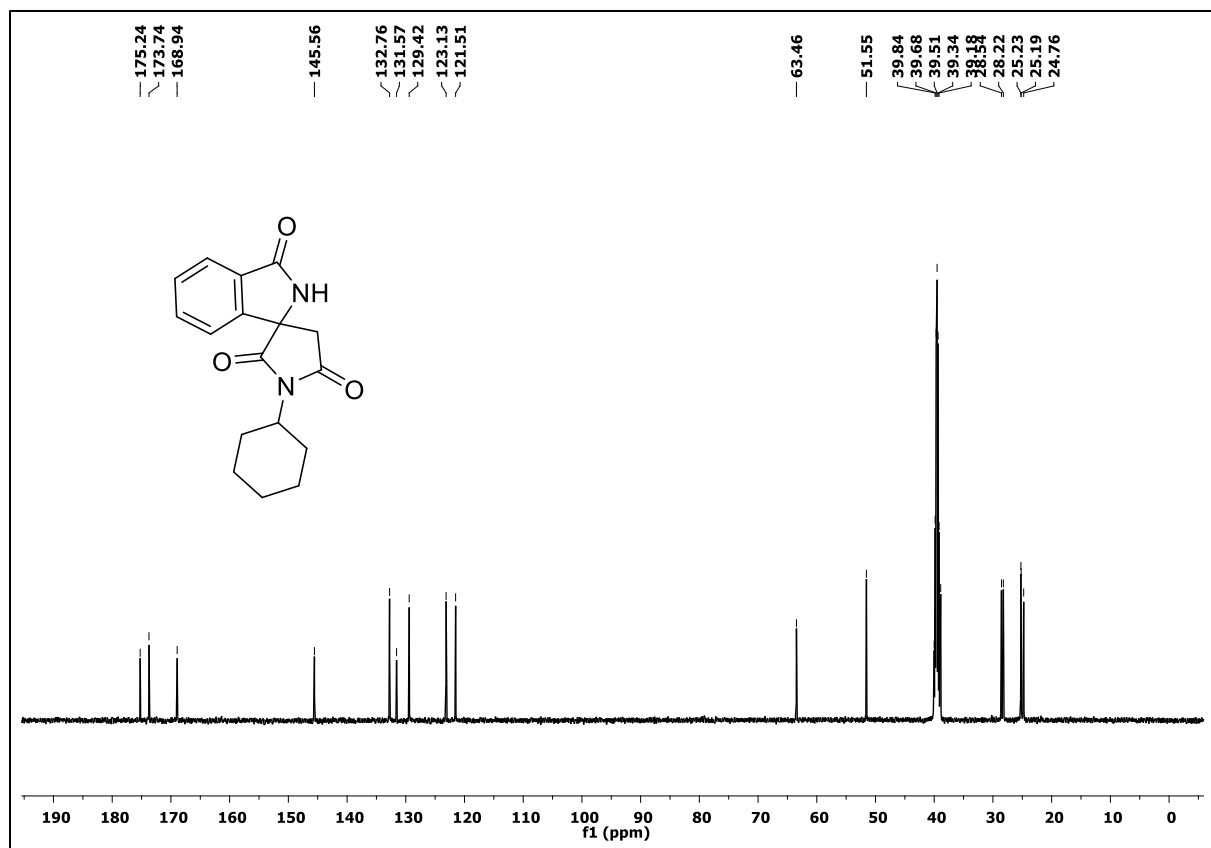
¹H and ¹³C{¹H} NMR Spectra of Compound 3ae.



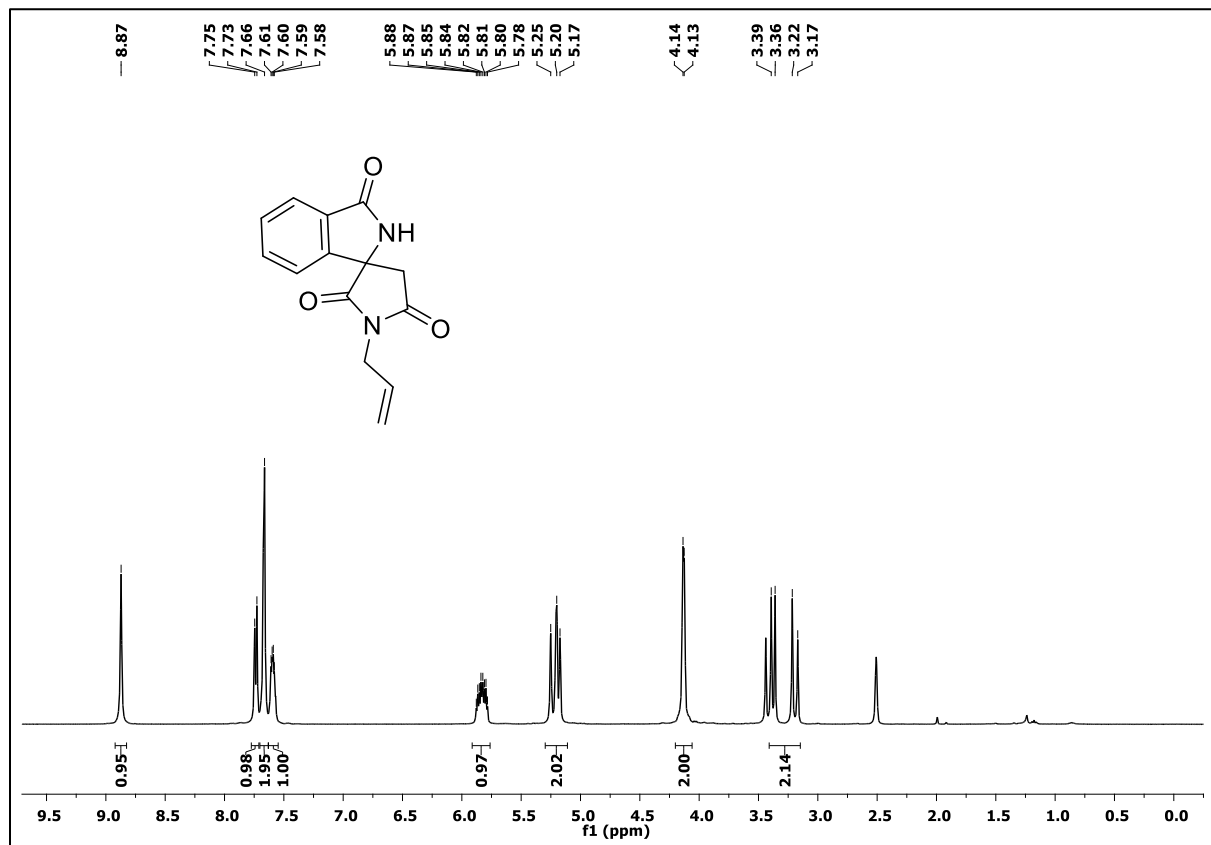


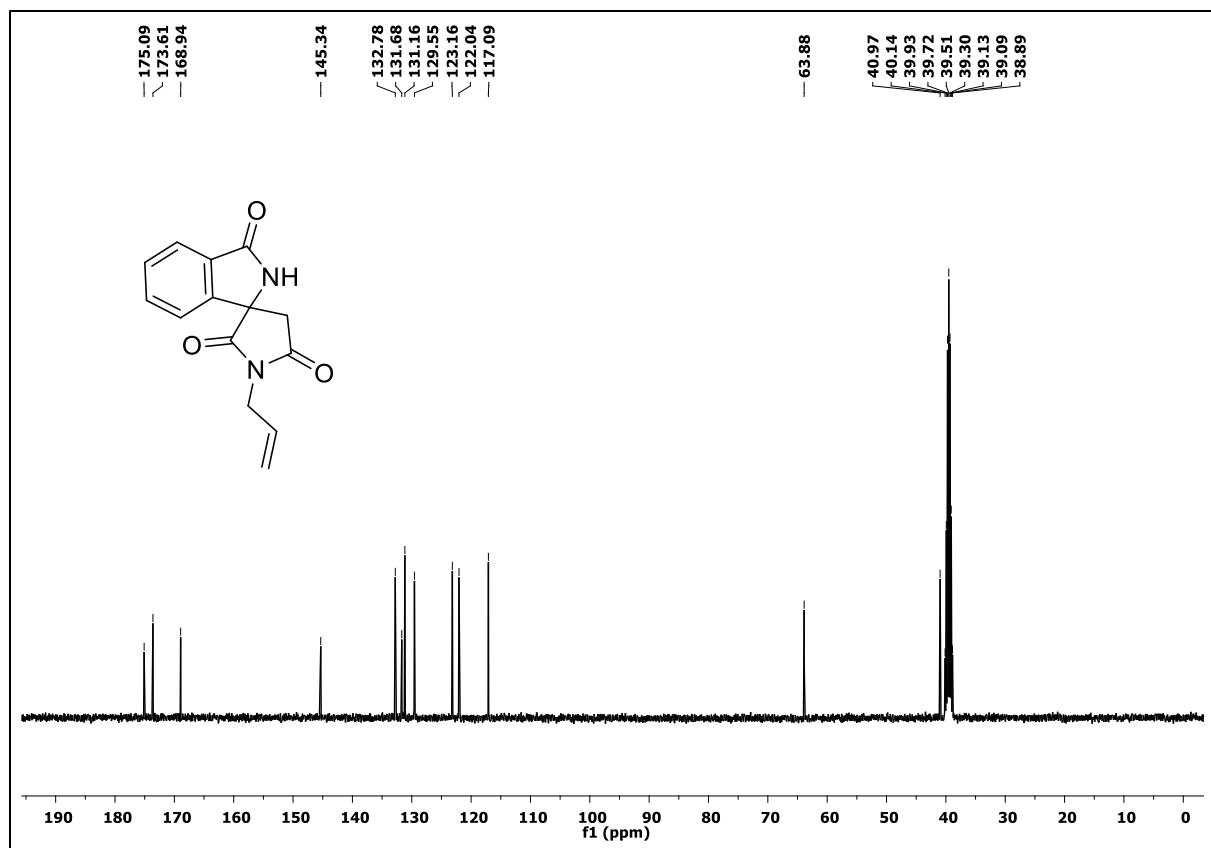
¹H and ¹³C{¹H} NMR Spectra of Compound **3af**.



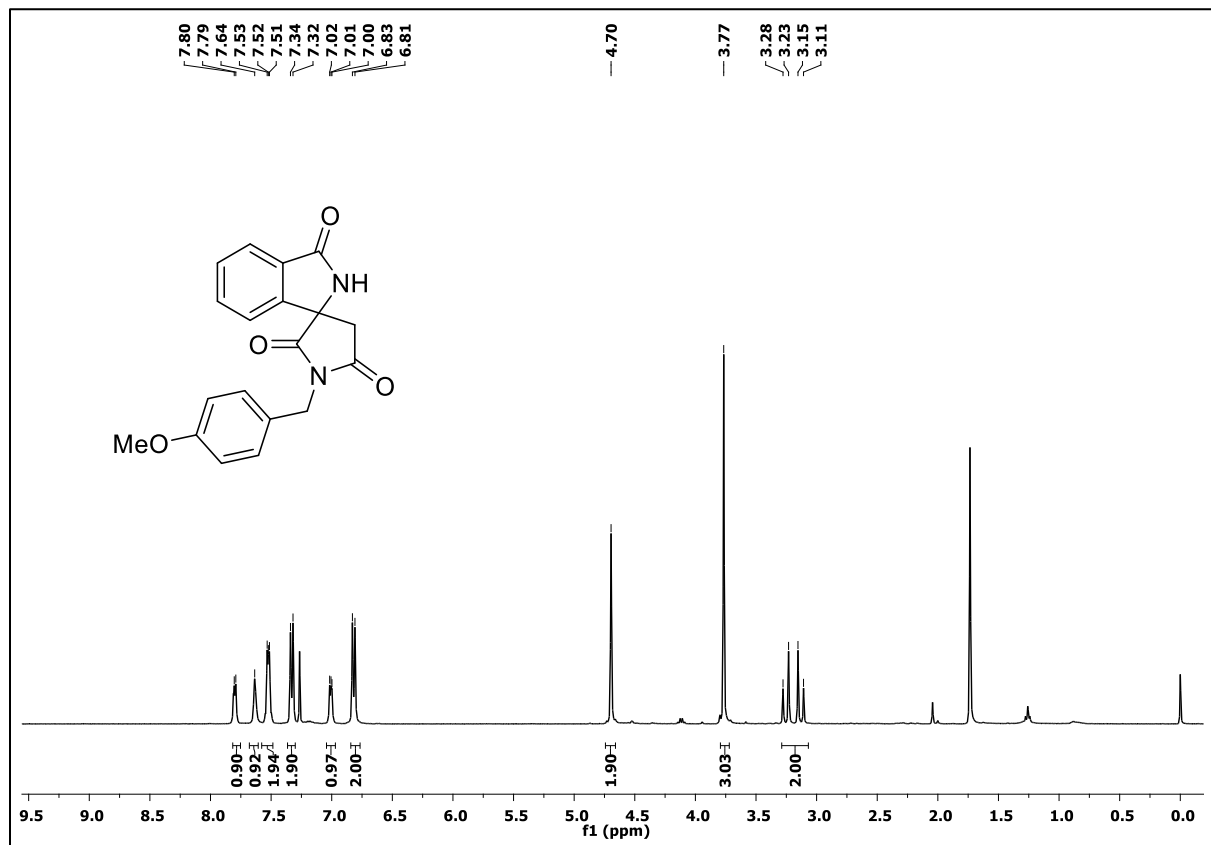


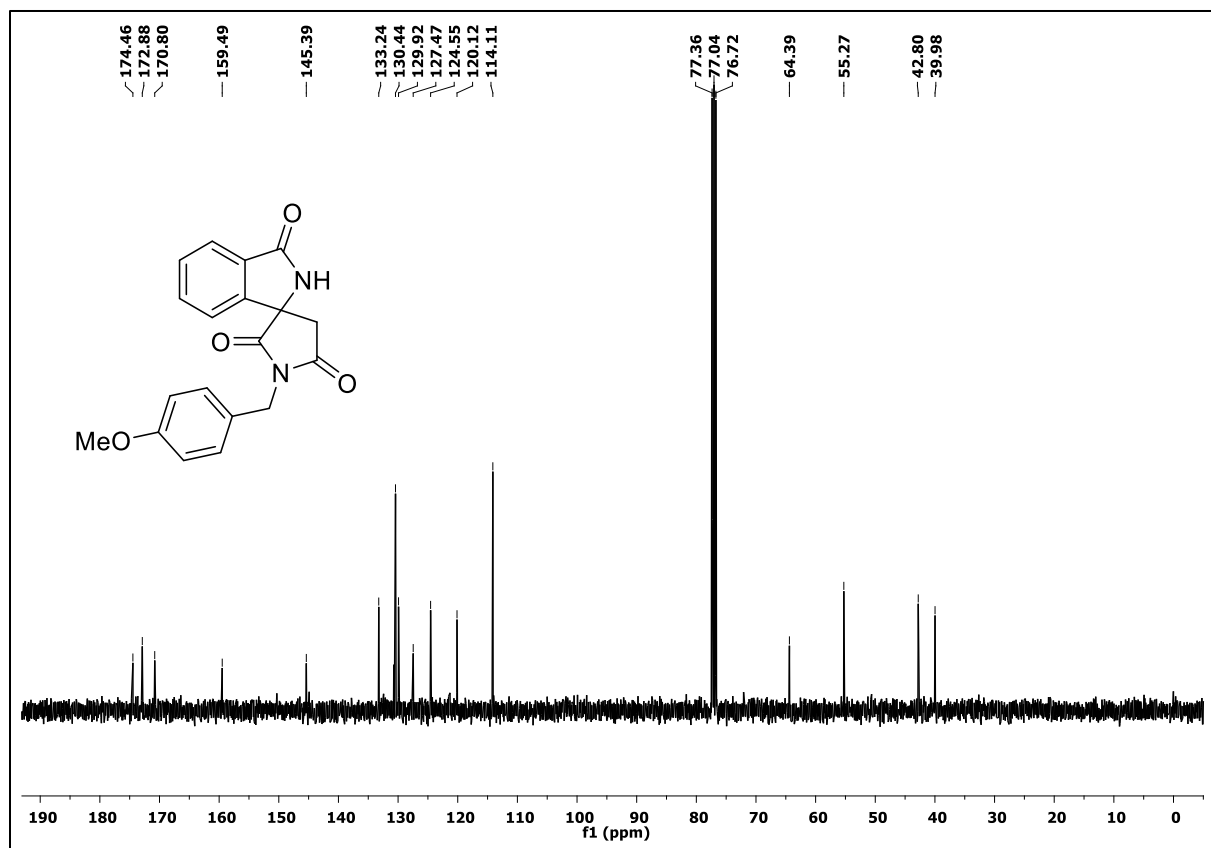
¹H and ¹³C{¹H} NMR Spectra of Compound 3ag.





¹H and ¹³C{¹H} NMR Spectra of Compound **3ah**.





¹H and ¹³C{¹H} NMR Spectra of Compound **3ai**.

