

Supporting Information

CATALYST-FREE GREEN SYNTHESIS OF PHTHALAZINONES AT ROOM TEMPERATURE

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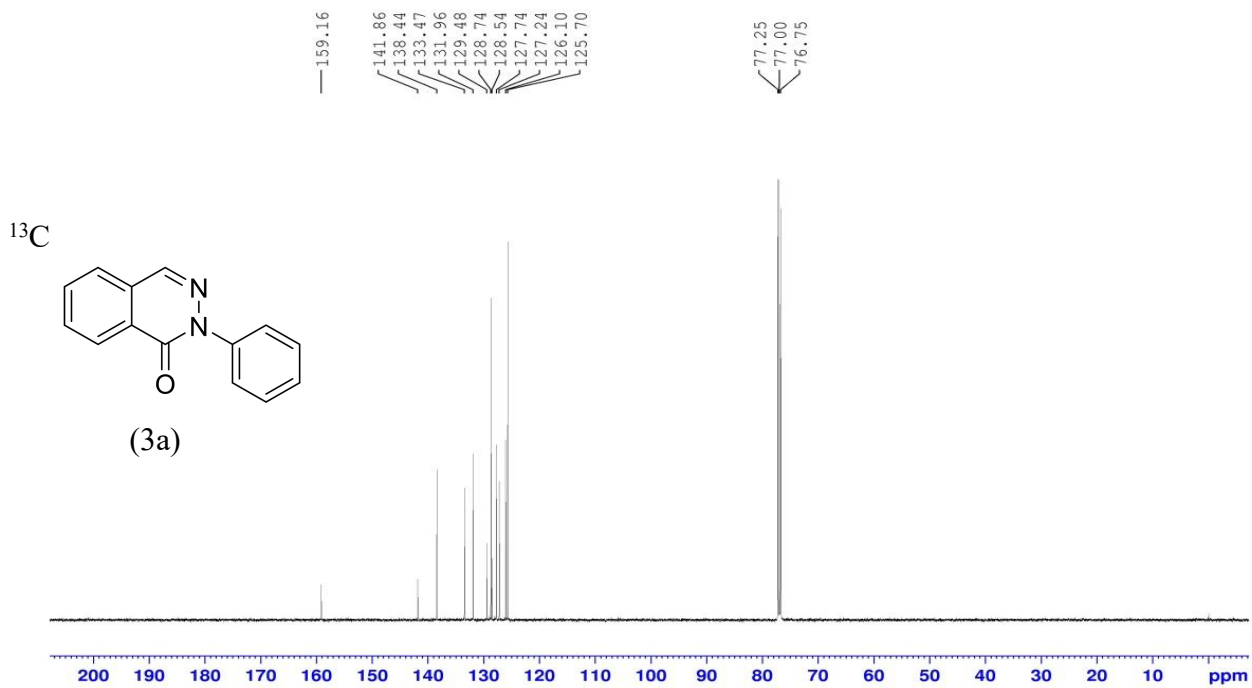
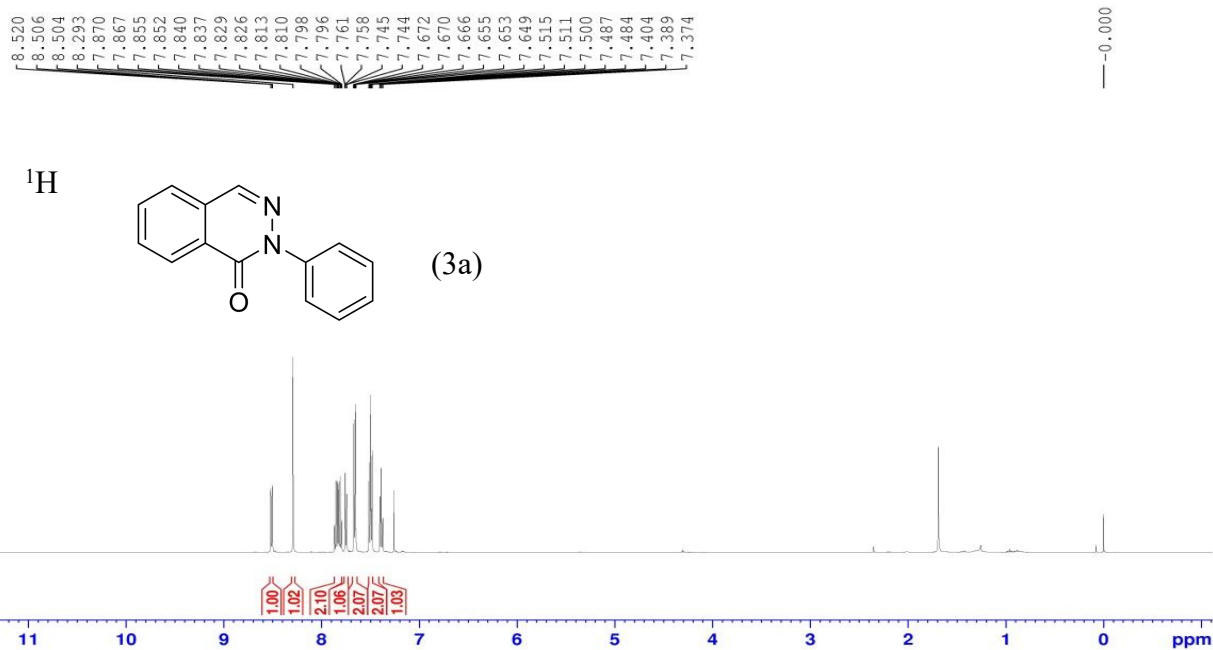
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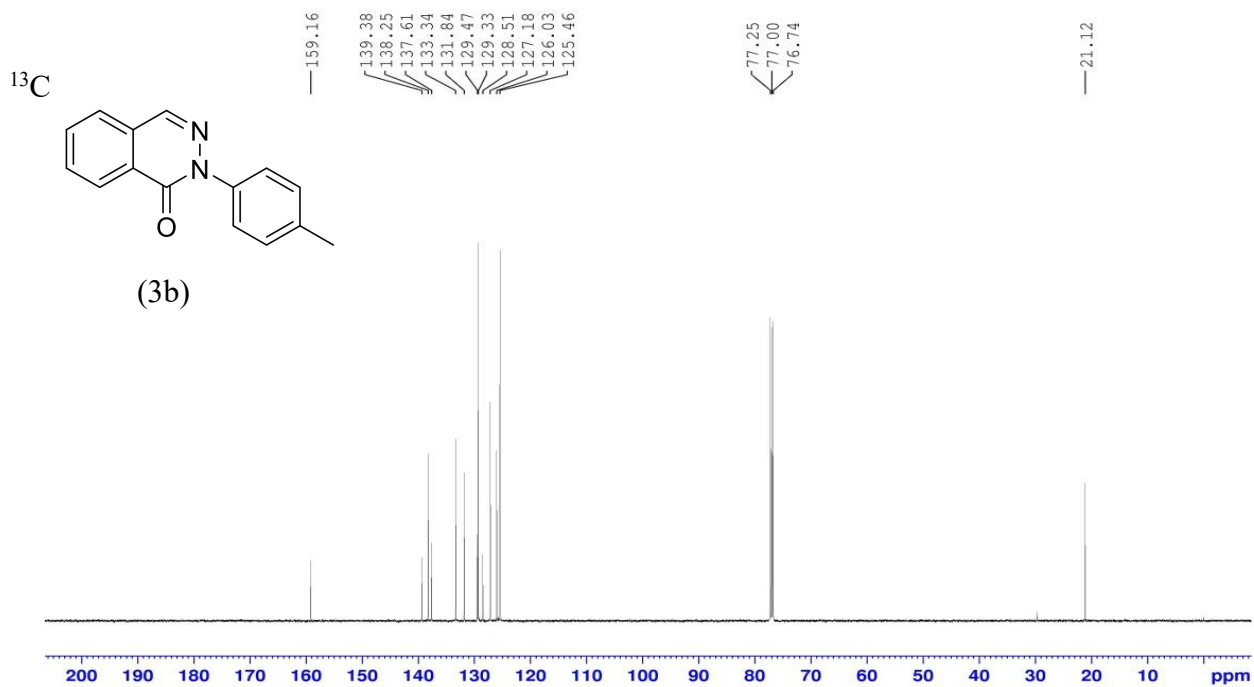
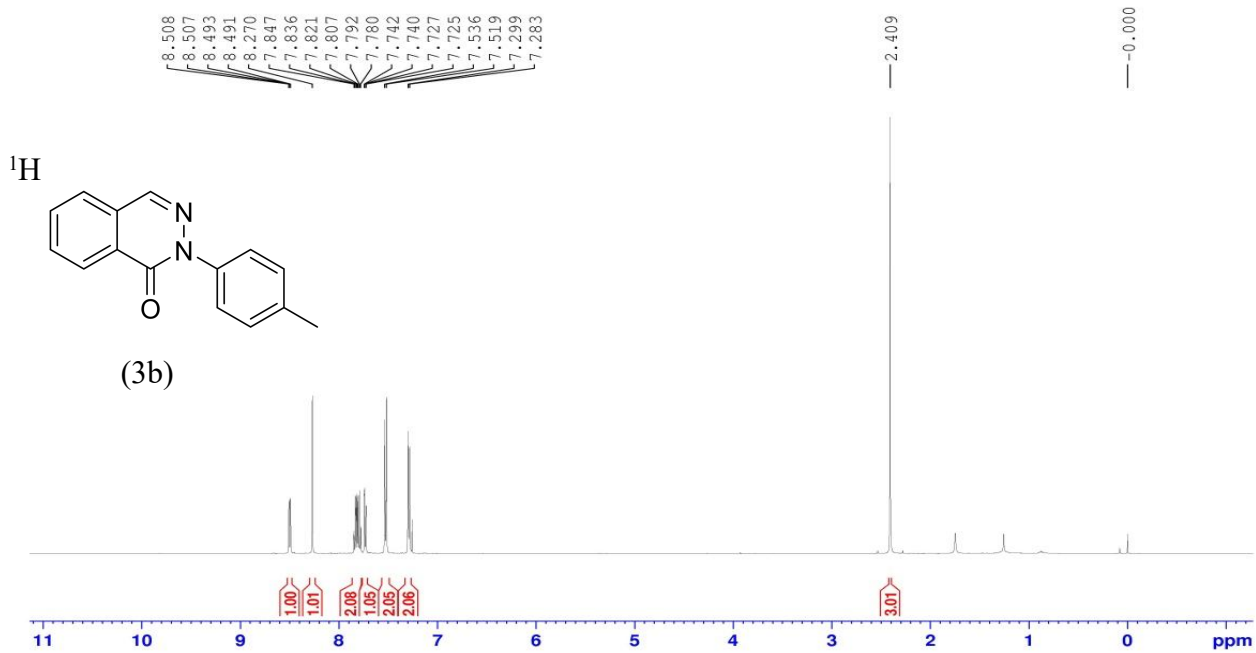
^bDepartment of Chemistry and Material Science, College of Science, Nanjing Forestry University, Nanjing 210037, China; E-mail: mengtao@njfu.edu.cn

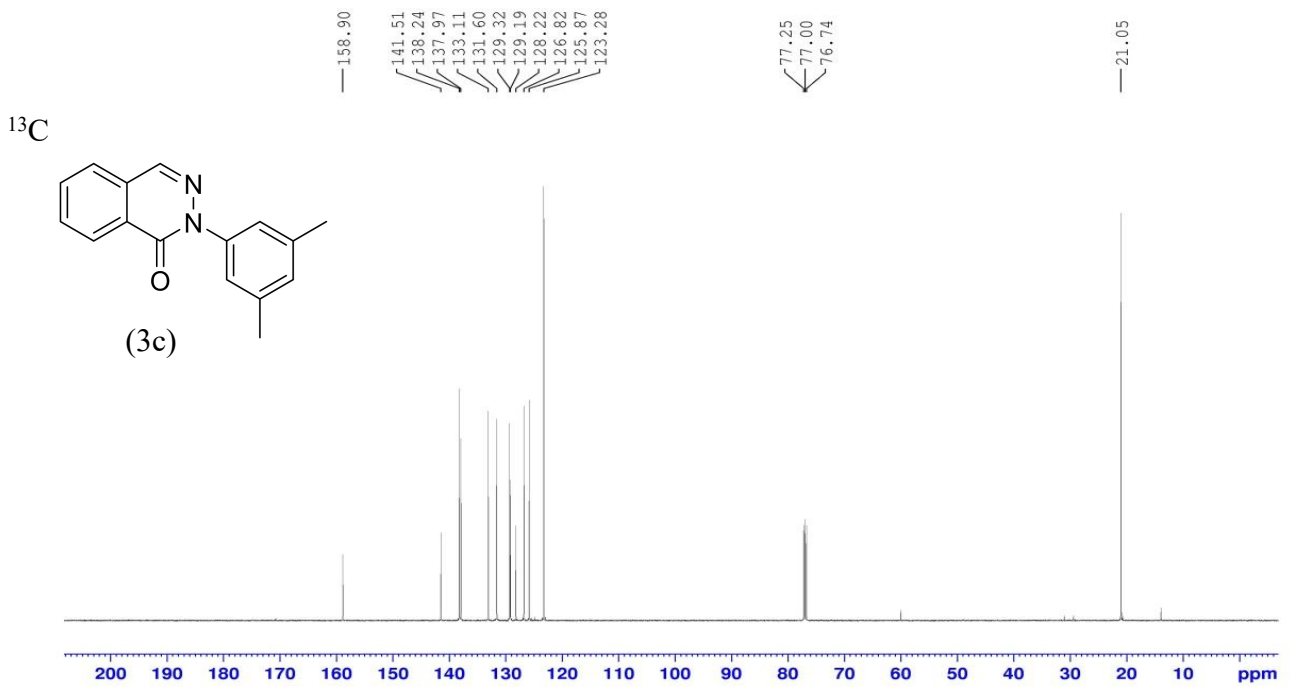
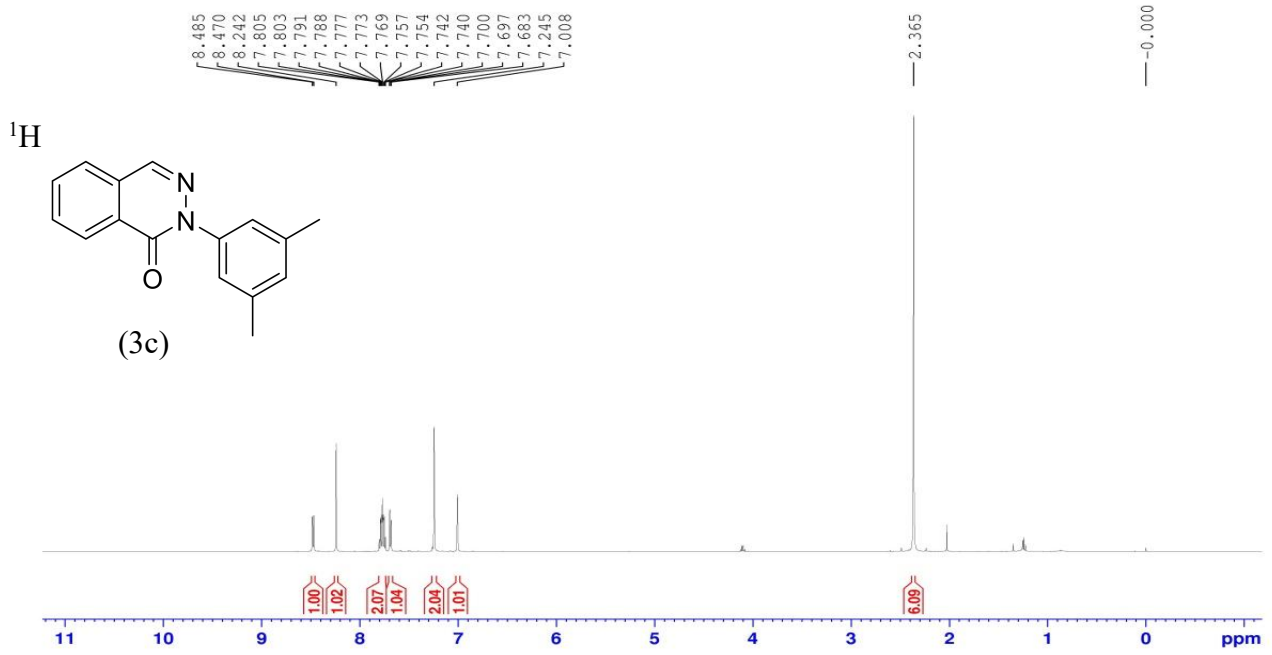
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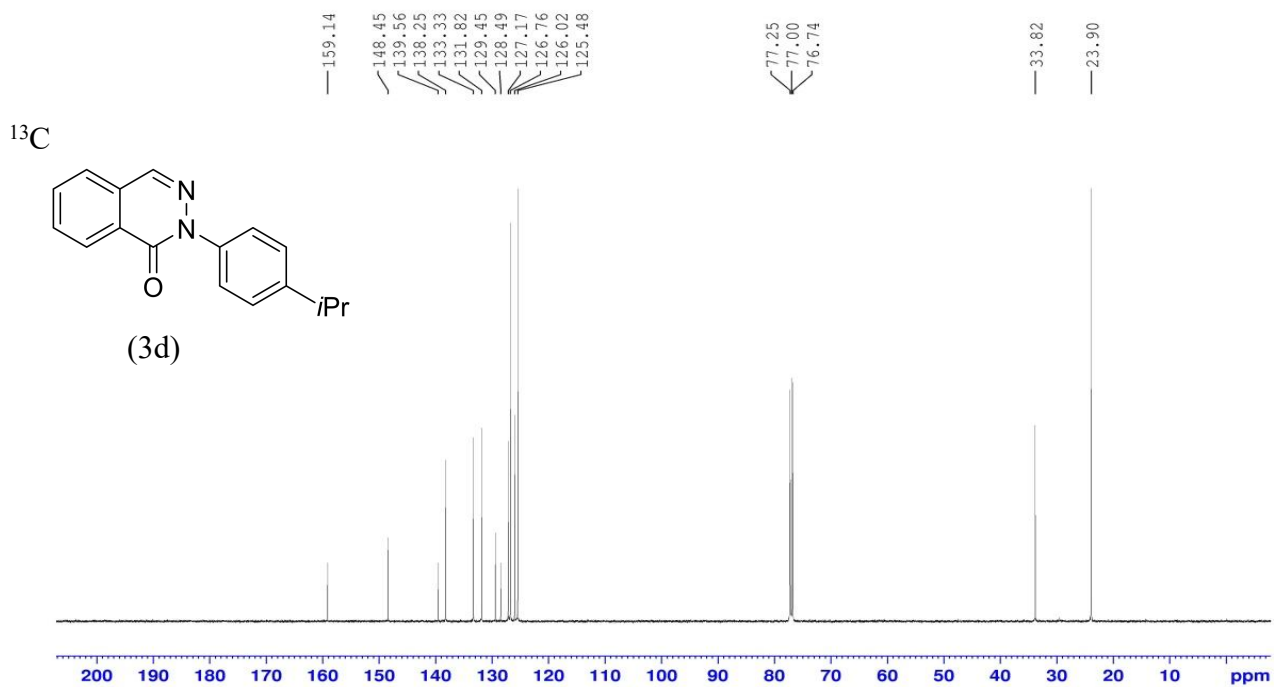
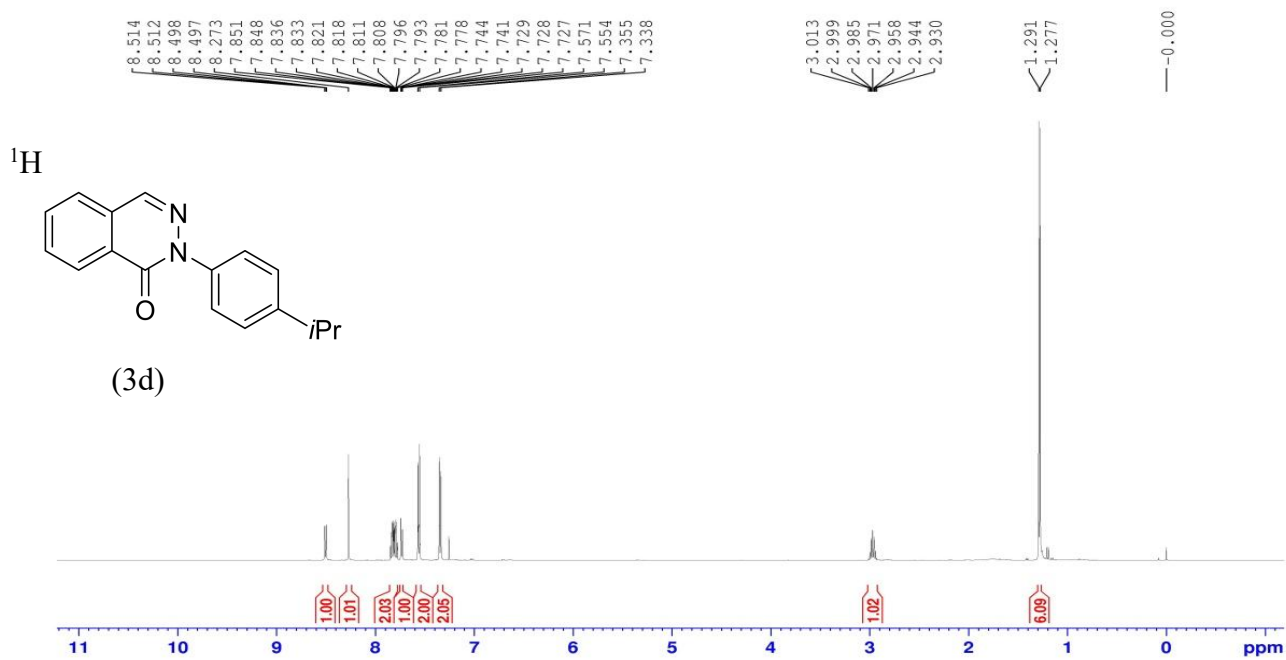
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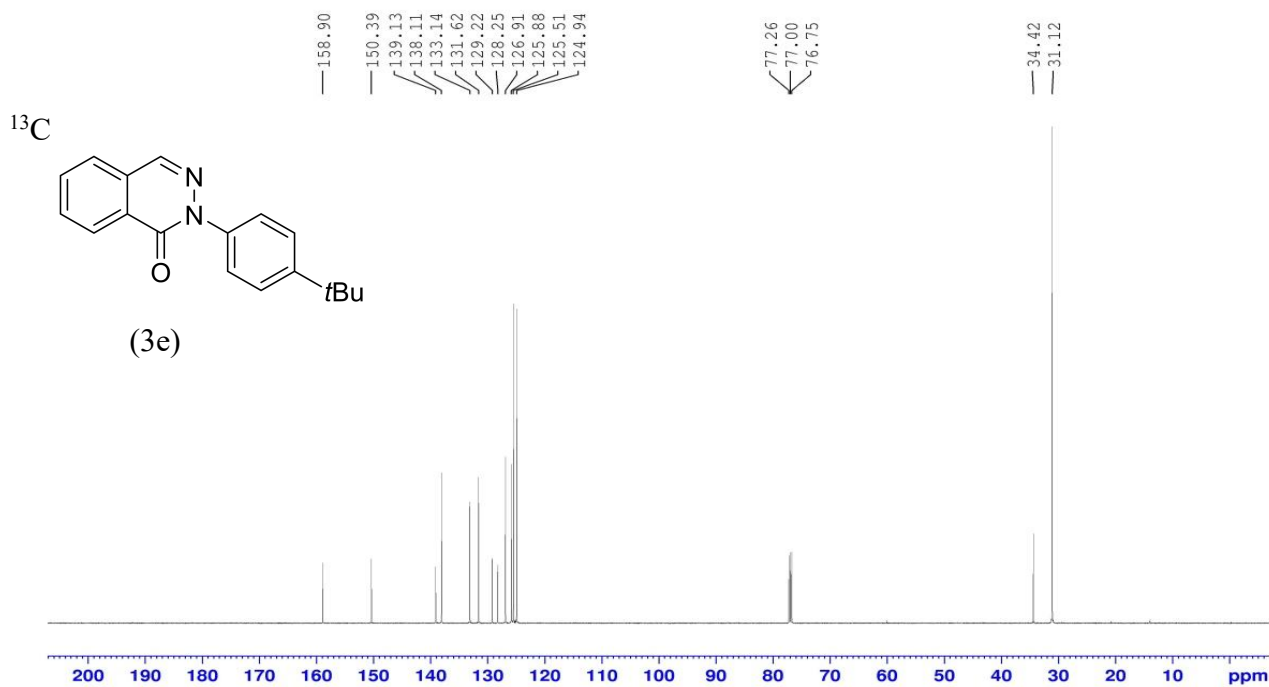
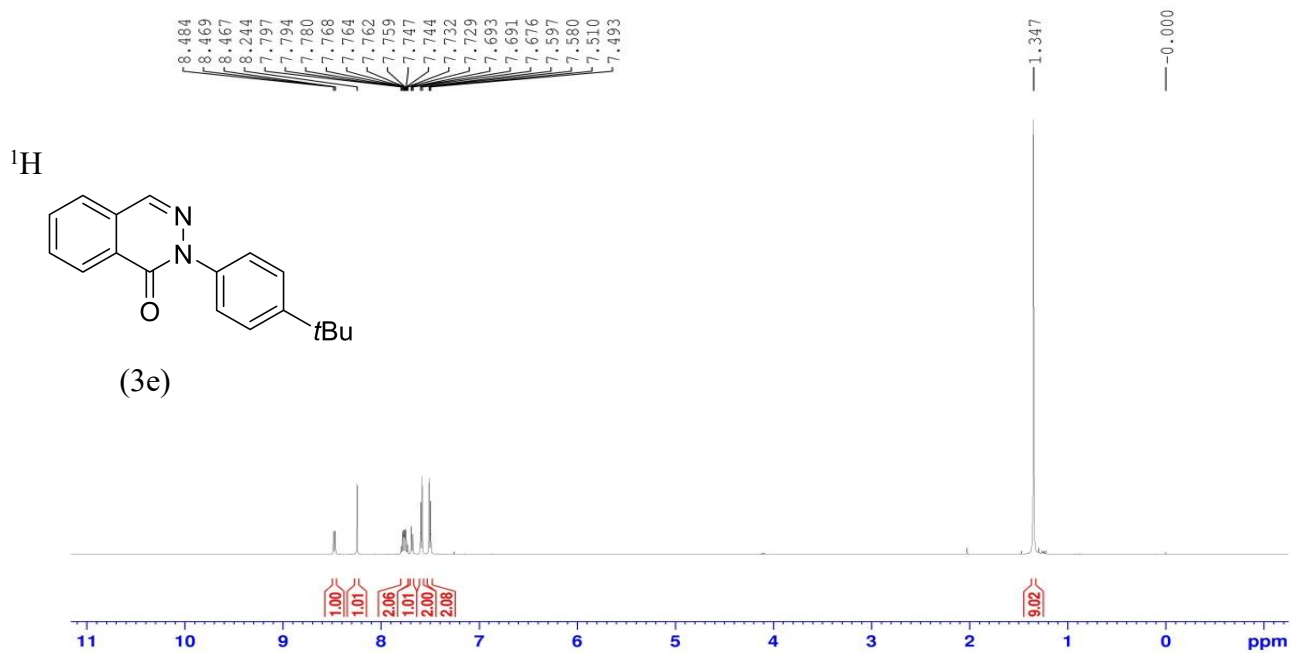
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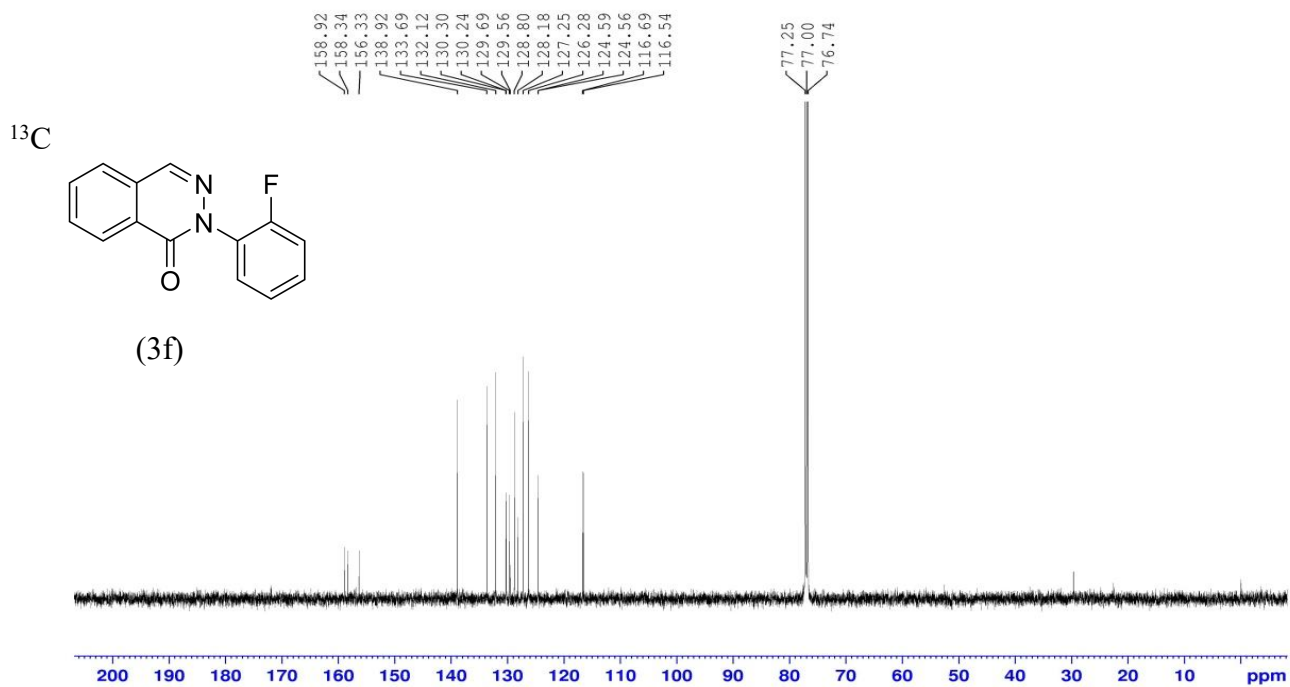
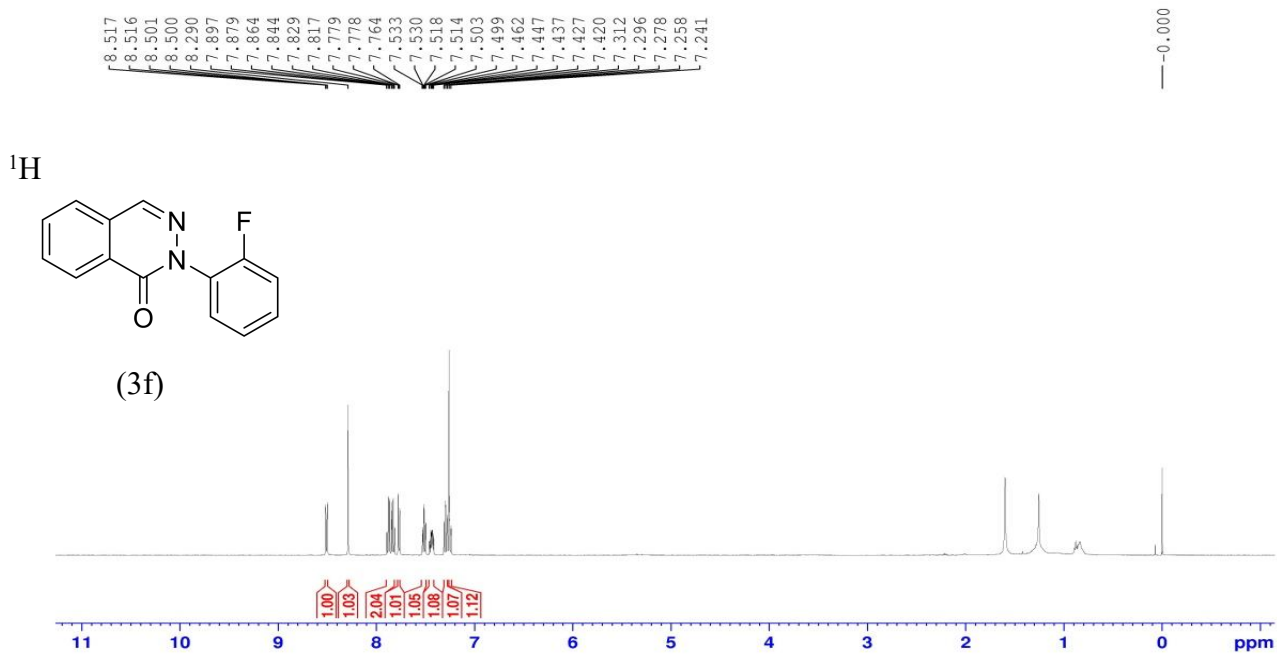


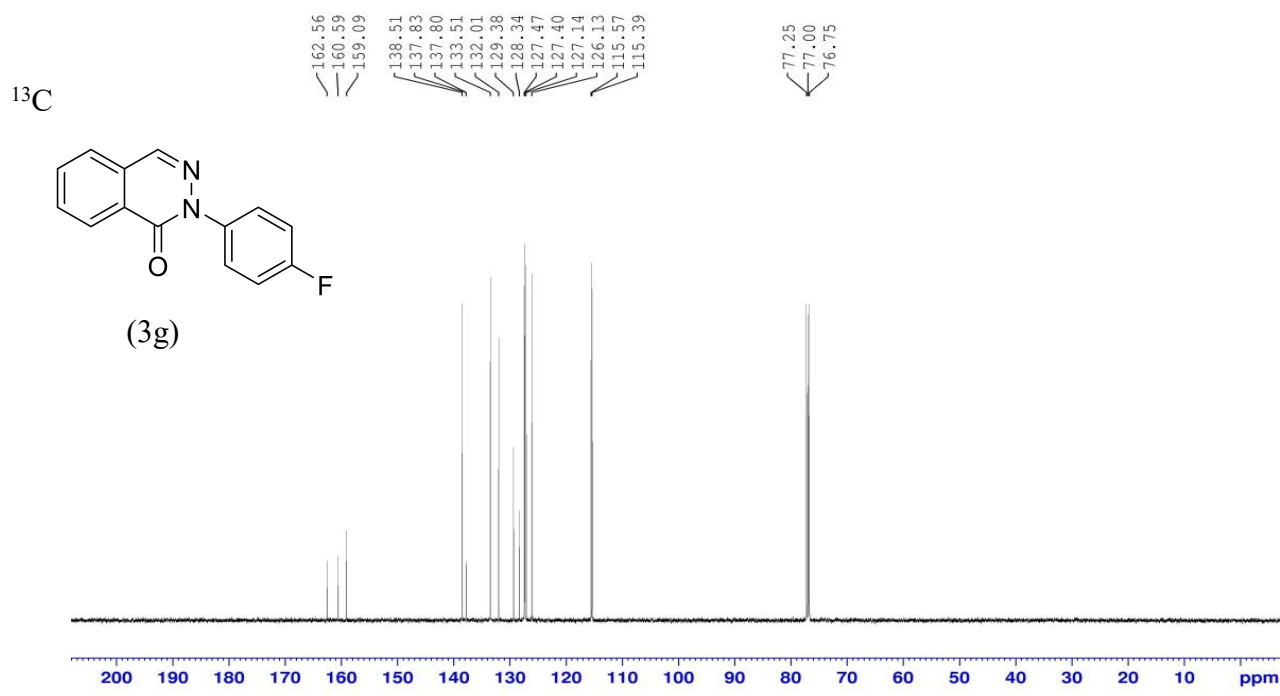
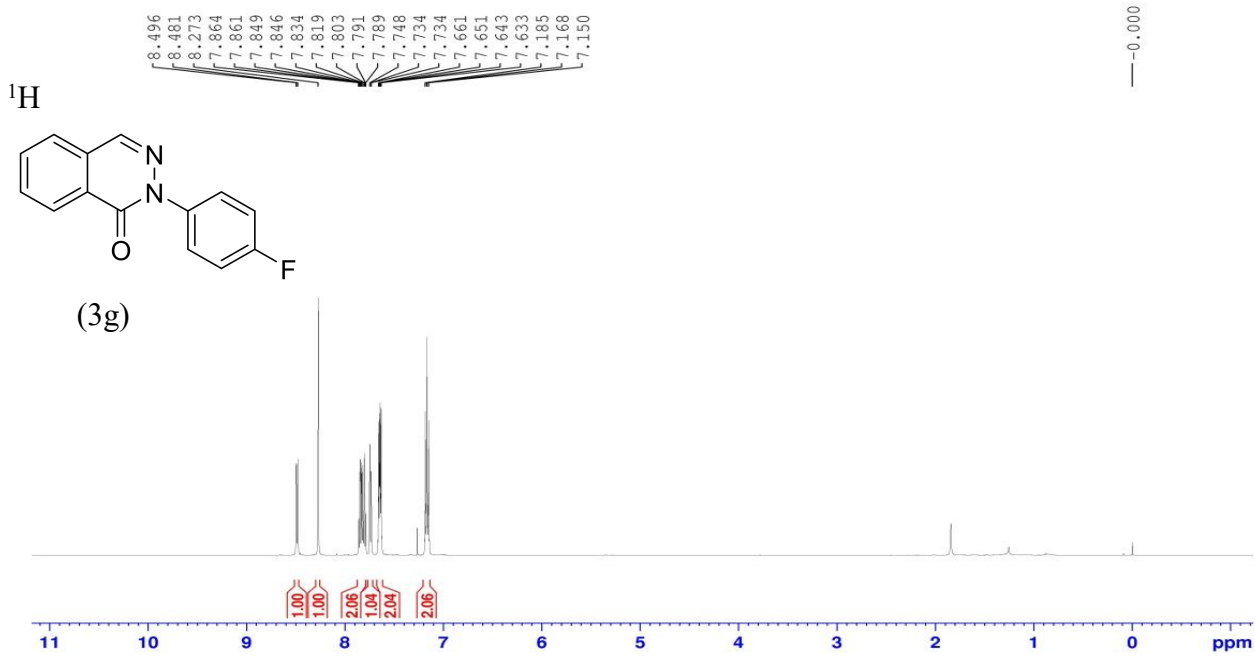


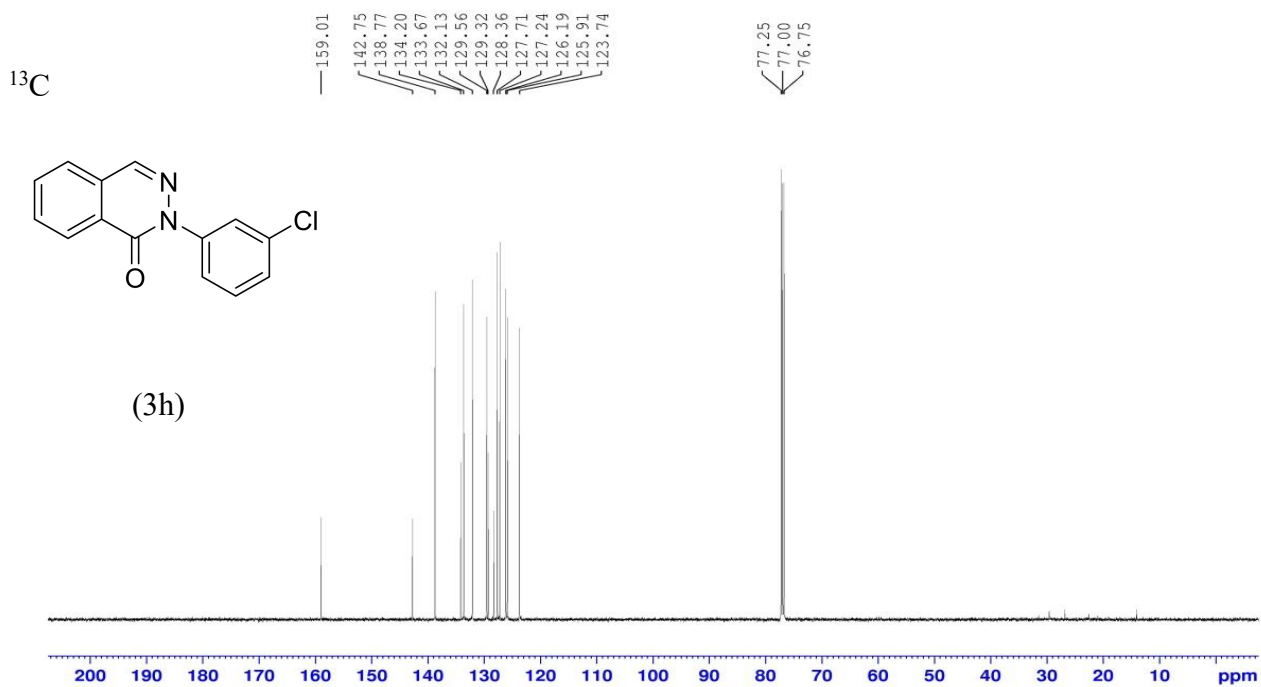
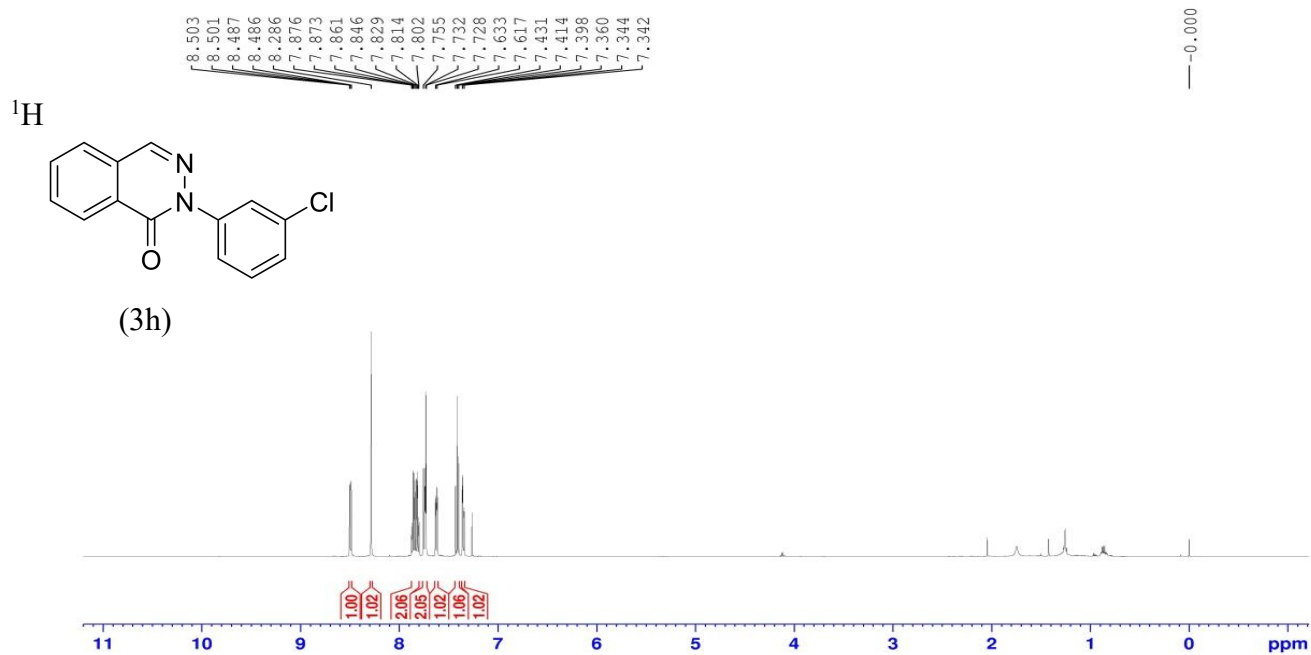


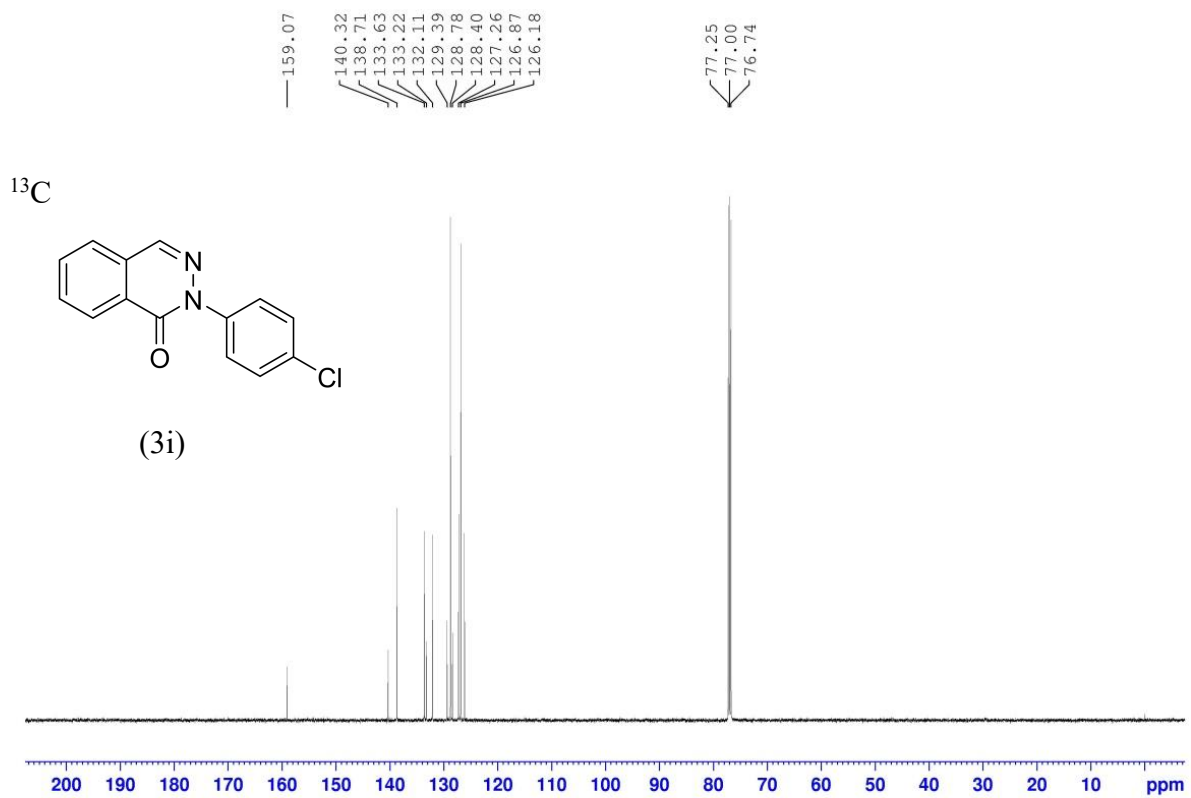
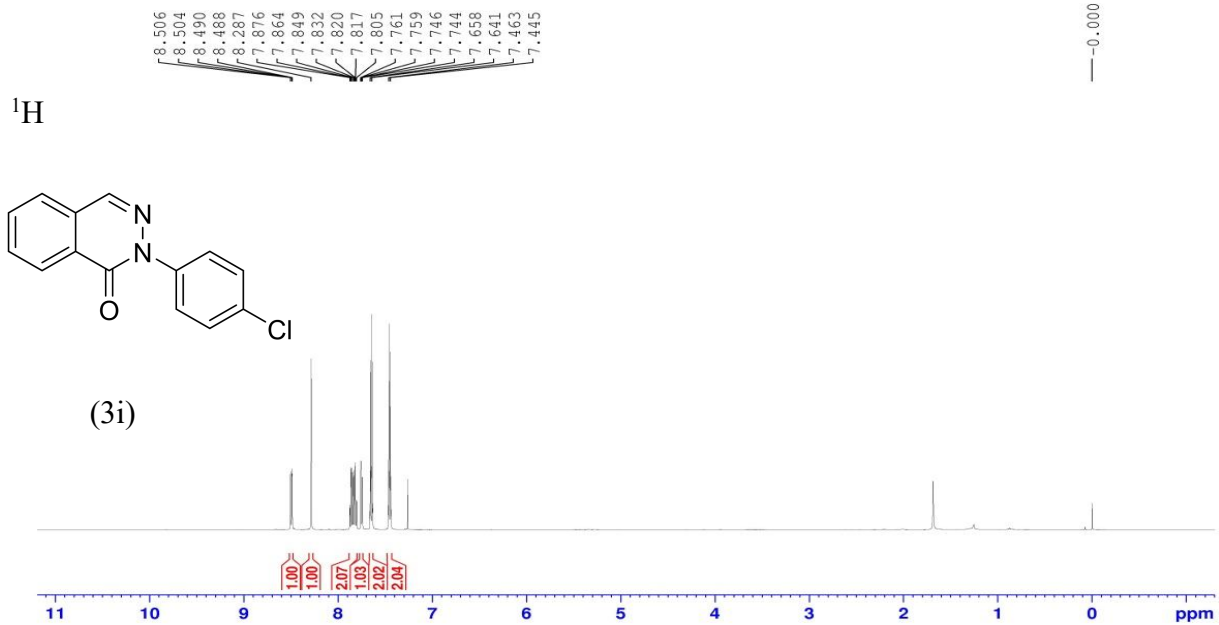


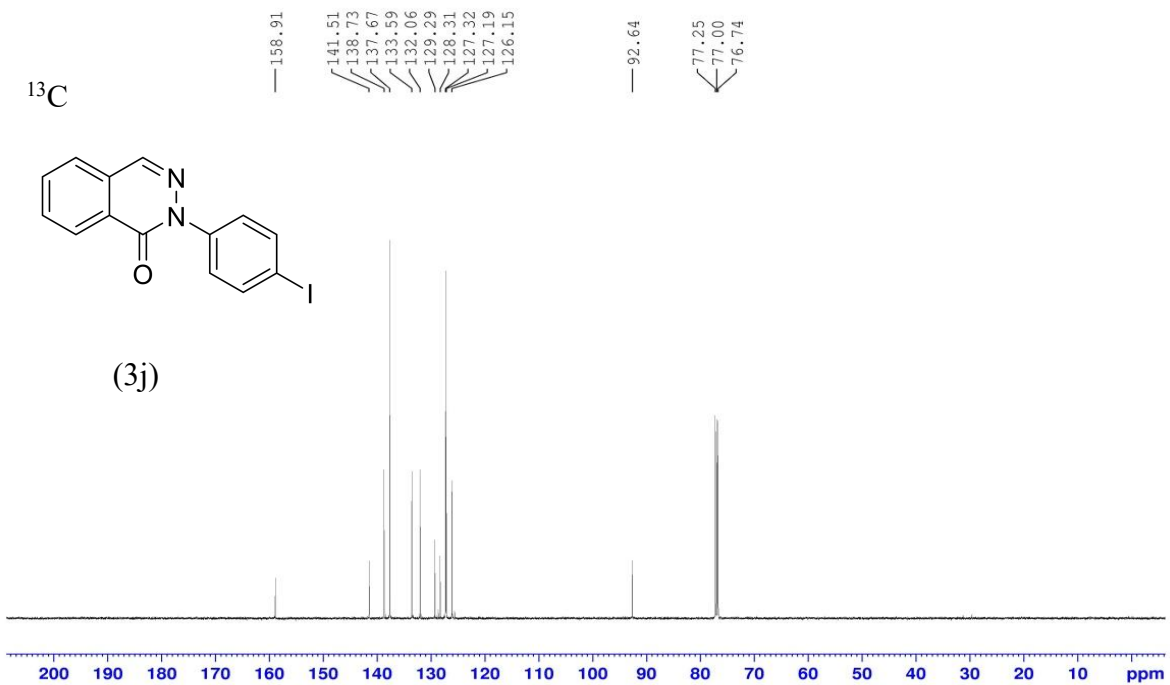
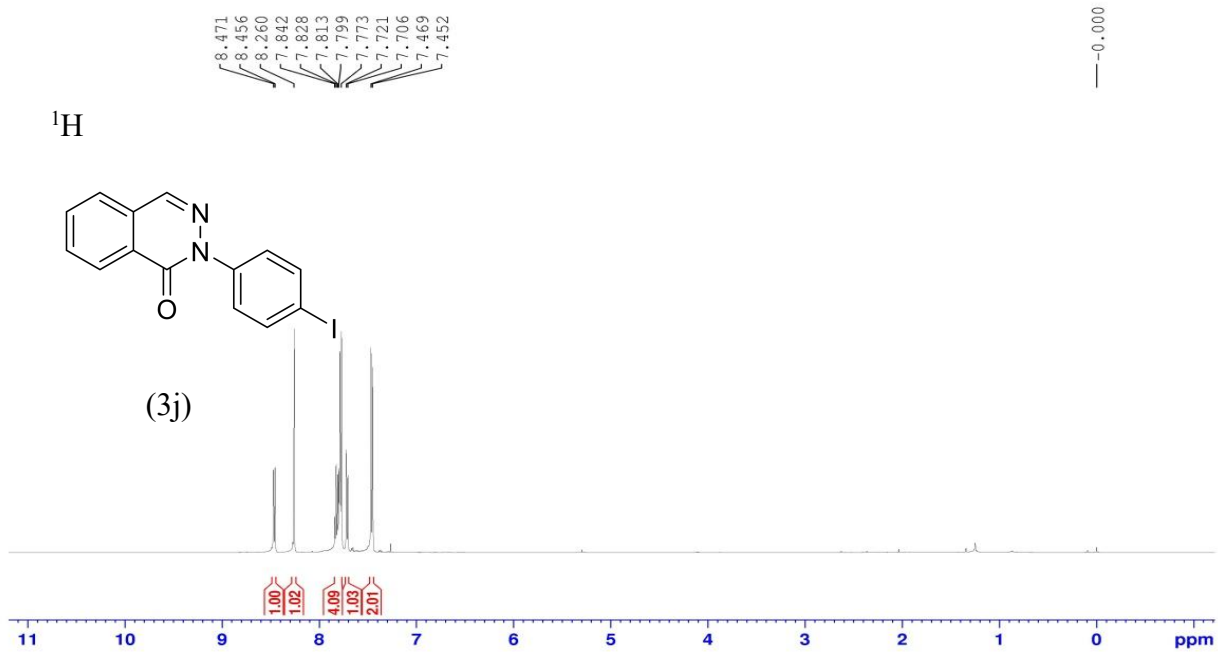


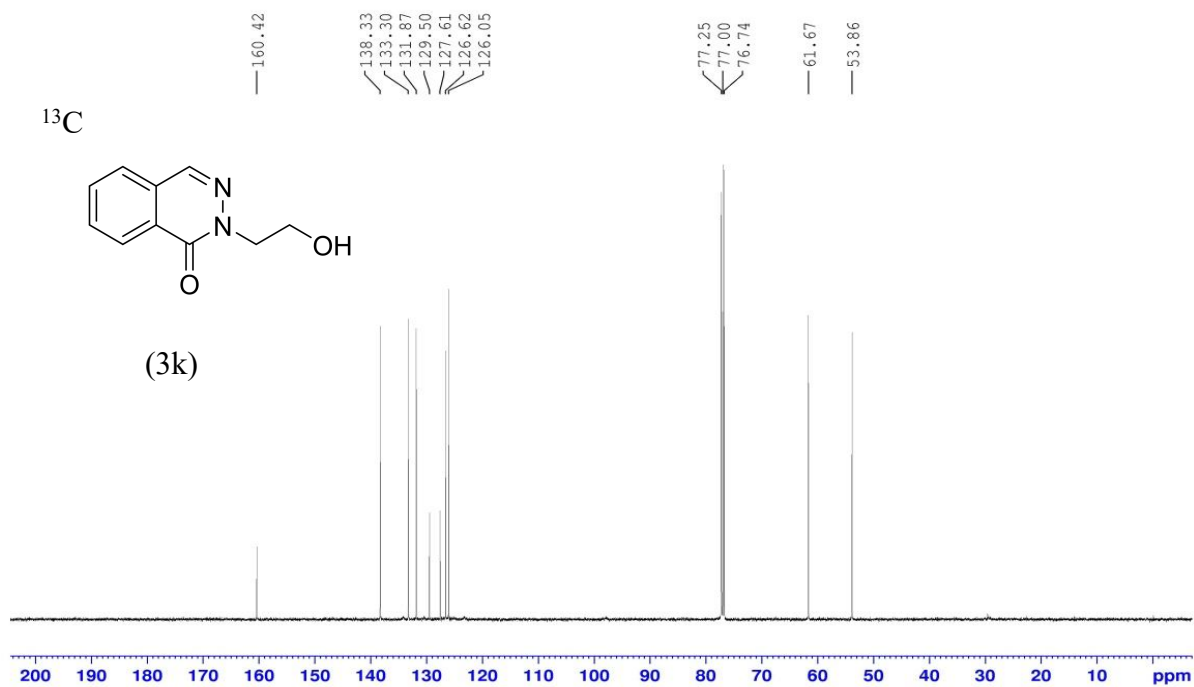
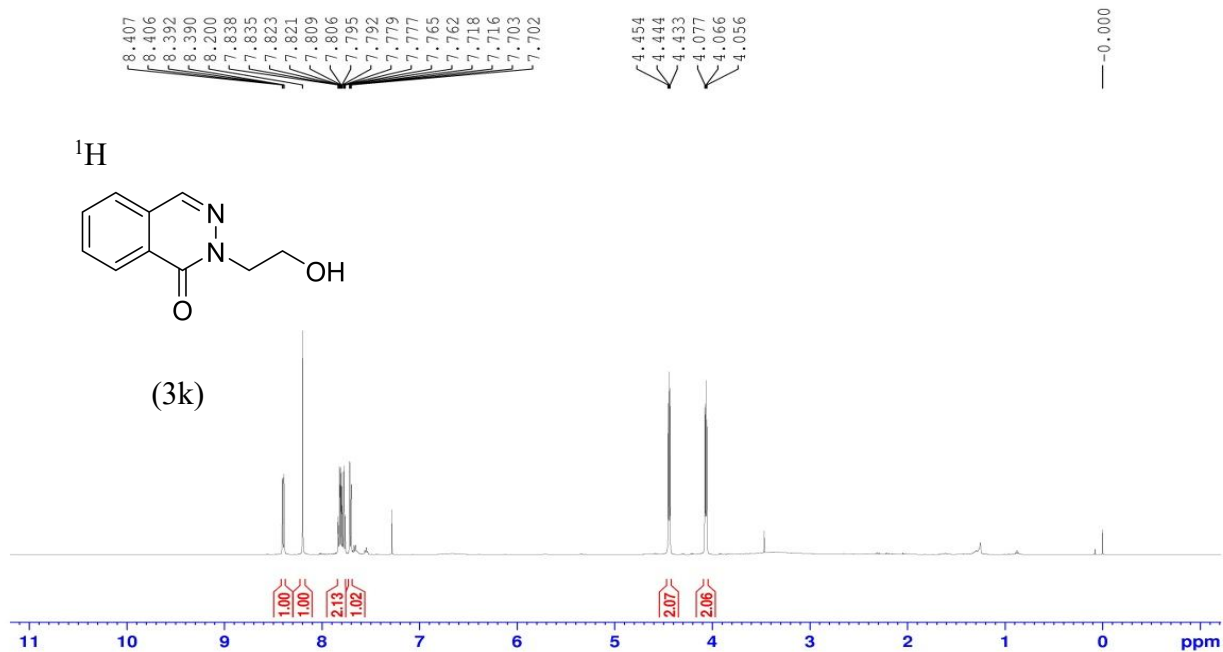


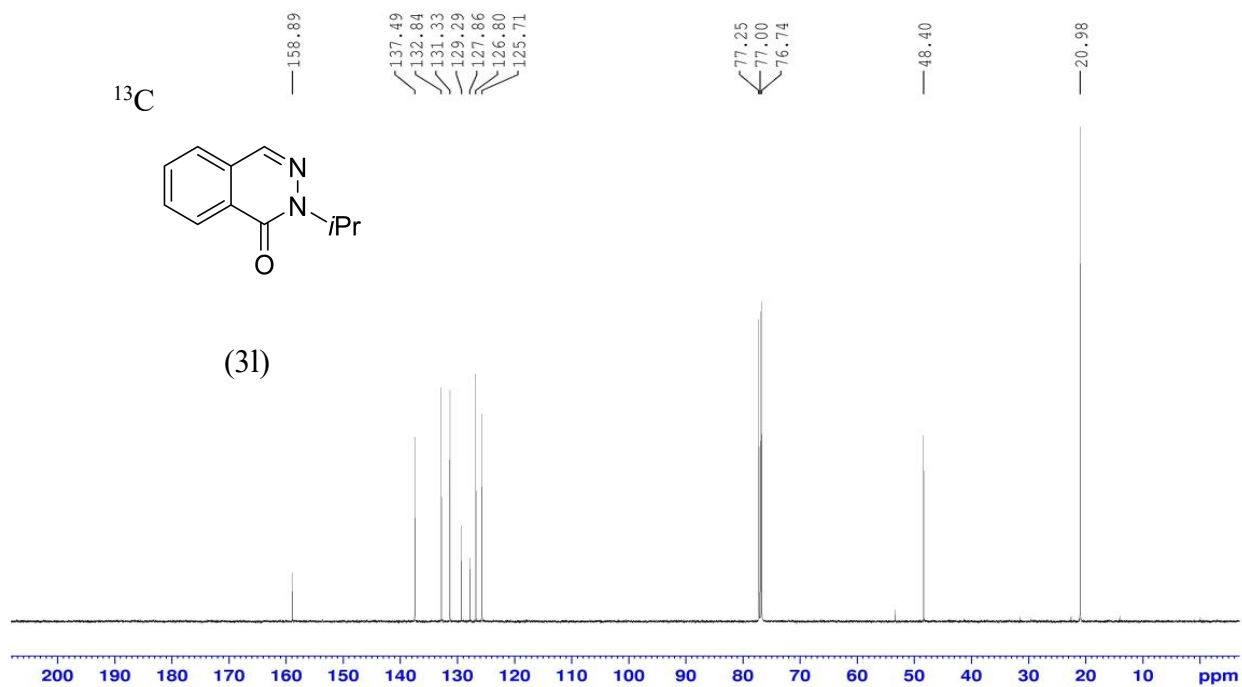
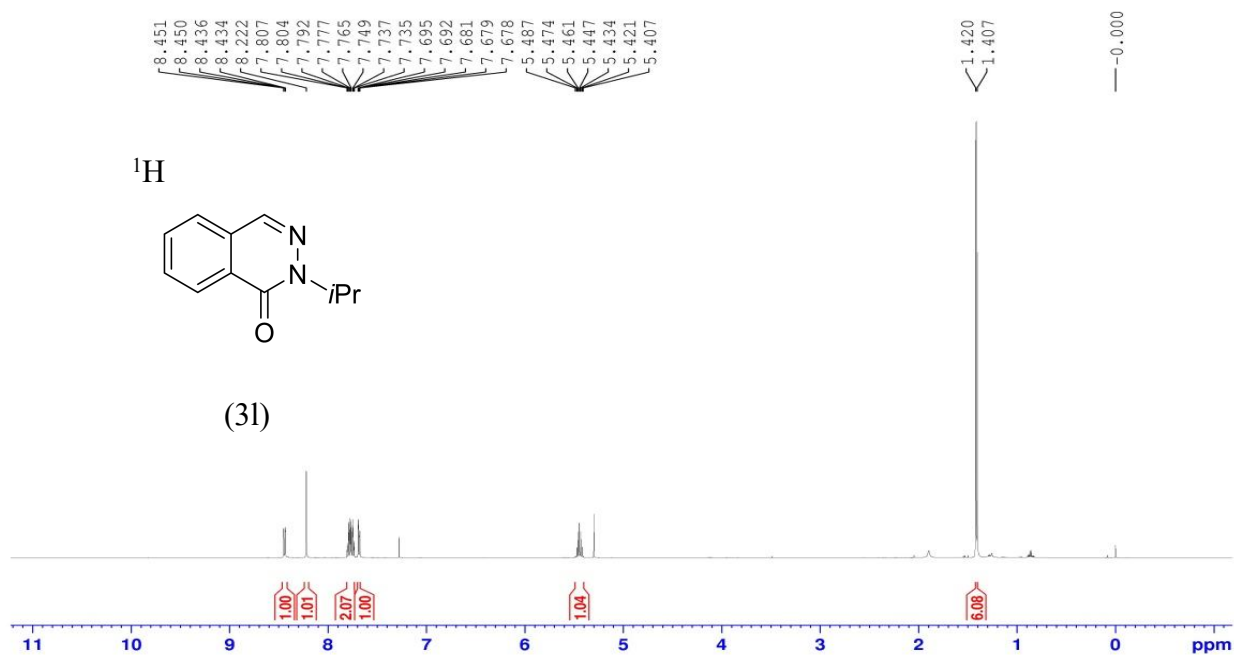


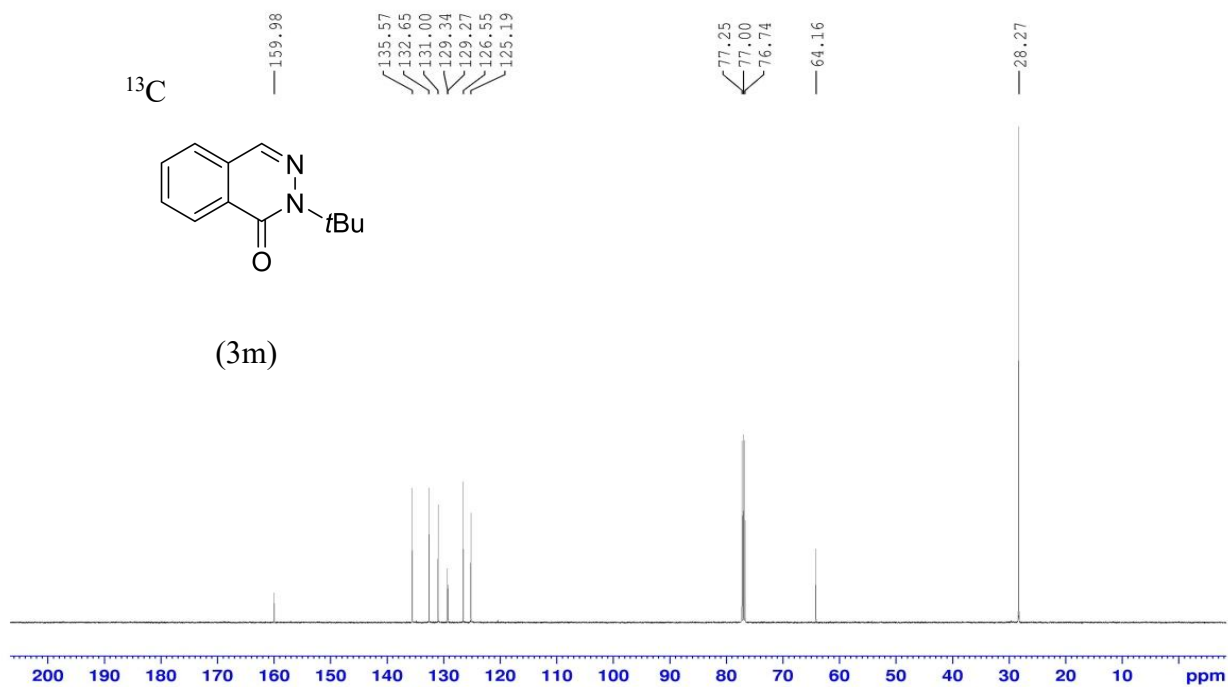
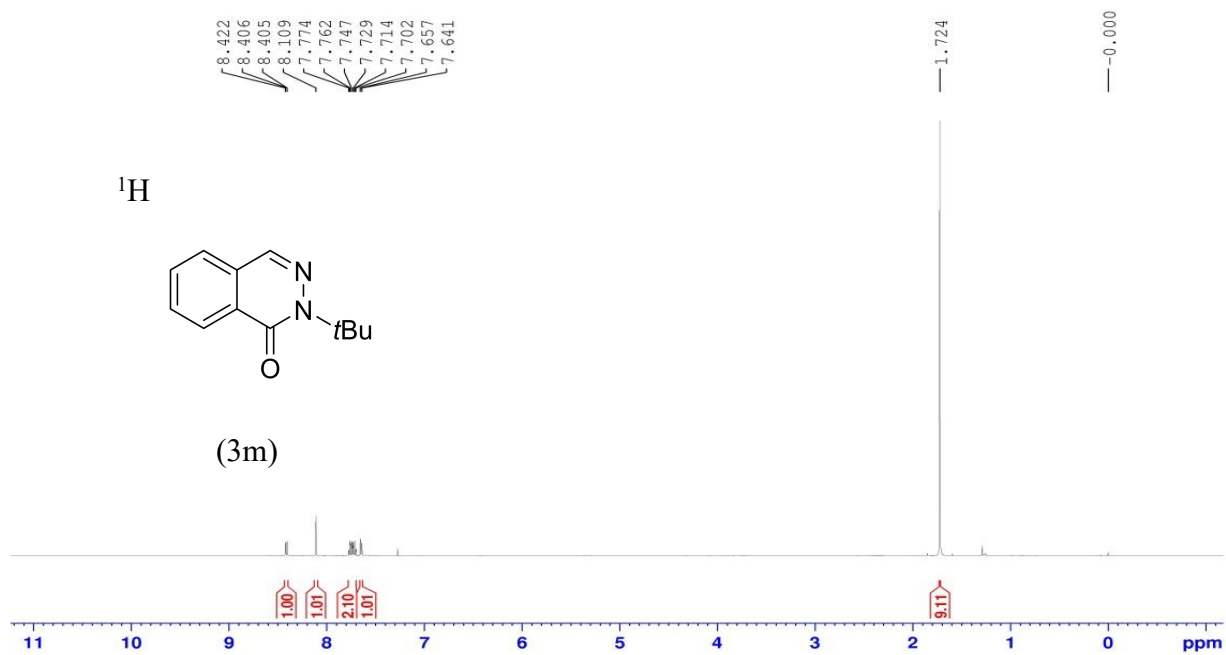


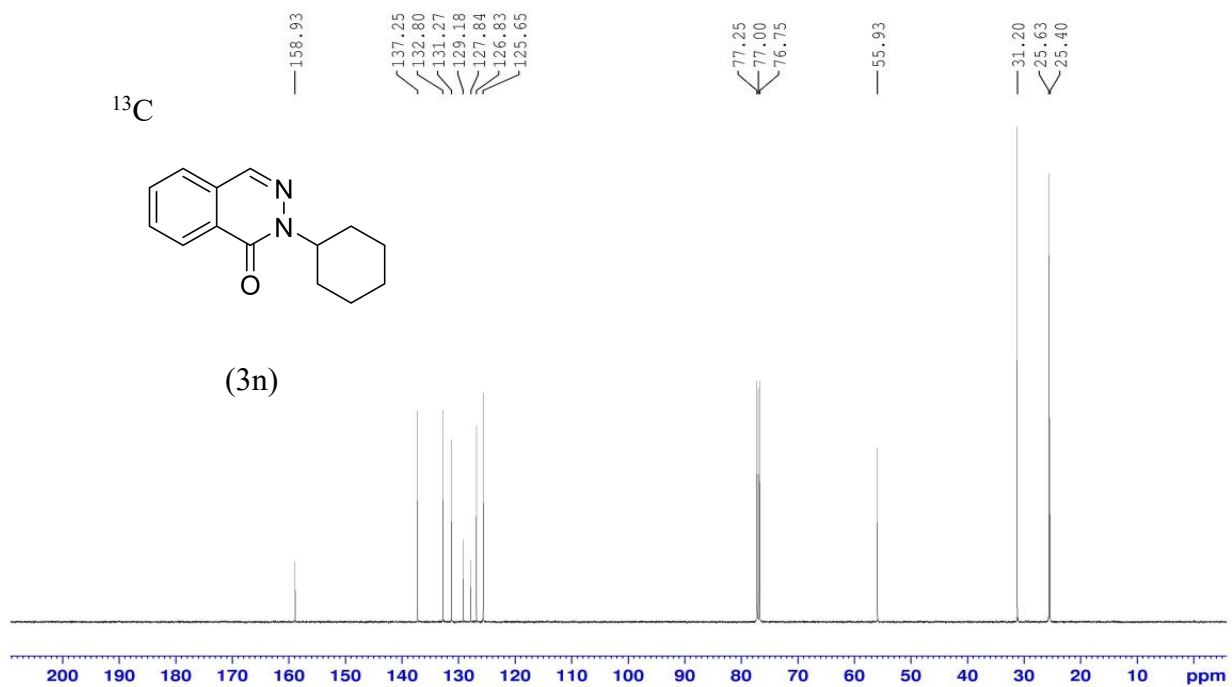
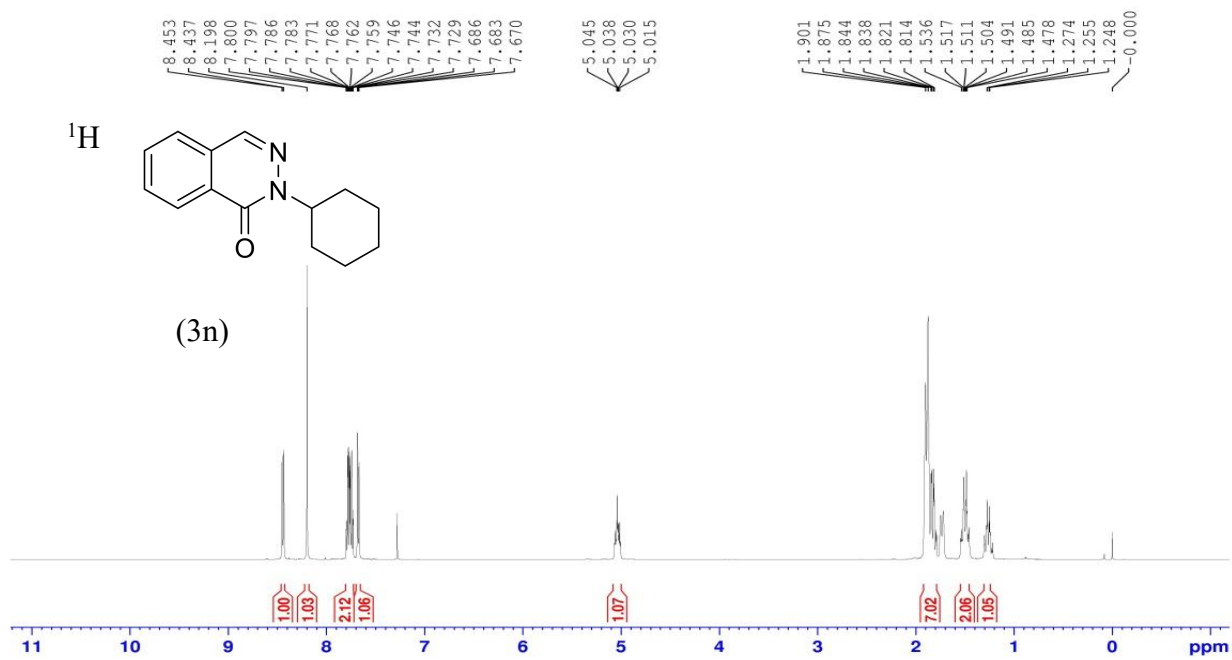


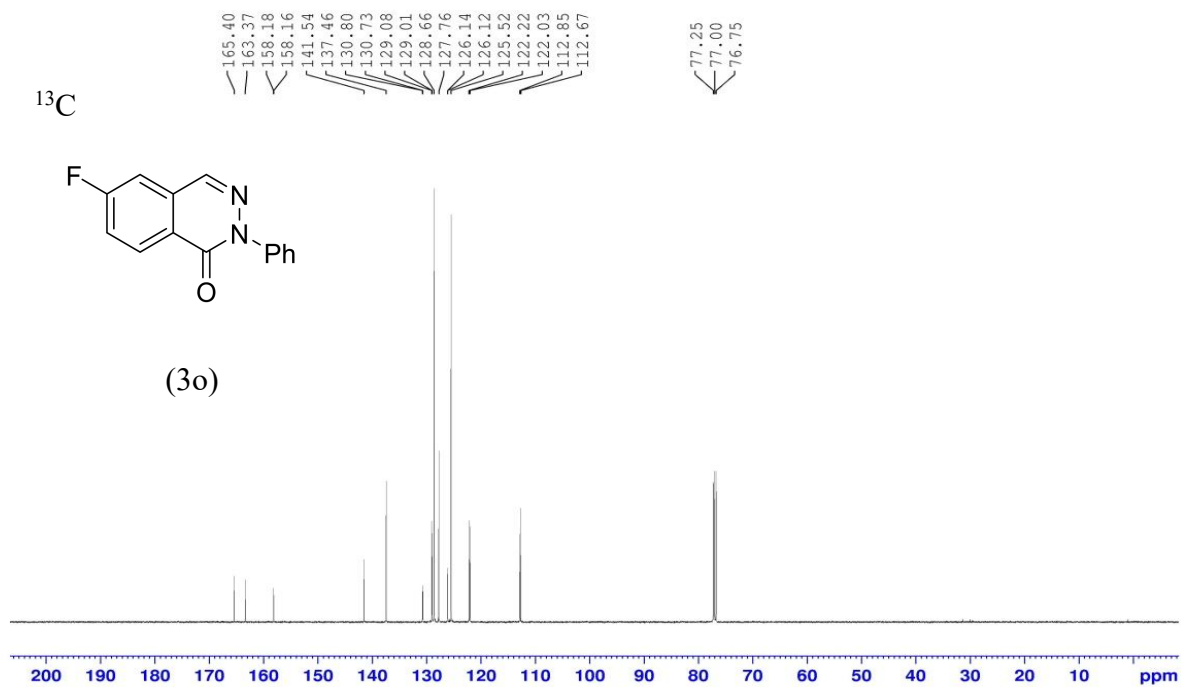
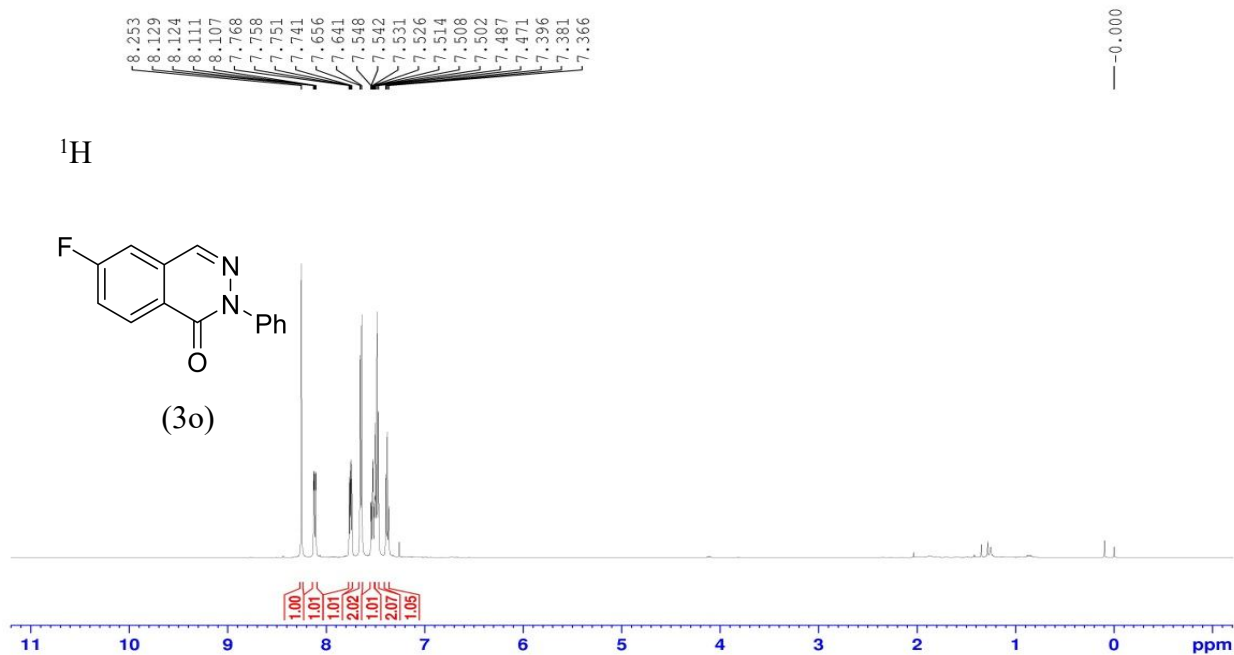


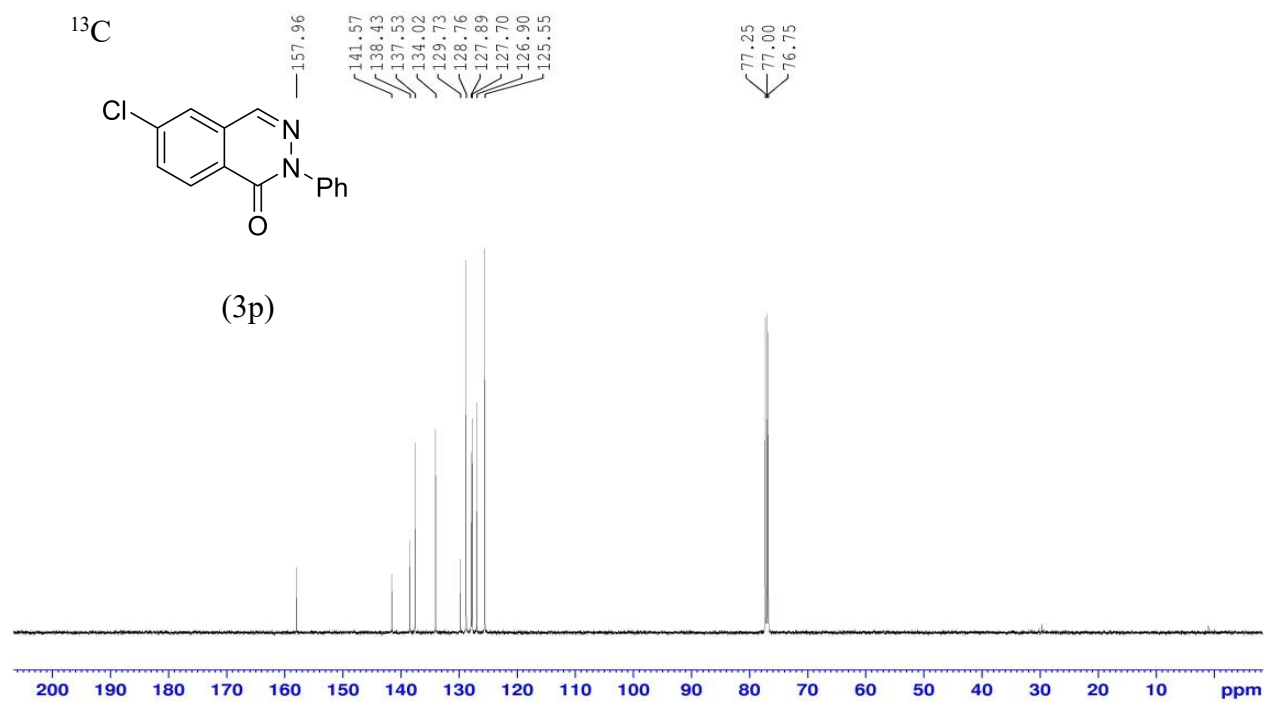
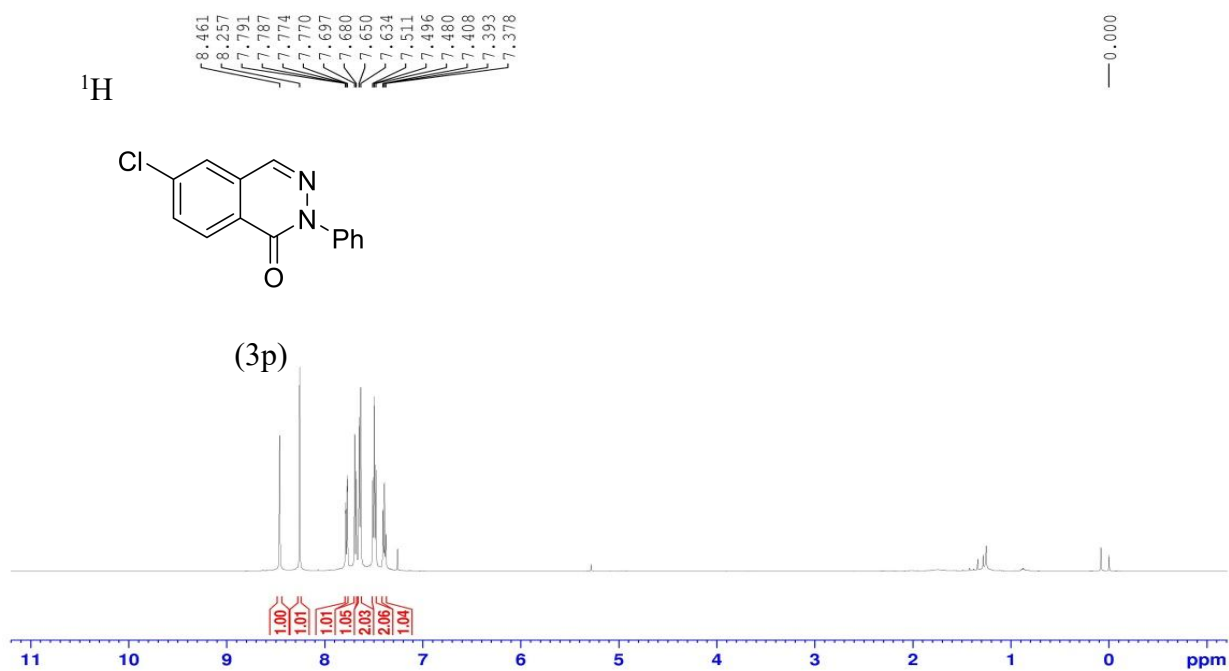


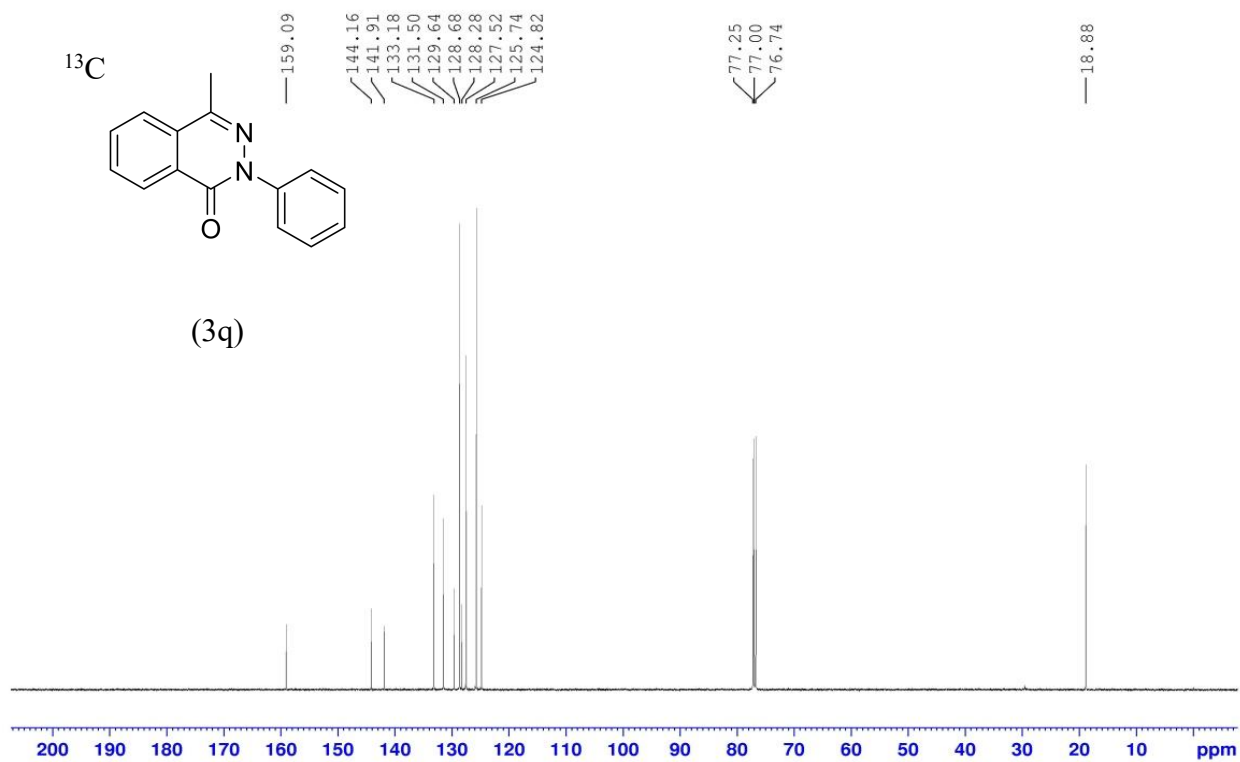
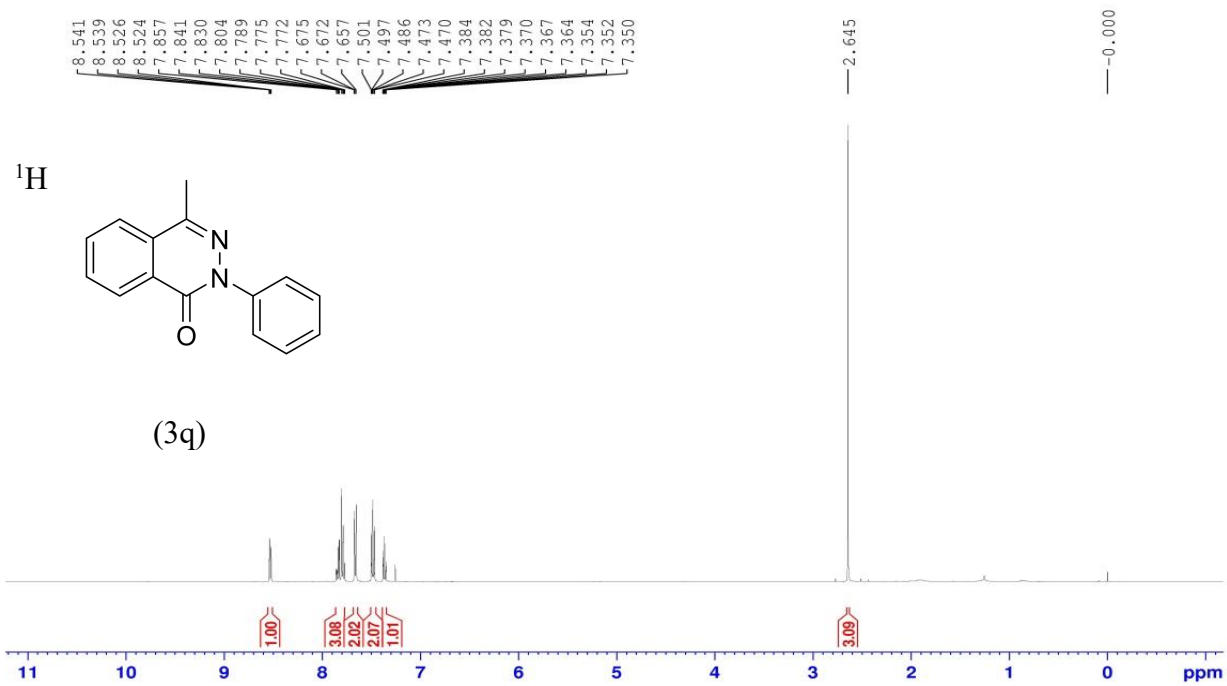


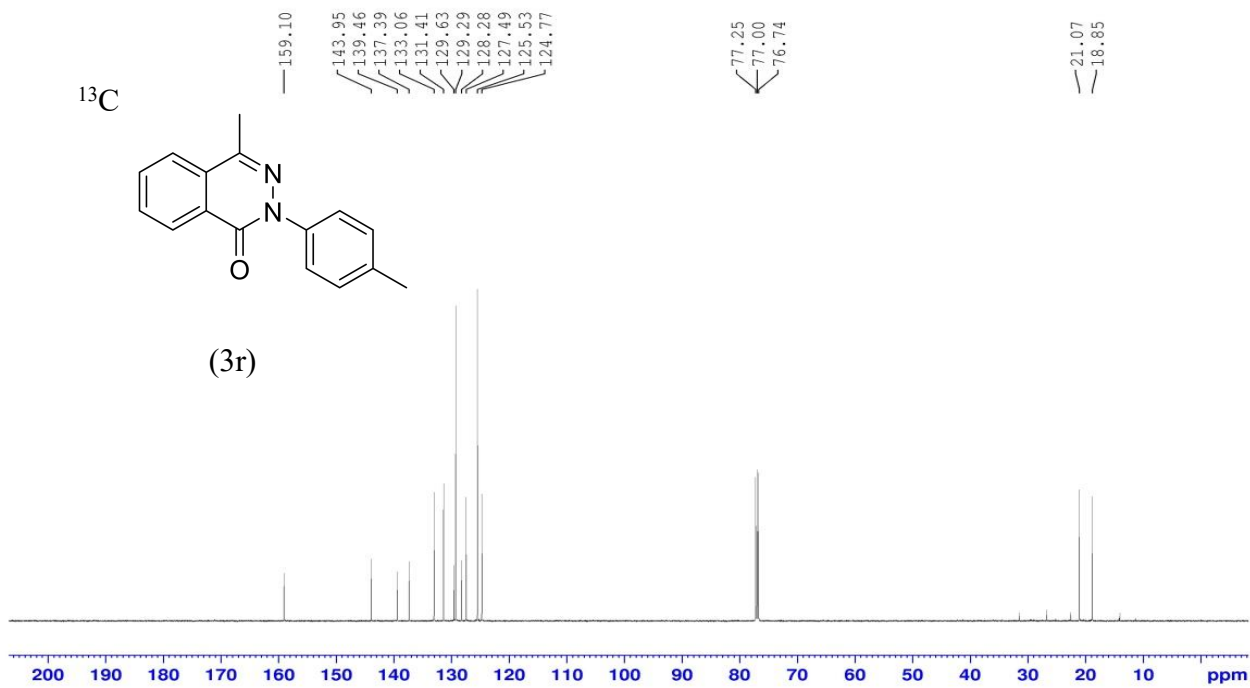
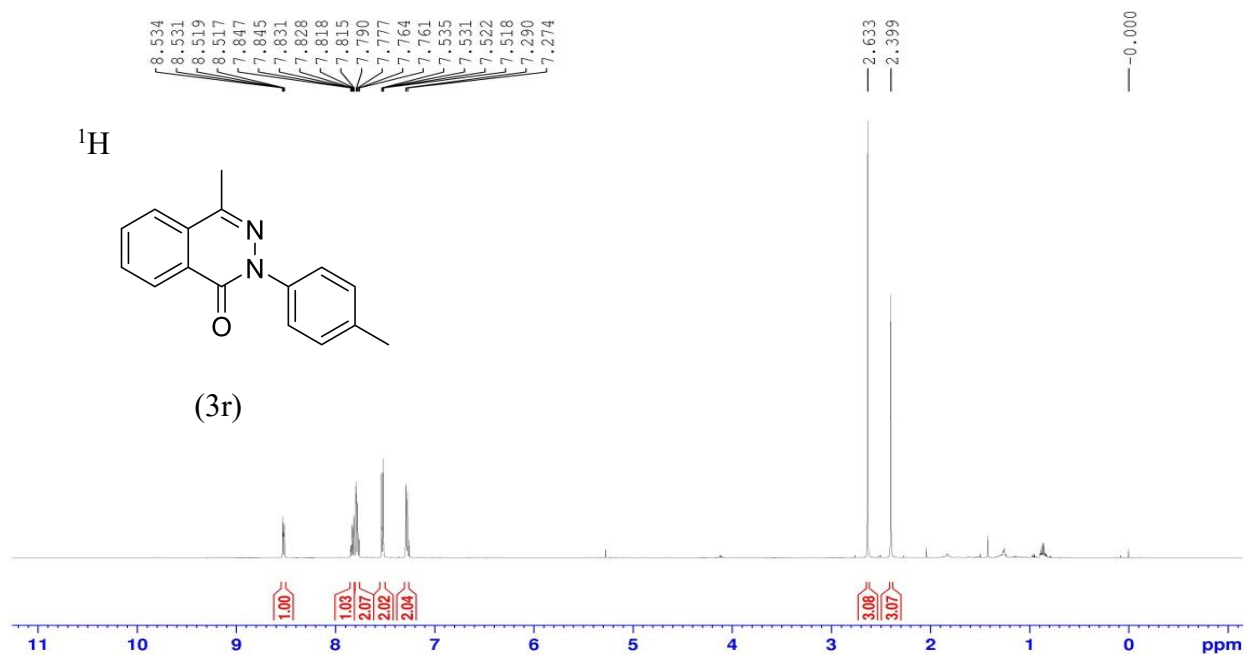


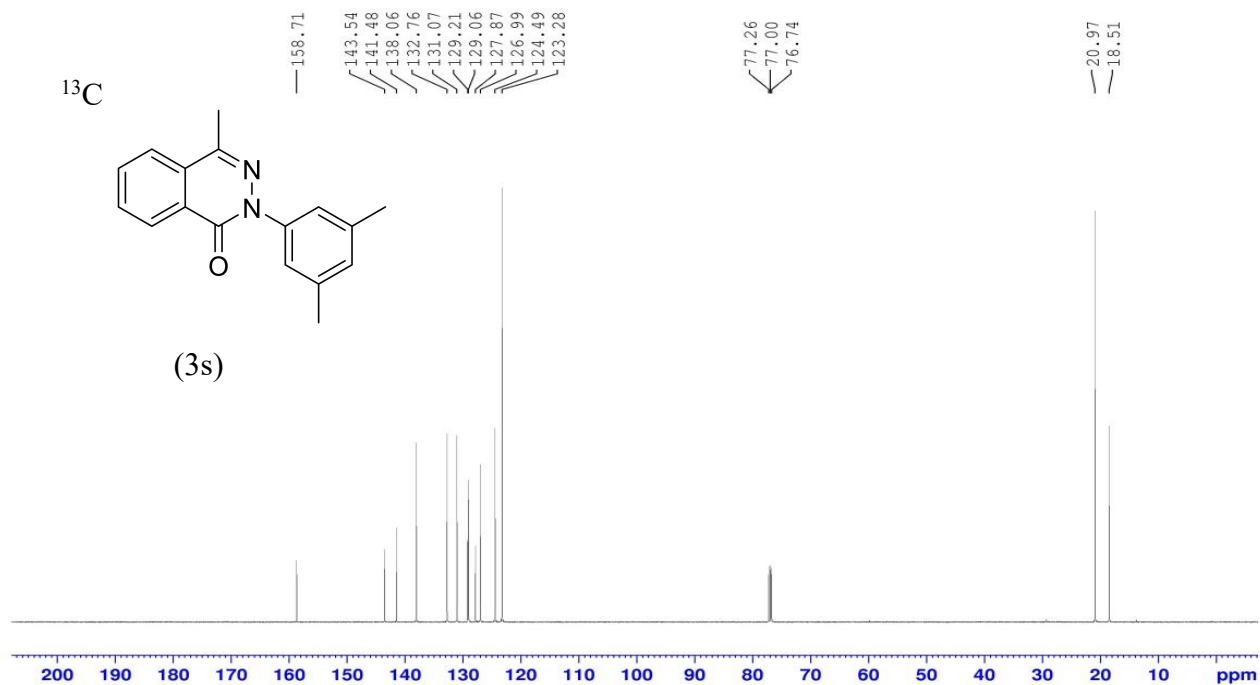
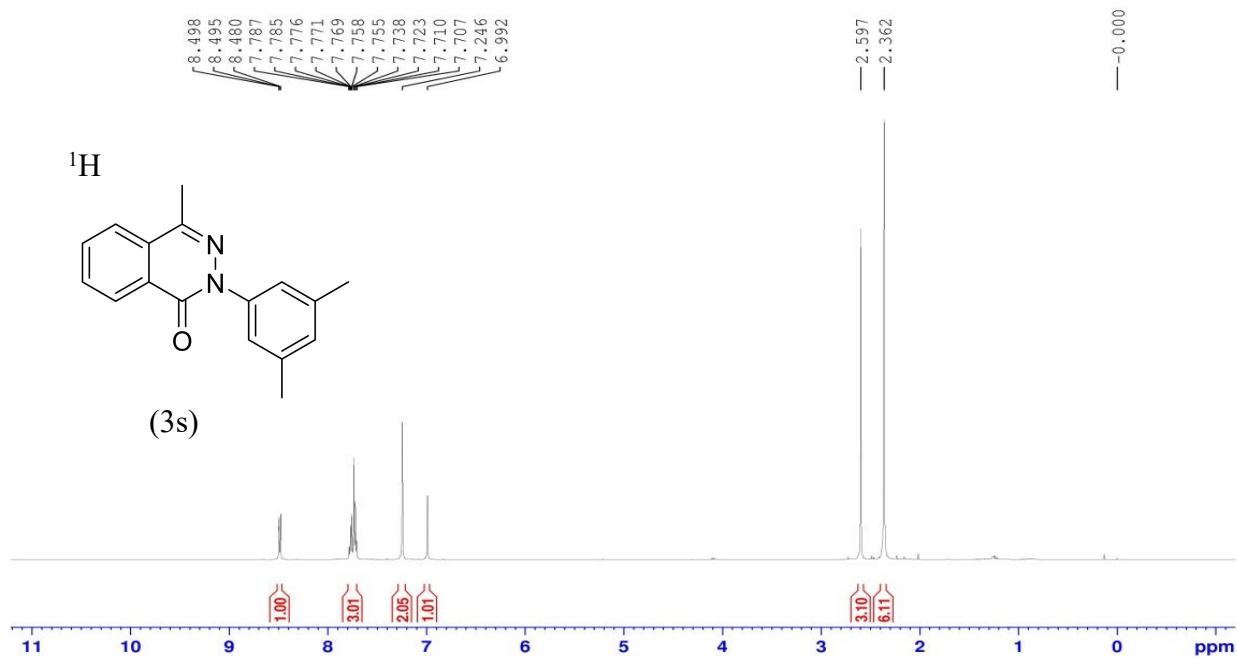


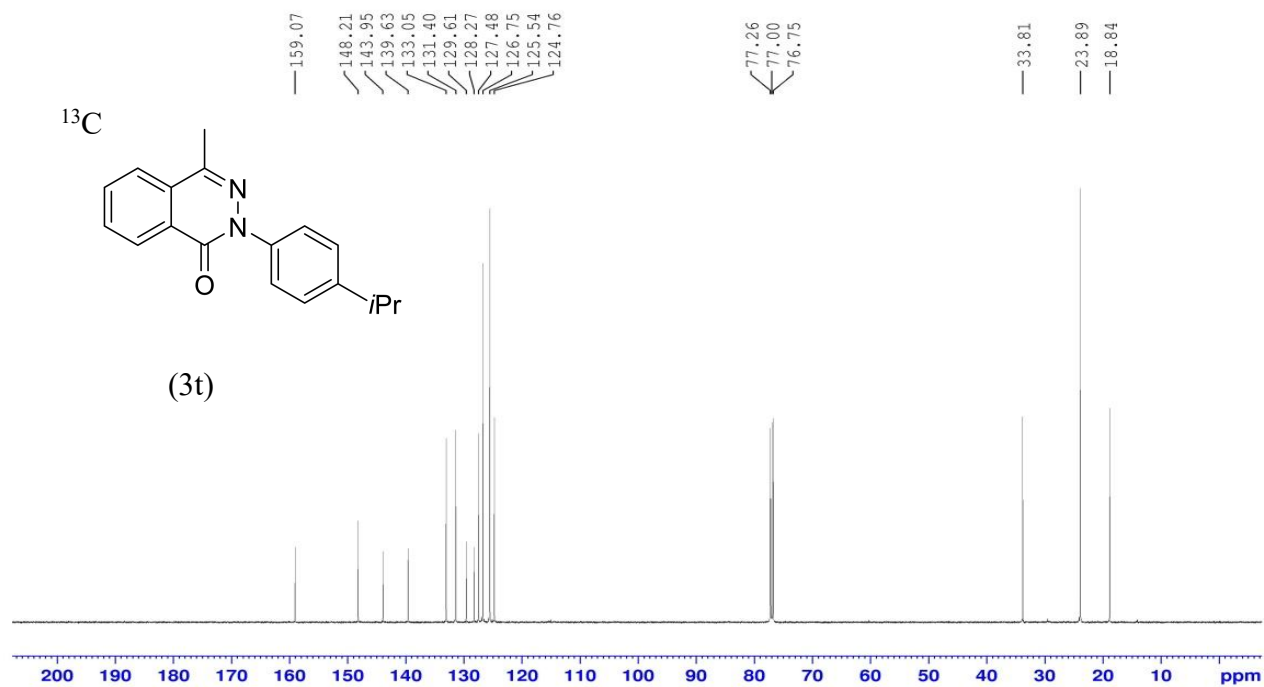
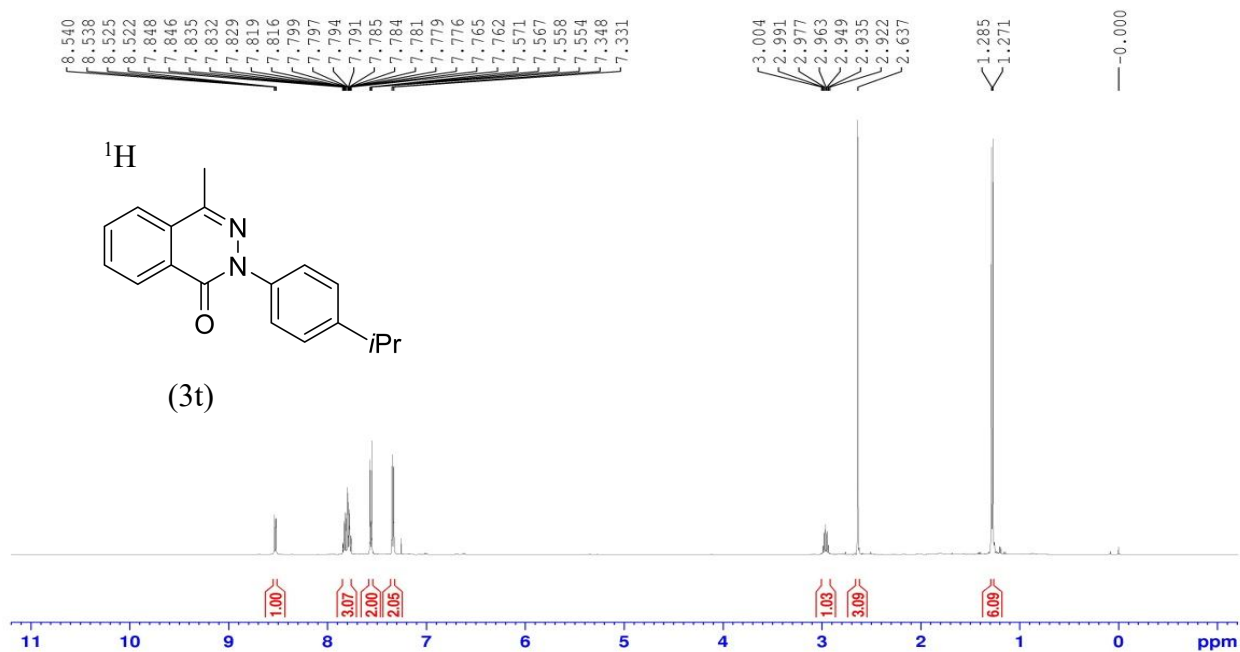


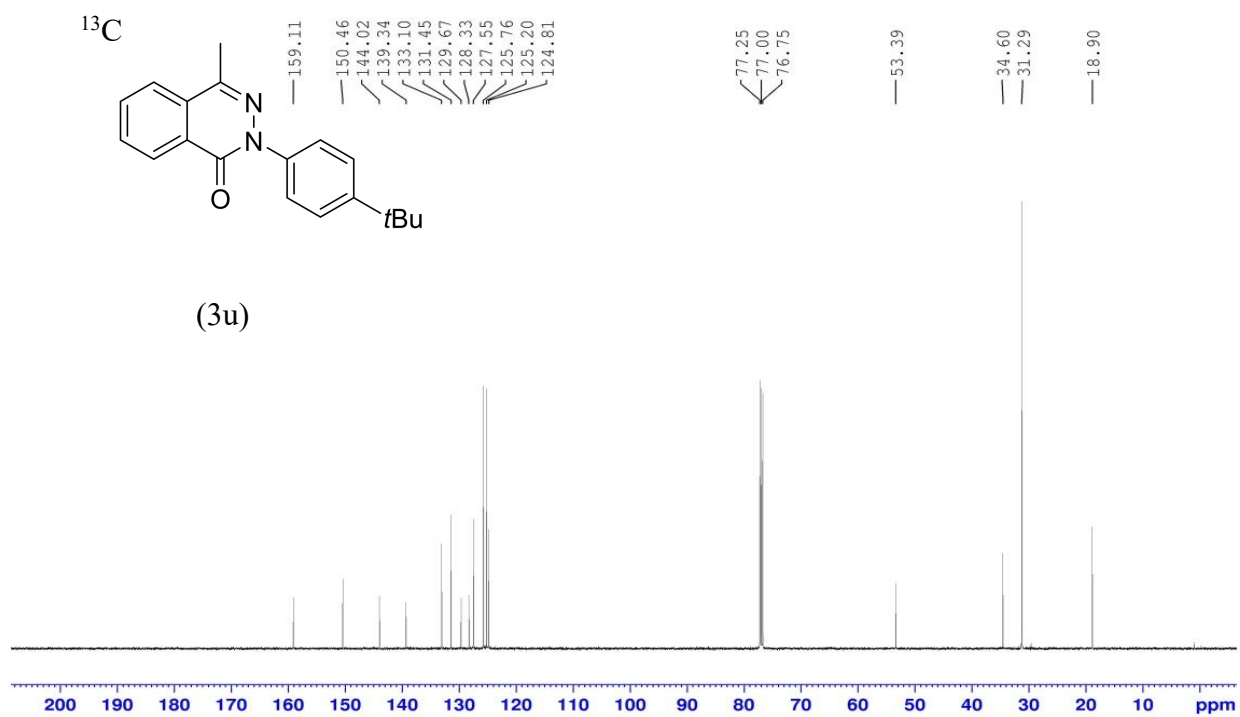
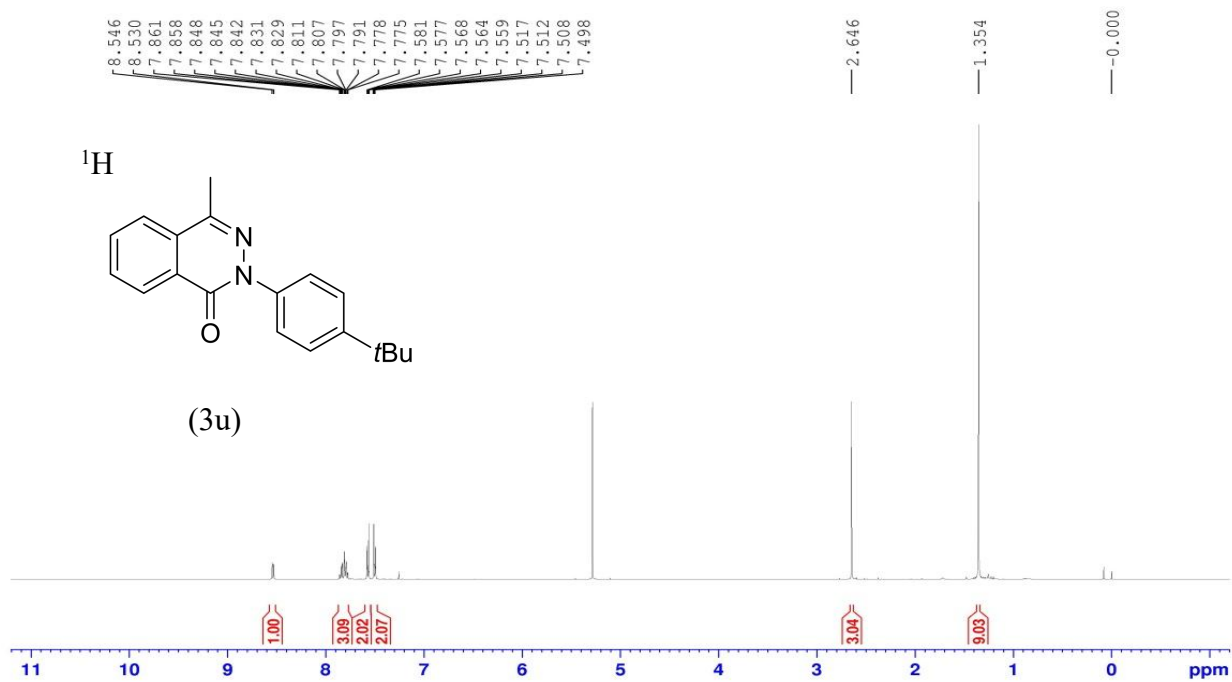


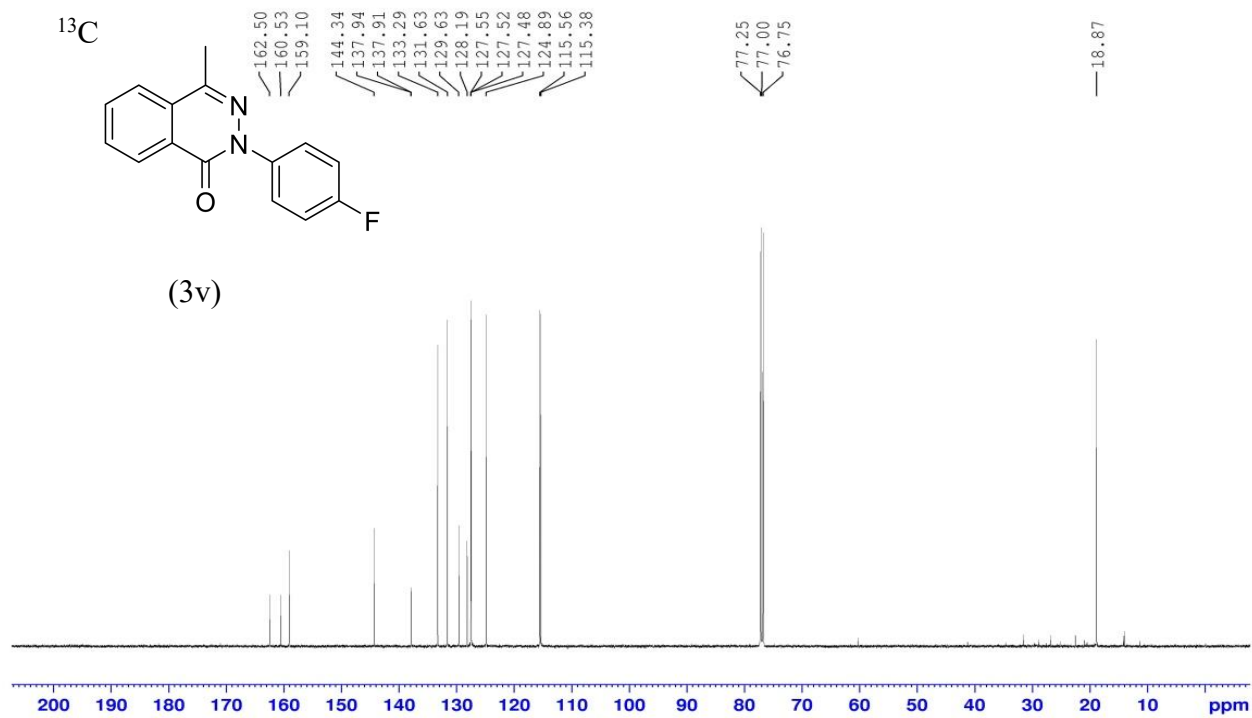
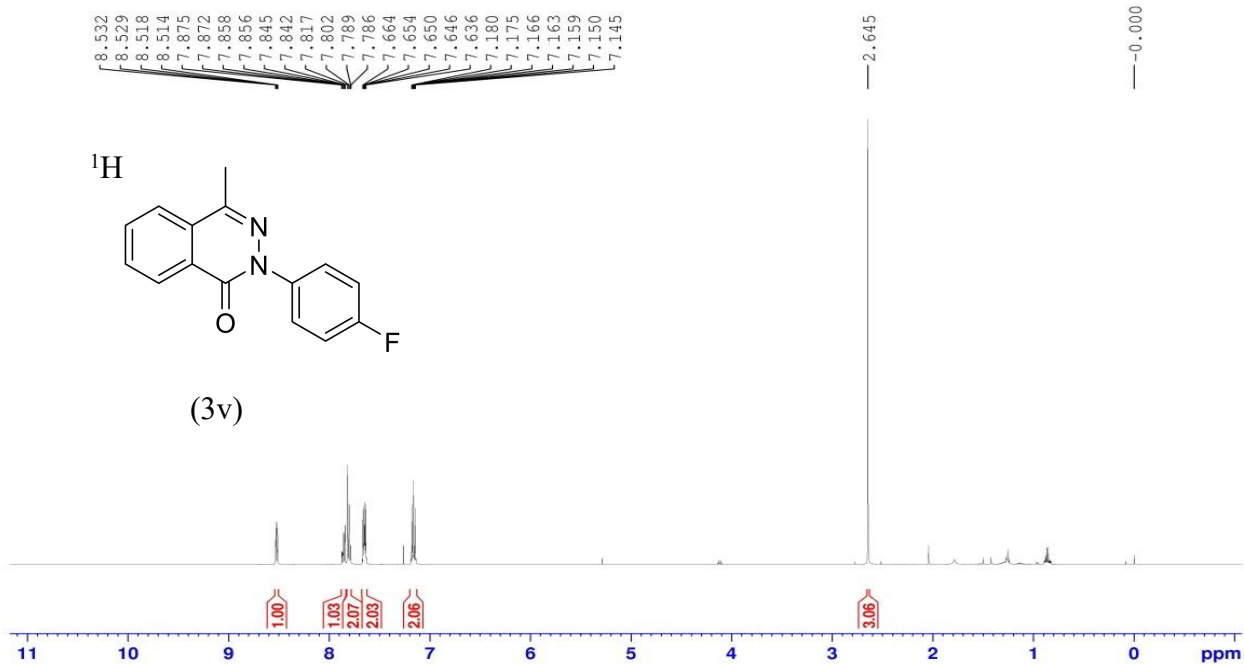


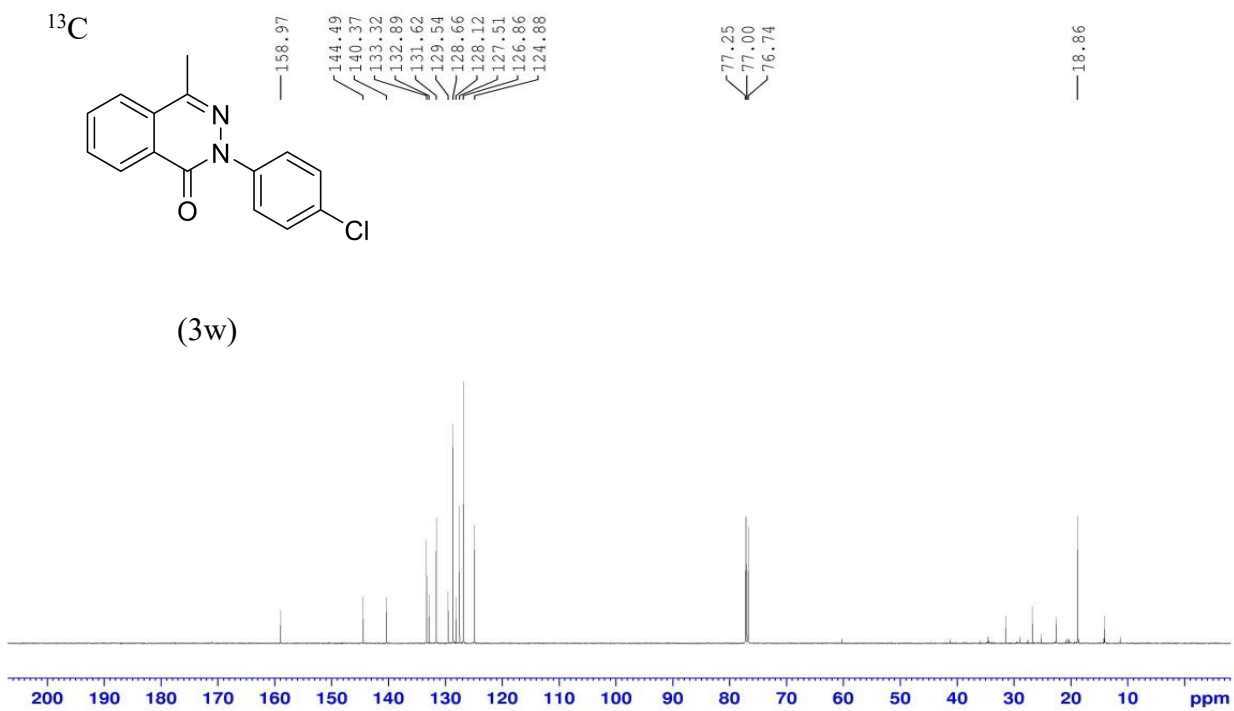
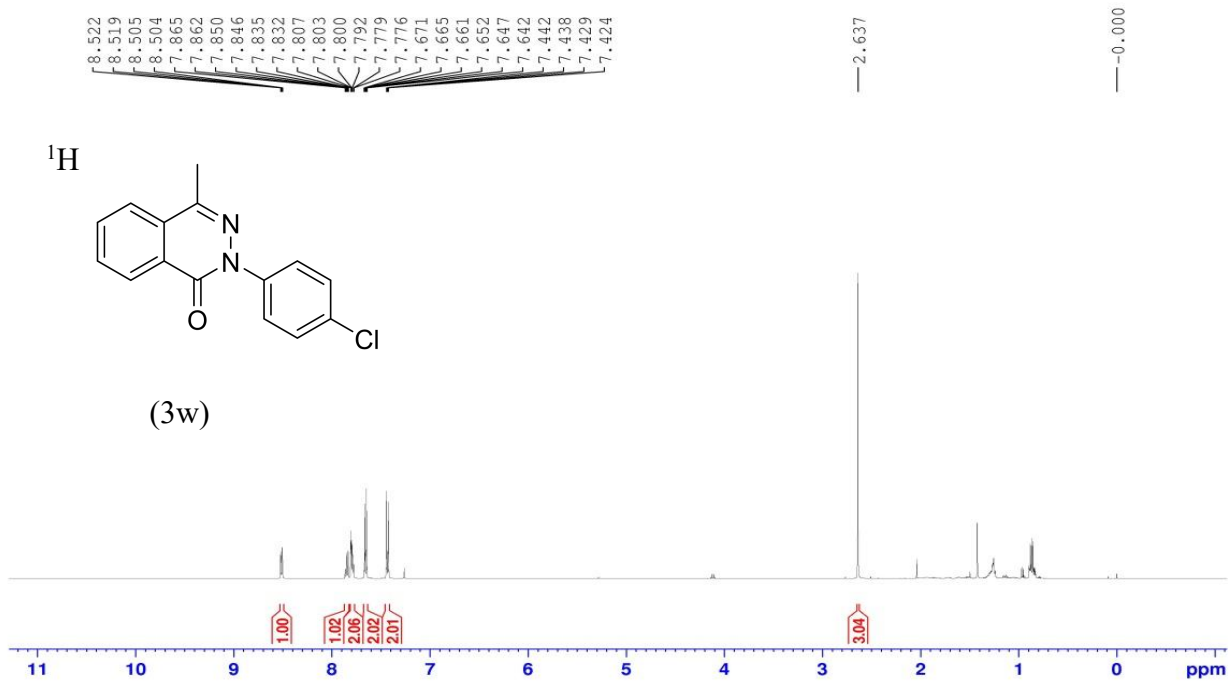


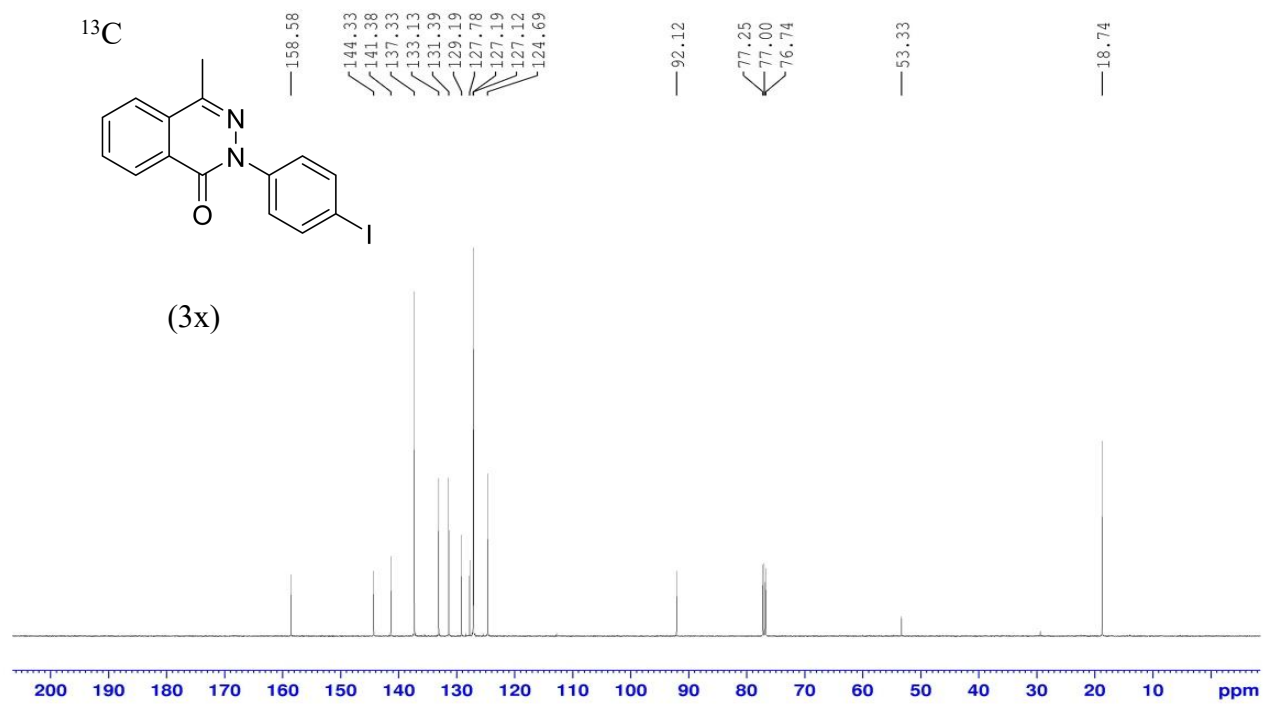
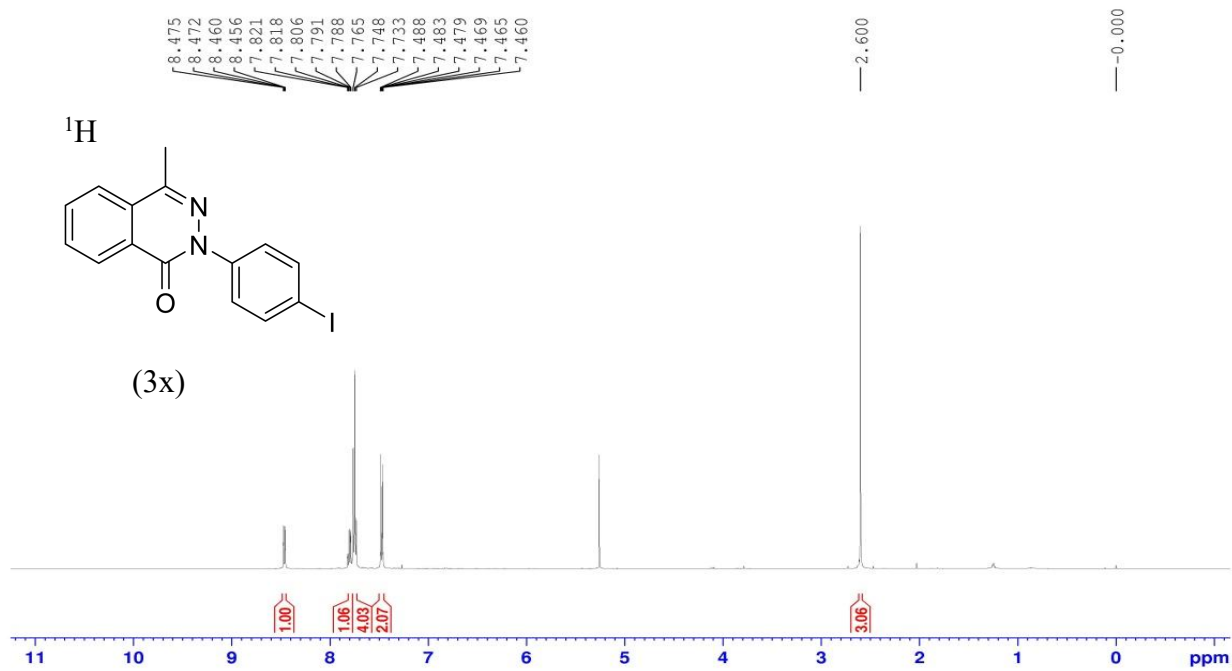


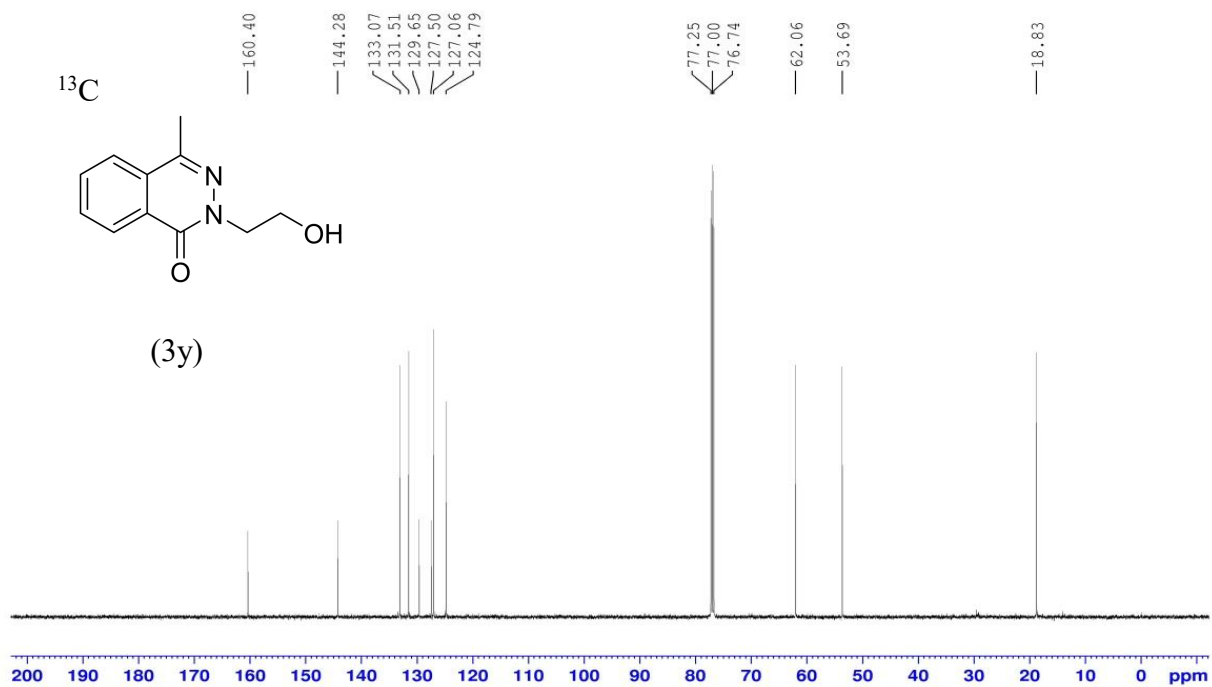
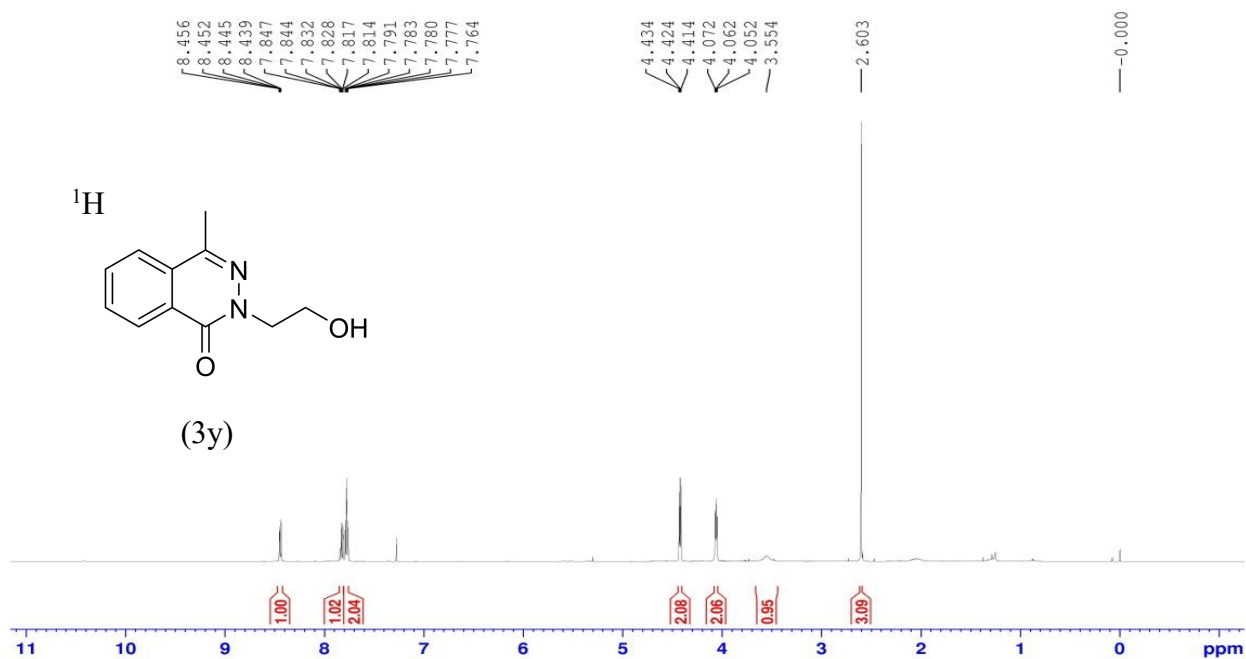


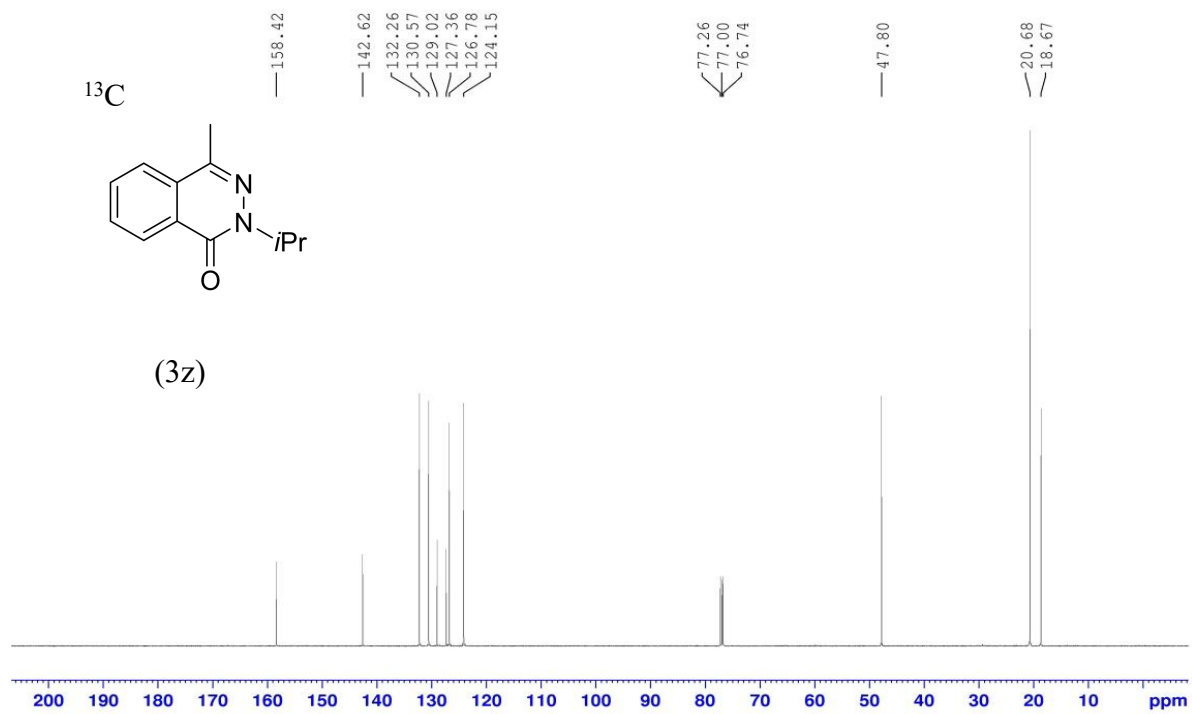
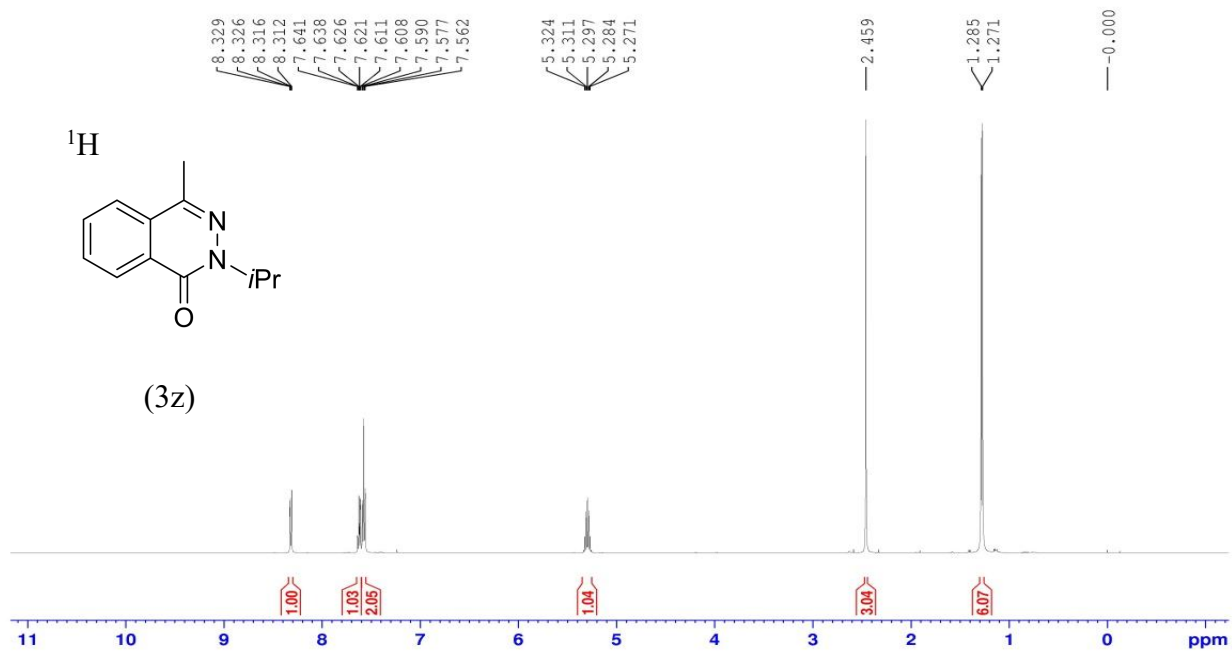


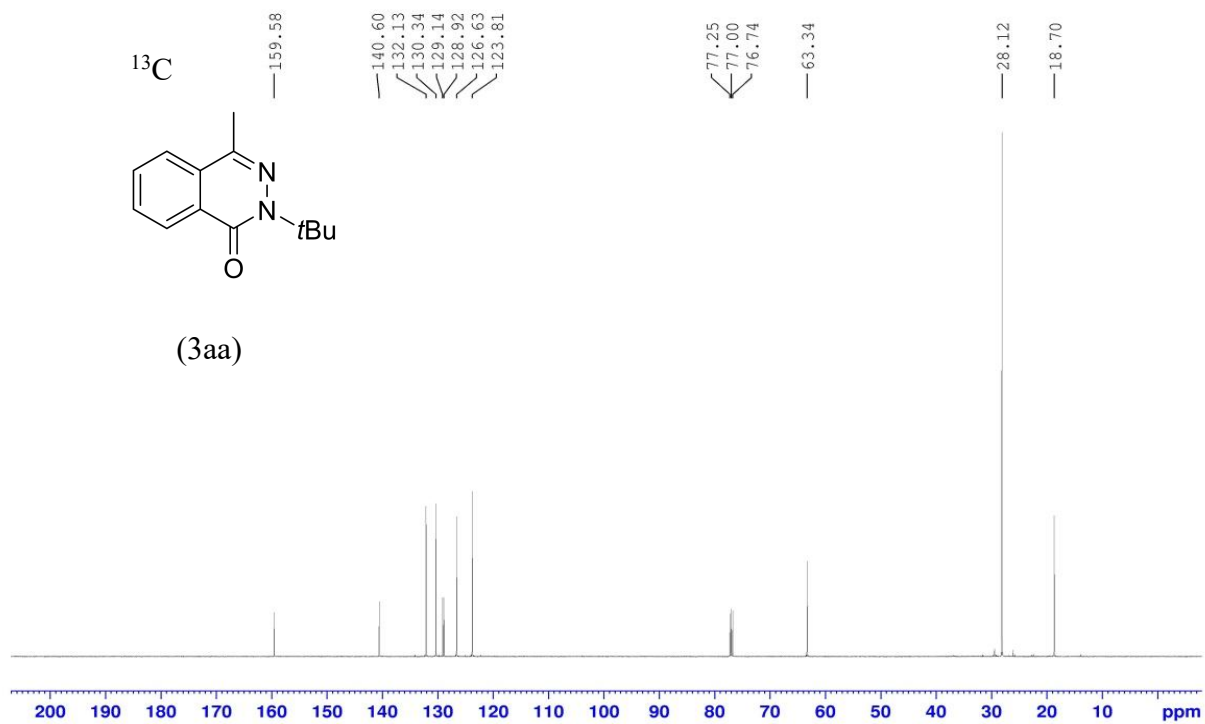
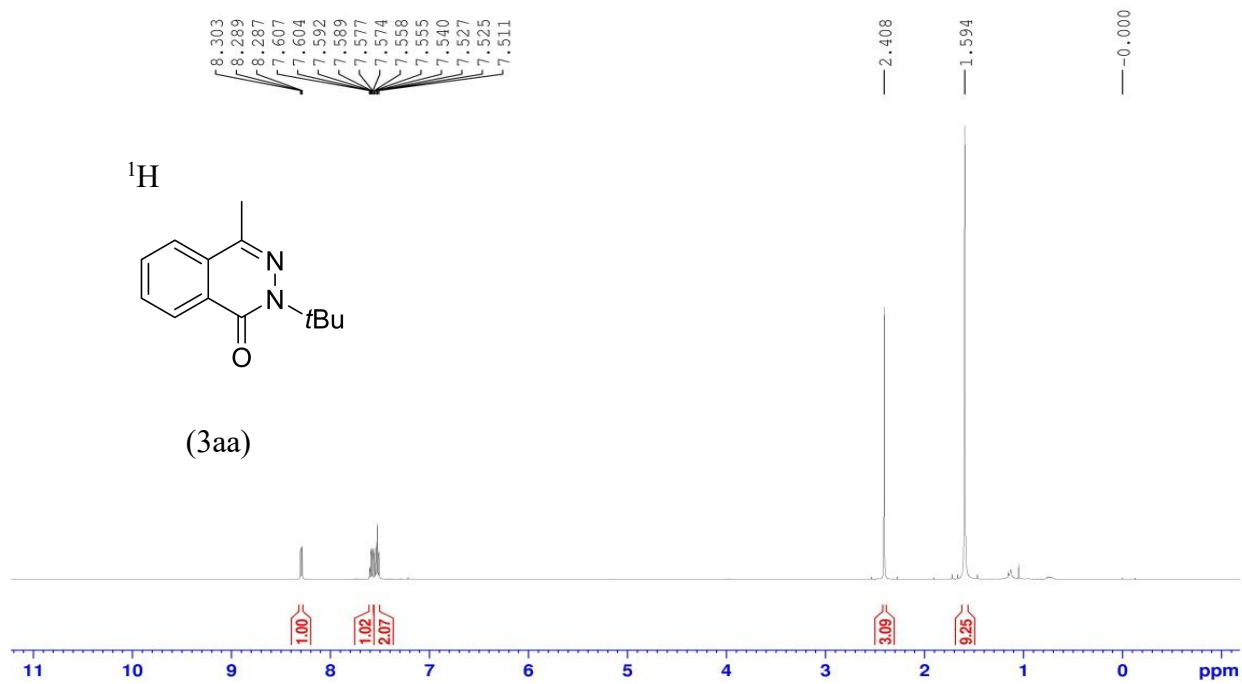


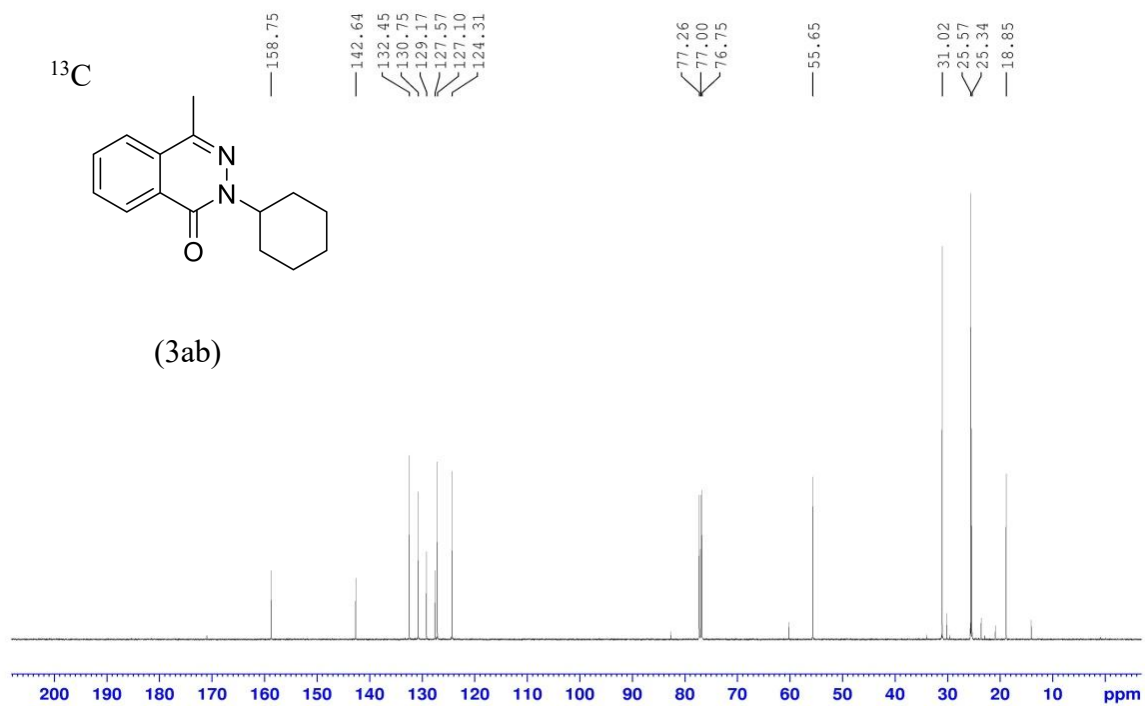
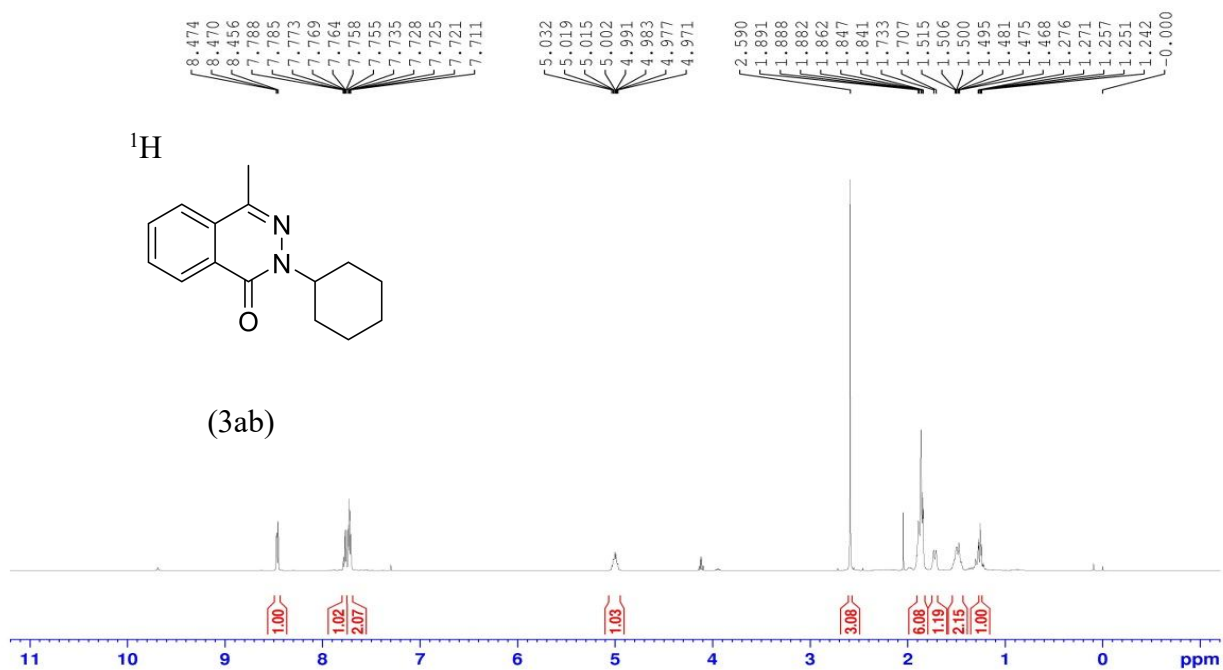


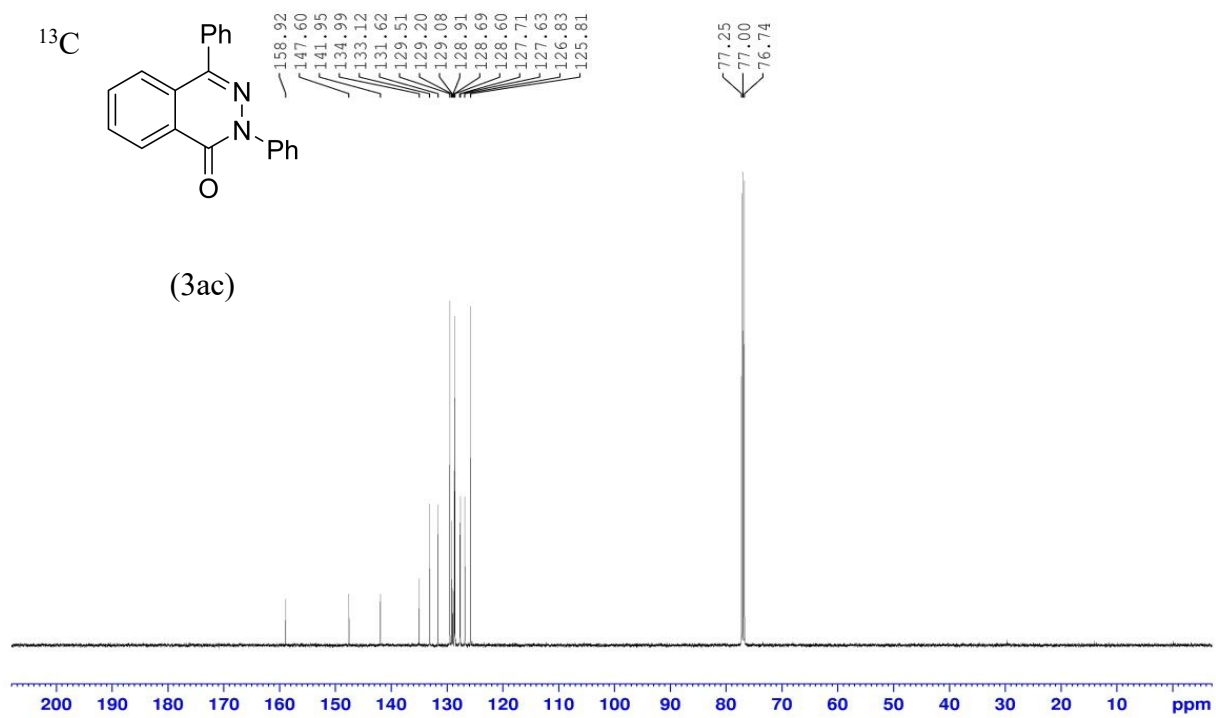
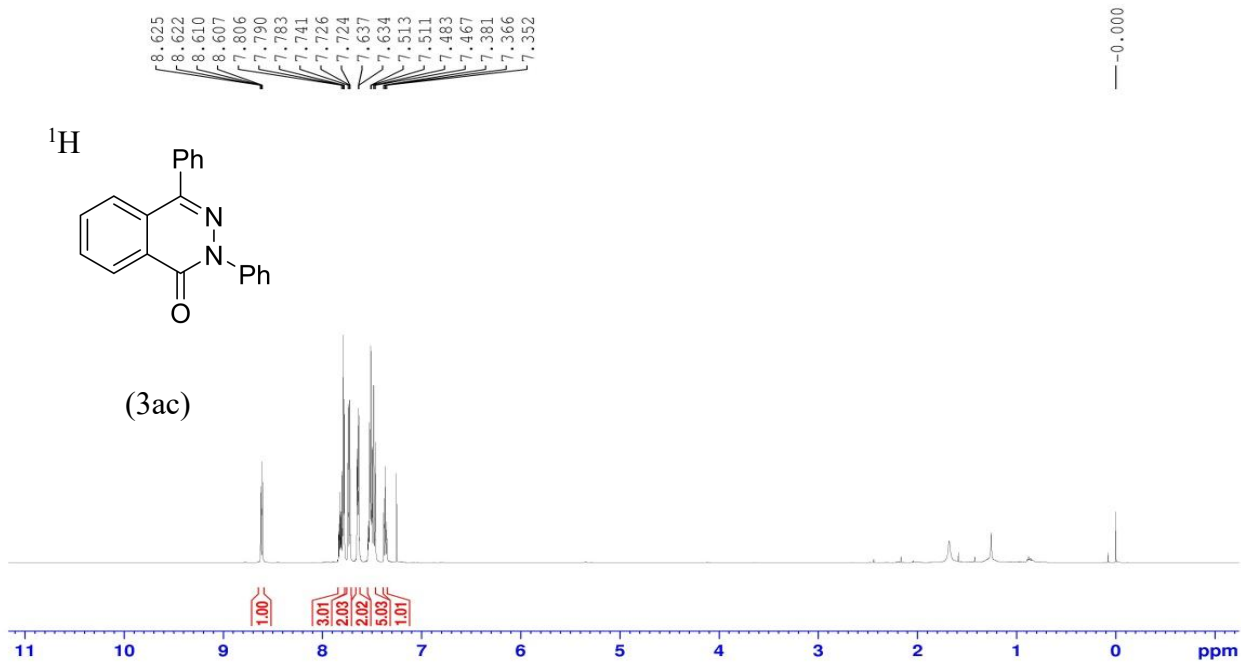


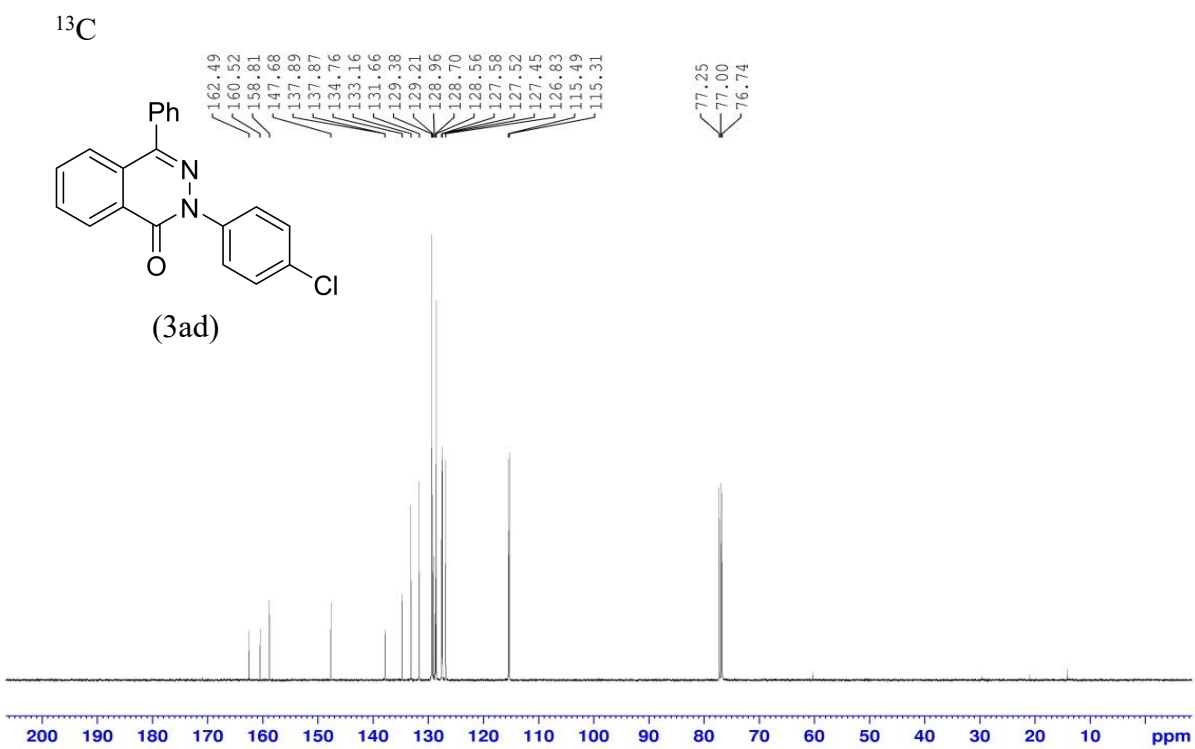
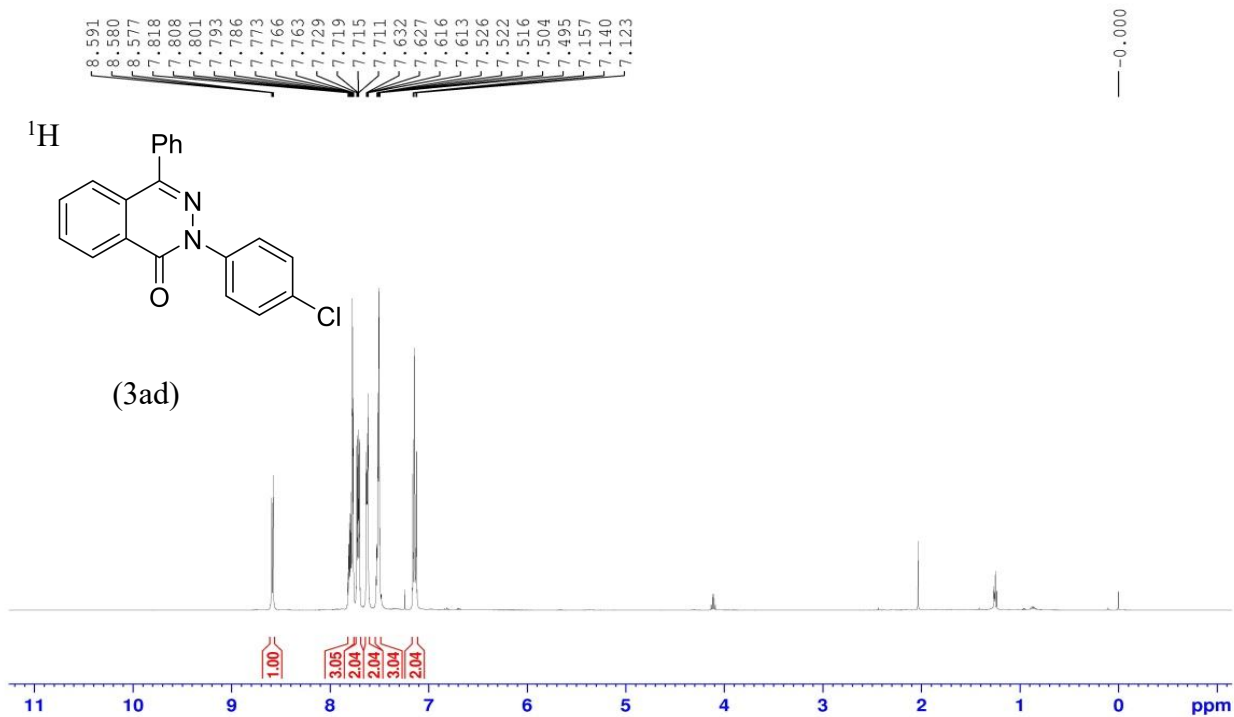


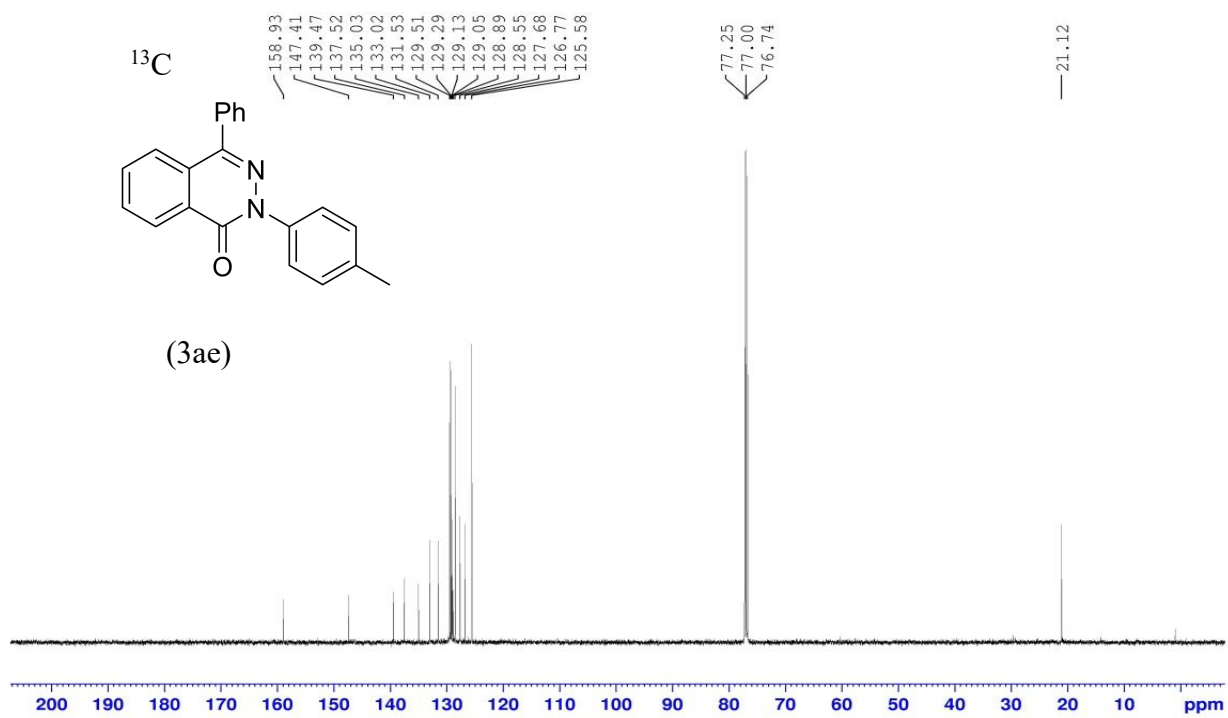
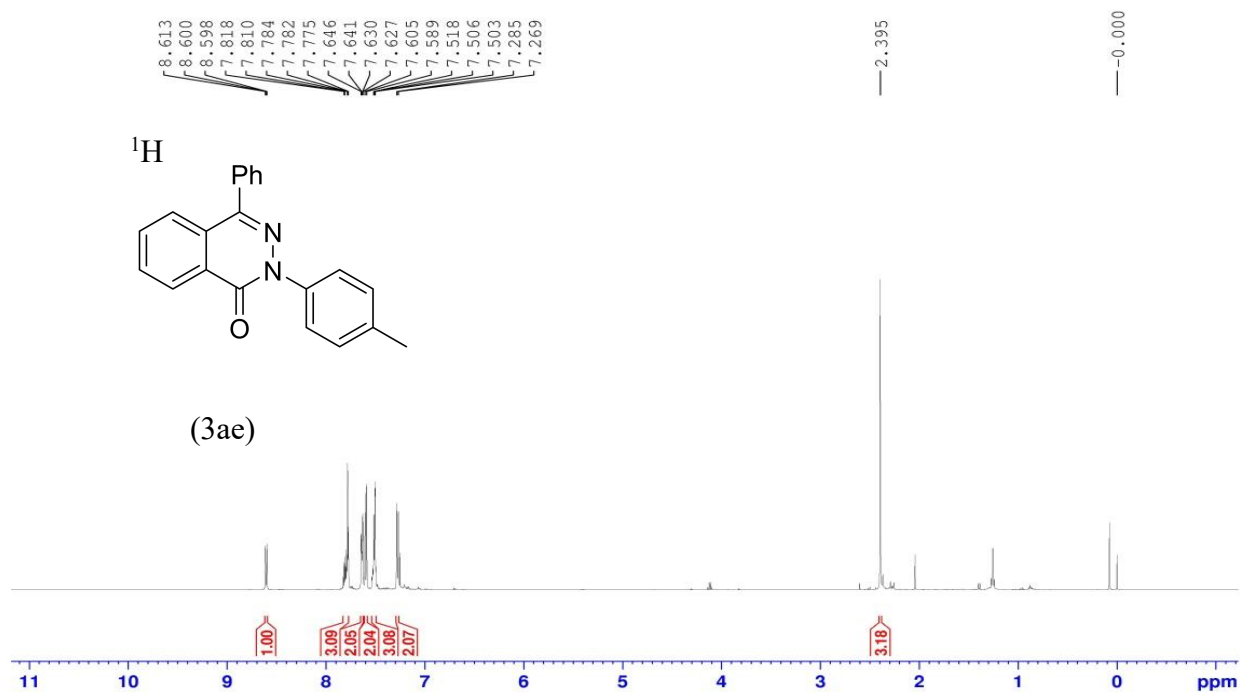


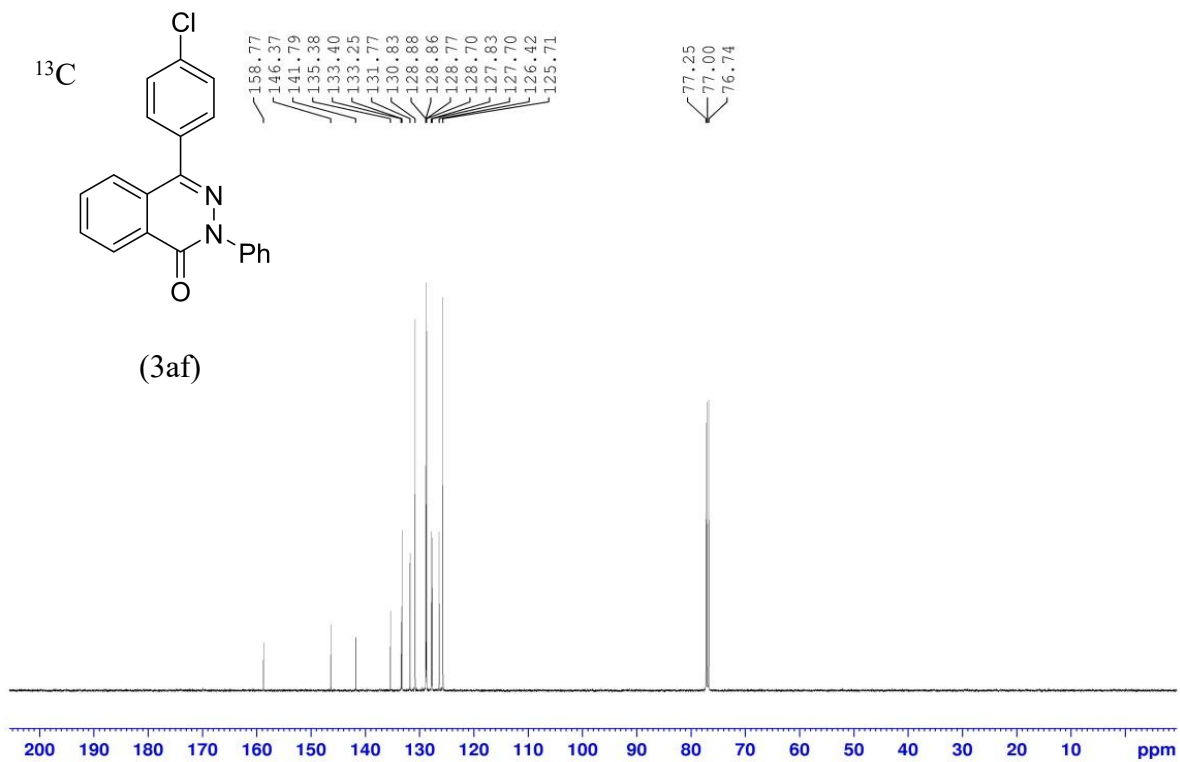
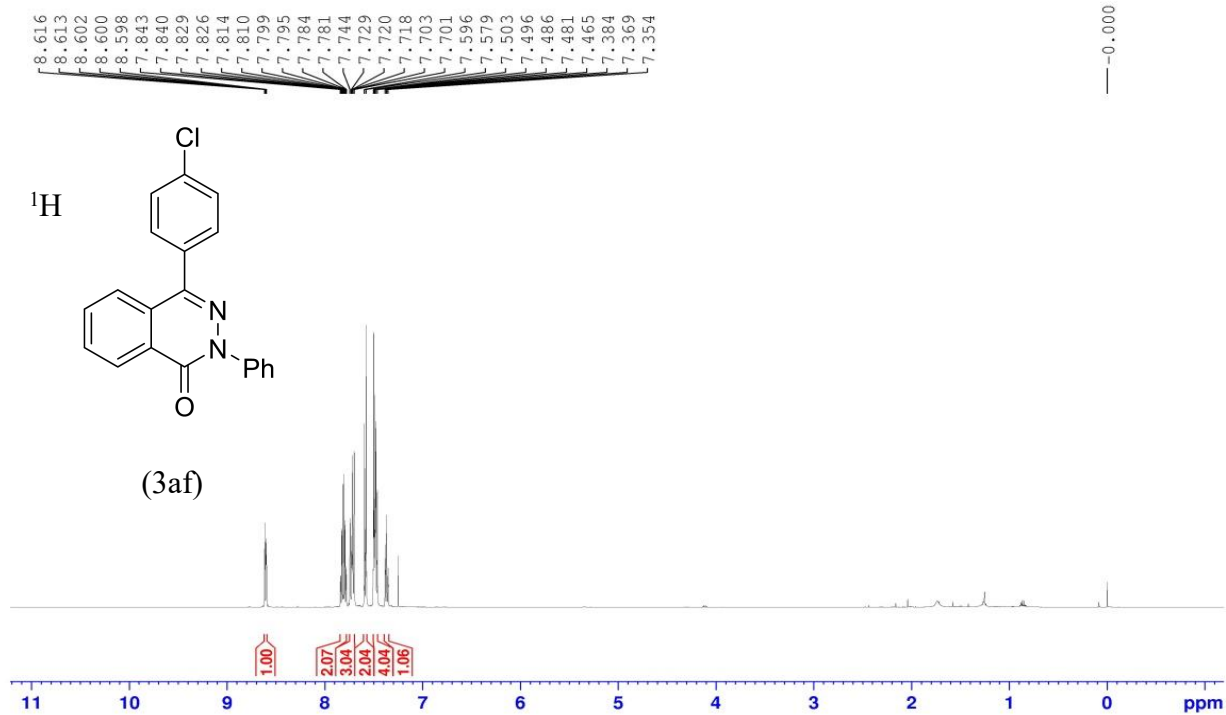


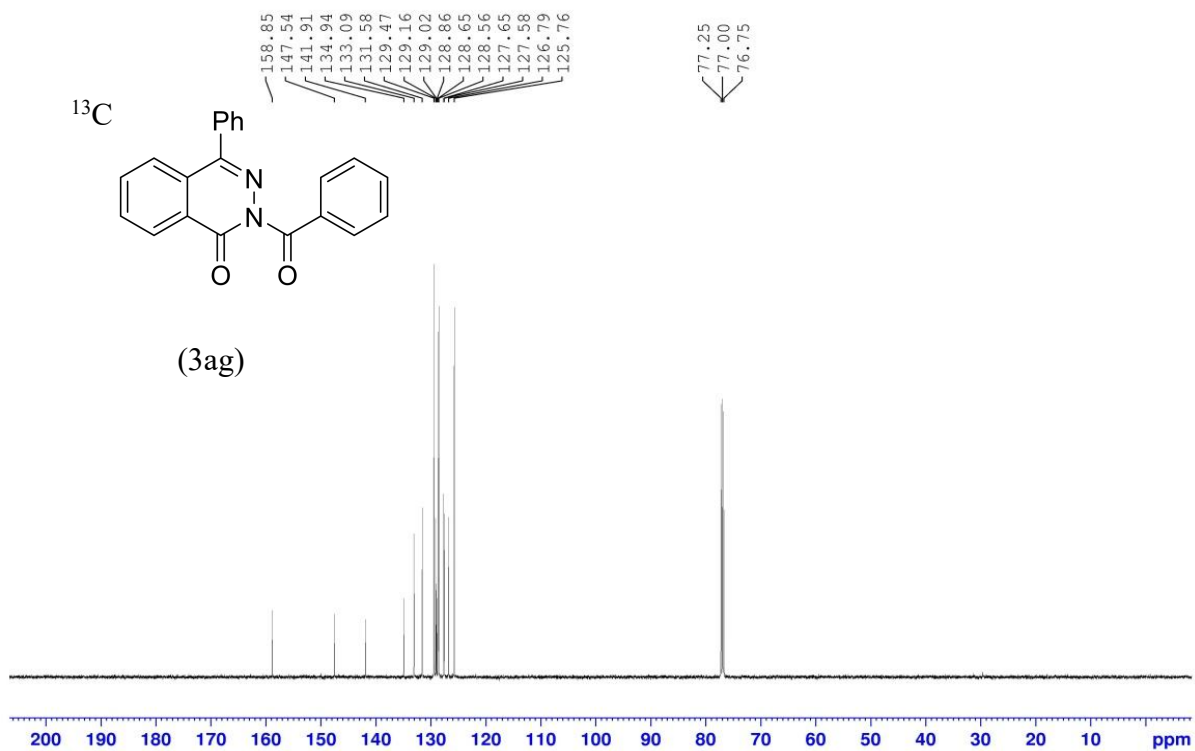
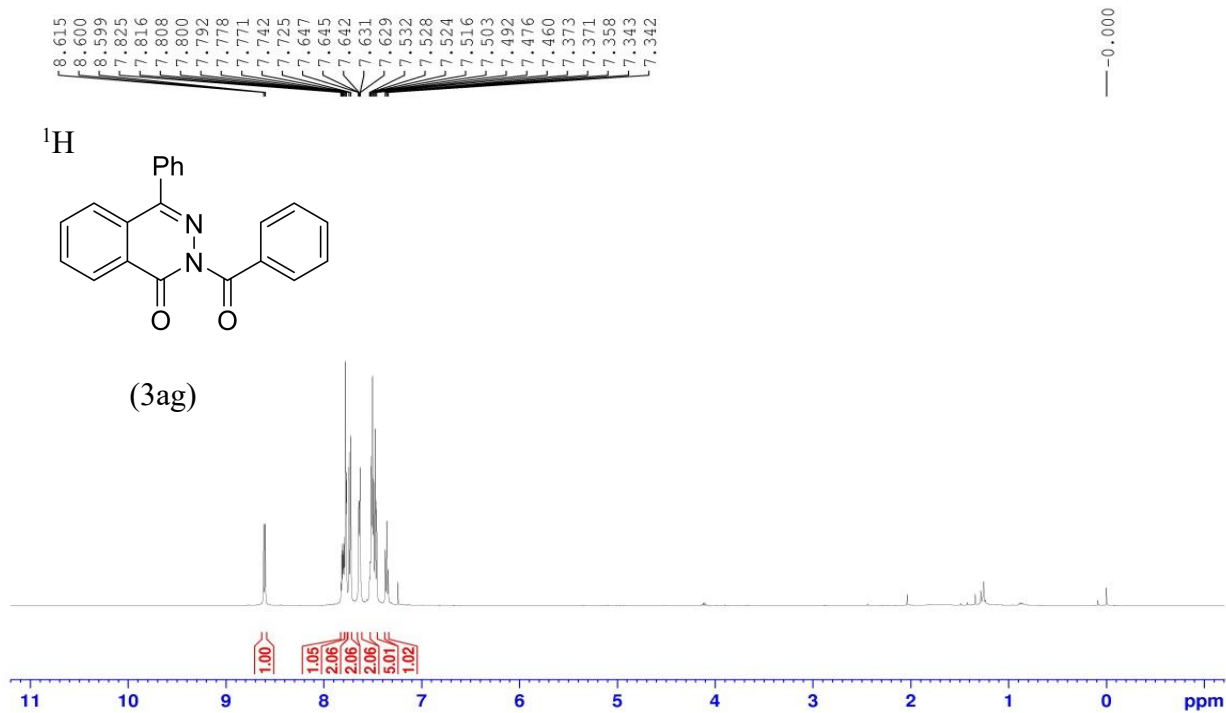












Computational details

Computational method

In this work, all density functional theory (DFT) calculations are performed by Gaussian 09 software package¹. First, all structures are optimized to the minimum points or transition states in the potential energy surface at the level of M06-2X-D3/def2-SVP²⁻⁵ with the dichloromethane solvent that is simulated by IEFPCM implicit solvent model⁶⁻⁸. At the same level, the vibration frequency of each structure is calculated to ensure that the structure at minimum point has no imaginary frequency and the transition state has only one imaginary frequency. Based on the structure of each transition state, Intrinsic Reaction Coordinate (IRC) is calculated to check whether the transition state connected the reactant and product rightly.

Then, the Solvation Gibbs free energy is calculated by **Eq. (S1)**. The gas electronic energies (E_{gas}) and the solution electronic energies (E_{sol}) are calculated at the level of M05-2X/6-31G(d)⁹⁻¹¹ and the dichloromethane solvent is simulated by solvation model based on density (SMD)¹².

$$\Delta G_{\text{solv}} = (E_{\text{sol}} - E_{\text{gas}}) + RT \cdot \ln \frac{V_{m,g}}{V_{m,\text{solv}}} = \Delta E + 1.89 \text{ kcal} \cdot \text{mol}^{-1} \# \mathbf{Eq. (S1)}$$

At last, high quality single point energy is calculated by double-hybrid functional of rev-DSDPBEP86-D3(BJ)¹³ and basis sets of def2-TZVP^{4,5} for all structures in gas phase. Therefore, Gibbs free energy are calculated as sum of thermal correction for Gibbs free energy, solvation Gibbs free energy change and single point energy calculated under double-hybrid functional level.

Structures, energies and cartesian coordinates

Table S1: This table is used to record the calculation results about energy data.

Event	Unit	Mean
ZPE (M05-2X/Gas)	a.u.	The gas electronic energy (E_{gas})
ZPE (M05-2X/SMD)	a.u.	The solution electronic energy (E_{sol})
Solvation ΔG	kJ/mol	$E_{\text{sol}} - E_{\text{gas}}$
ZPE (M06-2X/IEFPCM)	a.u.	The electronic energy of hybrid functional

ZPE (double hybrid)	a.u.	The electronic energy of double hybrid functional
ZPE_corr	a.u.	Zero point energy
U_corr	a.u.	Thermal correction to Energy
H_corr	a.u.	Thermal correction to Enthalpy
G_corr	a.u.	Thermal correction to Gibbs Free Energy
U(T)	a.u.	ZPE (double hybrid)+ U_corr
H(T)	a.u.	ZPE (double hybrid)+ H_corr
G(T)	a.u.	ZPE (double hybrid)+ G_corr

H₂O

Energies:

ZPE (M05-2X/Gas)	a.u.	-76.3938676
ZPE (M05-2X/SMD)	a.u.	-76.4016241
Solvation ΔG	kJ/mol	-20.3646908
ZPE (M06-2X/IEFPCM)	a.u.	-76.3290933
ZPE (double hybrid)	a.u.	-76.3450612
ZPE_corr	a.u.	0.021503
U_corr	a.u.	0.024338
H_corr	a.u.	0.025283
G_corr	a.u.	0.003847
U(T)	a.u.	-76.3207232
H(T)	a.u.	-76.3197782
G(T)	a.u.	-76.3412142

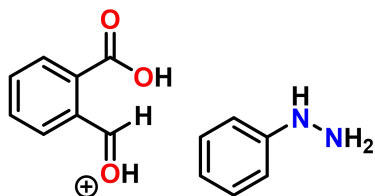
Cartesian coordinate:

O	0.00000000	0.00000000	0.12007900
H	0.00000000	0.75438100	-0.48031700
H	0.00000000	-0.75438100	-0.48031700

Path A

a-IM1

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.3257104
ZPE (M05-2X/SMD)	a.u.	-877.4108834
Solvation ΔG	kJ/mol	-223.6217115
ZPE (M06-2X/IEFPCM)	a.u.	-876.5039913
ZPE (double hybrid)	a.u.	-876.1850673
ZPE_corr	a.u.	0.2749570
U_corr	a.u.	0.2917820
H_corr	a.u.	0.2927270
G_corr	a.u.	0.2304590
U(T)	a.u.	-875.8932853
H(T)	a.u.	-875.8923403
G(T)	a.u.	-875.9546083

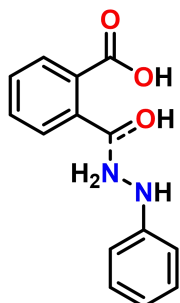
Cartesian coordinate:

C	-2.72219000	0.57780300	-1.23465700
C	-1.49400900	-0.04063900	-1.47244700
C	-1.12694100	-1.16608600	-0.72502600
C	-2.01151400	-1.66994100	0.24394000
C	-3.23455400	-1.04646000	0.46514700
C	-3.59782400	0.08640900	-0.26843100

H	-2.99469200	1.45792600	-1.82033000
H	-0.81109700	0.34774500	-2.22642600
H	-1.72510500	-2.54715100	0.82856100
H	-3.91070300	-1.44934100	1.22099000
H	-4.55715700	0.57360500	-0.09185500
N	0.12941300	-1.77315600	-0.85948200
H	0.08808600	-2.78562500	-0.73596000
N	0.93049200	-1.33603000	-1.92213900
H	0.60003900	-1.71305500	-2.81530500
H	1.87166100	-1.69786300	-1.77712700
C	0.51256900	2.50761200	-0.29125000
C	1.27322300	1.35049400	-0.09758600
C	0.88322600	0.43444200	0.92129000
C	-0.24509000	0.71518700	1.69074200
C	-0.98298700	1.88463700	1.48526500
C	-0.60552700	2.78293500	0.49659700
H	0.80627000	3.20738600	-1.07530100
H	-0.55460300	0.01069200	2.46074100
H	-1.86079300	2.07877100	2.10177800
H	-1.17974200	3.69345800	0.32614400
C	2.42775600	1.23977300	-0.99663700
H	2.49807100	2.01734600	-1.77519200
C	1.56077800	-0.85219400	1.17644800
O	3.32586000	0.40437100	-0.94151900
O	2.65776600	-1.20227400	0.68133900
O	1.00232500	-1.62076600	2.05513000
H	1.53047700	-2.42922500	2.18740200
H	3.07084100	-0.47485400	-0.05674200

a-TS1

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.3257934
ZPE (M05-2X/SMD)	a.u.	-877.4121443
Solvation ΔG	kJ/mol	-226.7142880
ZPE		
(M06-2X/IEFPCM)	a.u.	-876.5026479
ZPE (double hybrid)	a.u.	-876.1846172
ZPE_corr	a.u.	0.276378
U_corr	a.u.	0.292282
H_corr	a.u.	0.293226
G_corr	a.u.	0.232403
U(T)	a.u.	-875.8923352
H(T)	a.u.	-875.8913912
G(T)	a.u.	-875.9522142

Cartesian coordinate:

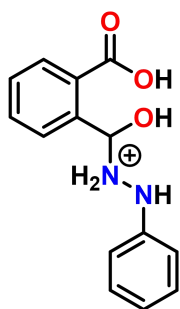
C	-2.84033800	0.59633100	-0.99819400
C	-1.58266300	0.13471600	-1.39486300
C	-1.07676500	-1.05277000	-0.85631800
C	-1.85093400	-1.77755600	0.06514200
C	-3.10318200	-1.31093300	0.44406200

C	-3.60662800	-0.11629000	-0.08109100
H	-3.21905300	1.52882100	-1.42064900
H	-0.99496700	0.71141000	-2.10838000
H	-1.45437800	-2.70341700	0.48668000
H	-3.69281700	-1.88533000	1.16023200
H	-4.58837900	0.24877600	0.22139600
N	0.20986300	-1.53081300	-1.16334600
H	0.22428000	-2.54542600	-1.26665400
N	0.88577100	-0.85684200	-2.19652900
H	0.32959800	-0.83574800	-3.05984000
H	1.73835900	-1.37584000	-2.40192500
C	0.63622100	2.39947200	-0.41351000
C	1.27162000	1.18330700	-0.13525500
C	0.86179000	0.43333600	0.99857800
C	-0.18206500	0.91247300	1.78784300
C	-0.78935000	2.13797100	1.50450000
C	-0.37191700	2.89040700	0.41243300
H	0.93762500	2.96713900	-1.29550500
H	-0.51751400	0.32205900	2.63915100
H	-1.59676900	2.49651600	2.14332200
H	-0.84303800	3.84682600	0.18636400
C	2.28858800	0.80023000	-1.11446200
H	2.33628000	1.39888900	-2.03130900
C	1.47318600	-0.86854600	1.37538800
O	3.23735800	0.00383900	-0.92488200
O	2.57776500	-1.26105900	1.00407200
O	0.75754900	-1.57752900	2.20586100
H	1.23815900	-2.39126000	2.44141900

H 3.08643100 -0.56473500 -0.02110900

a-IM2

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.3507784
ZPE (M05-2X/SMD)	a.u.	-877.4448290
Solvation ΔG	kJ/mol	-246.9298503
ZPE		
(M06-2X/IEFPCM)	a.u.	-876.5238303
ZPE (double hybrid)	a.u.	-876.2040685
ZPE_corr	a.u.	0.281671
U_corr	a.u.	0.297601
H_corr	a.u.	0.298545
G_corr	a.u.	0.237022
U(T)	a.u.	-875.9064675
H(T)	a.u.	-875.9055235
G(T)	a.u.	-875.9670465

Cartesian coordinate:

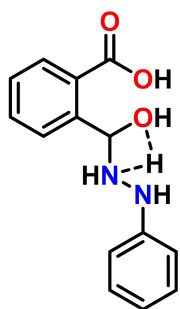
C	4.29940000	-0.36237700	0.92324200
C	2.96865800	-0.67078900	0.62516900
C	2.40000900	-0.19617200	-0.55969400
C	3.16399700	0.58696300	-1.43607000

C	4.48619100	0.87970100	-1.12878800
C	5.06294300	0.40852800	0.05435500
H	4.73219100	-0.73848100	1.85084500
H	2.41063600	-1.27949100	1.33841900
H	2.71200000	0.96326600	-2.35539600
H	5.07217800	1.48594300	-1.82062900
H	6.09998600	0.64404700	0.29323900
N	1.05560500	-0.44271400	-0.92519700
H	0.90859600	-0.60615600	-1.91796400
N	0.33850300	-1.35521400	-0.14320400
H	0.91479900	-2.14709600	0.19522300
H	-0.44179700	-1.77898900	-0.68427700
C	-0.87605500	1.69450200	1.02543100
C	-1.26641900	0.41298700	0.63713600
C	-2.47384400	0.27019100	-0.08647200
C	-3.24786400	1.39671400	-0.38207400
C	-2.83949900	2.66724100	0.01588800
C	-1.64889400	2.81559700	0.71867100
H	0.05296500	1.82400000	1.58342500
H	-4.17630100	1.26721200	-0.93664800
H	-3.45238700	3.53569100	-0.22532200
H	-1.31393900	3.80362300	1.03552300
C	-0.34514800	-0.71319500	1.08062300
H	0.47772500	-0.26502300	1.64947600
C	-2.94088000	-1.05734000	-0.56824100
O	-0.86371900	-1.72590300	1.83291100
O	-2.26631800	-2.07414200	-0.49925100
O	-4.14667100	-1.05673000	-1.08772300

H	-4.36517700	-1.95586700	-1.38900100
H	-1.63213500	-2.10829300	1.37932400

a-TS2

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.2912486
ZPE (M05-2X/SMD)	a.u.	-877.3831156
Solvation ΔG	kJ/mol	-241.1968085
ZPE (M06-2X/IEFPCM)	a.u.	-876.4713024
ZPE (double hybrid)	a.u.	-876.1468688
ZPE_corr	a.u.	0.274765
U_corr	a.u.	0.290343
H_corr	a.u.	0.291287
G_corr	a.u.	0.229636
U(T)	a.u.	-875.8565258
H(T)	a.u.	-875.8555818
G(T)	a.u.	-875.9172328

Cartesian coordinate:

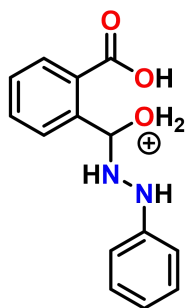
C	-4.47412800	-1.05673400	-0.80691000
C	-3.15715300	-0.71498100	-0.49629900
C	-2.90431600	0.35553700	0.36895100

C	-3.97619000	1.08485600	0.90127000
C	-5.28292700	0.73949700	0.57382200
C	-5.54225200	-0.33580500	-0.27880500
H	-4.65766100	-1.89567900	-1.47959000
H	-2.34294300	-1.28370400	-0.94746300
H	-3.77921300	1.92020200	1.57596000
H	-6.10766700	1.31402600	0.99791400
H	-6.56811100	-0.60616900	-0.52931200
N	-1.59539400	0.76560200	0.67763800
H	-1.50455100	1.41553100	1.45153700
N	-0.57839300	-0.17663100	0.62163800
H	-0.59210500	-1.42312300	0.12742500
H	-0.02860400	-0.18022700	1.48820900
C	1.59140800	1.86228300	-0.71415100
C	1.64637400	0.49034400	-0.44618400
C	2.87453200	-0.05679500	0.00536100
C	3.98222500	0.78868100	0.16495600
C	3.90117700	2.15086200	-0.10110600
C	2.69817000	2.69046100	-0.54246200
H	0.65295900	2.29425400	-1.06579300
H	4.92459600	0.35895600	0.49935500
H	4.77939200	2.78254600	0.03046000
H	2.61481900	3.75481200	-0.76309000
C	0.29825100	-0.17464300	-0.60113600
H	-0.27283000	0.34074100	-1.38210700
C	3.09904500	-1.50231100	0.28964600
O	0.20003800	-1.57937400	-0.80989800
O	2.30368800	-2.40592200	0.05641700

O	4.26368100	-1.77187000	0.82208700
H	4.34388400	-2.73331600	0.95266100
H	1.08998500	-2.05182500	-0.50167000

a-IM3

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.3405279
ZPE (M05-2X/SMD)	a.u.	-877.4302273
Solvation ΔG	kJ/mol	-235.5057747
ZPE (M06-2X/IEFPCM)	a.u.	-876.5121174
ZPE (double hybrid)	a.u.	-876.2029431
ZPE_corr	a.u.	0.275573
U_corr	a.u.	0.294048
H_corr	a.u.	0.294992
G_corr	a.u.	0.227904
U(T)	a.u.	-875.9088951
H(T)	a.u.	-875.9079511
G(T)	a.u.	-875.9750391

Cartesian coordinate:

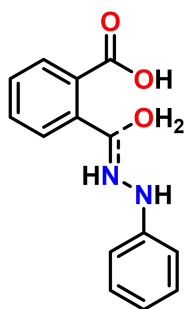
C	4.26148100	-1.30971900	0.24327900
C	3.01351200	-0.69183100	0.31282400

C	2.88158700	0.63385800	-0.11341900
C	3.99098600	1.33850300	-0.58969600
C	5.23520700	0.71430400	-0.63260900
C	5.37515900	-0.61289800	-0.22454800
H	4.36234300	-2.34478700	0.57249100
H	2.15143100	-1.22078900	0.72409900
H	3.87914200	2.37107100	-0.92601500
H	6.09908100	1.26908800	-1.00090800
H	6.34927700	-1.10047200	-0.26953100
N	1.62641400	1.29116800	-0.02214000
H	1.59912000	2.18796200	-0.50650100
N	0.54240100	0.51952600	-0.40478200
H	-0.28662700	-1.89250000	2.47036600
H	0.60969700	-0.01360300	-1.28201400
C	-1.42453200	-1.72373400	-0.40708000
C	-1.65867800	-0.38138500	-0.09683600
C	-2.97093300	0.12579800	-0.11733800
C	-4.03478300	-0.71487600	-0.43674300
C	-3.79647400	-2.05508700	-0.74238400
C	-2.49595800	-2.55579900	-0.73096600
H	-0.41161800	-2.12626000	-0.35272700
H	-5.04553800	-0.30830800	-0.45957400
H	-4.63111600	-2.70910700	-0.99544000
H	-2.30980200	-3.60367800	-0.96702300
C	-0.52966500	0.46871000	0.30308600
H	-0.54246700	1.06902600	1.21153300
C	-3.16827000	1.58436500	0.12461500
O	0.25848400	-1.19345700	2.08648100

O	-2.24631000	2.36372200	0.18366100
O	-4.43724300	1.93289900	0.25619000
H	-4.48827500	2.89487400	0.38640100
H	0.81238200	-0.89393800	2.81951800

a-TS3

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.3326592
ZPE (M05-2X/SMD)	a.u.	-877.4215649
Solvation ΔG	kJ/mol	-233.4219154
ZPE (M06-2X/IEFPCM)	a.u.	-876.5057624
ZPE (double hybrid)	a.u.	-876.1876199
ZPE_corr	a.u.	0.277486
U_corr	a.u.	0.293701
H_corr	a.u.	0.294645
G_corr	a.u.	0.232899
U(T)	a.u.	-875.8939189
H(T)	a.u.	-875.8929749
G(T)	a.u.	-875.9547209

Cartesian coordinate:

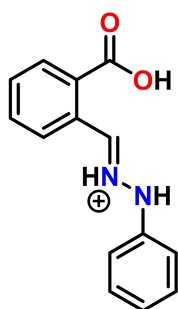
C	-3.79555000	1.33406000	0.40857100
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C	-2.62101300	0.62378600	0.14667800
C	-2.69969000	-0.67439000	-0.36820300
C	-3.95397700	-1.24416700	-0.63032500
C	-5.11255500	-0.52321600	-0.36749500
C	-5.04272200	0.77023500	0.15775400
H	-3.72199800	2.34634000	0.80870200
H	-1.65731700	1.09844100	0.32974800
H	-4.01228500	-2.25647900	-1.03457600
H	-6.08212300	-0.97829900	-0.57497500
H	-5.95419500	1.33158800	0.36357900
N	-1.55338600	-1.46270300	-0.60340600
H	-1.64382400	-2.11856300	-1.37664500
N	-0.32719900	-0.83632700	-0.59767100
H	-0.75492300	-0.48246300	2.20003400
H	-0.17282100	-0.04626700	-1.22672400
C	2.89512300	-1.83111300	0.24686600
C	1.99384400	-0.76822800	0.16826300
C	2.48335500	0.52362600	-0.13685700
C	3.84691600	0.70025700	-0.38304300
C	4.73227100	-0.37473500	-0.31578600
C	4.25658000	-1.64017600	0.00589200
H	2.52721400	-2.82926400	0.48770800
H	4.21527400	1.69928300	-0.61249200
H	5.79355400	-0.21459000	-0.50550800
H	4.93908600	-2.48759600	0.07206500
C	0.56385500	-1.15620500	0.33176500
H	0.39197600	-2.13465200	0.78230300
C	1.61513900	1.73792600	-0.12201200

O	0.16130100	-0.29812600	1.93254300
O	0.54293100	1.80446000	0.45311900
O	2.12082500	2.75950600	-0.77536300
H	1.52950600	3.52662700	-0.67773600
H	0.19706800	0.64642000	1.63725800

a-IM4

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.9236326
ZPE (M05-2X/SMD)	a.u.	-801.0148446
Solvation ΔG	kJ/mol	-239.4771060
ZPE (M06-2X/IEFPCM)	a.u.	-800.1662634
ZPE (double hybrid)	a.u.	-799.8415788
ZPE_corr	a.u.	0.251643
U_corr	a.u.	0.266360
H_corr	a.u.	0.267304
G_corr	a.u.	0.208010
U(T)	a.u.	-799.5752188
H(T)	a.u.	-799.5742748
G(T)	a.u.	-799.6335688

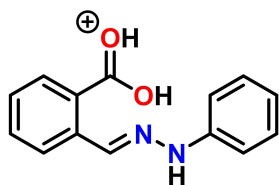
Cartesian coordinate:

C	-4.27658600	-1.35679700	0.25013300
C	-2.92638300	-1.21543200	-0.07010400
C	-2.32504400	0.04279300	0.03106900
C	-3.06187100	1.14743200	0.47162100
C	-4.40187100	0.98603500	0.80858600
C	-5.01702100	-0.26251100	0.69246700
H	-4.74439900	-2.33839400	0.16662800
H	-2.34358900	-2.08766300	-0.37178800
H	-2.58499700	2.12640900	0.54361200
H	-4.97352900	1.84839800	1.15354700
H	-6.06963400	-0.38063700	0.95033700
N	-0.95590700	0.20776900	-0.27396500
H	-0.59219400	1.16381900	-0.31245200
N	-0.49363900	-0.50701800	-1.33536300
H	-1.18385000	-0.75489200	-2.05735100
C	2.41653800	-2.02602100	-0.26719700
C	1.82797300	-0.78298500	-0.54072000
C	2.32470300	0.37312200	0.10092300
C	3.34531400	0.24295600	1.04503200
C	3.87215200	-1.00772700	1.36115700
C	3.41463100	-2.14238300	0.69711500
H	2.06855000	-2.91469100	-0.79599300
H	3.73570300	1.13970600	1.52369700
H	4.66095600	-1.08918900	2.10908000
H	3.84039400	-3.12158000	0.91630800
C	0.72690300	-0.87947900	-1.50750900
H	0.89661500	-1.44032900	-2.43124900
C	1.87584600	1.73831800	-0.30589300

O	0.96167300	1.94922000	-1.07236900
O	2.59018000	2.70555100	0.24010000
H	2.25027300	3.56170500	-0.07100700

a-IM5

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.8942156
ZPE (M05-2X/SMD)	a.u.	-800.9839289
Solvation ΔG	kJ/mol	-235.5422691
ZPE (M06-2X/IEFPCM)	a.u.	-800.1419814
ZPE (double hybrid)	a.u.	-799.8127967
ZPE_corr	a.u.	0.249963
U_corr	a.u.	0.264685
H_corr	a.u.	0.265629
G_corr	a.u.	0.206816
U(T)	a.u.	-799.5481117
H(T)	a.u.	-799.5471677
G(T)	a.u.	-799.6059807

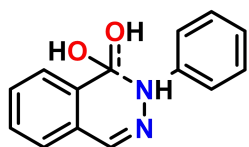
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C	4.55268000	-0.23471200	-0.60063800
C	3.20579800	-0.41718900	-0.90559200
C	2.25409800	-0.31701700	0.11493800
C	2.65271900	-0.03212100	1.42550600

C	4.00310300	0.14823200	1.71316800
C	4.96093100	0.04781200	0.70374500
H	5.29274400	-0.31587200	-1.39823600
H	2.88351800	-0.63849300	-1.92164900
H	1.90419600	0.04712200	2.21664800
H	4.30622200	0.36779800	2.73779800
H	6.01769800	0.18862200	0.93166000
N	0.88280700	-0.48403000	-0.14125000
H	0.25352200	-0.50364600	0.66292700
N	0.45320100	-0.84569100	-1.33138400
H	-0.51460200	0.96610800	-1.78946700
C	-2.62241600	-1.92218400	-0.16358000
C	-1.89808600	-0.80138500	-0.56649100
C	-2.24007500	0.45569200	-0.00005500
C	-3.26323500	0.55058800	0.96053200
C	-3.95736500	-0.58434100	1.35511000
C	-3.64040900	-1.81765300	0.78650900
H	-2.37637300	-2.89235500	-0.59662900
H	-3.51590300	1.52249800	1.38252400
H	-4.74955200	-0.50521600	2.09878700
H	-4.18790600	-2.71229800	1.08541100
C	-0.80779300	-0.98806100	-1.56893200
H	-1.07302000	-1.34933500	-2.56637300
C	-1.61142100	1.70320400	-0.41923300
O	-0.73895800	1.81973200	-1.34301000
O	-1.96327600	2.78257200	0.17285800
H	-1.50590700	3.56948500	-0.18366500

a-TS4

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.8894378
ZPE (M05-2X/SMD)	a.u.	-800.9820217
Solvation ΔG	kJ/mol	-243.0790295
ZPE (M06-2X/IEFPCM)	a.u.	-800.1375668
ZPE (double hybrid)	a.u.	-799.8076141
ZPE_corr	a.u.	0.249818
U_corr	a.u.	0.263817
H_corr	a.u.	0.264761
G_corr	a.u.	0.208532
U(T)	a.u.	-799.5437971
H(T)	a.u.	-799.5428531
G(T)	a.u.	-799.5990821

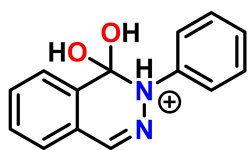
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C	2.80049100	1.01699600	0.43141200
C	1.95032300	0.33784600	-0.44773200
C	2.44440000	-0.70049200	-1.24753600
C	3.79052800	-1.04812400	-1.17165200
C	4.64872300	-0.36937900	-0.30508100
H	4.80963000	1.19799400	1.17031200
H	2.40162900	1.81913000	1.05062900

H	1.77451500	-1.22715000	-1.93086400
H	4.17085700	-1.85408500	-1.80069500
H	5.70288700	-0.64224100	-0.25067200
N	0.57252800	0.61751300	-0.48209300
H	0.07940000	0.28053400	-1.31122200
N	0.14438700	1.82543900	0.00518800
H	-0.67615500	0.49909100	2.30438600
C	-3.36511300	1.21876900	-0.60544300
C	-2.13602700	0.89484000	-0.03765900
C	-1.89418700	-0.45655800	0.30466200
C	-2.84244500	-1.44673600	0.04973800
C	-4.06495500	-1.09810100	-0.52762800
C	-4.32526300	0.22998200	-0.84615600
H	-3.56785600	2.25529100	-0.87803300
H	-2.63158400	-2.48253500	0.31728900
H	-4.80842800	-1.87027600	-0.72361500
H	-5.28028000	0.50663300	-1.29353300
C	-1.11602700	1.95437700	0.17885800
H	-1.46091500	2.93442600	0.52300300
C	-0.65383700	-0.86977600	0.98758400
O	-0.19016800	-0.30442600	2.04240300
O	-0.11850700	-1.97553100	0.63700300
H	0.63770600	-2.22705800	1.20509700

a-IM6

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.9161112
ZPE (M05-2X/SMD)	a.u.	-801.0038966
Solvation ΔG	kJ/mol	-230.4805677
ZPE (M06-2X/IEFPCM)	a.u.	-800.1533868
ZPE (double hybrid)	a.u.	-799.8308778
ZPE_corr	a.u.	0.251944
U_corr	a.u.	0.265890
H_corr	a.u.	0.266835
G_corr	a.u.	0.211176
U(T)	a.u.	-799.5649878
H(T)	a.u.	-799.5640428
G(T)	a.u.	-799.6197018

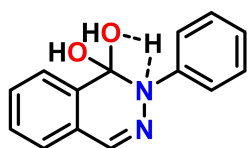
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C	3.92262800	0.75553300	0.81615000
C	2.55386900	0.94384400	0.64241300
C	1.90756000	0.20632200	-0.34387600
C	2.57679800	-0.70516700	-1.15351400
C	3.94706600	-0.88238600	-0.96581900
C	4.61693900	-0.15417000	0.01638100
H	4.44923500	1.32678800	1.58077700
H	1.99393200	1.65265800	1.25057000
H	2.04290300	-1.26966900	-1.91980000
H	4.48828800	-1.58830700	-1.59565300

H	5.68930300	-0.29239200	0.15735700
N	0.45481500	0.35348400	-0.51176000
H	0.21666800	0.04873900	-1.46960700
N	0.07123200	1.74269100	-0.39760600
H	-0.73877600	-0.27279000	2.28313100
C	-3.56330900	1.17595100	-0.35184200
C	-2.20892400	0.89413100	-0.16389700
C	-1.79822100	-0.41925500	0.10697400
C	-2.72060300	-1.45337000	0.17858000
C	-4.07418700	-1.16636600	-0.02626800
C	-4.49333400	0.13859000	-0.28445300
H	-3.88343900	2.19834900	-0.55731600
H	-2.38336700	-2.46855200	0.38725900
H	-4.80658900	-1.97276100	0.01974900
H	-5.55192000	0.35040200	-0.43497300
C	-1.18340200	1.93369900	-0.25537200
H	-1.48290700	2.98628300	-0.21562800
C	-0.34081700	-0.63251700	0.42936400
O	0.02238600	-0.24356200	1.68503800
O	0.05164100	-1.88908200	0.11239200
H	0.83974800	-2.11986100	0.63132100

a-TS5

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.8522172
ZPE (M05-2X/SMD)	a.u.	-800.9408024
Solvation ΔG	kJ/mol	-232.5804426
ZPE (M06-2X/IEFPCM)	a.u.	-800.0985381
ZPE (double hybrid)	a.u.	-799.7713739
ZPE_corr	a.u.	0.246559
U_corr	a.u.	0.260177
H_corr	a.u.	0.261121
G_corr	a.u.	0.205836
U(T)	a.u.	-799.5111969
H(T)	a.u.	-799.5102529
G(T)	a.u.	-799.5655379

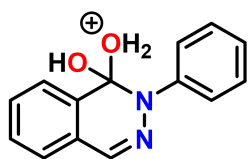
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C	3.22005300	1.25984600	1.40285100
C	1.98655000	1.10747600	0.77728500
C	1.86751300	0.18522500	-0.26245900
C	2.95072200	-0.57893900	-0.68730000
C	4.18239100	-0.42143000	-0.04894100
C	4.31516100	0.49499700	0.99208700
H	3.32728900	1.97807900	2.21594200
H	1.12276900	1.69744900	1.08860400
H	2.84264500	-1.27621300	-1.52040300
H	5.03842400	-1.01144500	-0.37659800
H	5.27916800	0.61878400	1.48646100
N	0.57770700	-0.00546700	-0.90087300
H	0.40517000	-1.05763800	-1.76926000
N	0.09863400	1.18652700	-1.46891300

H	1.11144900	-1.88463700	0.64520200
C	-3.36185000	1.31132200	-0.21080100
C	-2.09714300	0.77479700	-0.47659000
C	-1.69982600	-0.40442800	0.16159700
C	-2.52836600	-1.03559400	1.08662600
C	-3.78632100	-0.49346400	1.34382000
C	-4.20453800	0.67038800	0.69172000
H	-3.67005200	2.23576000	-0.70165500
H	-2.19444500	-1.94200300	1.59151000
H	-4.44817000	-0.98396600	2.05796200
H	-5.19143000	1.08441000	0.89948800
C	-1.13368100	1.48525100	-1.31272800
H	-1.45230100	2.40626000	-1.81046500
C	-0.37179900	-0.97171500	-0.20312300
O	0.17006600	-1.68298800	0.78824800
O	-0.48204400	-1.77776400	-1.46202700
H	-0.44227100	-2.74864800	-1.35231600

a-IM7

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.9314304
ZPE (M05-2X/SMD)	a.u.	-801.0169953
Solvation ΔG	kJ/mol	-224.6506450
ZPE	a.u.	-800.1739374

(M06-2X/IEFPCM)		
ZPE (double hybrid)	a.u.	-799.8594687
ZPE_corr	a.u.	0.247984
U_corr	a.u.	0.264185
H_corr	a.u.	0.265129
G_corr	a.u.	0.203790
U(T)	a.u.	-799.5952837
H(T)	a.u.	-799.5943397
G(T)	a.u.	-799.6556787

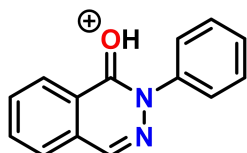
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C	-4.09165100	0.79455800	-0.99926400
C	-2.70944300	0.97188200	-1.01639600
C	-1.93139500	0.20444600	-0.15621600
C	-2.48364500	-0.72255200	0.72349800
C	-3.86687700	-0.89023000	0.72638800
C	-4.66741700	-0.13583100	-0.13284500
H	-4.71938000	1.38613300	-1.66604700
H	-2.23710000	1.69606900	-1.68086300
H	-1.82886100	-1.27937900	1.39517200
H	-4.32067100	-1.60941300	1.40878300
H	-5.74957400	-0.27090600	-0.12414000
N	-0.49802700	0.41349700	-0.14388100
H	-0.07354600	-0.11605200	2.92816500
N	-0.11316100	1.62430100	0.31239600
H	0.43932200	-2.32940100	-1.17957600
C	3.54430900	1.20267300	0.18074000
C	2.17235100	0.91724900	0.06750500
C	1.75523400	-0.34663600	-0.39669900

C	2.70610500	-1.32869700	-0.73528600
C	4.05021500	-1.03184700	-0.61665600
C	4.46940800	0.23427400	-0.16201500
H	3.86229000	2.18294200	0.53751100
H	2.41374800	-2.32167000	-1.07989100
H	4.79295900	-1.78602800	-0.87593800
H	5.53531200	0.44736500	-0.07813000
C	1.15024000	1.86371500	0.41482400
H	1.41807200	2.85497900	0.78757900
C	0.33933100	-0.56238200	-0.48167200
O	-0.21058400	-1.66918400	-0.89462500
O	0.36028000	-0.69174800	2.28541600
H	0.92758300	-1.25549000	2.82599100

a-IM8

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-724.5194770
ZPE (M05-2X/SMD)	a.u.	-724.6059160
Solvation ΔG	kJ/mol	-226.9455945
ZPE (M06-2X/IEFPCM)	a.u.	-723.8296350
ZPE (double hybrid)	a.u.	-723.5006502
ZPE_corr	a.u.	0.224483
U_corr	a.u.	0.236814

H_corr	a.u.	0.237759
G_corr	a.u.	0.185103
U(T)	a.u.	-723.2638362
H(T)	a.u.	-723.2628912
G(T)	a.u.	-723.3155472

Cartesian coordinate:

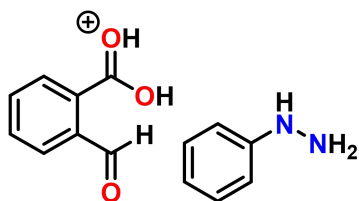
C	4.03012800	-0.81278000	-0.82528600
C	2.64554200	-0.95934300	-0.79616300
C	1.90320400	-0.13536900	0.04560200
C	2.50354700	0.81737200	0.86434900
C	3.88959300	0.95198900	0.82434300
C	4.65084400	0.14187400	-0.01870800
H	4.62463800	-1.44873000	-1.48144400
H	2.14092000	-1.70480100	-1.41085600
H	1.90192400	1.44118900	1.52502500
H	4.37472500	1.69120100	1.46200100
H	5.73538400	0.25252000	-0.04419900
N	0.46638000	-0.32707500	0.08401600
N	0.08574300	-1.60368400	0.31860400
H	-0.50187400	2.51275900	-0.62979300
C	-3.57490900	-1.20051800	0.21825600
C	-2.20473200	-0.88964600	0.16228600
C	-1.79510600	0.43821100	-0.08672300
C	-2.75401400	1.45507400	-0.27193400
C	-4.09490100	1.13056200	-0.21243300
C	-4.50534800	-0.19605900	0.03008000
H	-3.88726900	-2.22768700	0.40893600
H	-2.46983100	2.49321100	-0.45036100

H	-4.84360500	1.91002100	-0.35202300
H	-5.56980800	-0.42793300	0.07100100
C	-1.17547500	-1.87293200	0.34881800
H	-1.43275700	-2.91804700	0.53500500
C	-0.38136100	0.67750800	-0.14059800
O	0.15507700	1.83324500	-0.41287200

Path B

b-IM1

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.3246031
ZPE (M05-2X/SMD)	a.u.	-877.4106769
Solvation ΔG	kJ/mol	-225.9867619
ZPE (M06-2X/IEFPCM)	a.u.	-876.4992511
ZPE (double hybrid)	a.u.	-876.1818319
ZPE_corr	a.u.	0.275498
U_corr	a.u.	0.292236
H_corr	a.u.	0.293180
G_corr	a.u.	0.230445
U(T)	a.u.	-875.8895959
H(T)	a.u.	-875.8886519
G(T)	a.u.	-875.9513869

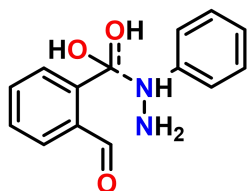
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C	-3.62661900	-0.30216300	-0.78276100
C	-2.59742500	0.35897100	-0.10434200
C	-1.62071300	-0.41671800	0.58474200
C	-1.72851300	-1.80624500	0.57858600
C	-2.77656700	-2.44227400	-0.09316700
C	-3.72375100	-1.69380900	-0.77980400
H	-4.37165100	0.28906700	-1.31723900
H	-0.98083500	-2.40167600	1.10034400
H	-2.83901100	-3.53042600	-0.07815400
H	-4.53826300	-2.18360900	-1.31275000
C	-2.68352500	1.82373300	-0.17316100
H	-3.48181700	2.22186000	-0.82117300
C	-0.44219100	0.15897800	1.27513400
O	-1.98869800	2.62882900	0.43866700
O	0.39868600	-0.69455500	1.75735700
O	-0.26600900	1.37918400	1.50892800
H	1.15483000	-0.24289400	2.17722800
H	-1.05825000	2.03459900	1.08483000
N	0.26025700	1.53519200	-1.44987900
N	0.67075700	0.27197300	-1.02749800
C	2.00727100	0.00392800	-0.70868700
C	2.41690200	-1.33495400	-0.58579700
C	2.91408100	1.03147400	-0.42012100
C	3.71387800	-1.63370900	-0.18683400
H	1.70503100	-2.13449600	-0.80506000
C	4.21336200	0.71566800	-0.01734400
H	2.61573500	2.07526200	-0.51580500
C	4.62202800	-0.61035800	0.10207800

H	4.02020200	-2.67736300	-0.10092300
H	4.91197400	1.52481000	0.20115400
H	5.63898500	-0.84831200	0.41463500
H	0.20263000	-0.46844200	-1.54322300
H	0.83422600	1.87079500	-2.22845200
H	0.38797100	2.19786300	-0.68452500

b-TS1

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.3274435
ZPE (M05-2X/SMD)	a.u.	-877.4122490
Solvation ΔG	kJ/mol	-222.6568403
ZPE (M06-2X/IEFPCM)	a.u.	-876.4979564
ZPE (double hybrid)	a.u.	-876.1816419
ZPE_corr	a.u.	0.276992
U_corr	a.u.	0.292801
H_corr	a.u.	0.293745
G_corr	a.u.	0.233095
U(T)	a.u.	-875.8888409
H(T)	a.u.	-875.8878969
G(T)	a.u.	-875.9485469

Cartesian coordinate:

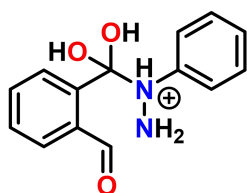
C	-3.78361300	-0.12377900	-0.63059600
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C	-2.62969600	0.44616300	-0.08013400
C	-1.63212800	-0.40972600	0.46362900
C	-1.84495900	-1.78762000	0.44662100
C	-3.01263800	-2.33248400	-0.09408600
C	-3.98312400	-1.50297900	-0.64084700
H	-4.54648700	0.53388600	-1.05050200
H	-1.08497700	-2.44831700	0.86104100
H	-3.15121000	-3.41376800	-0.08703900
H	-4.89285900	-1.92013400	-1.07196600
C	-2.63107200	1.92063800	-0.09567700
H	-3.46498700	2.37852500	-0.65748800
C	-0.31639200	0.05204800	1.00756500
O	-1.83845900	2.65883500	0.46868600
O	0.40131300	-0.88741600	1.56878900
O	-0.08640400	1.25234900	1.40038500
H	1.18222300	-0.49916800	2.00211600
H	-0.82129200	1.93141300	1.08152100
N	0.18919100	1.31208800	-1.42194300
N	0.64962400	0.11957200	-0.85012000
C	2.03995300	-0.05622000	-0.60379600
C	2.54348000	-1.35996300	-0.52642400
C	2.86817800	1.03874900	-0.34597000
C	3.87982200	-1.56414600	-0.19786000
H	1.88505800	-2.20765800	-0.72802400
C	4.20593400	0.82009800	-0.01566800
H	2.48711600	2.05745300	-0.41192600
C	4.71530400	-0.47500000	0.05990900
H	4.27107700	-2.58073400	-0.14618600

H	4.85302500	1.67577500	0.18022700
H	5.76276600	-0.63722500	0.31526200
H	0.24697100	-0.67783700	-1.34414500
H	0.72548800	1.53194100	-2.26416100
H	0.35049400	2.06941800	-0.75716600

b-IM2

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.3257347
ZPE (M05-2X/SMD)	a.u.	-877.4146233
Solvation ΔG	kJ/mol	-233.3770193
ZPE (M06-2X/IEFPCM)	a.u.	-876.4995920
ZPE (double hybrid)	a.u.	-876.1806642
ZPE_corr	a.u.	0.278689
U_corr	a.u.	0.294654
H_corr	a.u.	0.295599
G_corr	a.u.	0.236273
U(T)	a.u.	-875.8860102
H(T)	a.u.	-875.8850652
G(T)	a.u.	-875.9443912

Cartesian coordinate:

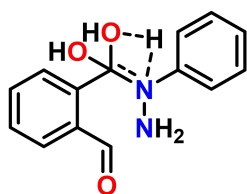
C	1.88709000	2.20947700	-0.20354100
C	1.07088000	1.14535700	-0.60657600

C	1.49357600	-0.18637200	-0.34163500
C	2.72315300	-0.38333400	0.28690300
C	3.52921700	0.69381400	0.66681000
C	3.10987000	1.99590600	0.42896000
H	1.55541200	3.22964200	-0.40495200
H	3.05452200	-1.40144700	0.48528600
H	4.48545300	0.50109700	1.15368100
H	3.72741300	2.84321800	0.72630900
C	-0.14448700	1.58433700	-1.33656200
H	-0.33771300	2.67345900	-1.28338500
C	0.68696600	-1.44021100	-0.64024000
O	-0.89227900	0.88639300	-1.99378300
O	1.43417200	-2.55309100	-0.54841800
O	-0.11168300	-1.46974100	-1.69395700
H	1.07789500	-3.21309700	-1.16429200
H	-0.48479300	-0.55497900	-1.92170000
N	0.37275000	-1.70742100	1.90443900
N	-0.38136900	-1.59055800	0.71537500
C	-1.46154700	-0.61350300	0.68781700
C	-2.57016000	-0.87919000	-0.11408500
C	-1.34257600	0.58482900	1.38896200
C	-3.56566200	0.08703300	-0.23586200
H	-2.64886300	-1.82727200	-0.64857000
C	-2.34541900	1.54527100	1.25596000
H	-0.48675500	0.78309100	2.03371500
C	-3.45019100	1.30168400	0.44018900
H	-4.43412200	-0.11298900	-0.86353500
H	-2.26005200	2.48613100	1.80016200

H	-4.22998700	2.05708100	0.34051800
H	-0.77284700	-2.51991000	0.51951700
H	-0.27425100	-1.78091000	2.69129200
H	0.92307500	-0.85633900	2.02392400

b-TS2

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-877.2635500
ZPE (M05-2X/SMD)	a.u.	-877.3505631
Solvation ΔG	kJ/mol	-228.4528941
ZPE (M06-2X/IEFPCM)	a.u.	-876.4404378
ZPE (double hybrid)	a.u.	-876.1198663
ZPE_corr	a.u.	0.273150
U_corr	a.u.	0.288781
H_corr	a.u.	0.289725
G_corr	a.u.	0.229877
U(T)	a.u.	-875.8310853
H(T)	a.u.	-875.8301413
G(T)	a.u.	-875.8899893

Cartesian coordinate:

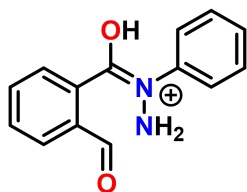
C	2.76295100	1.87470100	0.06138900
C	1.63764500	1.15344700	-0.35974300
C	1.65542300	-0.26358100	-0.26858700

C	2.79419700	-0.89436300	0.22365400
C	3.91693300	-0.15655300	0.60807100
C	3.90354900	1.23124900	0.53378700
H	2.74140400	2.96430100	0.00106200
H	2.80445200	-1.97888900	0.31773000
H	4.79830300	-0.67961900	0.98004900
H	4.77150100	1.81281700	0.84365500
C	0.54964300	2.00310700	-0.90017100
H	0.67843200	3.08536500	-0.70438800
C	0.44632600	-1.11020100	-0.61060300
O	-0.41644500	1.63295700	-1.54019000
O	0.75735800	-2.54651600	-0.64352000
O	-0.18848000	-0.84971600	-1.75028800
H	0.68984800	-2.88474500	-1.56007500
H	-0.37242300	0.14535400	-1.81283400
N	0.17192300	-1.37894700	1.77587200
N	-0.53116000	-1.30363700	0.55379600
C	-1.73799900	-0.50455200	0.50788600
C	-2.73837500	-0.86345900	-0.39700400
C	-1.89190400	0.61279700	1.32967700
C	-3.88673300	-0.08247100	-0.49770000
H	-2.61020600	-1.74805500	-1.01987100
C	-3.04716800	1.38607000	1.22471500
H	-1.12840900	0.89261600	2.05565900
C	-4.04188500	1.04489300	0.30955000
H	-4.66675800	-0.36207900	-1.20643700
H	-3.16675900	2.25983600	1.86590600
H	-4.94354700	1.65315300	0.23146900

H	-0.20552400	-2.57318500	0.00071900
H	-0.43228100	-1.84106300	2.45423900
H	0.40154900	-0.44801200	2.12789900

b-IM3

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.9110838
ZPE (M05-2X/SMD)	a.u.	-800.9963372
Solvation ΔG	kJ/mol	-223.8328017
ZPE (M06-2X/IEFPCM)	a.u.	-800.1507944
ZPE (double hybrid)	a.u.	-799.8303891
ZPE_corr	a.u.	0.250489
U_corr	a.u.	0.265805
H_corr	a.u.	0.266749
G_corr	a.u.	0.207159
U(T)	a.u.	-799.5645841
H(T)	a.u.	-799.5636401
G(T)	a.u.	-799.6232301

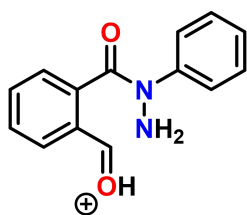
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C	-2.44759800	0.79587500	-0.00281800
C	-1.73918600	-0.40170300	0.21336300
C	-2.41278600	-1.61894200	0.27142300

C	-3.79853400	-1.65213200	0.08086100
C	-4.50368500	-0.47607900	-0.15050900
H	-4.37623400	1.67452300	-0.35305400
H	-1.86282100	-2.54569800	0.44381400
H	-4.32022200	-2.60868200	0.11470000
H	-5.58335700	-0.50502800	-0.29702200
C	-1.76113800	2.11167500	0.00487300
H	-2.40697500	2.98696600	-0.22100000
C	-0.27106300	-0.42874400	0.43895000
O	-0.58646000	2.24535900	0.25055100
O	0.19713800	-0.75920100	1.60172100
H	-0.51138000	-0.87746200	2.25709600
N	0.12146400	0.19245600	-1.75656300
N	0.59905200	-0.21336000	-0.50937900
C	2.01938000	-0.18537100	-0.23984500
C	2.79988100	-1.29279600	-0.55958100
C	2.56553400	0.98063600	0.29413900
C	4.17445900	-1.22514100	-0.33780400
H	2.33656300	-2.19039900	-0.97151000
C	3.94071700	1.03236300	0.51158200
H	1.91238100	1.82273200	0.53027700
C	4.74132200	-0.06673500	0.19538300
H	4.80296400	-2.08233600	-0.58028000
H	4.38732900	1.93467500	0.92998600
H	5.81724700	-0.02043800	0.36729400
H	0.55672800	-0.39618900	-2.46794100
H	0.43728400	1.15376100	-1.90673900

b-IM4

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.8865475
ZPE (M05-2X/SMD)	a.u.	-800.9777594
Solvation ΔG	kJ/mol	-239.4768434
ZPE (M06-2X/IEFPCM)	a.u.	-800.1300087
ZPE (double hybrid)	a.u.	-799.8056992
ZPE_corr	a.u.	0.250747
U_corr	a.u.	0.265397
H_corr	a.u.	0.266341
G_corr	a.u.	0.208010
U(T)	a.u.	-799.5403022
H(T)	a.u.	-799.5393582
G(T)	a.u.	-799.5976892

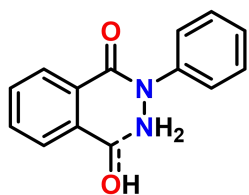
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C	-2.42445200	0.74380900	-0.14080600
C	-1.73120000	-0.50177900	-0.12139000
C	-2.46410100	-1.66972200	0.00889100
C	-3.85728000	-1.63113300	0.16968400
C	-4.54173300	-0.42056800	0.16520600
H	-4.35549900	1.71388500	-0.04410200

H	-1.94330900	-2.62721200	-0.01224400
H	-4.40530000	-2.56679500	0.28708800
H	-5.62459500	-0.39353400	0.27923900
C	-1.84288600	2.03672300	-0.35103800
C	-0.25236700	-0.69263500	-0.36271000
O	-0.62524900	2.33118200	-0.47372800
O	0.14760800	-1.51480700	-1.13711100
H	0.00428600	1.53939100	-0.33202600
N	0.11674000	0.51946900	1.62326600
N	0.61430600	0.17110500	0.35442000
C	2.03974800	0.00762100	0.17228100
C	2.87407500	-0.19199600	1.27029500
C	2.57168500	0.09556900	-1.11720500
C	4.25026900	-0.31525300	1.07292600
H	2.46886800	-0.24795900	2.27961400
C	3.94416800	-0.03328700	-1.30236100
H	1.91459900	0.25984500	-1.97140800
C	4.78830700	-0.23942200	-0.20908900
H	4.90028300	-0.47093900	1.93450400
H	4.35674200	0.03495700	-2.30946200
H	5.86414900	-0.33496900	-0.35842500
H	0.58175800	1.36953600	1.94093800
H	0.30022800	-0.22282200	2.29991400
H	-2.52012400	2.89584700	-0.43384300

b-TS3

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.8757847
ZPE (M05-2X/SMD)	a.u.	-800.9725025
Solvation ΔG	kJ/mol	-253.9325839
ZPE (M06-2X/IEFPCM)	a.u.	-800.1236719
ZPE (double hybrid)	a.u.	-799.7932410
ZPE_corr	a.u.	0.250863
U_corr	a.u.	0.265035
H_corr	a.u.	0.265980
G_corr	a.u.	0.209516
U(T)	a.u.	-799.5282060
H(T)	a.u.	-799.5272610
G(T)	a.u.	-799.5837250

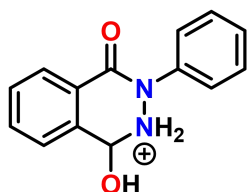
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C	-3.77272100	-0.78237900	-0.14343700
C	-2.40295800	-0.68926100	0.14269700
C	-1.73058300	0.55511500	0.07217900
C	-2.47714700	1.68880200	-0.21159200
C	-3.85680200	1.60007900	-0.44764300
C	-4.50465500	0.37022500	-0.42374700
H	-4.26579700	-1.75534500	-0.11673700
H	-1.96641200	2.65020500	-0.26735700
H	-4.41901200	2.50736900	-0.67110800
H	-5.57230400	0.30110700	-0.62928900

C	-1.77391600	-1.91990500	0.53525900
C	-0.24155600	0.78146600	0.24079600
O	-0.84282600	-2.06289700	1.38171800
O	0.14780400	1.80108200	0.76205200
H	-0.47951700	-1.22852900	1.73950000
N	0.10856700	-1.18183900	-1.08173800
N	0.62171300	-0.18480200	-0.24461800
C	2.04199800	-0.00685600	-0.16896400
C	2.83661800	-0.32893600	-1.27197400
C	2.63717300	0.43940900	1.01650600
C	4.22226200	-0.19313700	-1.19159700
H	2.38493500	-0.68460600	-2.19765200
C	4.02041700	0.57534900	1.08287600
H	2.01857300	0.68282700	1.87801700
C	4.81913000	0.26186500	-0.01823900
H	4.83413200	-0.44469200	-2.05861800
H	4.47764200	0.92390000	2.00972600
H	5.90268100	0.36794800	0.04165600
H	0.69064600	-2.01490700	-0.99159400
H	0.12219700	-0.88286600	-2.05920200
H	-2.18310700	-2.87240600	0.17827100

b-IM5

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.9157402
ZPE (M05-2X/SMD)	a.u.	-801.0198523
Solvation ΔG	kJ/mol	-273.3463186
ZPE (M06-2X/IEFPCM)	a.u.	-800.1662966
ZPE (double hybrid)	a.u.	-799.8305708
ZPE_corr	a.u.	0.254313
U_corr	a.u.	0.268274
H_corr	a.u.	0.269218
G_corr	a.u.	0.212589
U(T)	a.u.	-799.5622968
H(T)	a.u.	-799.5613528
G(T)	a.u.	-799.6179818

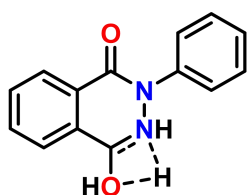
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C	-3.57090900	0.88520400	0.33133500
C	-2.20576600	0.62816100	0.23048000
C	-1.75219100	-0.65682100	-0.09829800
C	-2.66807900	-1.68674700	-0.32103900
C	-4.03182700	-1.42983000	-0.21297000
C	-4.48147400	-0.14795200	0.11100400
H	-3.92052800	1.88761200	0.58342500
H	-2.29242000	-2.67740500	-0.57859800
H	-4.75011700	-2.23209000	-0.38263500
H	-5.55045500	0.04907100	0.19586300
C	-1.20242200	1.73469300	0.39981300
C	-0.29864300	-0.95421100	-0.26207400
O	-0.85229200	2.40668800	-0.73389300
O	0.13067300	-1.96134600	-0.76048400

H	-0.95900400	1.84564200	-1.51637400
N	0.06299800	1.09024000	0.97778800
N	0.57228400	0.05485600	0.15873000
C	2.00129800	-0.05810700	0.08521300
C	2.66162900	-1.06530100	0.78899400
C	2.69898400	0.86788800	-0.69061500
C	4.05002100	-1.14165500	0.70908400
H	2.08996400	-1.78306600	1.37808500
C	4.08946700	0.79375400	-0.74760500
H	2.15083400	1.63082600	-1.24744900
C	4.76137700	-0.21153600	-0.05166700
H	4.57933200	-1.92839300	1.24718300
H	4.64555400	1.51420400	-1.34774300
H	5.84885400	-0.27381400	-0.10525700
H	0.78809800	1.82278600	1.02832400
H	-0.10614900	0.76428100	1.94555700
H	-1.50678700	2.45668300	1.16908400

b-TS4

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-800.8542781
ZPE (M05-2X/SMD)	a.u.	-800.9558259
Solvation ΔG	kJ/mol	-266.6137489

ZPE (M06-2X/IEFPCM)	a.u.	-800.1113549
ZPE (double hybrid)	a.u.	-799.7721824
ZPE_corr	a.u.	0.248703
U_corr	a.u.	0.262423
H_corr	a.u.	0.263368
G_corr	a.u.	0.207278
U(T)	a.u.	-799.5097594
H(T)	a.u.	-799.5088144
G(T)	a.u.	-799.5649044

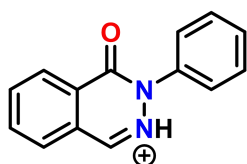
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C	2.22528900	0.56557300	-0.25572800
C	1.72927700	-0.70044600	0.06951400
C	2.61615200	-1.74019400	0.35311800
C	3.98786000	-1.50722600	0.31609600
C	4.47969700	-0.24003100	-0.00720400
H	3.98206800	1.78769000	-0.56549600
H	2.20876100	-2.72016800	0.60171400
H	4.68137300	-2.31869000	0.53782300
H	5.55491400	-0.06299500	-0.03854100
C	1.26553800	1.65535800	-0.57553000
C	0.26443200	-0.98087200	0.14878100
O	0.98601700	2.61656500	0.50610500
O	-0.17704800	-2.03759000	0.53344200
H	1.27396900	2.32013800	1.39244800
N	-0.13928400	1.27476200	-0.75794600
N	-0.57882300	0.06724600	-0.17377700

C	-2.00470300	-0.04752000	-0.07242300
C	-2.67885900	-0.97797900	-0.86323700
C	-2.69717300	0.78637600	0.80564400
C	-4.06549900	-1.07448700	-0.76692400
H	-2.11536400	-1.62316200	-1.53792400
C	-4.08496200	0.69281100	0.88530500
H	-2.15375100	1.49824200	1.43007700
C	-4.76789600	-0.23820300	0.10167000
H	-4.59910700	-1.80331300	-1.37767200
H	-4.63193700	1.34237300	1.56918100
H	-5.85372500	-0.31373500	0.17006800
H	-0.12189400	2.30387800	0.15787800
H	-0.46494700	1.34477200	-1.72924300
H	1.57434500	2.26134000	-1.43348400

b-IM6

Structure:



Energies:

ZPE (M05-2X/Gas)	a.u.	-724.5141549
ZPE (M05-2X/SMD)	a.u.	-724.6092607
Solvation ΔG	kJ/mol	-249.7002779
ZPE (M06-2X/IEFPCM)	a.u.	-723.8303989
ZPE (double hybrid)	a.u.	-723.4950751

ZPE_corr	a.u.	0.225134
U_corr	a.u.	0.237470
H_corr	a.u.	0.238414
G_corr	a.u.	0.185624
U(T)	a.u.	-723.2576051
H(T)	a.u.	-723.2566611
G(T)	a.u.	-723.3094511

Cartesian coordinate:

N	-0.49431600	0.24938000	-0.12928600
N	-0.02934100	1.49762600	-0.36847700
C	-1.92132200	0.10482000	-0.04728400
C	1.22127900	1.83786900	-0.39797600
H	-0.76616300	2.18515300	-0.55322600
C	0.38189100	-0.82761900	0.10354300
C	-2.63409200	0.91695700	0.83509800
C	-2.56040600	-0.83603300	-0.85427900
C	2.23219200	0.85466600	-0.16720900
H	1.43242300	2.88555100	-0.61384100
C	1.81790900	-0.47137800	0.07437900
O	-0.04857600	-1.93114200	0.31576800
C	-4.02184300	0.79745700	0.89119500
H	-2.11270900	1.62437000	1.48292900
C	-3.94455000	-0.95786300	-0.77250200
H	-1.97772900	-1.46248300	-1.52872900
C	3.59890200	1.18203500	-0.18378400
C	2.76721300	-1.46694400	0.30314400
C	-4.67478200	-0.14016900	0.09247400
H	-4.58881900	1.43018600	1.57420500

H	-4.45621500	-1.69169000	-1.39557400
C	4.53298500	0.18307200	0.04308600
H	3.91076600	2.20976800	-0.37255600
C	4.11814900	-1.13518400	0.28561900
H	2.42982200	-2.48628500	0.49025600
H	-5.75947300	-0.23809200	0.14609200
H	5.59606700	0.42314000	0.03333800
H	4.86508100	-1.90964300	0.46228300

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