

Pd-catalyzed one-pot cascade consisting C-C/C-O/N-N bond formation to access benzoxazine fused 1,2,3-triazoles

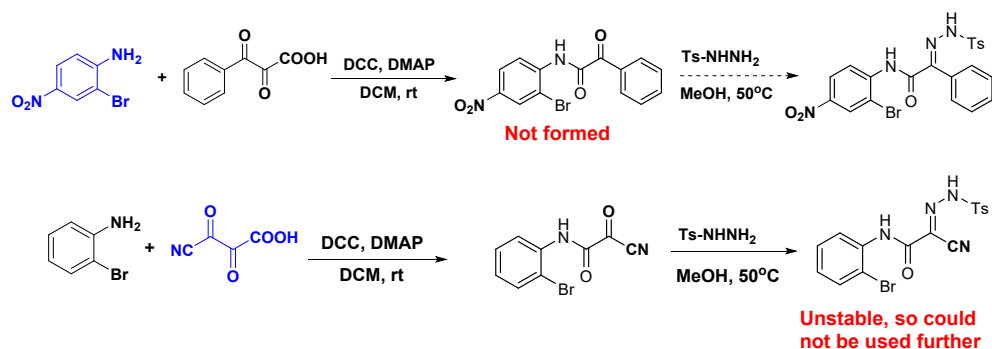
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Scheme S1: Reaction of 4-nitroaniline and cyanoacetic acid

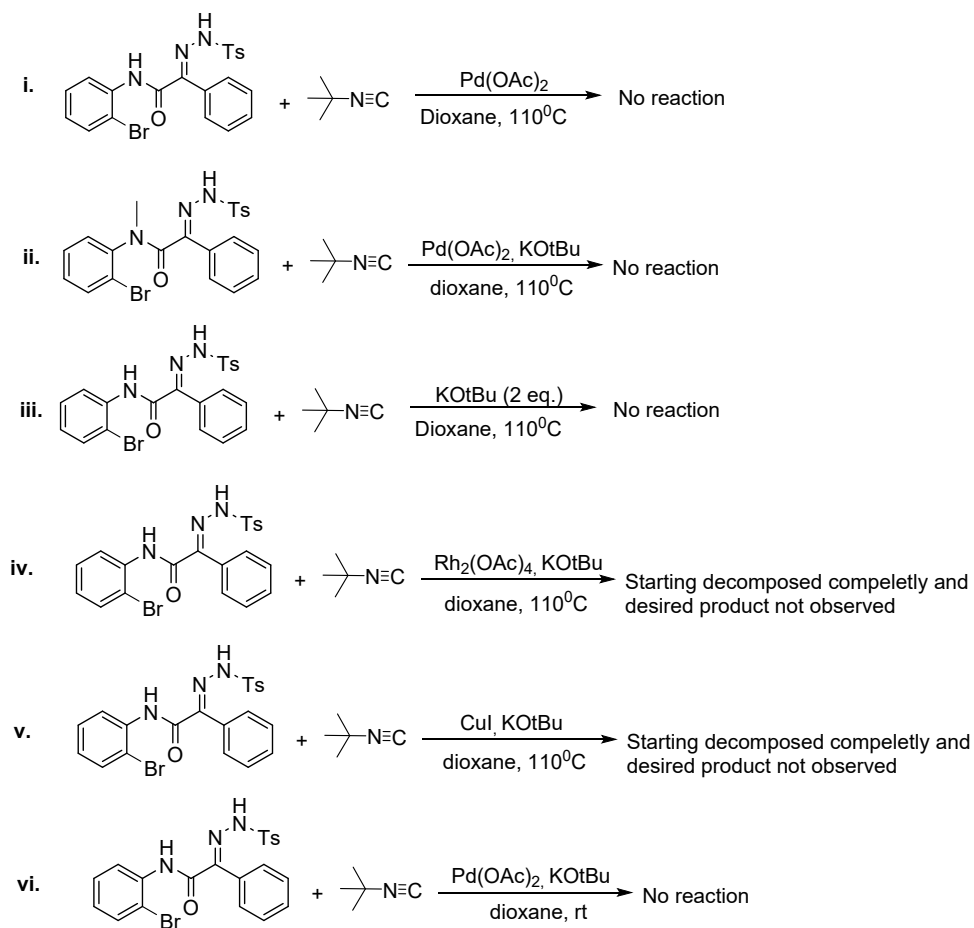


Figure S1: Control experiments

PES and Transition state

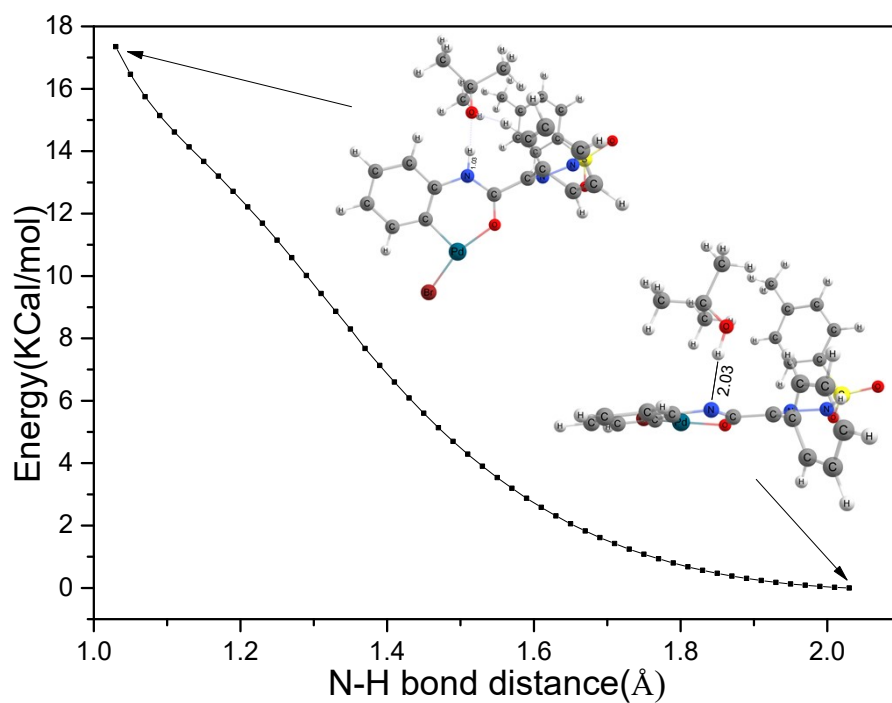


Figure S2: Relaxed potential energy surface scan for N-H proton abstraction from N-aryl amide in presence of strong base (KOtBu)

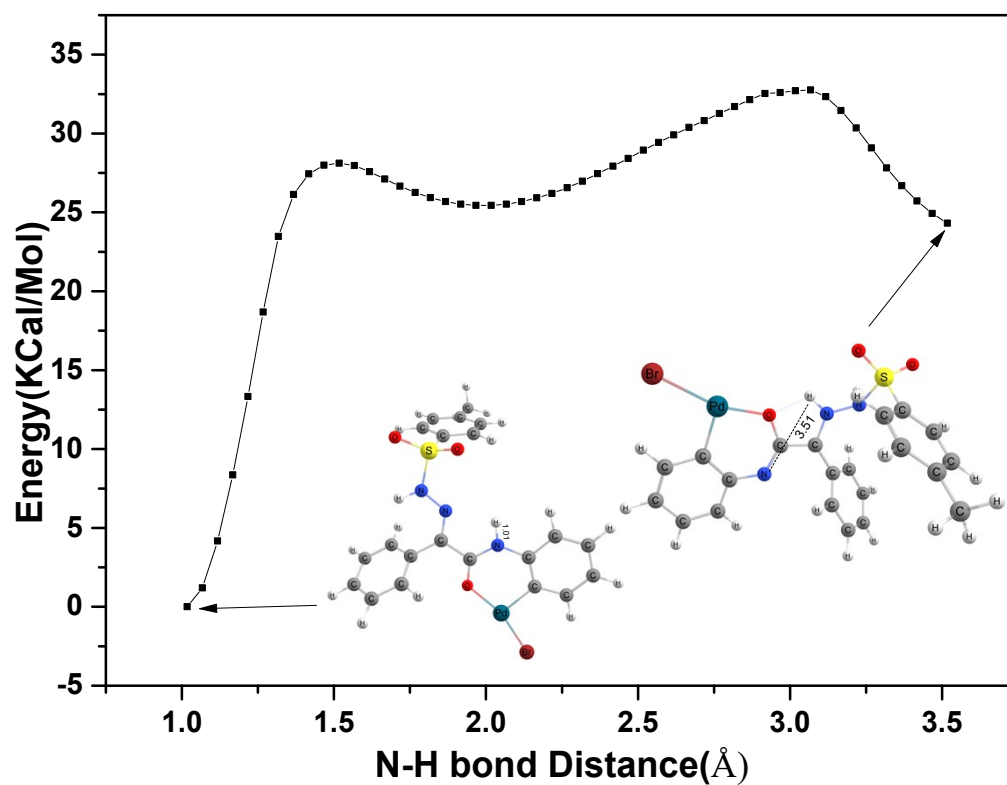


Figure S3: Relaxed potential energy surface scan for N-H proton abstraction from N-aryl amide in absence of strong base

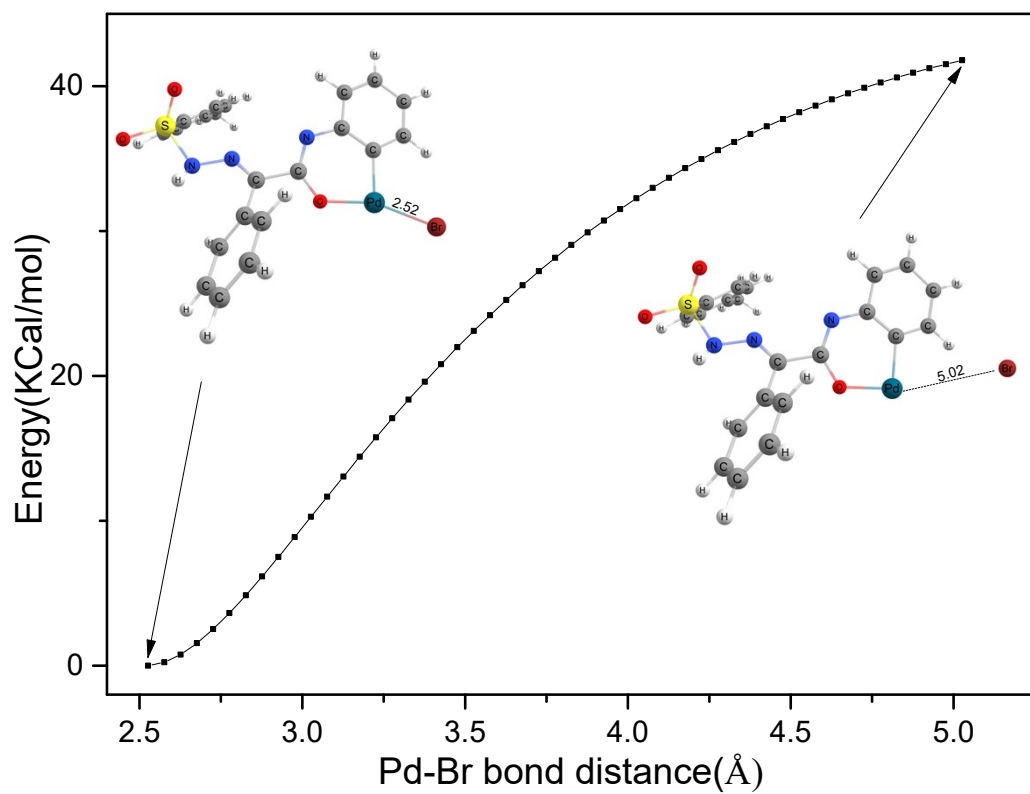


Figure S4: Relaxed potential energy surface scan for Pd-Br bond breaking

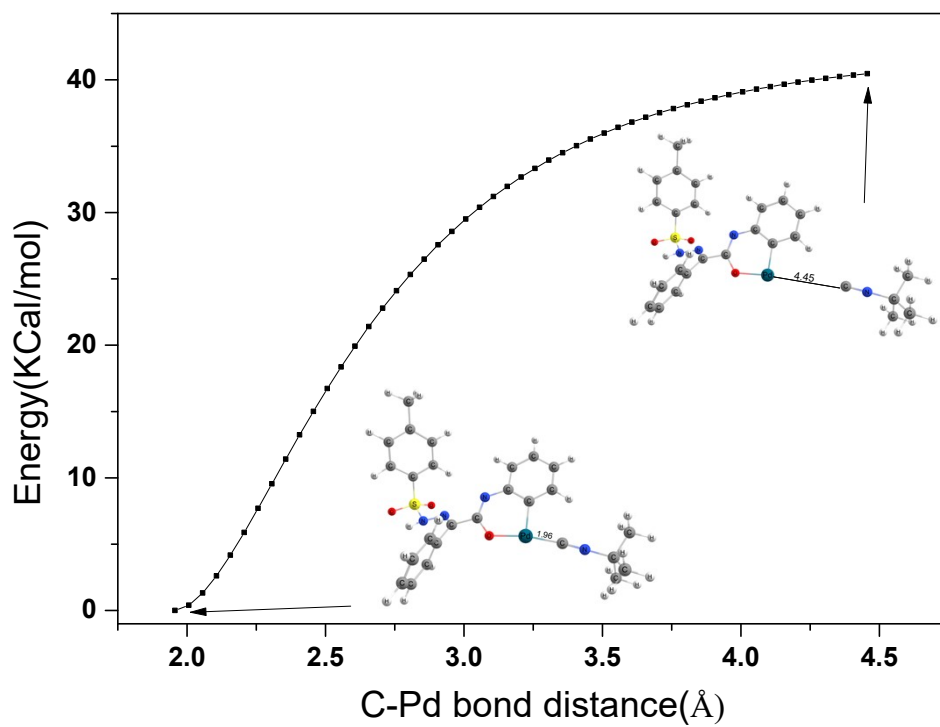


Figure S5: Relaxed potential energy surface for C-Pd bond formation

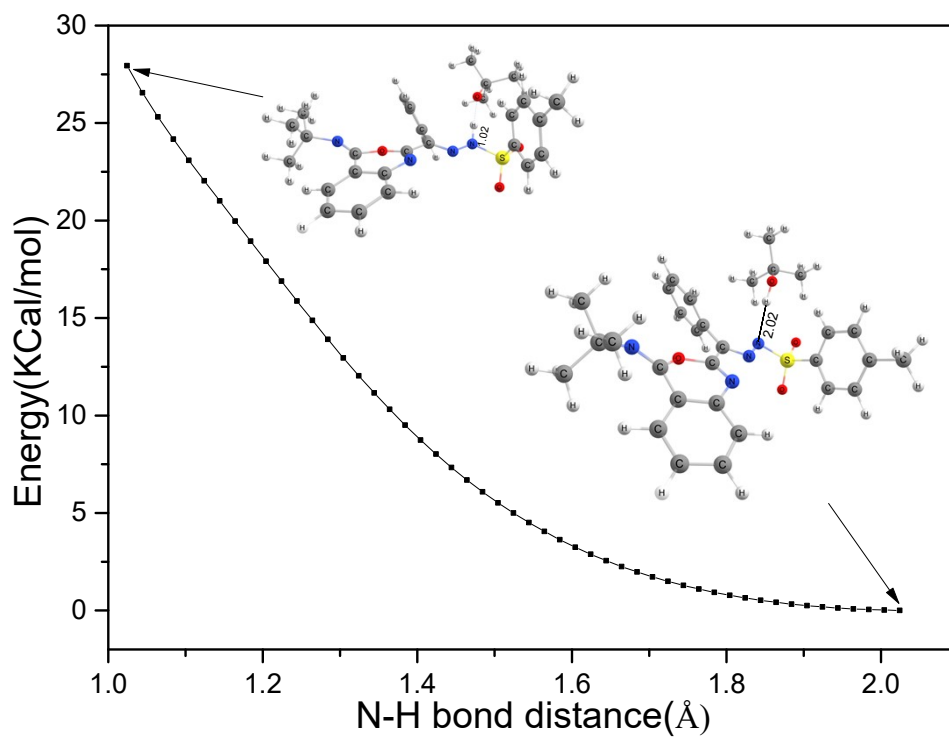


Figure S6: PES Scan for N-H proton abstraction from tosyl hydrazone in presence of base

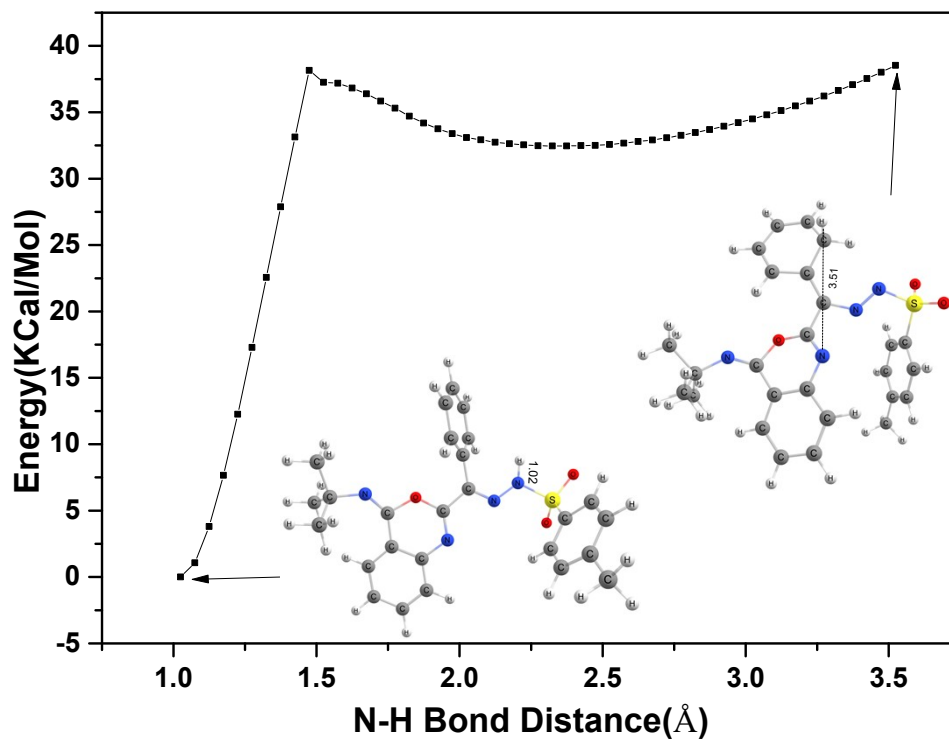


Figure S7: PES Scan for N-H proton abstraction from tosyl hydrazone in absence of base

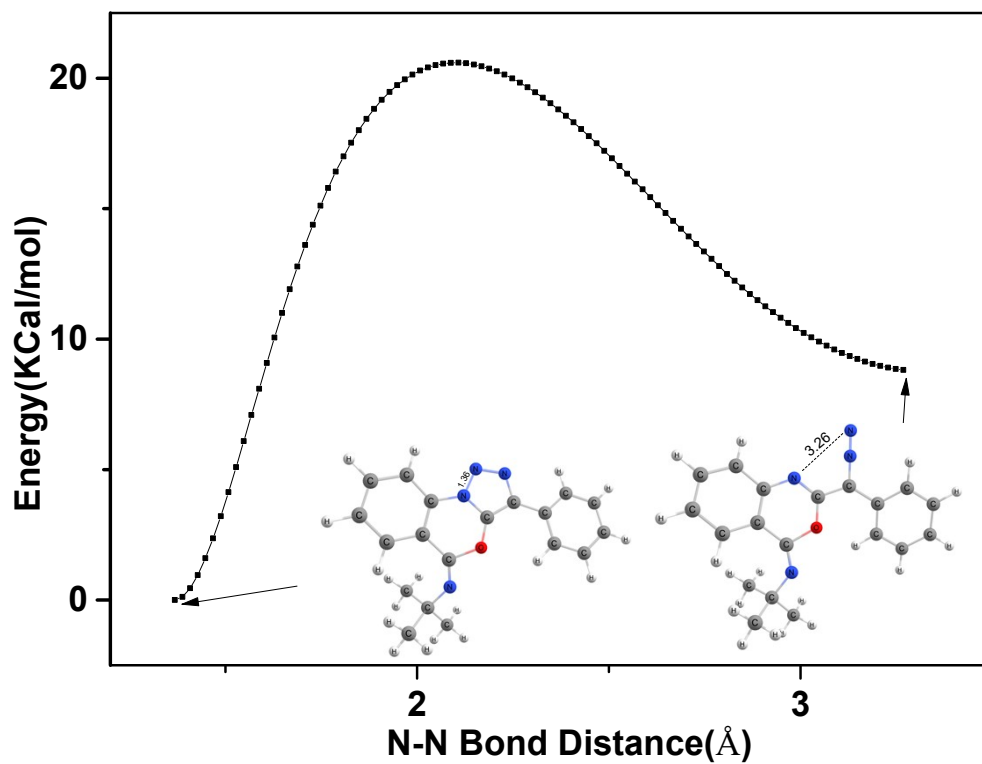


Figure S8: PES scan calculation for TS₁₁₋₁₂

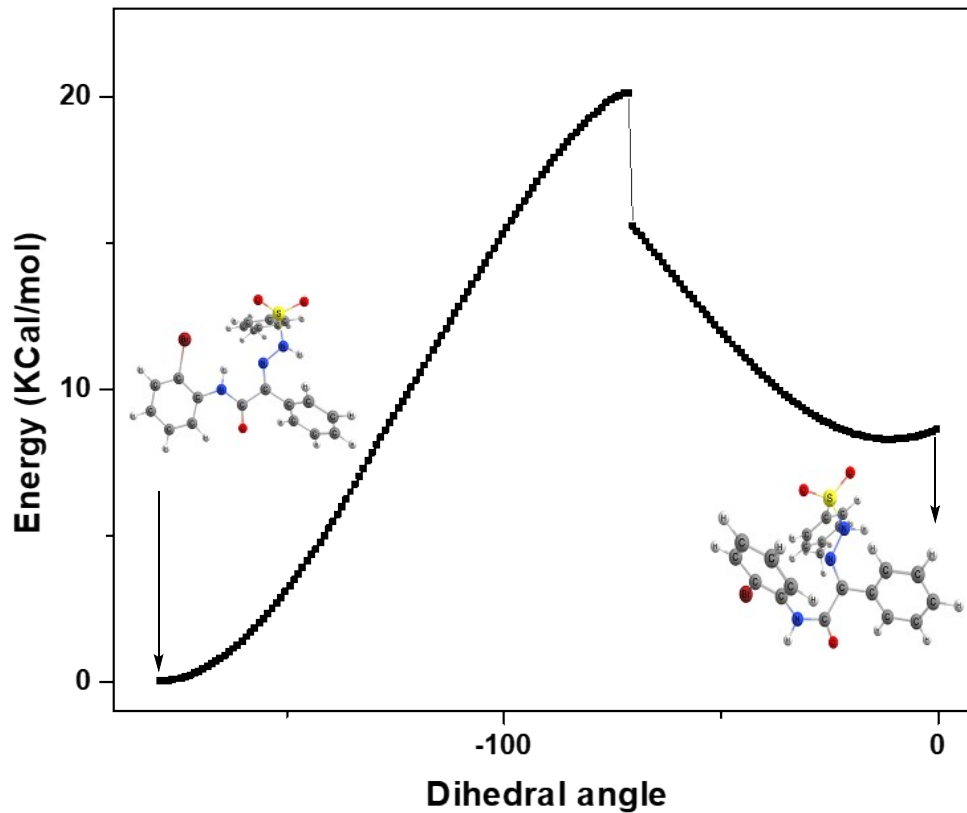


Figure S9: PES Scan for rotation along O-C-N-H dihedral

Characterization Data of compounds (1a-1h)

1a. Mixture of (*E*) & (*Z*)- *N*-(2-bromophenyl)-2-phenyl-2-(2-tosylhydrazono)acetamide

Solid (Trans: Cis=3:1), ¹H NMR (500 MHz, CDCl₃): δ 8.56 (d, *J* = 10.0 Hz, 1H), δ 8.41-8.39 (m, 2H), δ 8.18-8.16 (m, 1H), δ 7.86 (t, *J* = 10.0 Hz, 2H), δ 7.72-7.46 (m, 7H), δ 7.37-7.32 (m, 2H), δ 7.28 (d, *J* = 6.5 Hz, 2H), δ 2.43 (s, 1H), δ 2.36 (s, 3H) ppm.

1b. (*E*)-*N*-(2-bromo-4-chlorophenyl)-2-phenyl-2-(2-tosylhydrazono)acetamide

Solid, ¹H NMR (500 MHz, CDCl₃): δ 9.54 (s, 1H), δ 8.38 (d, 1H), δ 8.24 (s, 1H), δ 7.89 (d, *J* = 10.0 Hz, 2H), δ 7.59-7.52 (m, 4H), δ 7.37 (d, *J* = 10.0 Hz, 2H), δ 7.29-7.26 (m, 2H), δ 2.45 (s, 3H) ppm.

1c. (*E*)-*N*-(2-bromo-4-fluorophenyl)-2-phenyl-2-(2-tosylhydrazono)acetamide

Solid, ¹H NMR (500 MHz, CDCl₃): δ 8.33-8.30 (m, 1H), δ 8.00 (s, 1H), δ 7.87-7.85 (m, 2H), δ 7.55-7.45 (m, 5H), δ 7.31-7.26 (m, 2H), δ 7.11-7.07 (m, 1H), δ 2.41 (s, 3H) ppm.

1d. (*E*)-*N*-(2-bromo-4-methylphenyl)-2-phenyl-2-(2-tosylhydrazono)acetamide

Solid, ¹H NMR (500 MHz, CDCl₃): δ 8.19 (m, *J* = 8.5 Hz, 1H), δ 8.03 (s, 1H), δ 7.87 (d, *J* = 8.5, 2H), δ 7.56-7.54 (m, 2H), δ 7.47-7.44 (m, 3H), δ 7.31-7.29 (m, 3H), δ 7.15-7.13 (m, 1H), δ 2.41 (s, 3H), δ 2.30 (s, 3H) ppm.

1e. (*E*)-*N*-(2-bromo-4,6-dimethylphenyl)-2-phenyl-2-(2-tosylhydrazono)acetamide

Solid, ¹H NMR (500 MHz, CDCl₃): δ 8.50 (s, 1H), δ 8.18 (s, 1H), δ 7.86 (d, *J* = 8.5, 2H), δ 7.51-7.49 (m, 4H), δ 7.36 (d, *J* = 8.0 Hz, 2H), δ 7.30-7.26 (m, 3H), δ 7.00 (s, 1H), δ 2.46 (s, 3H), δ 2.29 (s, 3H), δ 2.22 (s, 3H) ppm.

1f. (*E*)-*N*-(2-bromo-5-(trifluoromethyl)phenyl)-2-phenyl-2-(2-tosylhydrazono)acetamide

Solid, ¹H NMR (500 MHz, CDCl₃): δ 9.70 (s, 1H), δ 8.78 (s, 1H), δ 8.27 (s, 1H), δ 7.89 (d, *J* = 8.0 Hz, 2H), δ 7.55-7.53 (m, 3H), δ 7.37 (d, *J* = 8.0 Hz, 2H), δ 7.28-7.26 (m, 2H), δ 7.25-7.23 (m, 1H), δ 2.45 (s, 3H) ppm.

1g. (*E*)-*N*-(2-iodophenyl)-2-phenyl-2-(2-tosylhydrazono)acetamide

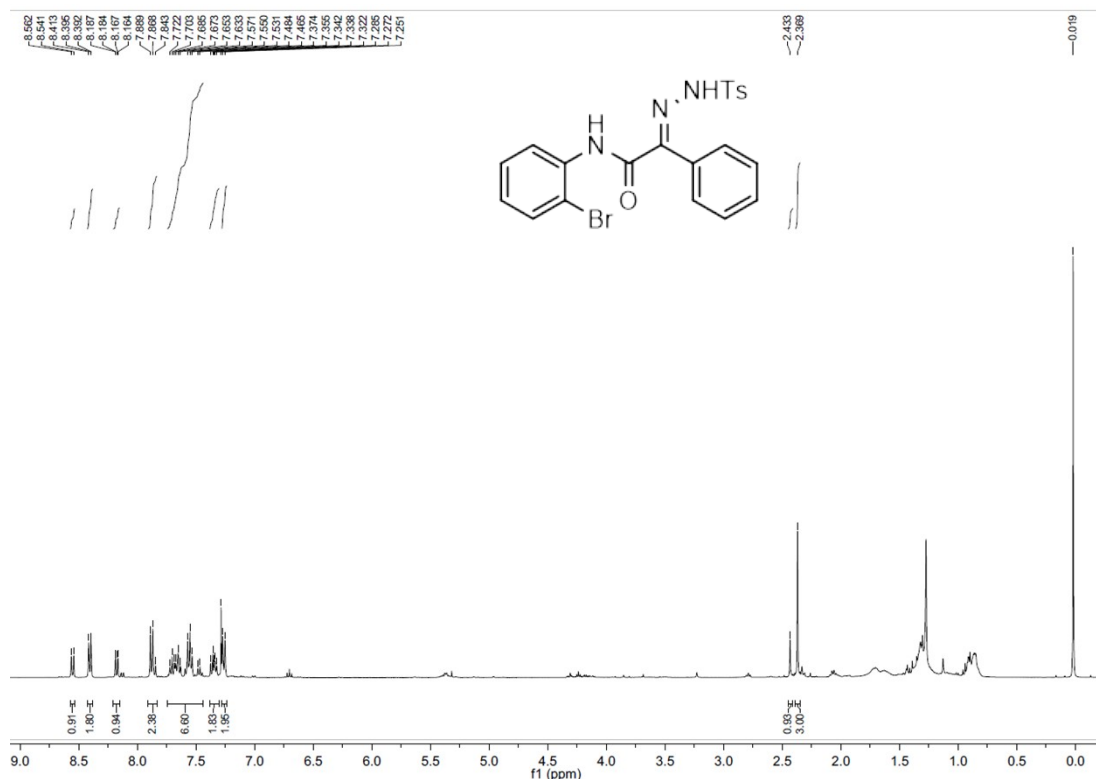
Solid, ¹H NMR (500 MHz, CDCl₃): δ 9.41 (s, 1H), δ 8.33-8.21 (m, 2H), δ 7.93-7.81 (m, 3H), δ 7.54-7.51 (m, 3H), δ 7.36-7.26 (m, 5H), δ 6.86-6.83 (m, 1H), δ 2.44 (s, 3H) ppm.

1h. Mixture of (*Z*) & (*E*)-*N*,2-diphenyl-2-(2-tosylhydrazono)acetamide

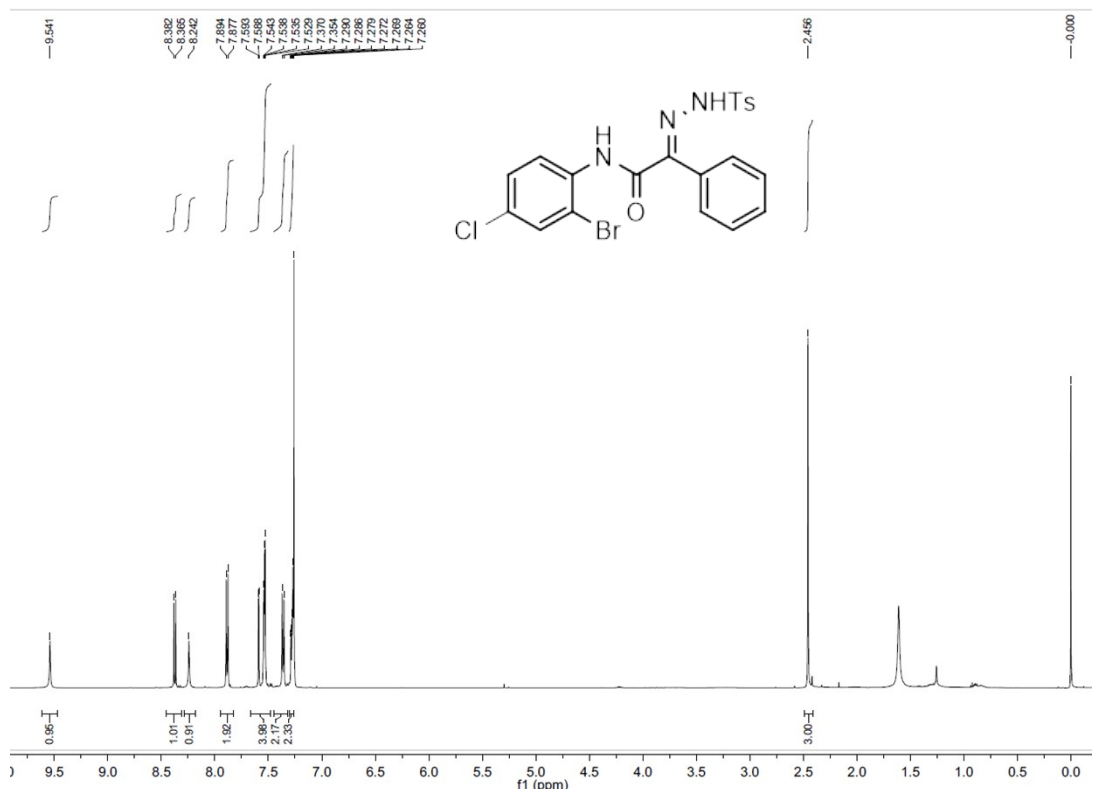
Solid (Trans: Cis = 1.5:1), ¹H NMR (500 MHz, CDCl₃): δ 8.83 (s, 1H), δ 8.15 (s, 1H), δ 7.86-7.81 (m, 3H), δ 7.59-7.50 (m, 6H), δ 7.44-7.43 (m, 2H), δ 7.38-7.28 (m, 6H), δ 7.24-7.13 (m, 3H), δ 2.45 (s, 3H), δ 2.40 (s, 2H) ppm.

Copies of ¹H NMR spectra of compounds (1a-1h)

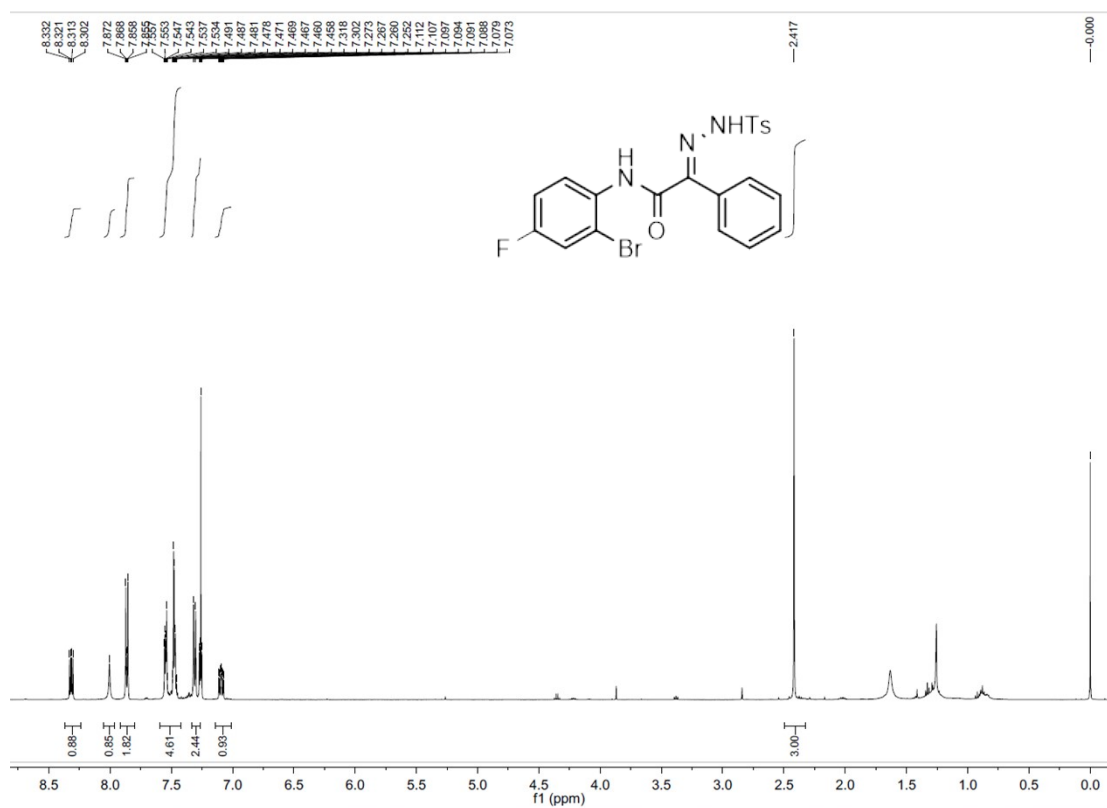
¹H NMR spectra of 1a



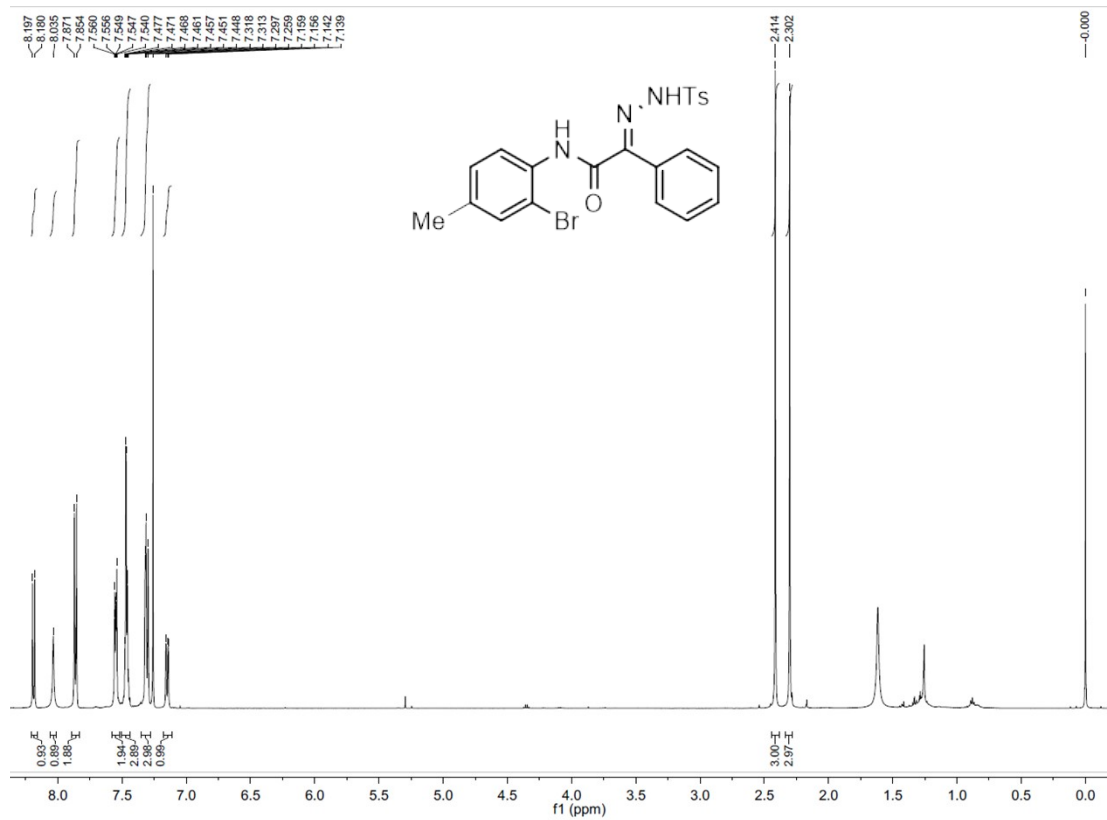
¹H NMR spectra of 1b



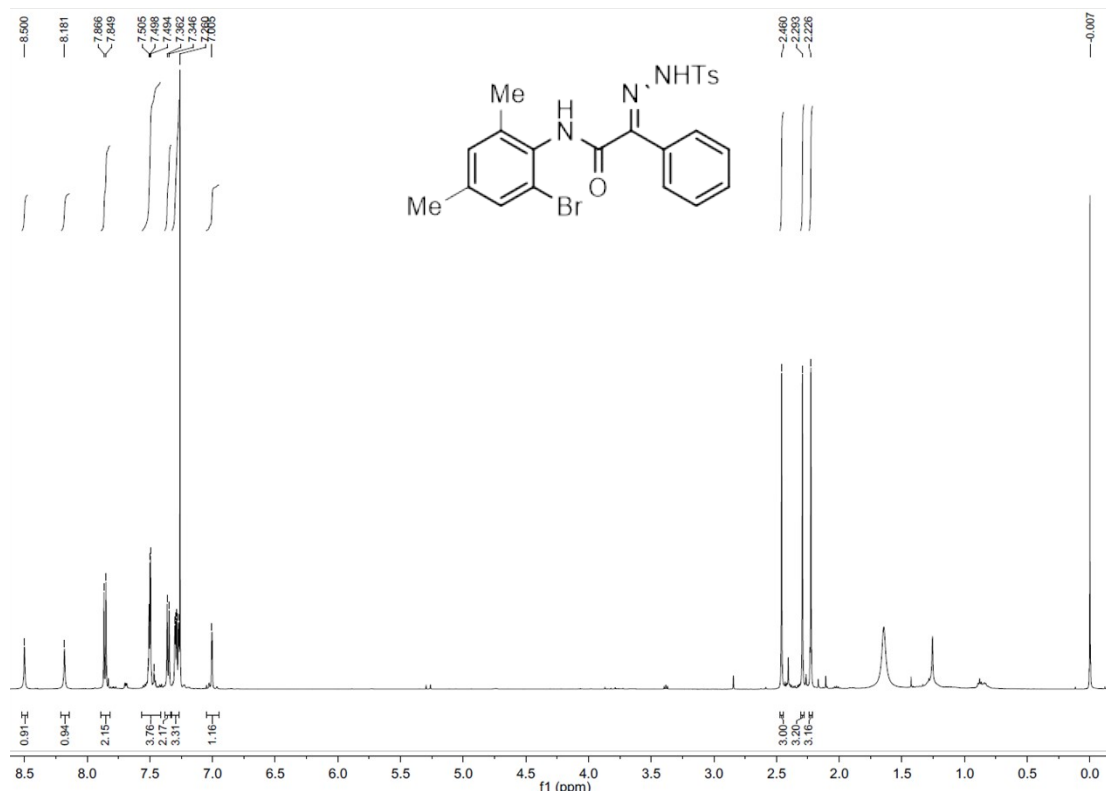
¹H NMR spectra of 1c



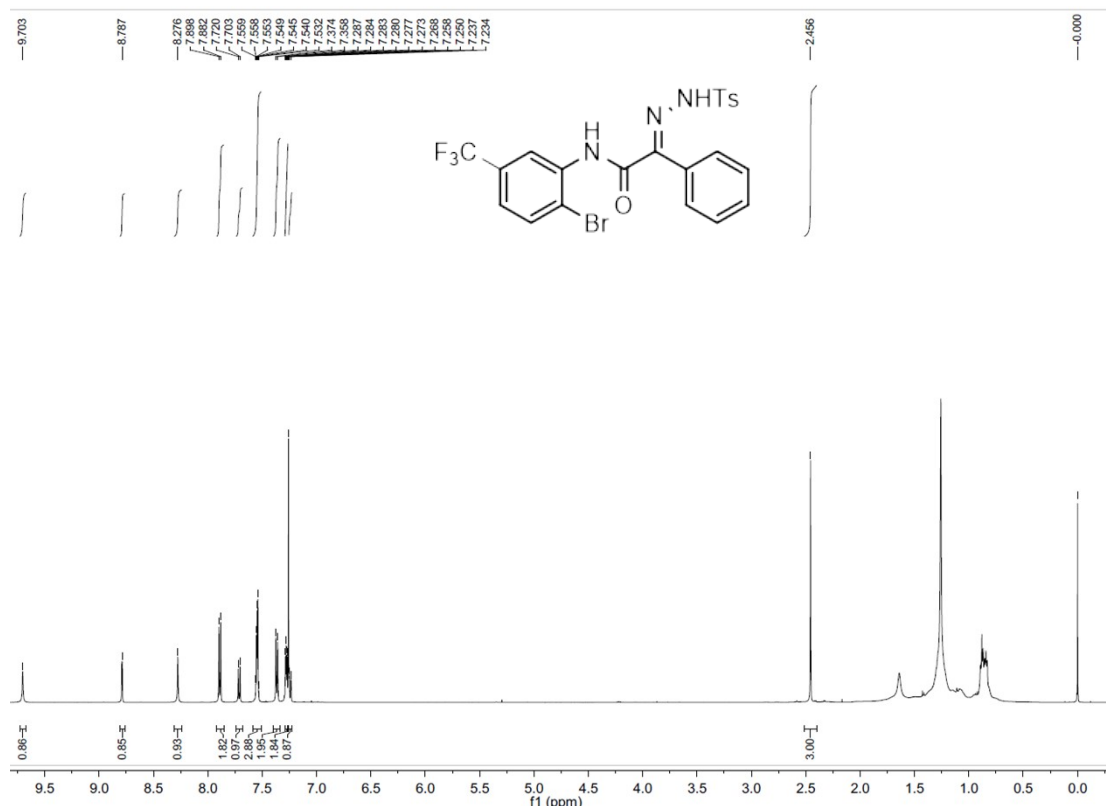
¹H NMR spectra of 1d



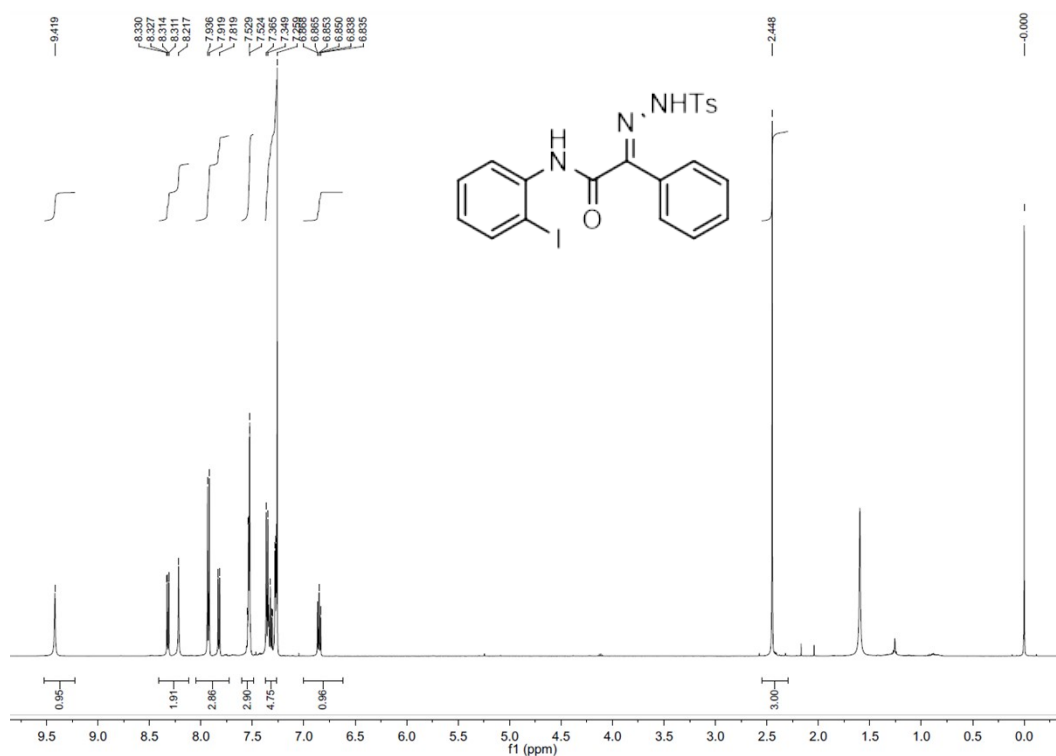
¹H NMR spectra of 1e



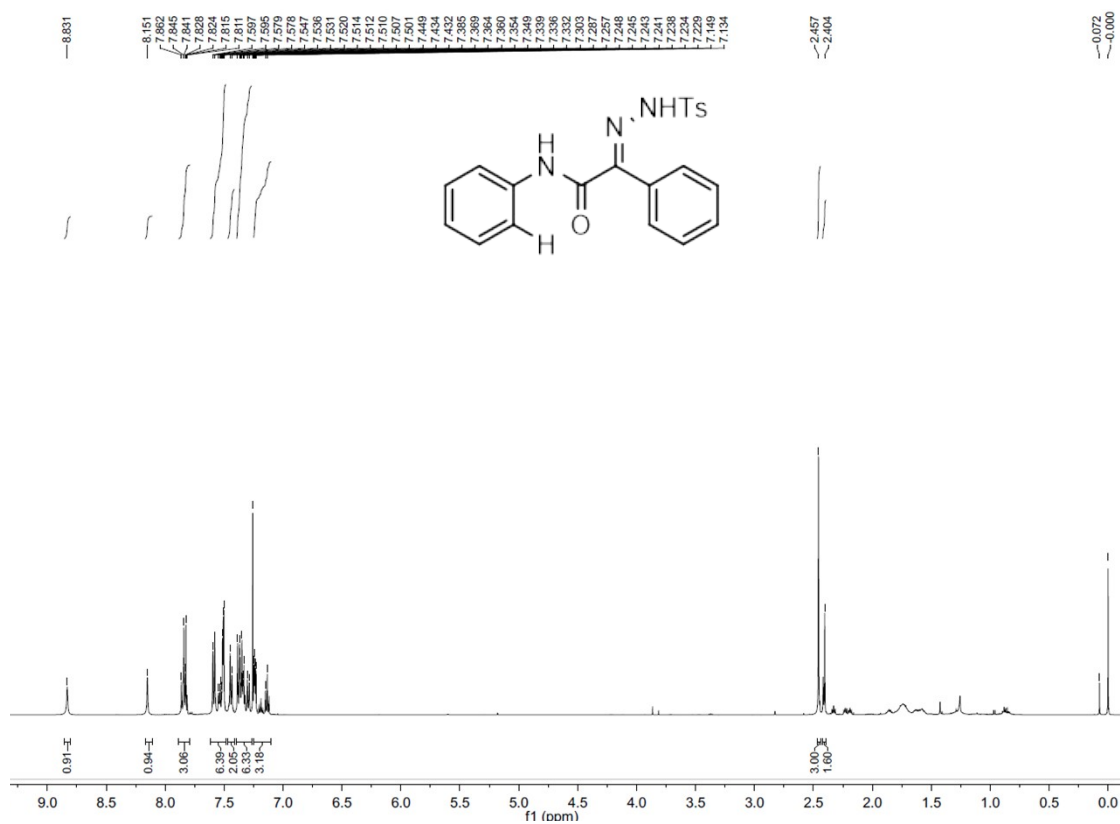
¹H NMR spectra of 1f



¹H NMR spectra of 1g

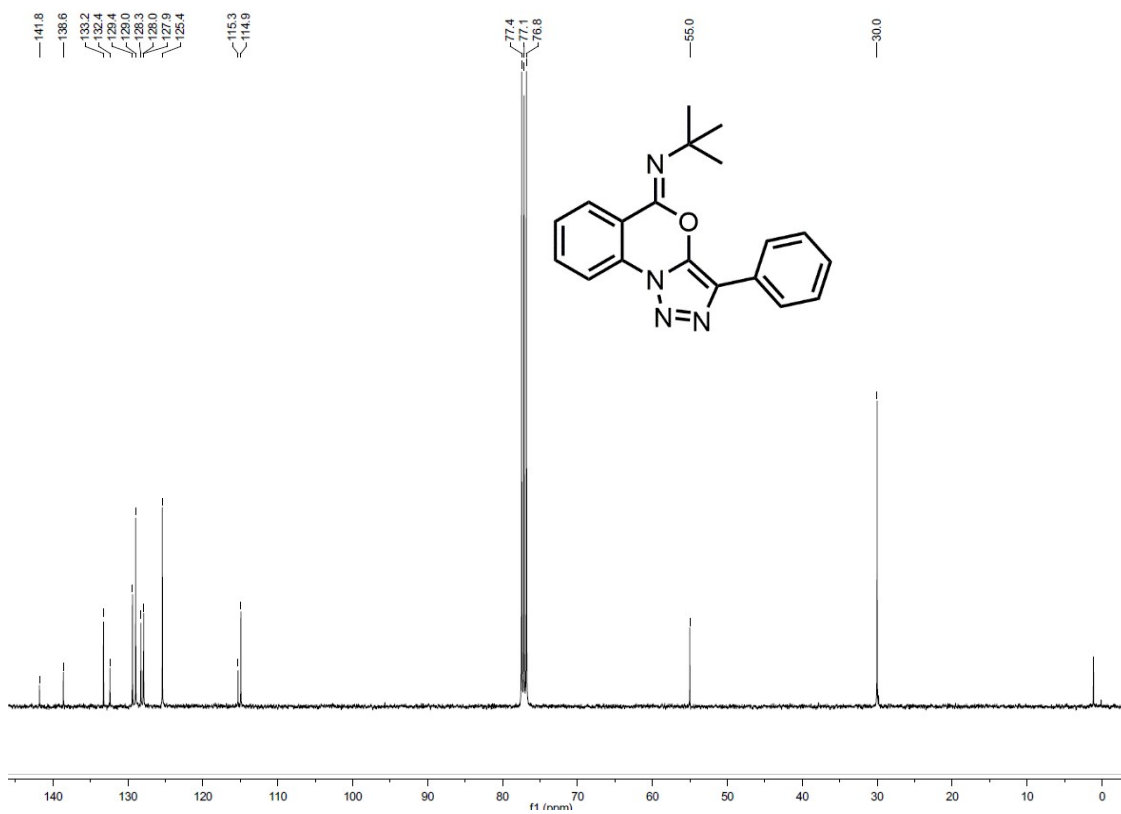
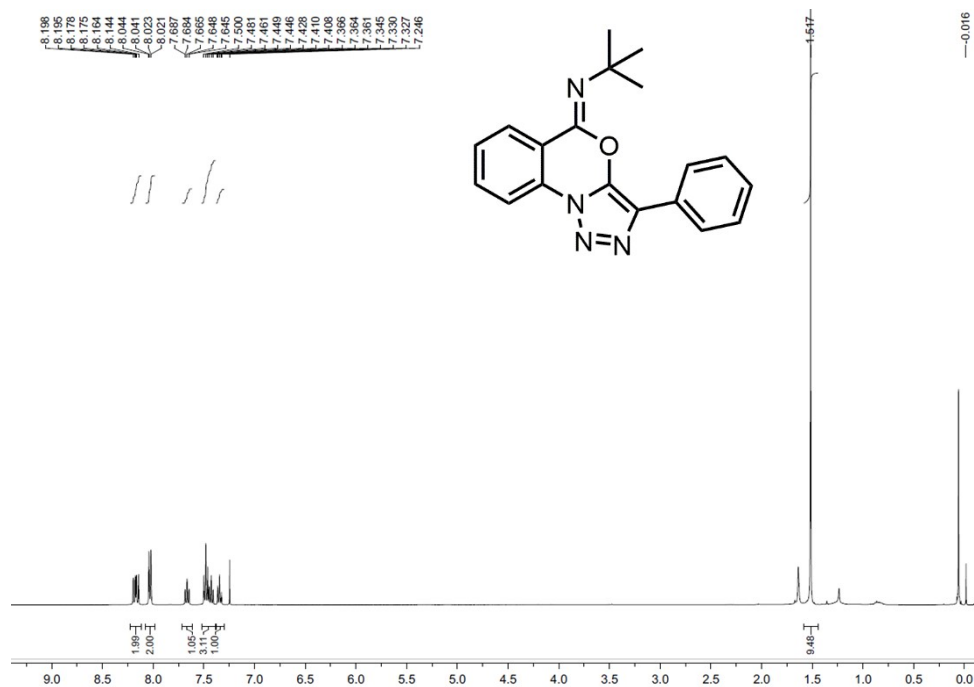


¹H NMR spectra of 1h

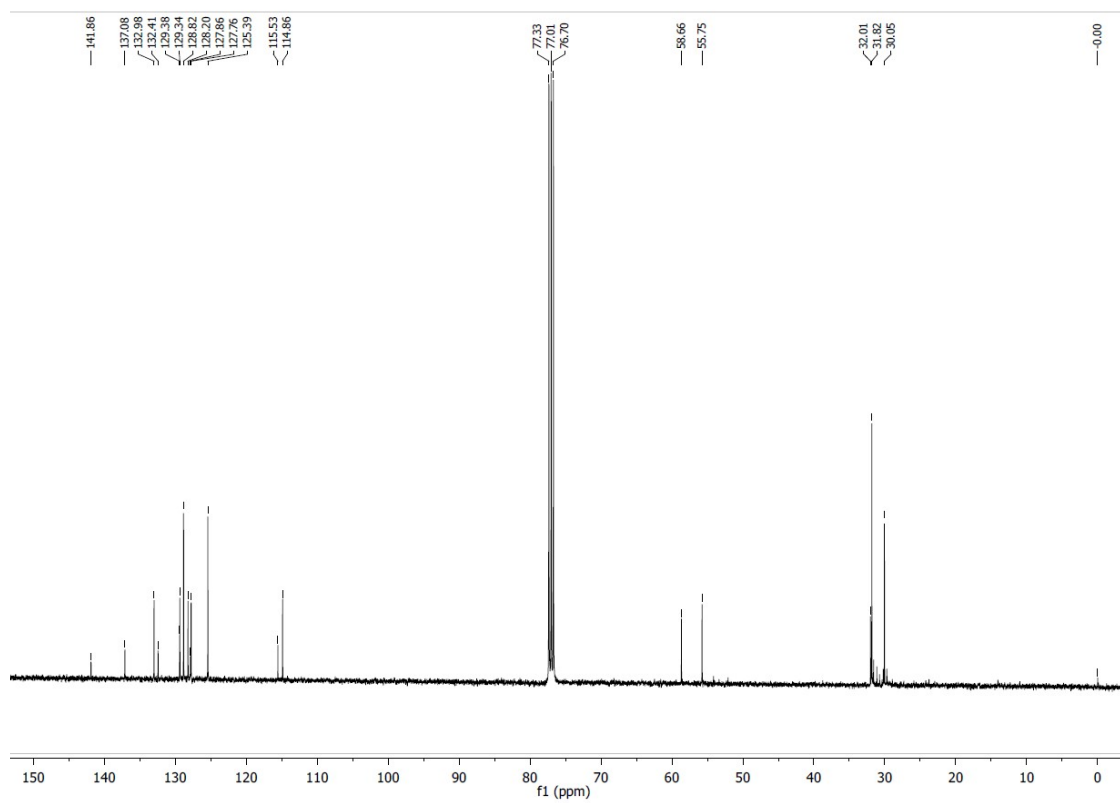
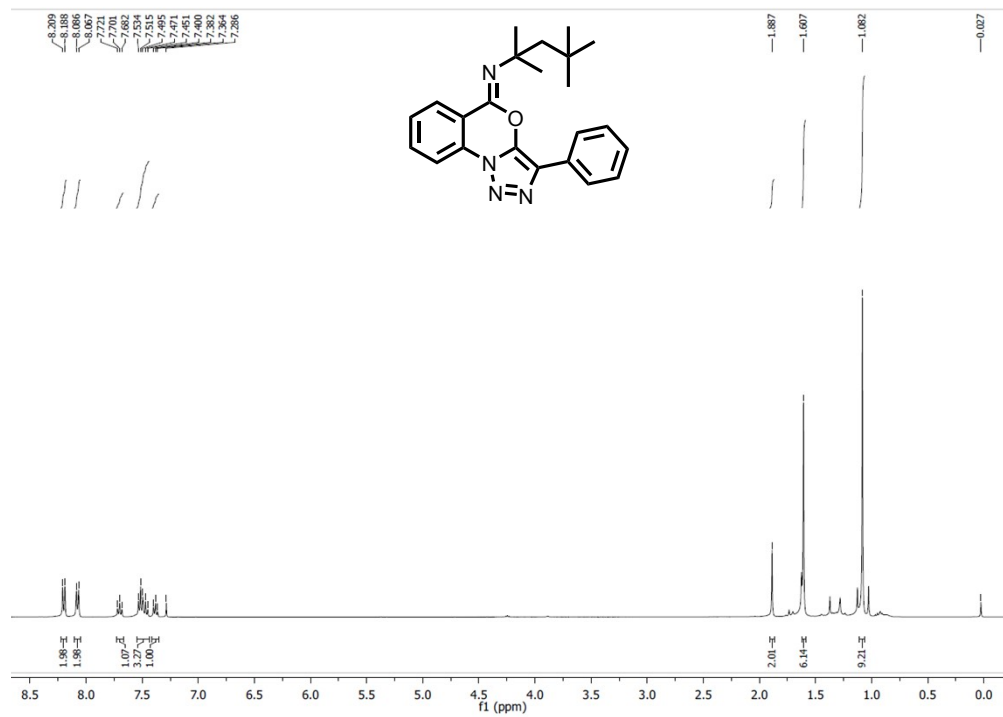


Copy of NMR spectra of synthesized compounds (3a-3m)

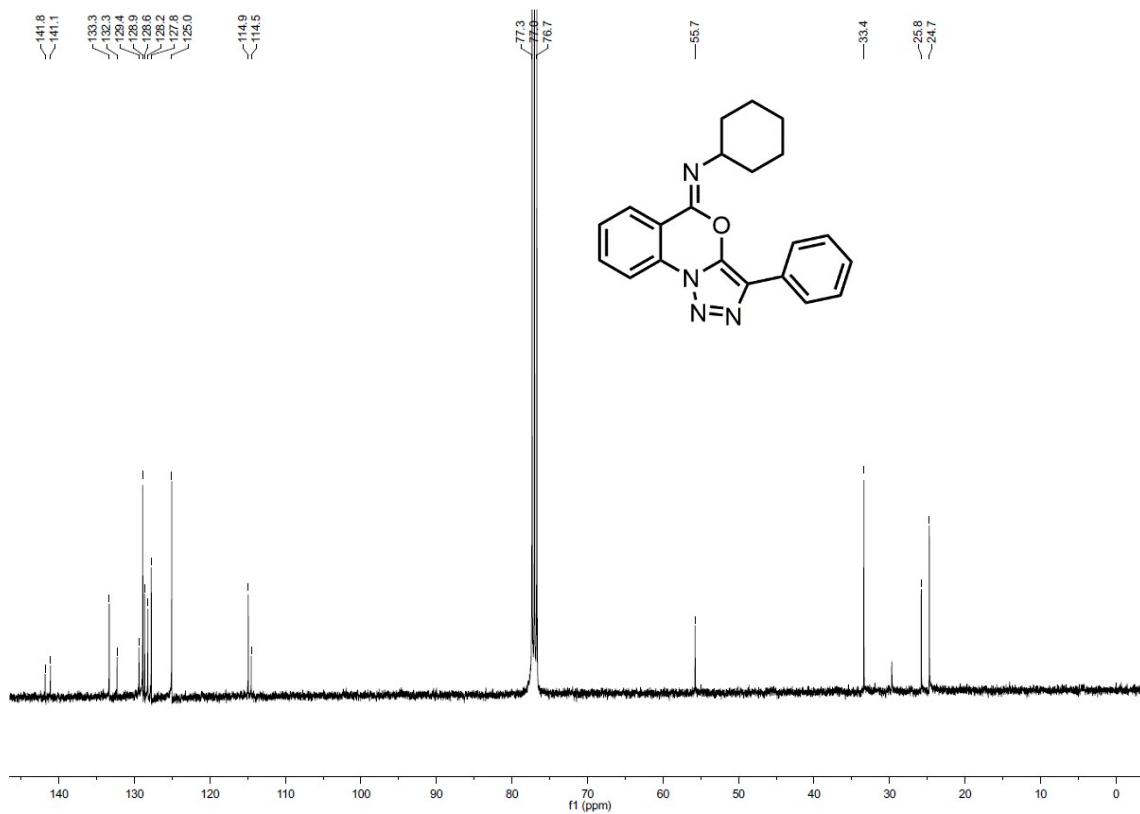
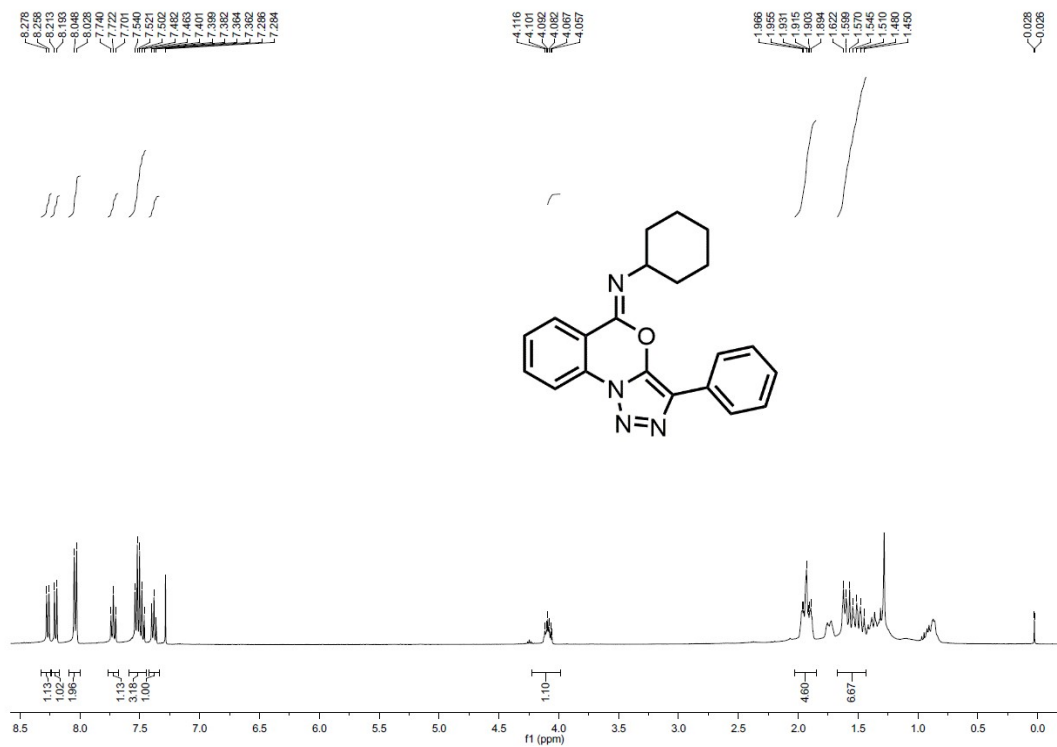
¹H NMR and ¹³C NMR spectra of 3a



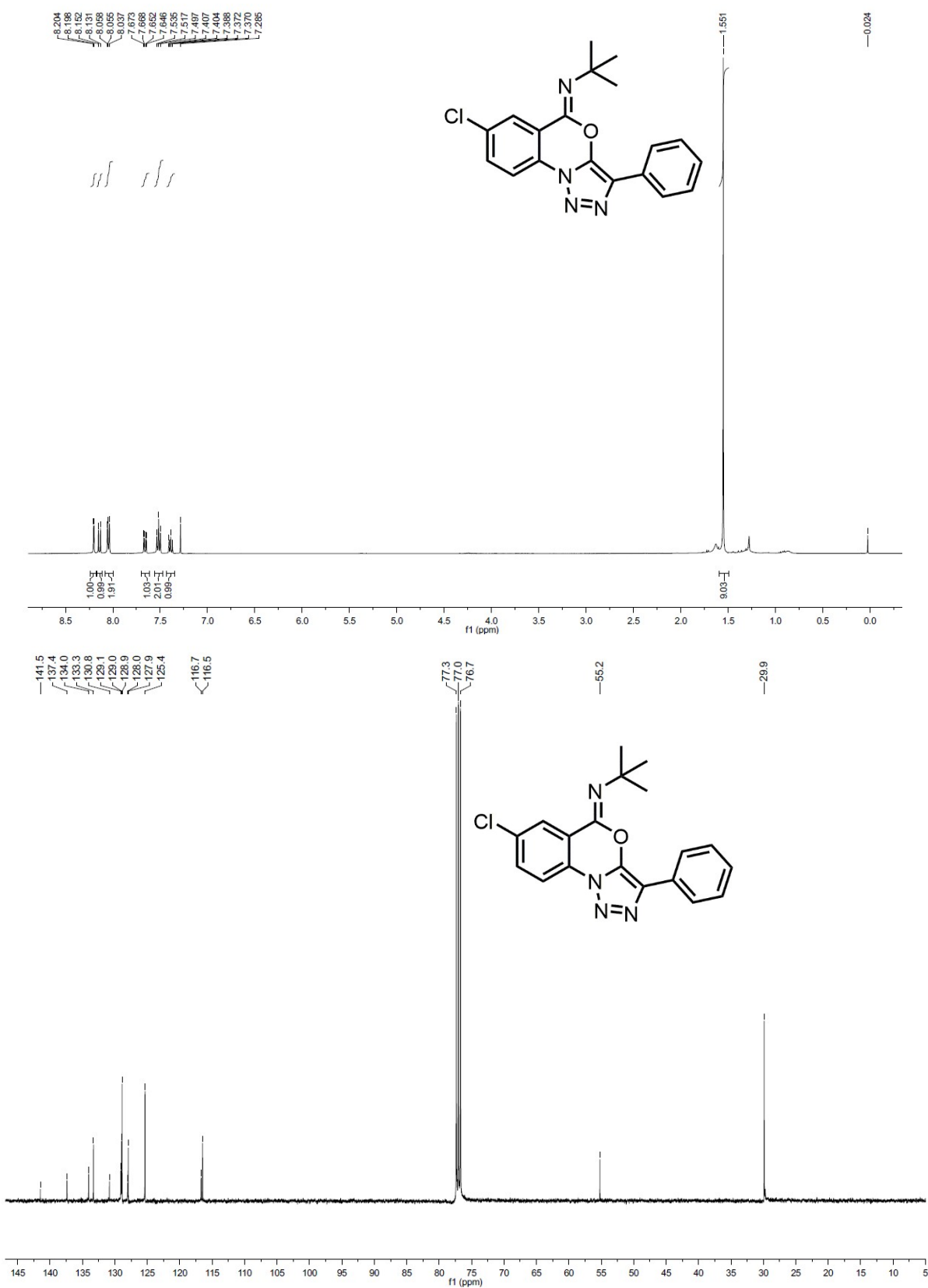
¹H NMR and ¹³C NMR spectra of 3b



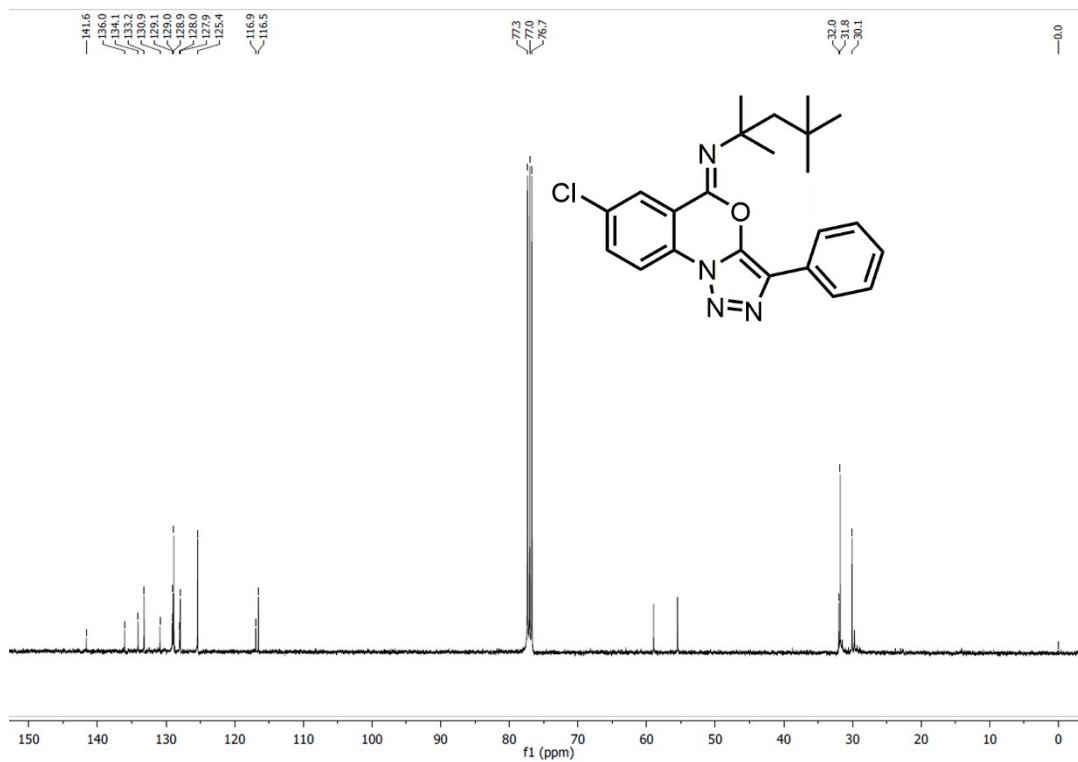
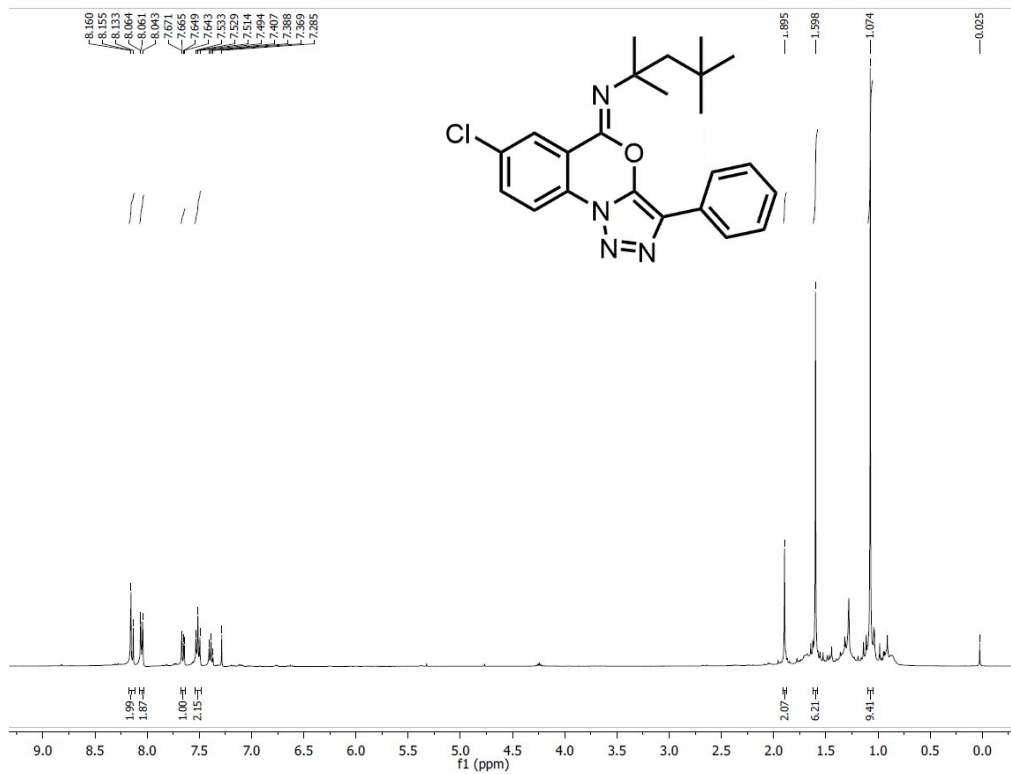
¹H NMR and ¹³C NMR spectra of 3c



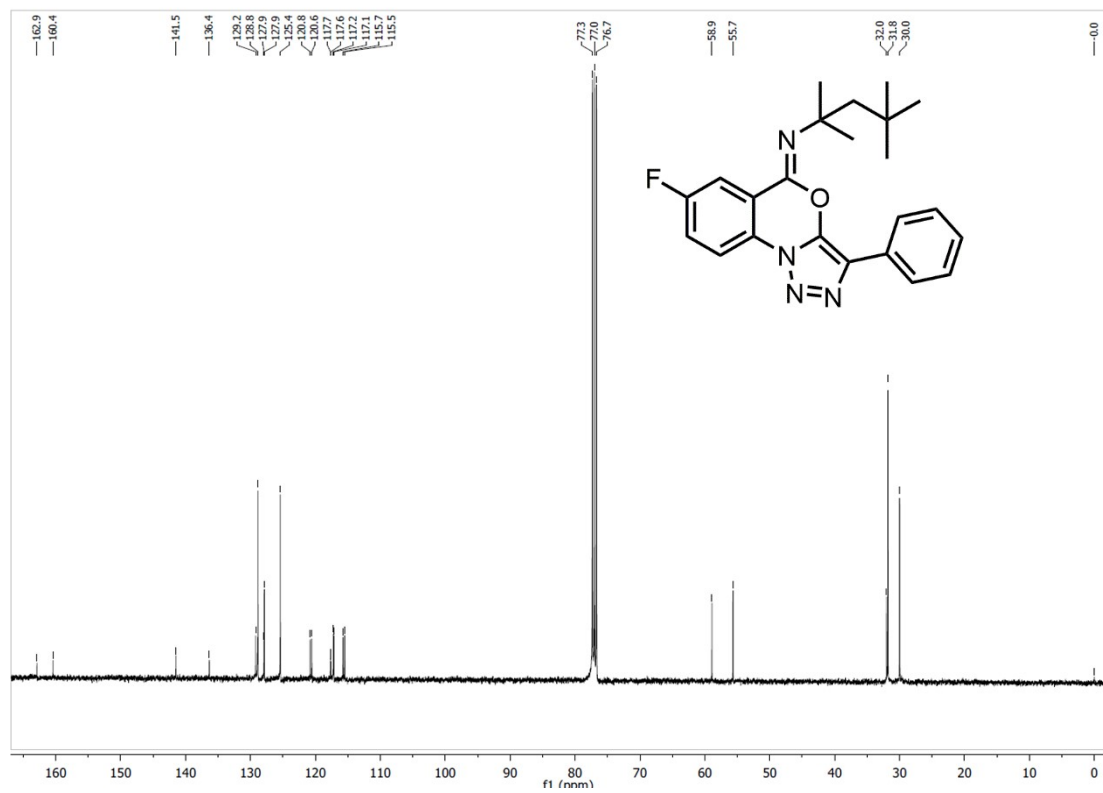
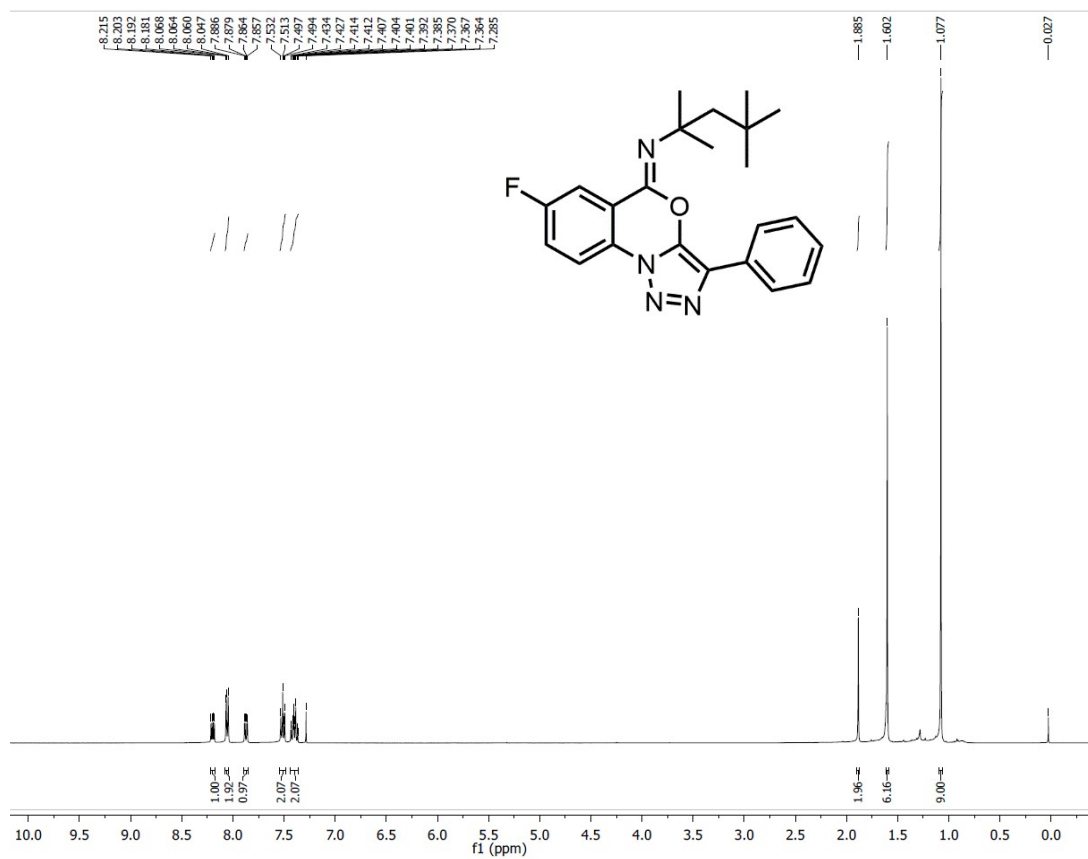
¹H NMR and ¹³C NMR spectra of 3d



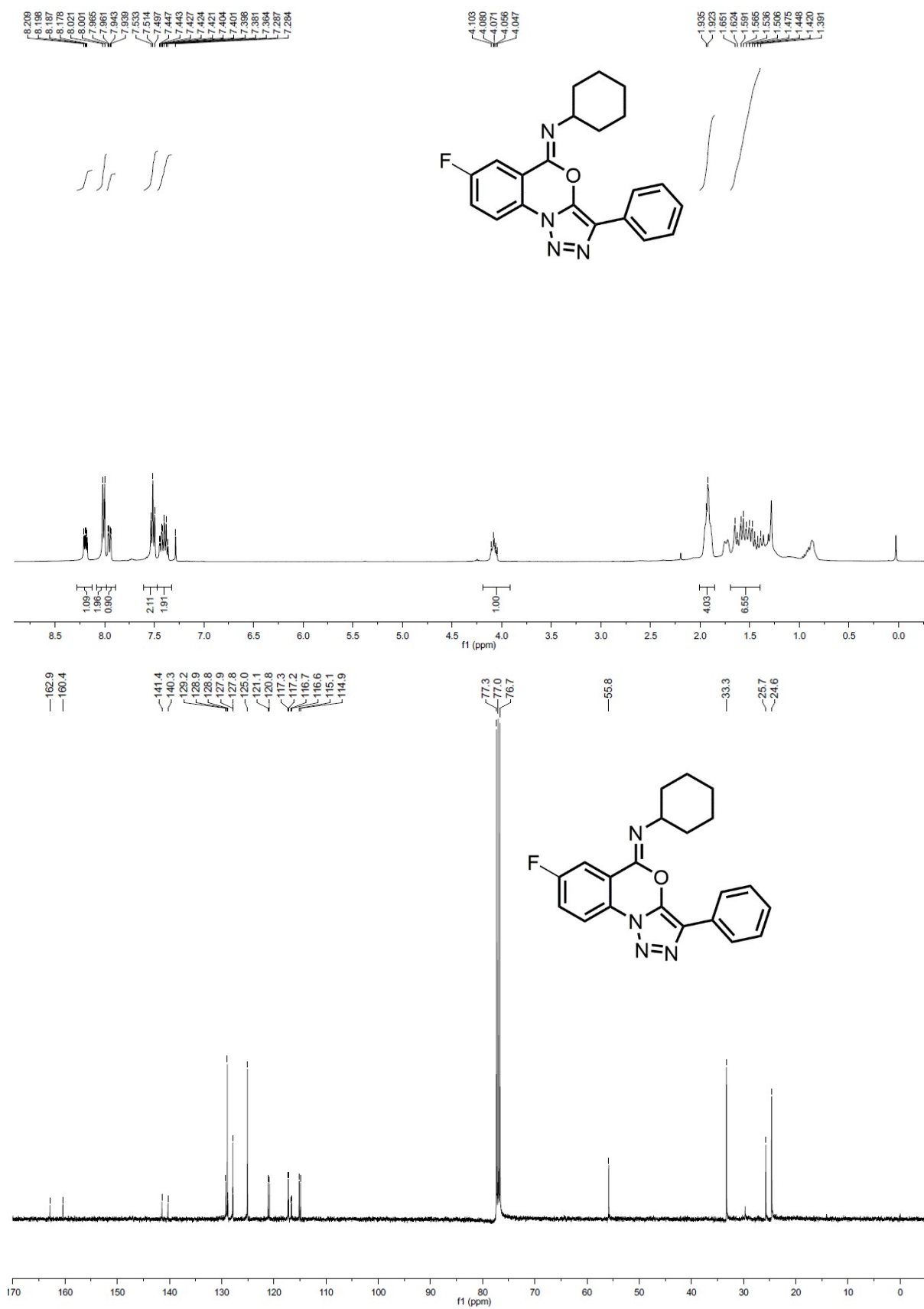
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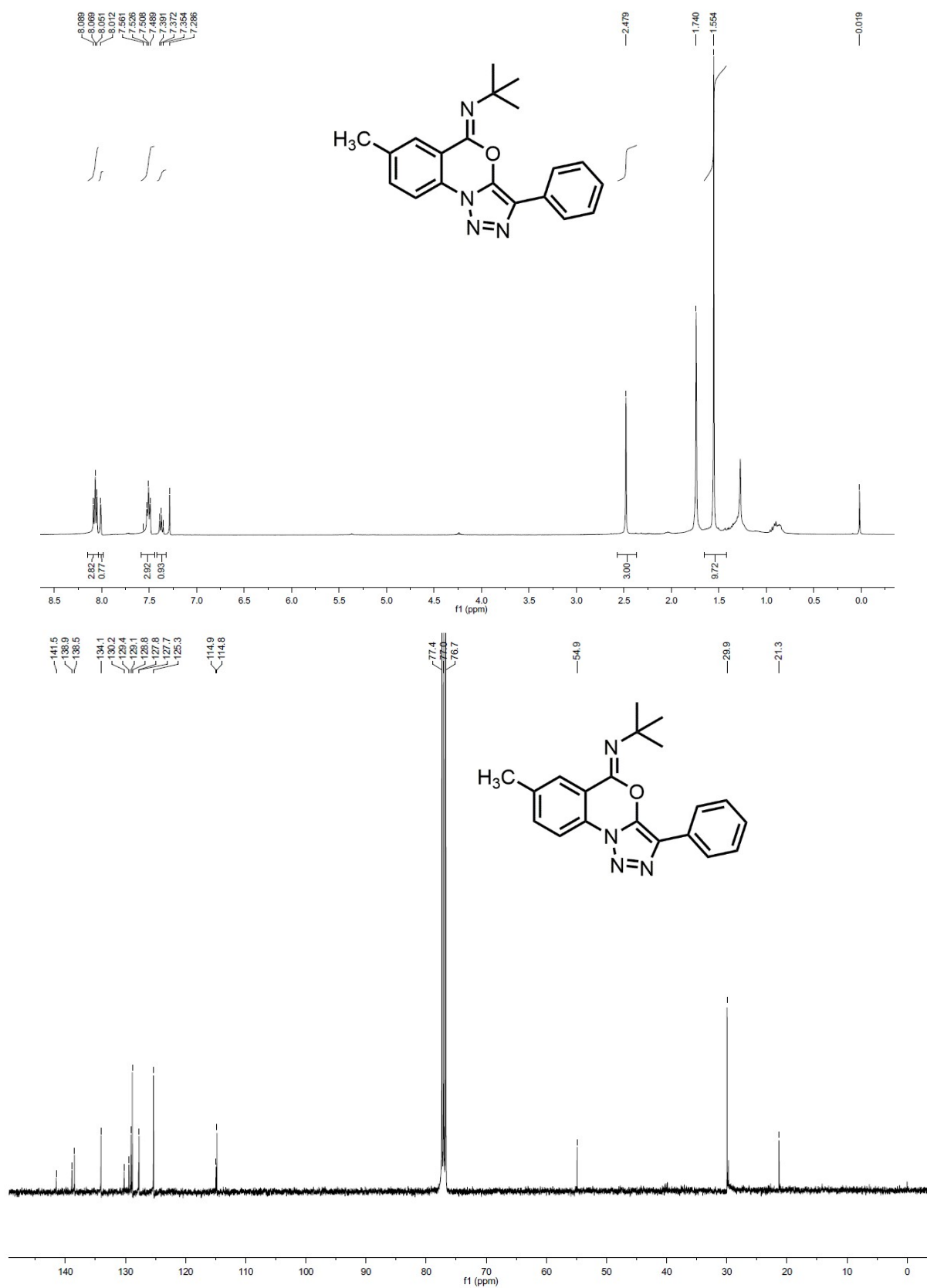
¹H NMR and ¹³C NMR spectra of 3f



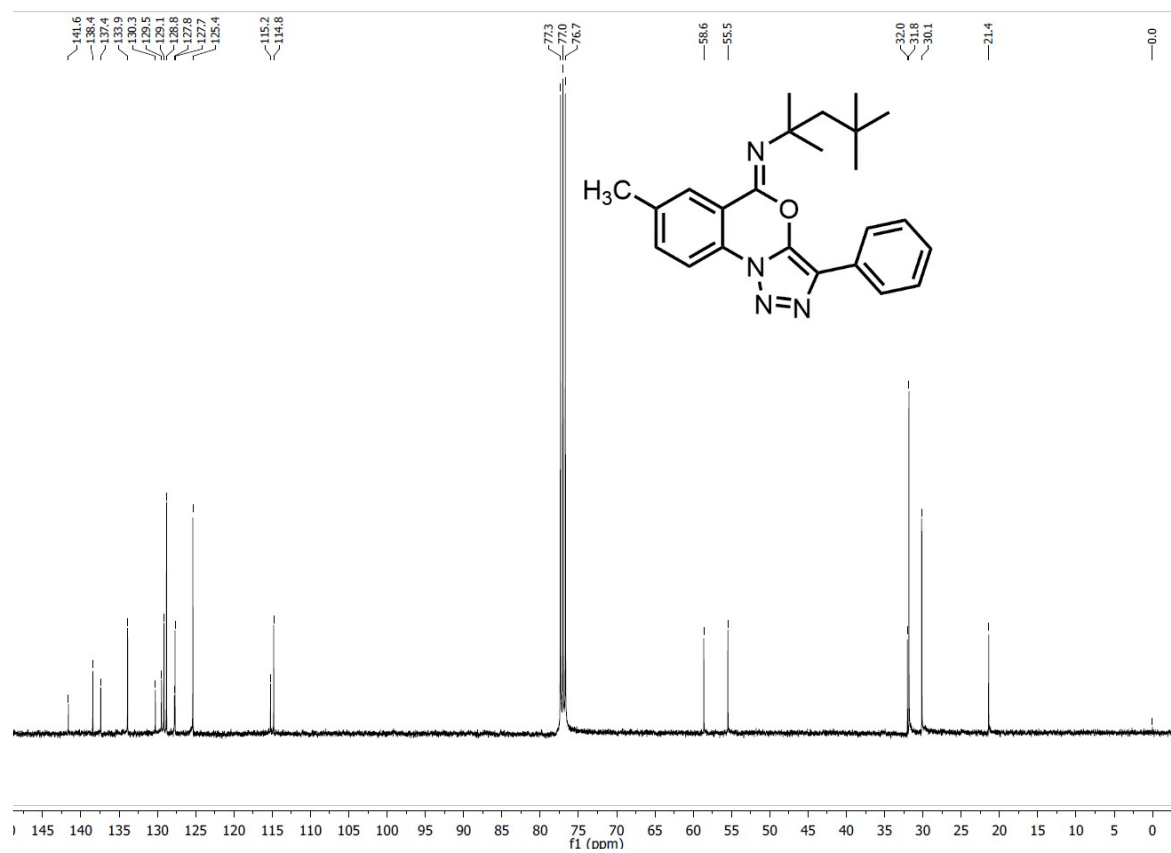
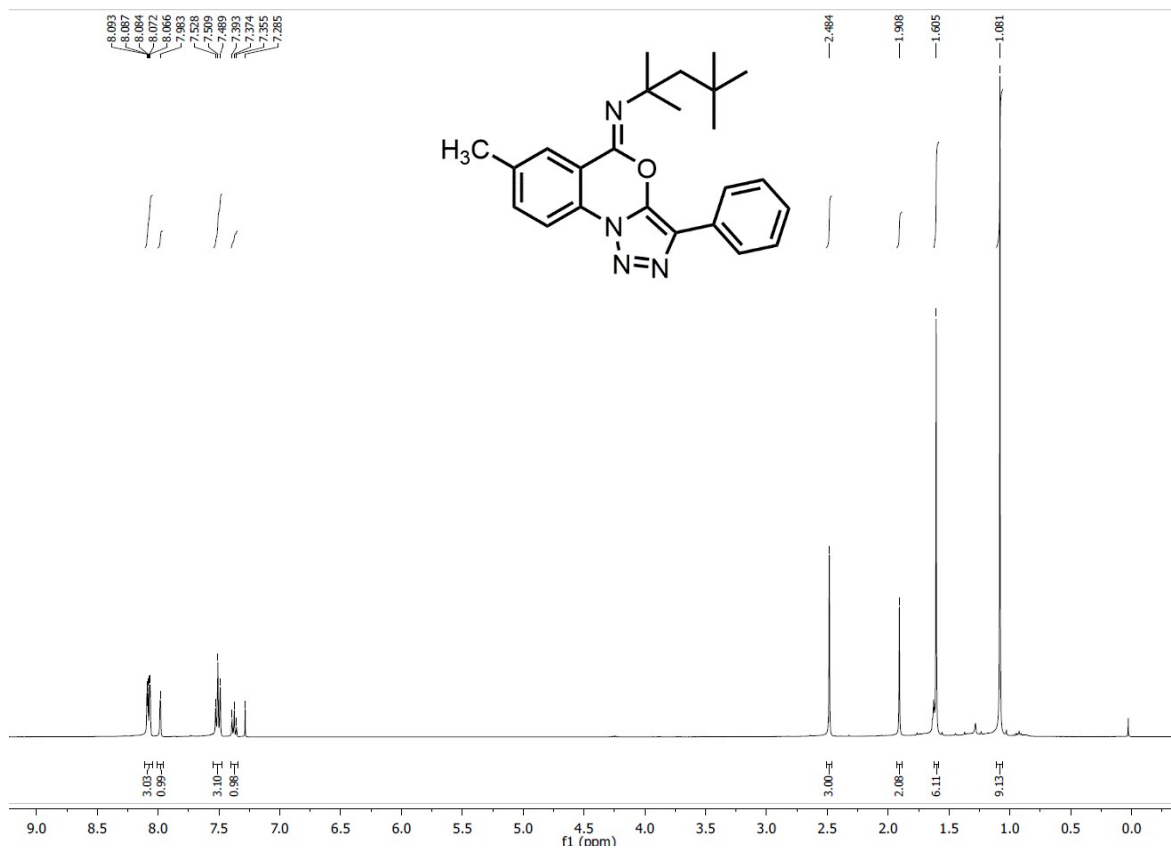
¹H and ¹³C NMR spectra of 3g



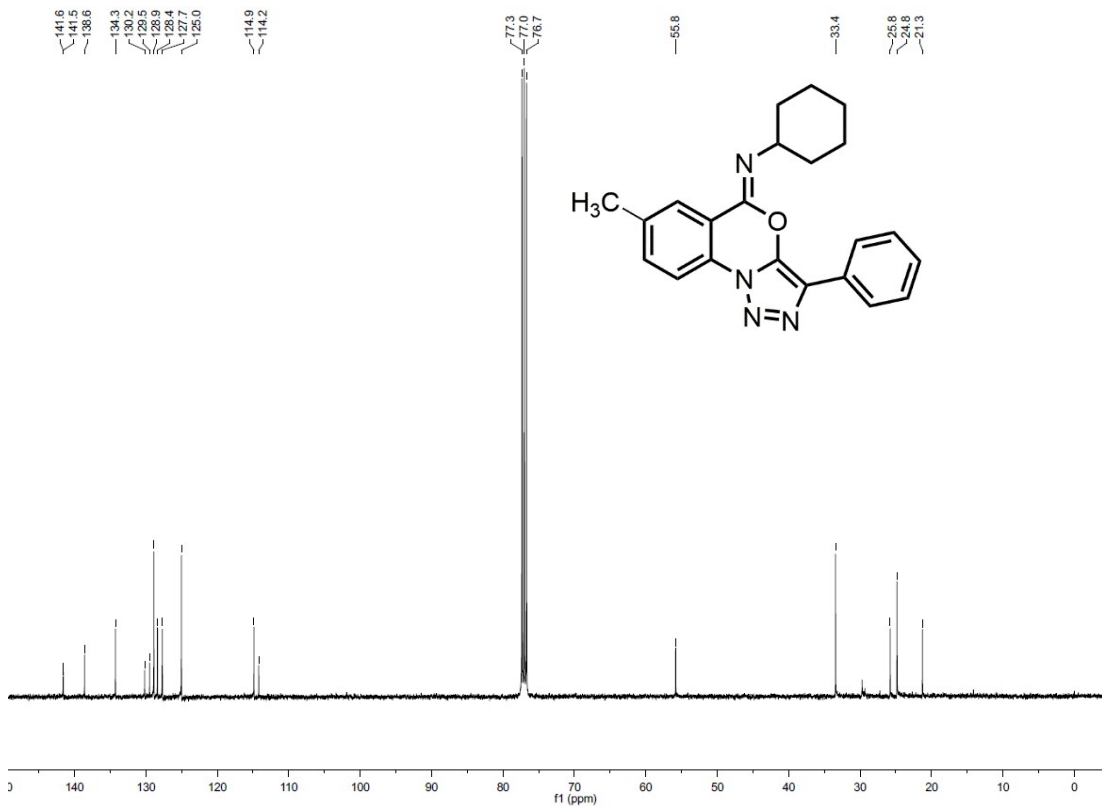
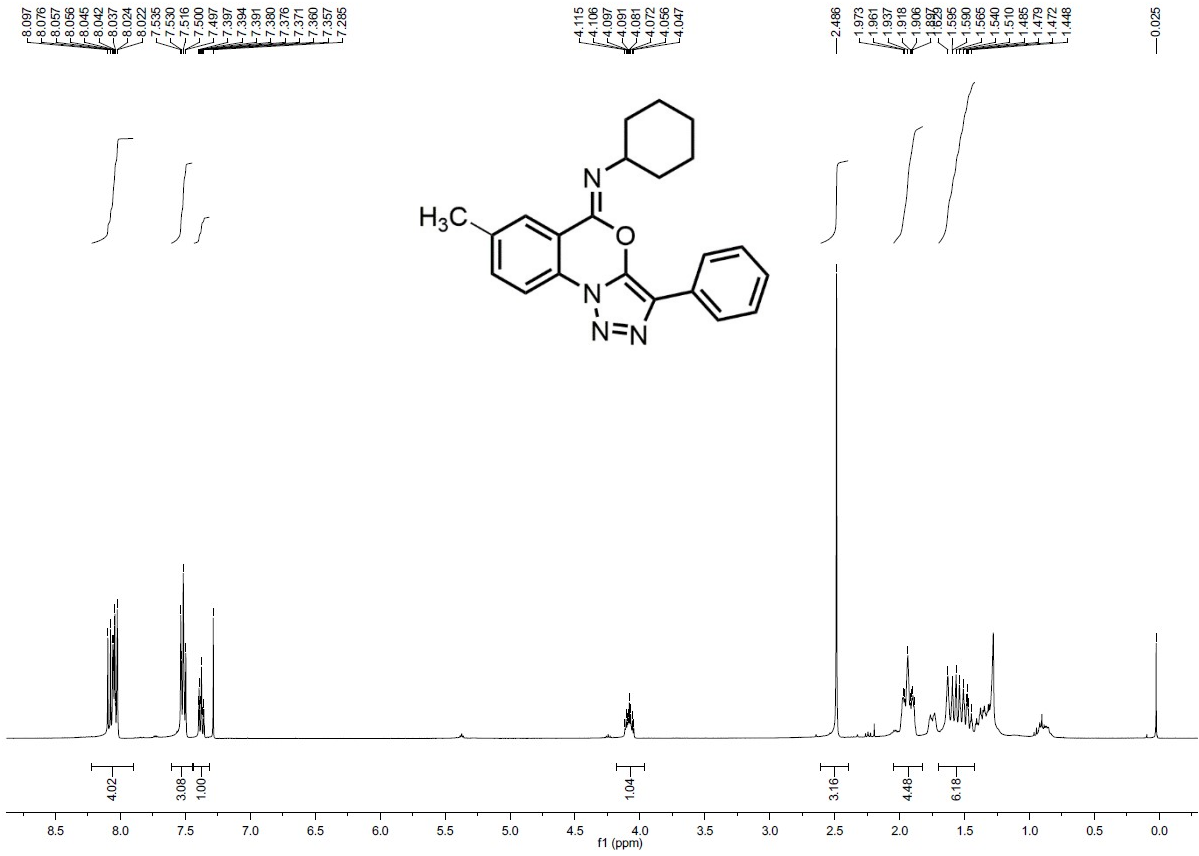
^1H and ^{13}C NMR spectra of 3h



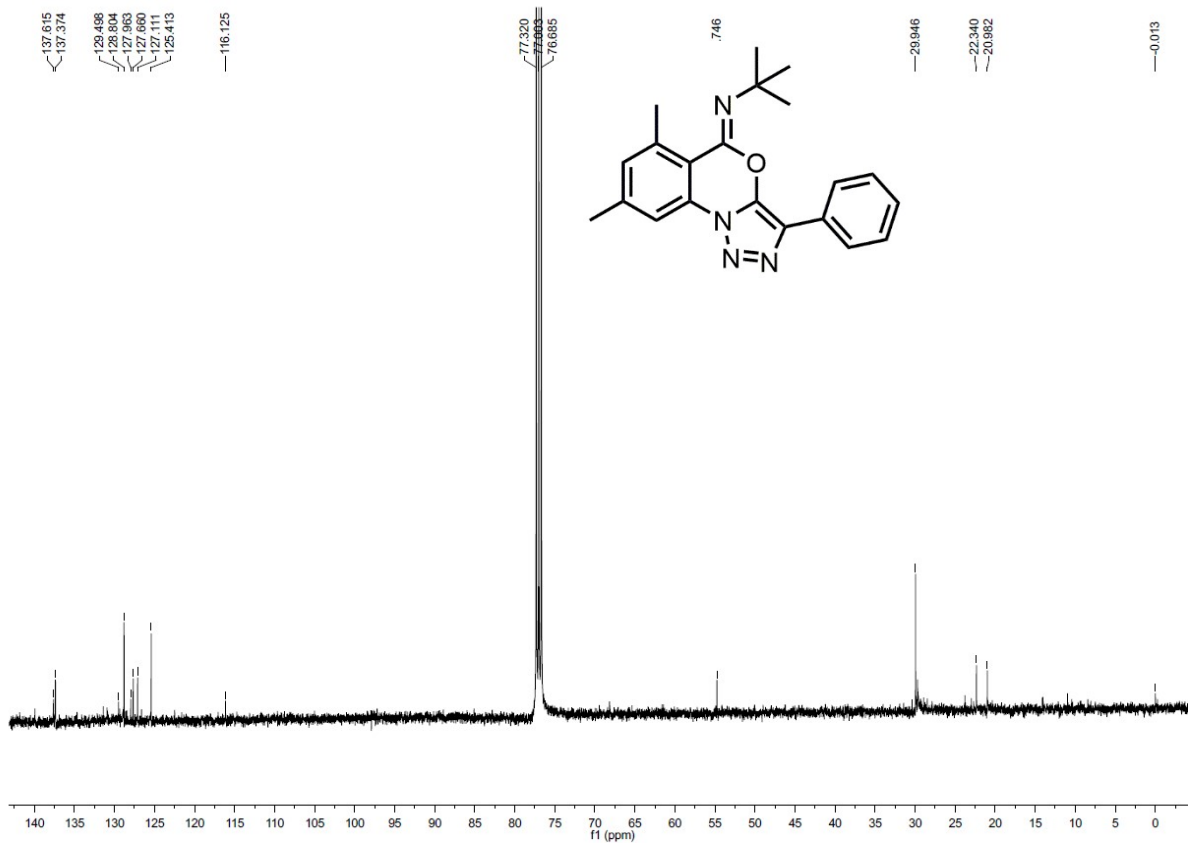
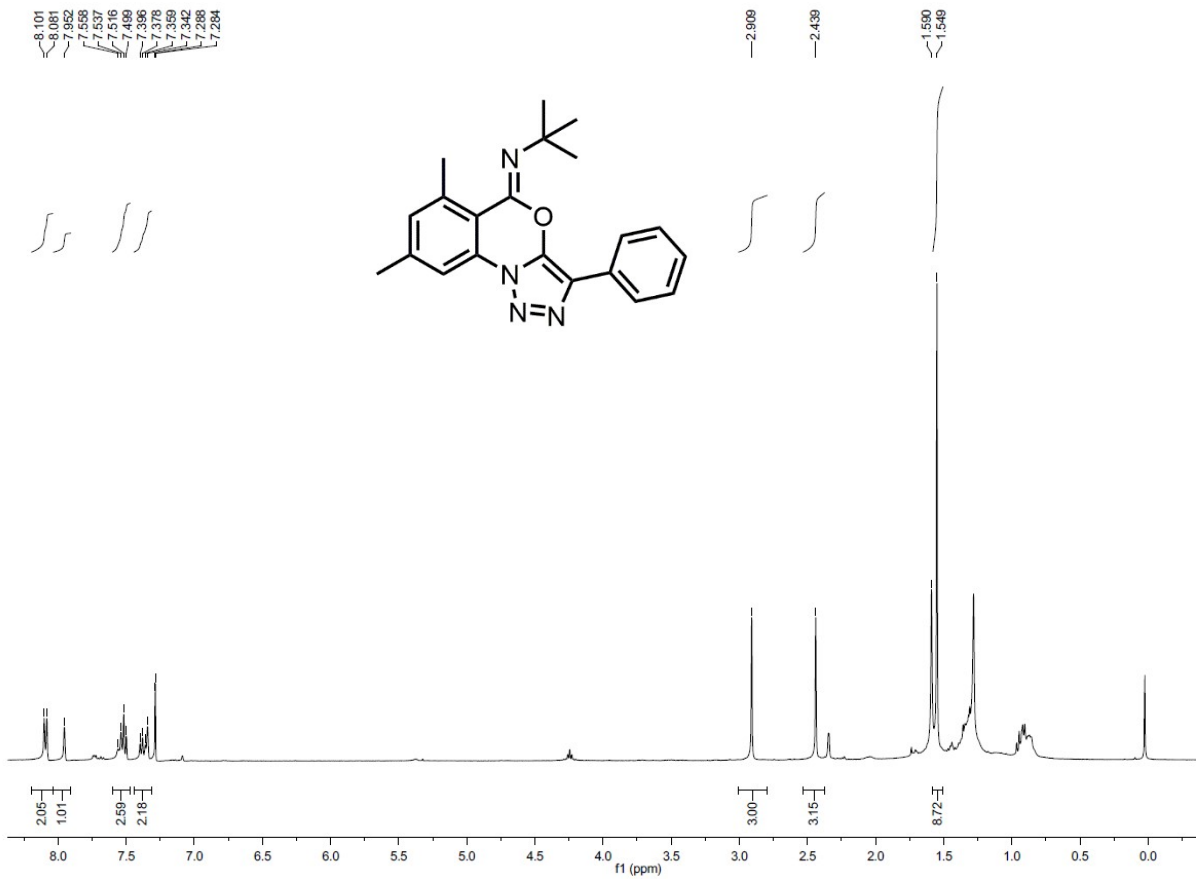
^1H and ^{13}C NMR spectra of 3i



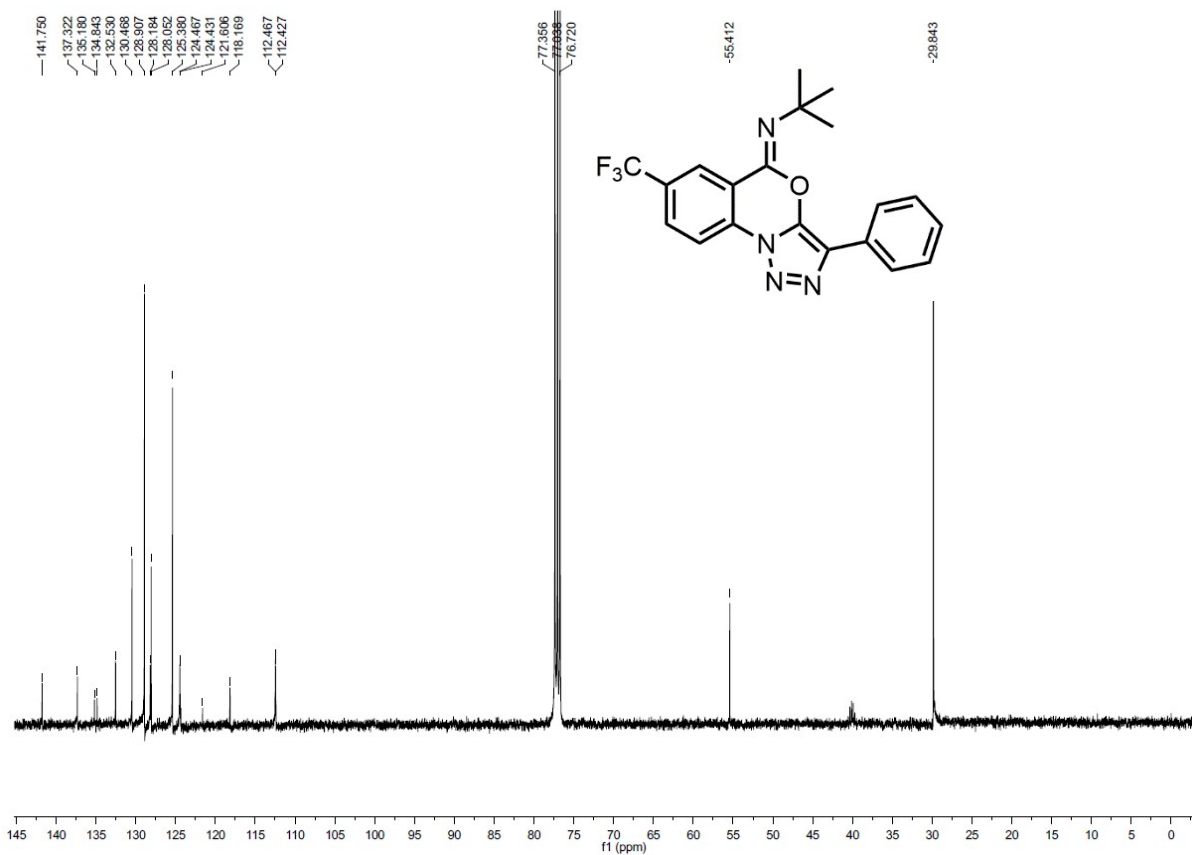
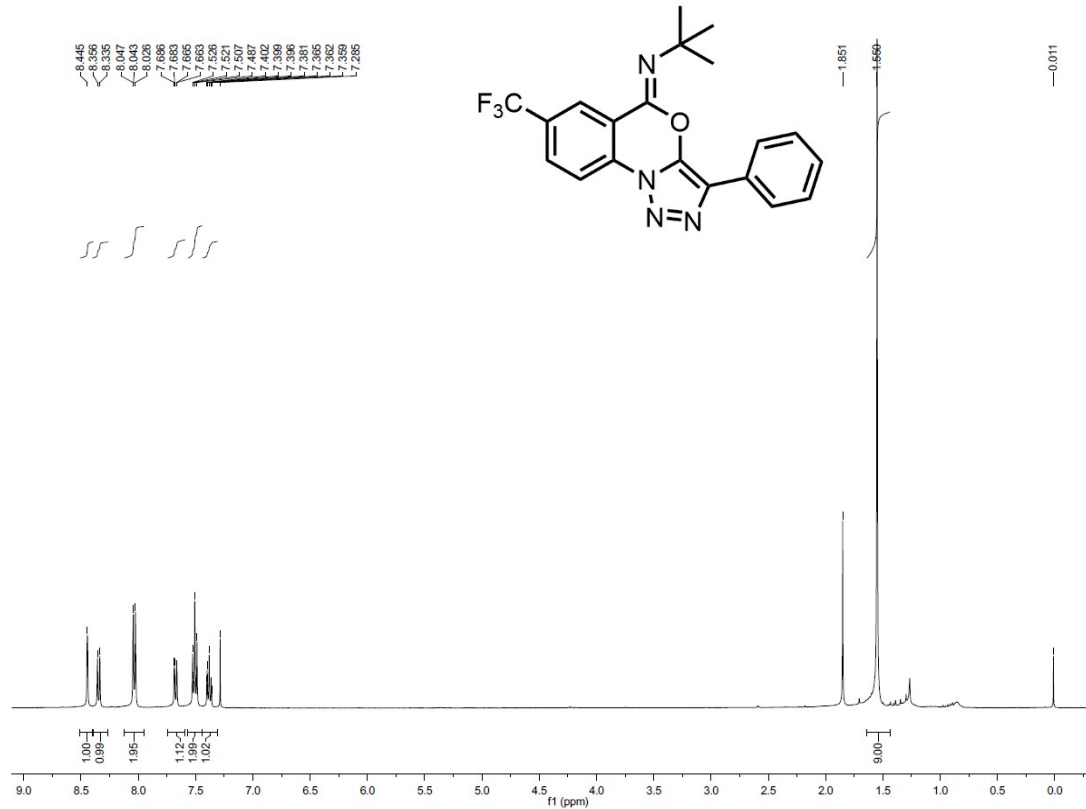
¹H and ¹³C NMR spectra of 3j



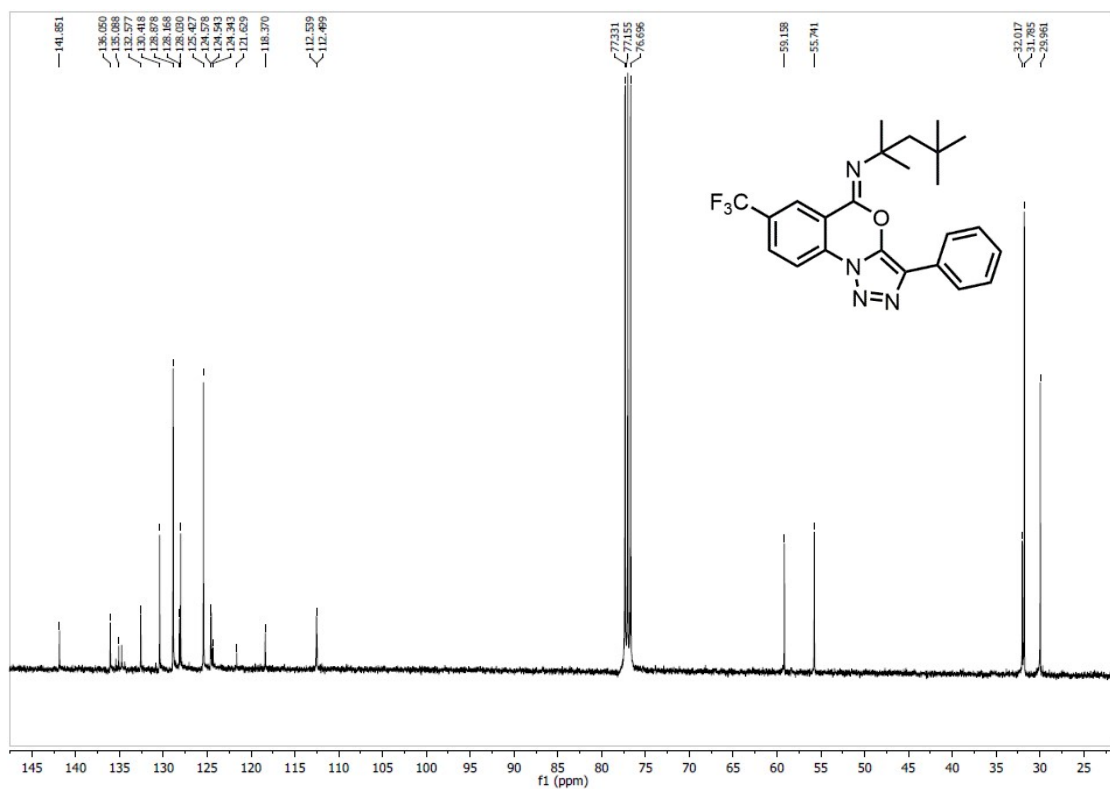
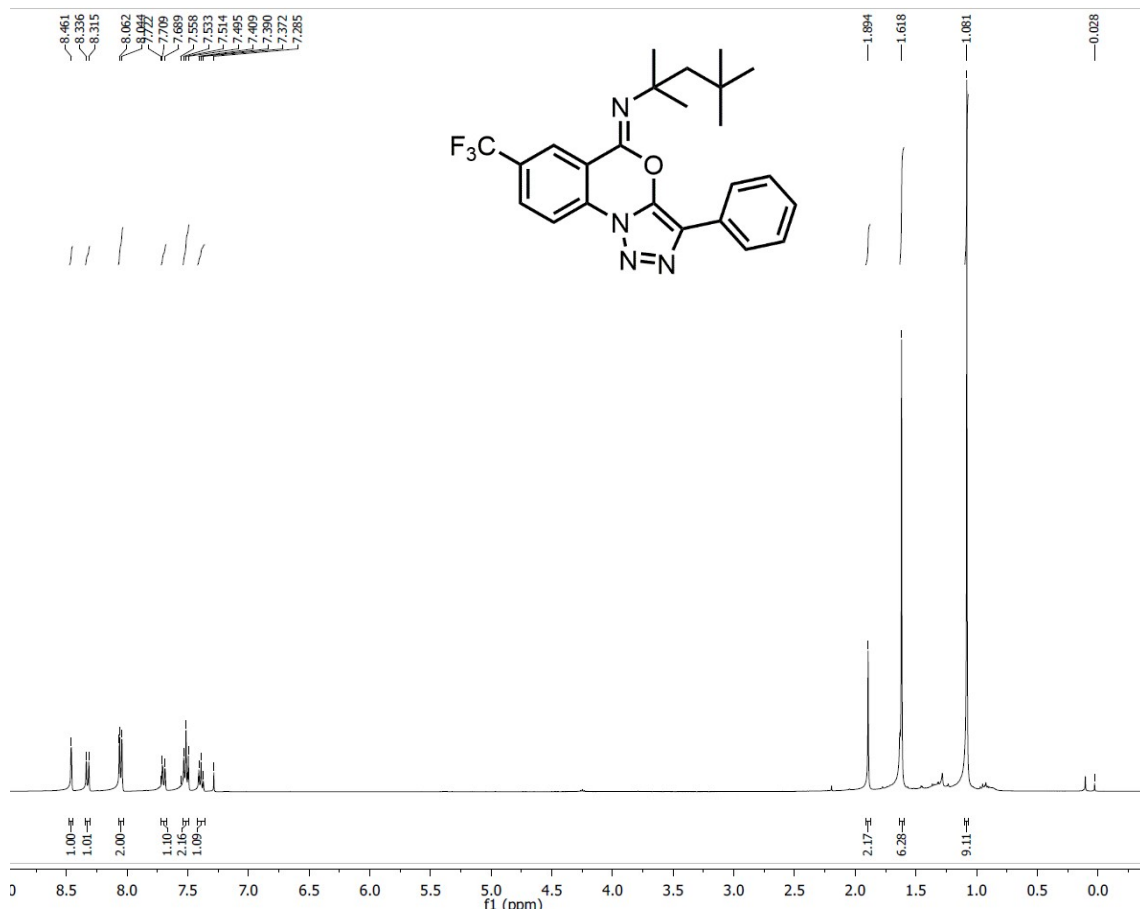
¹H and ¹³C NMR spectra of 3k



¹H and ¹³C NMR spectra of 3l



¹H and ¹³C NMR spectra of 3m



Comparison of theoretical and experimental NMR data of N-(tert-butyl)-5H-benzo[d][1,2,3] triazolo[5,1-b] [1,3] oxazin-5-imine (3a)

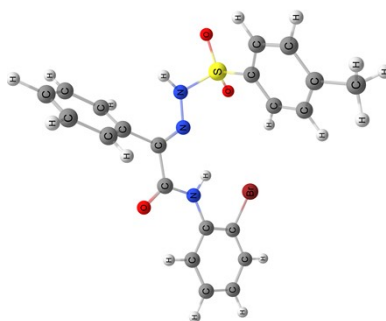
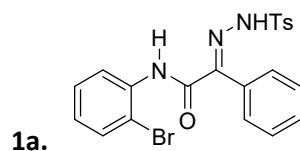
Experimentally ^1H NMR and ^{13}C NMR of title compound was evaluated in CDCl_3 solvent using TMS as an internal standard. Theoretically it was calculated in PCM with Chloroform as solvent using GIAO method involving B3LYP/6-31+G** level of theory. Both theoretical and experimental ^1H NMR and ^{13}C NMR spectral data are presented in table. ^1H NMR revealed the presence of 6 resonances of 18 protons out of which 9 correspond to aromatic protons lies between 7.34-8.20 ppm and rest 9 corresponds to tertiary butyl group give sharp singlet at 1.52ppm. However, its theoretical ^1H NMR spectra displayed all the 18 resonances for 18 protons in similar region which revealed a good agreement. Similarly, ^{13}C NMR revealed the presence of 14 resonance of 19 carbons experimentally in which 11 resonance corresponds to 14 aromatic carbons lies in range of 114-138 ppm and 1 resonance for carbonyl carbon at approx. 142 ppm. 1 resonance for 3 methyl carbons and 1 quaternary carbon of tertiary butyl group lies at 30ppm and 55ppm respectively. However, DFT calculation for ^{13}C NMR spectra gives 19 resonance for each 19 carbon atoms which is again in good agreement with experimental results.

Table S1: Comparison of theoretical and experimental NMR data

^1H NMR		^{13}C NMR	
Experimental (δ ppm)	Theoretical	Experimental (δ ppm)	Theoretical

8.20-8.14 (m, 2H)	9.11 (s, 1H)	141.8	132.5
8.04-8.02 (m, 2H)	8.81 (s, 1H)	138.6	127.8
7.66 (t, 1H)	8.69 (s, 1H)	133.2	123.6
7.50-7.41 (m, 3H)	8.62 (s, 1H)	132.3	120.6
7.34 (t, 1H)	8.34 (s, 1H)	129.3	119.7
1.52 (s, 9H)	8.08 (s, 1H)	128.9	119.4
	8.08 (s, 1H)	128.2	116.8
	8.05 (s, 1H)	127.9	115.5
	7.90 (s, 1H)	127.8	115.3
	2.20 (s, 1H)	125.3	113.2
	2.00 (s, 1H)	115.3	113.1
	1.99 (s, 1H)	114.9	111.7
	1.93 (s, 1H)	55.0	111.0
	1.82 (s, 1H)	30.0	102.9
	1.73 (s, 1H)		101.9
	1.47 (s, 1H)		49.6
	1.45 (s, 1H)		26.8
	1.05 (s, 1H)		18.5
			13.9

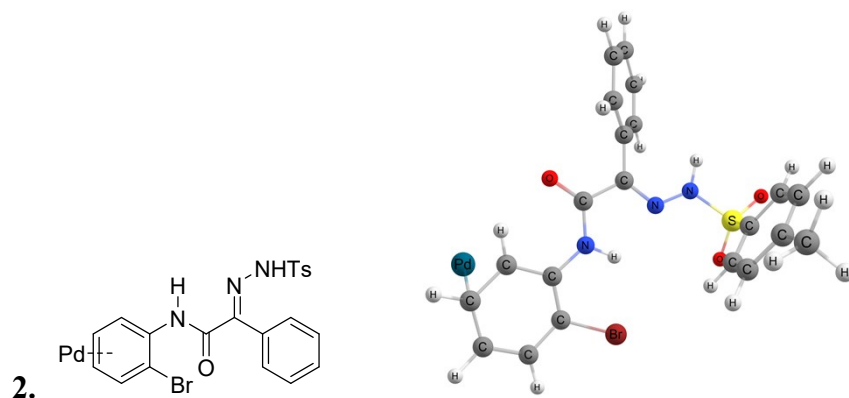
Optimized Cartesian Coordinates and electronic energies



Zero-point correction=	0.354593 (Hartree/Particle)
Thermal correction to Energy=	0.381260
Thermal correction to Enthalpy=	0.382204
Thermal correction to Gibbs free energy=	0.291742
Sum of electronic and zero-point Energies=	-1612.183338
Sum of electronic and thermal Energies=	-1612.156671
Sum of electronic and thermal Enthalpies=	-1612.155727
Sum of electronic and thermal Free Energies=	-1612.246189

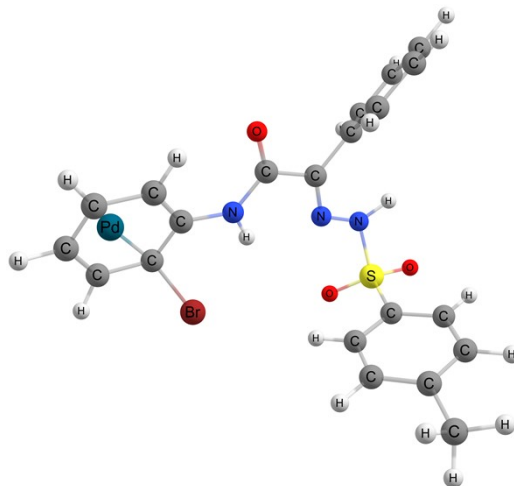
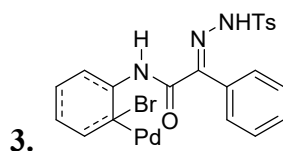
C	-5.759998000	0.824374000	1.004378000
C	-5.164263000	-0.107712000	0.151255000
C	-3.812215000	0.004988000	-0.151631000
C	-3.008834000	1.036910000	0.373106000
C	-3.629447000	1.967042000	1.231176000
C	-4.984966000	1.855974000	1.537110000
H	-6.815738000	0.739857000	1.242268000
H	-5.744276000	-0.916713000	-0.278544000
H	-3.030196000	2.767783000	1.641124000
H	-5.434604000	2.589309000	2.199900000
Br	-3.037295000	-1.324004000	-1.364585000
N	-1.651028000	1.098281000	0.032713000
H	-1.300242000	0.370826000	-0.583224000
C	-0.707584000	2.011316000	0.430252000
O	-0.916632000	2.971947000	1.166491000
C	0.680593000	1.745786000	-0.120763000
C	1.749000000	2.755676000	0.111463000
C	2.052963000	3.201151000	1.409284000
C	2.469369000	3.278550000	-0.978016000
C	3.067605000	4.137907000	1.610774000
H	1.486611000	2.822236000	2.252324000
C	3.476741000	4.223713000	-0.771972000
H	2.227216000	2.960016000	-1.988080000
C	3.780598000	4.651905000	0.523121000
H	3.295132000	4.473689000	2.618305000

H	4.018741000	4.625894000	-1.622816000
H	4.565074000	5.385833000	0.683731000
N	0.825312000	0.633369000	-0.761699000
N	2.018579000	0.283919000	-1.287791000
H	2.871076000	0.731711000	-0.941313000
S	2.232859000	-1.376127000	-1.696754000
O	3.630505000	-1.404229000	-2.135657000
O	1.117438000	-1.740055000	-2.563715000
C	2.083519000	-2.289481000	-0.163968000
C	0.825285000	-2.735568000	0.249911000
C	3.227930000	-2.534642000	0.599550000
C	0.720713000	-3.431754000	1.453622000
H	-0.048987000	-2.549477000	-0.364017000
C	3.100788000	-3.235086000	1.799243000
H	4.197941000	-2.197058000	0.249835000
C	1.850916000	-3.694075000	2.244893000
H	-0.255622000	-3.780131000	1.780153000
H	3.988238000	-3.433378000	2.394473000
C	1.727225000	-4.480518000	3.527981000
H	1.759978000	-5.558716000	3.326739000
H	2.543251000	-4.250518000	4.219172000
H	0.779840000	-4.272009000	4.034372000



Zero-point correction=		0.354601 (Hartree/Particle)	
Thermal correction to Energy=		0.383211	
Thermal correction to Enthalpy=		0.384155	
Thermal correction to Gibbs free energy=		0.288851	
Sum of electronic and zero-point Energies=		-1740.122683	
Sum of electronic and thermal Energies=		-1740.094073	
Sum of electronic and thermal Enthalpies=		-1740.093128	
Sum of electronic and thermal Free Energies=		-1740.188433	
C	-4.659641000	-1.962602000	0.952835000
C	-3.752244000	-2.509619000	0.058439000
C	-2.568689000	-1.820433000	-0.246457000
C	-2.249562000	-0.580725000	0.314804000
C	-3.181474000	-0.008640000	1.245768000
C	-4.383944000	-0.712547000	1.570818000

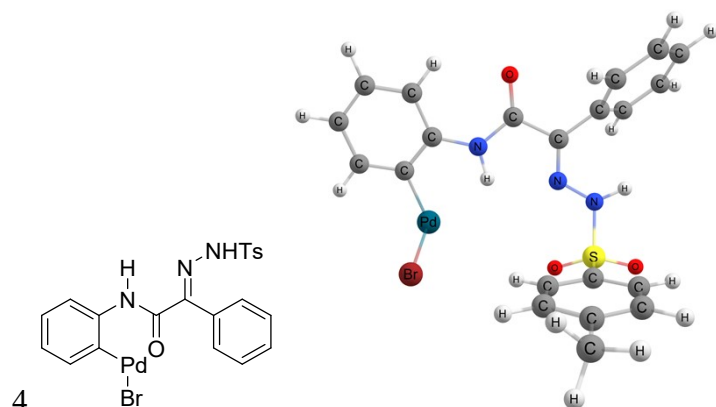
H	-5.563079000	-2.507827000	1.208872000
H	-3.949324000	-3.467387000	-0.410090000
H	-2.830577000	0.802727000	1.870636000
H	-4.941786000	-0.426534000	2.460125000
Br	-1.340727000	-2.669428000	-1.521136000
N	-1.032436000	0.038077000	0.005311000
H	-0.400276000	-0.478773000	-0.599644000
C	-0.583906000	1.284464000	0.355337000
O	-1.196601000	2.088702000	1.055986000
C	0.781967000	1.629215000	-0.206157000
C	1.308102000	3.009141000	-0.016222000
C	1.446026000	3.557536000	1.270211000
C	1.681726000	3.777769000	-1.133210000
C	1.958547000	4.845335000	1.433531000
H	1.148558000	2.978191000	2.137437000
C	2.184056000	5.070144000	-0.964805000
H	1.562187000	3.371789000	-2.134004000
C	2.326439000	5.604906000	0.318408000
H	2.063125000	5.258462000	2.432744000
H	2.459958000	5.656973000	-1.836244000
H	2.718559000	6.609620000	0.448918000
N	1.394231000	0.673240000	-0.821641000
N	2.617139000	0.873847000	-1.366483000
H	3.179676000	1.664643000	-1.038820000
S	3.551826000	-0.536852000	-1.679208000
O	4.802084000	0.026090000	-2.201749000
O	2.708540000	-1.430850000	-2.469933000
C	3.863791000	-1.292795000	-0.087767000
C	2.967416000	-2.243935000	0.407925000
C	4.987544000	-0.902681000	0.646248000
C	3.206838000	-2.805707000	1.661288000
H	2.107906000	-2.545362000	-0.180080000
C	5.208694000	-1.478633000	1.896935000
H	5.682426000	-0.173969000	0.242177000
C	4.326594000	-2.435784000	2.424355000
H	2.513070000	-3.546491000	2.050145000
H	6.084492000	-1.183347000	2.468627000
C	4.591111000	-3.076909000	3.763575000
H	5.122483000	-4.029232000	3.638290000
H	5.209816000	-2.437006000	4.399787000
H	3.658917000	-3.292378000	4.295313000
Pd	-4.866326000	0.902453000	0.192674000



Zero-point correction=	0.353983 (Hartree/Particle)
Thermal correction to Energy=	0.382858
Thermal correction to Enthalpy=	0.383802
Thermal correction to Gibbs Free Energy=	0.287324
Sum of electronic and zero-point Energies=	-1740.122007
Sum of electronic and thermal Energies=	-1740.093132
Sum of electronic and thermal Enthalpies=	-1740.092188
Sum of electronic and thermal Free Energies=	-1740.188665

C	-4.808698000	-0.211605000	2.079448000
C	-4.347571000	-0.876114000	0.911429000
C	-3.075087000	-0.517516000	0.360050000
C	-2.251108000	0.473049000	1.012054000
C	-2.756124000	1.096164000	2.155666000
C	-4.016007000	0.750827000	2.681677000
H	-5.763644000	-0.500256000	2.508677000
H	-4.825091000	-1.800636000	0.600786000
H	-2.156614000	1.857432000	2.634601000
H	-4.356417000	1.250545000	3.583861000
Br	-2.123182000	-1.943719000	-0.724421000
N	-0.979332000	0.739195000	0.485877000
H	-0.643502000	0.111167000	-0.238834000
C	-0.124398000	1.760681000	0.802311000
O	-0.355193000	2.644794000	1.626724000
C	1.182698000	1.743172000	0.035363000
C	2.108355000	2.901838000	0.174017000
C	2.598953000	3.286652000	1.433243000
C	2.509251000	3.619628000	-0.967039000
C	3.481662000	4.362019000	1.544348000
H	2.285670000	2.747847000	2.320793000
C	3.384200000	4.702014000	-0.849080000
H	2.123277000	3.341800000	-1.944044000
C	3.874400000	5.072952000	0.405907000
H	3.856669000	4.649590000	2.522470000
H	3.678712000	5.254154000	-1.736947000

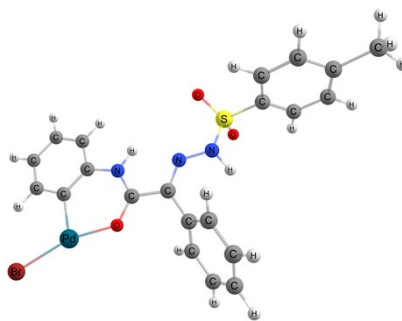
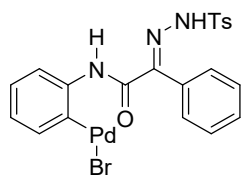
H	4.556388000	5.913684000	0.497096000
N	1.395416000	0.701323000	-0.697434000
N	2.532919000	0.594947000	-1.424896000
H	3.339288000	1.171473000	-1.167433000
S	2.973144000	-0.987981000	-1.933951000
O	4.246568000	-0.750710000	-2.623936000
O	1.808361000	-1.546611000	-2.617385000
C	3.277148000	-1.929694000	-0.443472000
C	2.217842000	-2.608377000	0.167009000
C	4.564416000	-1.955641000	0.099214000
C	2.461113000	-3.318928000	1.340721000
H	1.227508000	-2.587690000	-0.273501000
C	4.786109000	-2.675104000	1.273944000
H	5.378995000	-1.435776000	-0.393957000
C	3.743919000	-3.365587000	1.912434000
H	1.640844000	-3.848680000	1.818135000
H	5.787004000	-2.704193000	1.696192000
C	3.993534000	-4.162603000	3.168173000
H	4.024998000	-5.236989000	2.946483000
H	4.945894000	-3.892333000	3.633166000
H	3.196676000	-4.007664000	3.903327000
Pd	-4.448351000	0.383465000	-0.913597000.



Zero-point correction=	0.354415 (Hartree/Particle)
Thermal correction to Energy=	0.383379
Thermal correction to Enthalpy=	0.384323
Thermal correction to Gibbs Free Energy=	0.288546
Sum of electronic and zero-point Energies=	-1740.154753
Sum of electronic and thermal Energies=	-1740.125790
Sum of electronic and thermal Enthalpies=	-1740.124846
Sum of electronic and thermal Free Energies=	-1740.220622

C	-4.889902000	2.522997000	1.306117000
C	-4.571314000	1.428548000	0.492589000
C	-3.242661000	1.190085000	0.145568000

C	-2.186018000	1.970286000	0.668966000
C	-2.525891000	3.059588000	1.493549000
C	-3.861707000	3.327519000	1.798455000
H	-5.926511000	2.723027000	1.560526000
H	-5.357120000	0.770677000	0.133998000
H	-1.734234000	3.683466000	1.884835000
H	-4.092482000	4.171250000	2.442524000
Br	-2.979297000	-2.053095000	0.229517000
N	-0.859698000	1.643497000	0.334063000
H	-0.723742000	0.783332000	-0.190503000
C	0.279619000	2.375667000	0.537365000
O	0.334639000	3.439984000	1.151432000
C	1.525523000	1.786424000	-0.095561000
C	2.812703000	2.520187000	0.057237000
C	3.329705000	2.796327000	1.334178000
C	3.527485000	2.941627000	-1.077983000
C	4.544610000	3.469105000	1.470122000
H	2.779519000	2.487805000	2.217016000
C	4.738017000	3.624233000	-0.936614000
H	3.128317000	2.751876000	-2.070655000
C	5.250320000	3.885834000	0.336822000
H	4.936162000	3.675022000	2.462190000
H	5.276191000	3.952558000	-1.821183000
H	6.192504000	4.415394000	0.446438000
N	1.360245000	0.689123000	-0.756415000
N	2.399054000	0.111791000	-1.403321000
H	3.353357000	0.365814000	-1.132520000
S	2.233850000	-1.553677000	-1.806524000
O	3.488866000	-1.828056000	-2.515139000
O	0.928895000	-1.693880000	-2.451461000
C	2.227646000	-2.445004000	-0.256708000
C	1.013858000	-2.685608000	0.394651000
C	3.443794000	-2.858311000	0.294585000
C	1.030582000	-3.348969000	1.620028000
H	0.073909000	-2.374935000	-0.048028000
C	3.435641000	-3.522585000	1.521356000
H	4.376040000	-2.677857000	-0.230250000
C	2.235137000	-3.777564000	2.202951000
H	0.089110000	-3.539150000	2.128545000
H	4.377565000	-3.852513000	1.951179000
C	2.227722000	-4.512906000	3.519679000
H	1.612312000	-3.992134000	4.261572000
H	1.806988000	-5.519227000	3.401051000
H	3.237250000	-4.619291000	3.926748000
Pd	-2.940369000	-0.118002000	-1.263376000

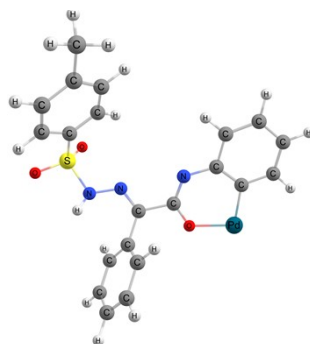
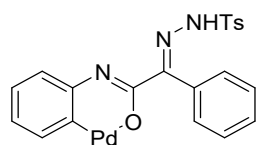


Zero-point correction=	0.355779 (Hartree/Particle)
Thermal correction to Energy=	0.384388
Thermal correction to Enthalpy=	0.385332
Thermal correction to Gibbs Free Energy=	0.289218
Sum of electronic and zero-point Energies=	-1740.184626
Sum of electronic and thermal Energies=	-1740.156018
Sum of electronic and thermal Enthalpies=	-1740.155074
Sum of electronic and thermal Free Energies=	-1740.251188

C	-4.425431000	-3.691753000	-0.058058000
C	-4.592506000	-2.306266000	-0.110759000
C	-3.491410000	-1.434857000	-0.070448000
C	-2.202138000	-1.998131000	0.026753000
C	-2.042501000	-3.397394000	0.080548000
C	-3.144286000	-4.241073000	0.037908000
H	-5.300898000	-4.333953000	-0.091995000
H	-5.590435000	-1.897515000	-0.184462000
H	-1.039213000	-3.810625000	0.158301000
H	-3.001848000	-5.316639000	0.080422000
Br	-6.209446000	0.787638000	-0.333826000
N	-0.998869000	-1.261574000	0.081806000
H	-0.137186000	-1.799616000	0.139457000
C	-0.813724000	0.061204000	0.059074000
O	-1.745648000	0.902026000	-0.017937000
C	0.601601000	0.552095000	0.128181000
C	0.872916000	2.013881000	0.188122000
C	0.311716000	2.802904000	1.206785000
C	1.709375000	2.617426000	-0.767631000
C	0.591061000	4.168330000	1.271366000
H	-0.340760000	2.349235000	1.945903000
C	1.977355000	3.986651000	-0.704077000
H	2.130990000	2.021067000	-1.572081000
C	1.421832000	4.763058000	0.316527000
H	0.154170000	4.768352000	2.064189000
H	2.614404000	4.445269000	-1.454765000
H	1.630963000	5.827884000	0.365218000
N	1.487913000	-0.387948000	0.128297000
N	2.806127000	-0.102218000	0.166765000
H	3.074764000	0.815326000	0.540696000

S	3.790792000	-1.399119000	0.799618000
O	3.313311000	-2.615376000	0.140426000
O	3.821811000	-1.308102000	2.265827000
C	5.374403000	-0.901428000	0.148353000
C	6.312160000	-0.316277000	1.000683000
C	5.655902000	-1.124523000	-1.205038000
C	7.553348000	0.056225000	0.480210000
H	6.080670000	-0.165261000	2.049590000
C	6.898779000	-0.745121000	-1.701948000
H	4.920685000	-1.591177000	-1.852270000
C	7.866747000	-0.150678000	-0.870920000
H	8.288474000	0.509330000	1.139385000
H	7.125843000	-0.917388000	-2.750781000
C	9.215603000	0.230139000	-1.426250000
H	9.809039000	-0.664924000	-1.650831000
H	9.115370000	0.792809000	-2.360876000
H	9.785274000	0.839582000	-0.719285000
Pd	-3.754982000	0.515525000	-0.149493000

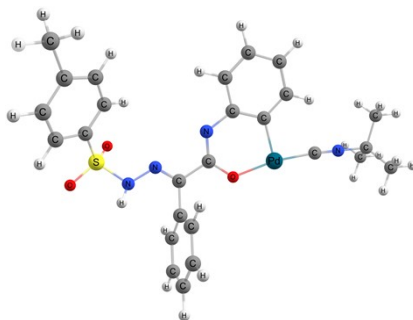
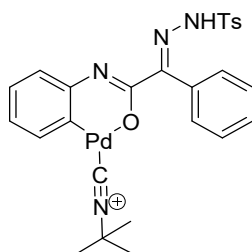
6.



Zero-point correction=	0.340563 (Hartree/Particle)
Thermal correction to Energy=	0.366837
Thermal correction to Enthalpy=	0.367781
Thermal correction to Gibbs Free Energy=	0.278458
Sum of electronic and zero-point Energies=	-1726.116248
Sum of electronic and thermal Energies=	-1726.089974
Sum of electronic and thermal Enthalpies=	-1726.089030
Sum of electronic and thermal Free Energies=	-1726.178353

C	-4.140182000	-3.805242000	0.130319000
C	-4.479080000	-2.460090000	-0.055965000
C	-3.468441000	-1.501120000	-0.100100000
C	-2.102116000	-1.809255000	0.031521000
C	-1.797296000	-3.180340000	0.219891000
C	-2.790095000	-4.153742000	0.267316000
H	-4.919197000	-4.561065000	0.166200000
H	-5.526229000	-2.174316000	-0.164081000

H	-0.749003000	-3.444646000	0.323964000
H	-2.513247000	-5.194516000	0.410897000
N	-1.029356000	-0.924670000	0.005556000
C	-1.181489000	0.350608000	-0.174443000
O	-2.273993000	1.060207000	-0.336644000
C	0.050838000	1.223212000	-0.206039000
C	0.018028000	2.514155000	0.543653000
C	-0.347789000	2.521211000	1.900688000
C	0.337399000	3.730868000	-0.083345000
C	-0.380276000	3.717586000	2.618516000
H	-0.602280000	1.586419000	2.393106000
C	0.293048000	4.928119000	0.635261000
H	0.603808000	3.742106000	-1.136139000
C	-0.061317000	4.924376000	1.987322000
H	-0.657025000	3.708144000	3.669098000
H	0.533577000	5.862673000	0.136241000
H	-0.090765000	5.855945000	2.545630000
N	1.035569000	0.777641000	-0.905801000
N	2.183982000	1.515345000	-0.990593000
H	2.419316000	2.151896000	-0.223599000
S	3.555929000	0.673777000	-1.574812000
O	4.630707000	1.663842000	-1.414602000
O	3.197902000	0.134677000	-2.886783000
C	3.850107000	-0.691994000	-0.455312000
C	3.132772000	-1.881711000	-0.619400000
C	4.784395000	-0.543988000	0.572001000
C	3.364962000	-2.932430000	0.265129000
H	2.408075000	-1.979715000	-1.419581000
C	5.003130000	-1.611156000	1.444951000
H	5.339460000	0.382112000	0.677113000
C	4.300950000	-2.817817000	1.307262000
H	2.810065000	-3.859148000	0.142663000
H	5.735696000	-1.503692000	2.240579000
C	4.549536000	-3.976128000	2.241418000
H	5.035841000	-4.806631000	1.714644000
H	5.194122000	-3.687760000	3.076663000
H	3.610171000	-4.361544000	2.653761000
Pd	-4.106914000	0.299665000	-0.358564000

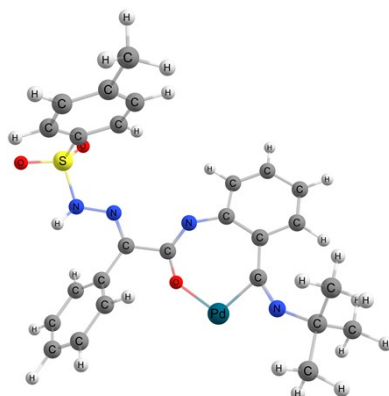
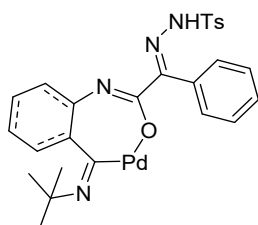


Zero-point correction=	0.473328 (Hartree/Particle)
Thermal correction to Energy=	0.508074
Thermal correction to Enthalpy=	0.509018
Thermal correction to Gibbs Free Energy=	0.400098
Sum of electronic and zero-point Energies=	-1976.736664
Sum of electronic and thermal Energies=	-1976.701918
Sum of electronic and thermal Enthalpies=	-1976.700974
Sum of electronic and thermal Free Energies=	-1976.809894

C	-2.786032000	-3.827591000	0.247987000
C	-3.184632000	-2.493953000	0.137686000
C	-2.242699000	-1.458724000	0.045292000
C	-0.848841000	-1.746631000	0.062572000
C	-0.486981000	-3.116493000	0.175666000
C	-1.422117000	-4.136504000	0.265868000
H	-3.537708000	-4.609151000	0.317521000
H	-4.244292000	-2.272468000	0.125465000
H	0.577144000	-3.332095000	0.186431000
H	-1.091614000	-5.168385000	0.348678000
N	0.240519000	-0.886384000	-0.009705000
C	0.123648000	0.401917000	-0.108518000
O	-0.965002000	1.118911000	-0.133622000
C	1.377637000	1.234834000	-0.195149000
C	1.403887000	2.540552000	0.531075000
C	1.116699000	2.579147000	1.906092000
C	1.705437000	3.739864000	-0.136464000
C	1.143187000	3.789182000	2.601118000
H	0.874484000	1.658130000	2.429477000
C	1.719872000	4.951295000	0.559432000
H	1.913910000	3.725993000	-1.202282000
C	1.443216000	4.978774000	1.929256000
H	0.926146000	3.803858000	3.665647000
H	1.946282000	5.872242000	0.029319000
H	1.459261000	5.921080000	2.469931000
N	2.334102000	0.758330000	-0.914737000
N	3.494256000	1.475300000	-1.038415000
H	3.760893000	2.114317000	-0.284051000
S	4.835133000	0.599693000	-1.638875000
O	5.937358000	1.563009000	-1.498596000
O	4.447189000	0.064599000	-2.944205000
C	5.111814000	-0.770155000	-0.519210000
C	4.355783000	-1.938474000	-0.663321000
C	6.071228000	-0.646744000	0.487714000
C	4.574414000	-2.992183000	0.220927000
H	3.612035000	-2.017622000	-1.447928000
C	6.275991000	-1.716925000	1.360734000
H	6.656616000	0.262228000	0.576535000
C	5.534120000	-2.901618000	1.243792000
H	3.989672000	-3.902361000	0.113909000

H	7.028955000	-1.629194000	2.139576000
C	5.753964000	-4.057920000	2.187782000
H	6.033723000	-4.966206000	1.640955000
H	6.546016000	-3.842102000	2.910516000
H	4.839392000	-4.287685000	2.747676000
Pd	-2.828486000	0.439077000	-0.114921000
C	-4.758245000	0.116272000	-0.137051000
N	-5.921744000	0.030206000	-0.163885000
C	-7.369660000	-0.084982000	-0.200867000
C	-7.926033000	0.644296000	1.034296000
H	-7.646624000	1.702129000	1.022795000
H	-9.017921000	0.574928000	1.032457000
H	-7.550916000	0.192673000	1.957470000
C	-7.855489000	0.571497000	-1.504772000
H	-7.430970000	0.067858000	-2.378278000
H	-8.945963000	0.500559000	-1.558737000
H	-7.575192000	1.628565000	-1.538973000
C	-7.717162000	-1.583304000	-0.167992000
H	-8.804476000	-1.700118000	-0.200199000
H	-7.288119000	-2.104272000	-1.029119000
H	-7.346821000	-2.052392000	0.748498000

8.



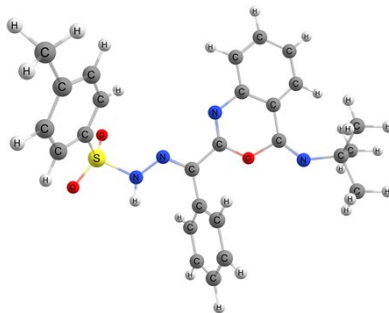
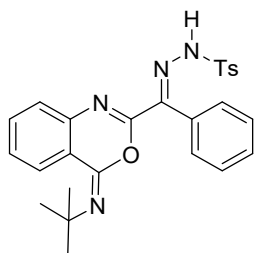
Zero-point correction=	0.474373 (Hartree/Particle)
Thermal correction to Energy=	0.507606
Thermal correction to Enthalpy=	0.508550
Thermal correction to Gibbs Free Energy=	0.405158
Sum of electronic and zero-point Energies=	-1976.715826
Sum of electronic and thermal Energies=	-1976.682593
Sum of electronic and thermal Enthalpies=	-1976.681648
Sum of electronic and thermal Free Energies=	-1976.785040

C	-2.954908000	-3.654730000	-2.146597000
C	-3.410518000	-2.670109000	-1.287362000
C	-2.602562000	-1.560189000	-0.933135000
C	-1.260550000	-1.453489000	-1.435107000
C	-0.836576000	-2.485348000	-2.313815000

C	-1.655614000	-3.543973000	-2.671985000
H	-3.596102000	-4.487800000	-2.417214000
H	-4.421619000	-2.719216000	-0.897189000
H	0.178317000	-2.419055000	-2.692922000
H	-1.280557000	-4.299981000	-3.356855000
N	-0.269508000	-0.570264000	-1.065096000
C	-0.199357000	0.727829000	-1.058911000
O	-1.099576000	1.620062000	-1.351581000
C	1.149869000	1.329389000	-0.714615000
C	1.176001000	2.649752000	-0.013782000
C	0.577664000	2.783578000	1.250242000
C	1.797509000	3.767427000	-0.594992000
C	0.605240000	4.007505000	1.921494000
H	0.092492000	1.925175000	1.707339000
C	1.814140000	4.994309000	0.073586000
H	2.254081000	3.679167000	-1.576653000
C	1.221237000	5.117007000	1.333339000
H	0.144498000	4.095923000	2.901647000
H	2.289563000	5.853051000	-0.392068000
H	1.238370000	6.070623000	1.853675000
N	2.194633000	0.671486000	-1.084210000
N	3.432768000	1.188457000	-0.827821000
H	3.546615000	1.845678000	-0.050910000
S	4.731129000	0.080019000	-0.938245000
O	5.880825000	0.881771000	-0.495269000
O	4.676613000	-0.511929000	-2.274876000
C	4.418853000	-1.204783000	0.270397000
C	3.534591000	-2.241970000	-0.042427000
C	5.051250000	-1.141793000	1.514549000
C	3.287647000	-3.226006000	0.913266000
H	3.045894000	-2.273889000	-1.009358000
C	4.793736000	-2.140638000	2.454373000
H	5.739729000	-0.333592000	1.737209000
C	3.912786000	-3.195941000	2.170873000
H	2.596848000	-4.031006000	0.676373000
H	5.290090000	-2.099701000	3.420457000
C	3.662351000	-4.289334000	3.179728000
H	4.301532000	-5.158601000	2.977317000
H	3.877944000	-3.953366000	4.198502000
H	2.624123000	-4.635065000	3.144840000
Pd	-2.852560000	1.368363000	-0.277992000
C	-3.226609000	-0.501156000	-0.183758000
N	-4.173336000	-0.155262000	0.550243000
C	-5.197521000	-0.696262000	1.471175000
C	-6.468878000	-0.980757000	0.651523000
C	-4.668505000	-1.969797000	2.150538000
C	-5.474206000	0.393950000	2.516702000
H	-6.815462000	-0.074305000	0.145500000
H	-6.293346000	-1.750835000	-0.105820000

H	-7.265952000	-1.330974000	1.316141000
H	-3.737178000	-1.766410000	2.688879000
H	-5.407812000	-2.332191000	2.872727000
H	-4.482858000	-2.770872000	1.429975000
H	-6.247817000	0.057630000	3.214181000
H	-4.569647000	0.623396000	3.089209000
H	-5.819275000	1.314238000	2.034748000

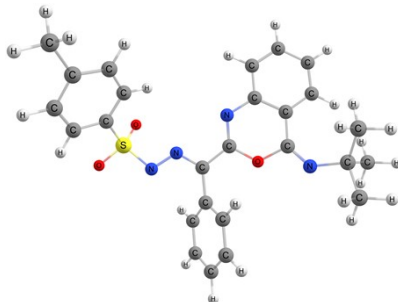
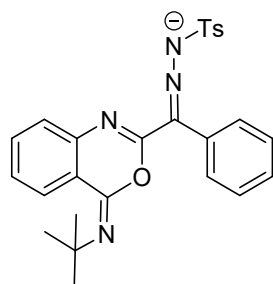
9.



Zero-point correction=	0.475408 (Hartree/Particle)
Thermal correction to Energy=	0.507032
Thermal correction to Enthalpy=	0.507976
Thermal correction to Gibbs Free Energy=	0.408224
Sum of electronic and zero-point Energies=	-1848.814367
Sum of electronic and thermal Energies=	-1848.782743
Sum of electronic and thermal Enthalpies=	-1848.781799
Sum of electronic and thermal Free Energies=	-1848.881552

C	-3.925443000	-3.786634000	-1.165992000
C	-4.146261000	-2.441137000	-0.884642000
C	-3.076324000	-1.579971000	-0.593182000
C	-1.754029000	-2.094335000	-0.648184000
C	-1.545814000	-3.461918000	-0.896661000
C	-2.622563000	-4.302510000	-1.150620000
H	-4.767127000	-4.431915000	-1.398242000
H	-5.156095000	-2.056911000	-0.916513000
H	-0.524492000	-3.828251000	-0.913579000
H	-2.451106000	-5.355018000	-1.356900000
N	-0.631633000	-1.282147000	-0.504684000
C	-0.831853000	-0.012683000	-0.534452000
O	-2.044081000	0.587214000	-0.549712000
C	0.281838000	0.975051000	-0.584437000
C	0.070644000	2.359549000	-0.068475000
C	-0.364174000	2.561843000	1.251586000
C	0.312453000	3.475577000	-0.887357000
C	-0.544024000	3.853922000	1.745514000
H	-0.564294000	1.706476000	1.890525000
C	0.122541000	4.767532000	-0.392399000
H	0.632064000	3.332557000	-1.915524000
C	-0.302011000	4.959533000	0.924783000

H	-0.879596000	3.996881000	2.768533000
H	0.303392000	5.621709000	-1.038355000
H	-0.448075000	5.965035000	1.308816000
N	1.383298000	0.527115000	-1.091795000
N	2.460812000	1.338492000	-1.170813000
H	2.534050000	2.155038000	-0.556784000
S	3.969188000	0.570119000	-1.463506000
O	4.911990000	1.694103000	-1.398083000
O	3.805741000	-0.235111000	-2.672250000
C	4.259024000	-0.521412000	-0.075708000
C	3.671956000	-1.790401000	-0.066912000
C	5.052921000	-0.080509000	0.985609000
C	3.891284000	-2.622889000	1.028496000
H	3.054690000	-2.116179000	-0.896297000
C	5.262797000	-0.933011000	2.069546000
H	5.506773000	0.904218000	0.957758000
C	4.689666000	-2.213361000	2.109367000
H	3.434822000	-3.609005000	1.042175000
H	5.886000000	-0.597662000	2.894197000
C	4.945094000	-3.141619000	3.270273000
H	5.733667000	-3.863890000	3.023107000
H	5.268417000	-2.592775000	4.159552000
H	4.048889000	-3.715243000	3.527883000
C	-3.229652000	-0.154342000	-0.230430000
N	-4.107264000	0.588274000	0.277222000
C	-5.446462000	0.366615000	0.838126000
C	-6.491745000	0.339295000	-0.295661000
C	-5.541312000	-0.877244000	1.744404000
C	-5.720076000	1.612645000	1.709580000
H	-6.405427000	1.240019000	-0.911959000
H	-6.380785000	-0.526884000	-0.953016000
H	-7.501235000	0.311604000	0.128869000
H	-4.763375000	-0.845005000	2.515191000
H	-6.512670000	-0.886943000	2.250766000
H	-5.441354000	-1.819543000	1.204397000
H	-6.720788000	1.566358000	2.153258000
H	-4.985877000	1.683208000	2.519091000
H	-5.644017000	2.522893000	1.106953000



Zero-point correction=
Thermal correction to Energy=

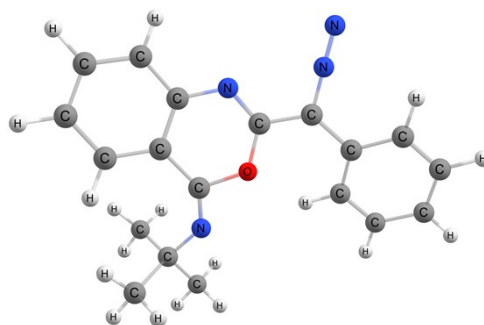
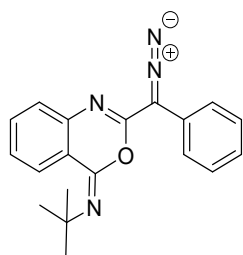
0.461859 (Hartree/Particle)
0.493033

Thermal correction to Enthalpy=	0.493977
Thermal correction to Gibbs Free Energy=	0.396334
Sum of electronic and zero-point Energies=	-1848.331844
Sum of electronic and thermal Energies=	-1848.300671
Sum of electronic and thermal Enthalpies=	-1848.299726
Sum of electronic and thermal Free Energies=	-1848.397369

C	-3.831014000	-3.709741000	-1.485674000
C	-4.078527000	-2.408949000	-1.059076000
C	-3.026895000	-1.554139000	-0.688600000
C	-1.684180000	-2.009556000	-0.817349000
C	-1.452665000	-3.347072000	-1.210995000
C	-2.509413000	-4.183733000	-1.537742000
H	-4.657634000	-4.350956000	-1.777179000
H	-5.097789000	-2.047331000	-1.037067000
H	-0.422552000	-3.681915000	-1.282390000
H	-2.310892000	-5.203588000	-1.857140000
N	-0.594633000	-1.197241000	-0.593640000
C	-0.810719000	0.085257000	-0.520954000
O	-2.072049000	0.622220000	-0.483214000
C	0.239438000	1.095416000	-0.515417000
C	-0.042265000	2.504184000	-0.114996000
C	-0.813283000	2.795876000	1.025838000
C	0.479818000	3.586171000	-0.848955000
C	-1.061959000	4.113157000	1.413743000
H	-1.229672000	1.983337000	1.612183000
C	0.229595000	4.904265000	-0.462691000
H	1.089001000	3.391120000	-1.723499000
C	-0.541354000	5.176978000	0.670971000
H	-1.663581000	4.306569000	2.298407000
H	0.643595000	5.720156000	-1.049938000
H	-0.732748000	6.203755000	0.972430000
N	1.429459000	0.637980000	-0.884955000
N	2.459437000	1.444835000	-0.899882000
S	3.854079000	0.591779000	-1.398484000
O	4.920139000	1.615927000	-1.461793000
O	3.621476000	-0.259863000	-2.588509000
C	4.266856000	-0.520867000	-0.033952000
C	3.577176000	-1.729781000	0.110121000
C	5.244640000	-0.147408000	0.887587000
C	3.883467000	-2.564258000	1.183819000
H	2.807590000	-2.003320000	-0.603353000
C	5.543695000	-0.998447000	1.955144000
H	5.767329000	0.794807000	0.761875000
C	4.870336000	-2.216086000	2.121761000
H	3.343882000	-3.501984000	1.296945000
H	6.312461000	-0.708218000	2.667553000
C	5.186107000	-3.134082000	3.278865000
H	5.491354000	-4.127576000	2.928343000

H	5.995105000	-2.734215000	3.897927000
H	4.309922000	-3.275310000	3.923683000
C	-3.194844000	-0.180601000	-0.177434000
N	-4.077603000	0.468925000	0.455452000
C	-5.361022000	0.089436000	1.056206000
C	-6.482733000	0.154714000	-0.001505000
C	-5.344544000	-1.266647000	1.792830000
C	-5.639696000	1.188904000	2.107618000
H	-6.482881000	1.134680000	-0.490190000
H	-6.372506000	-0.604301000	-0.780318000
H	-7.459559000	0.008875000	0.474197000
H	-4.509916000	-1.301668000	2.501823000
H	-6.273202000	-1.385970000	2.362888000
H	-5.253393000	-2.124832000	1.126372000
H	-6.609466000	1.031668000	2.594315000
H	-4.861339000	1.186384000	2.878064000
H	-5.637628000	2.175639000	1.634153000

11.

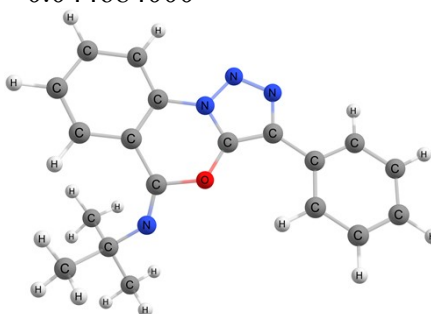
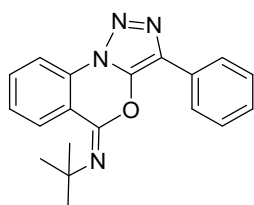


Zero-point correction=	0.333833 (Hartree/Particle)
Thermal correction to Energy=	0.355203
Thermal correction to Enthalpy=	0.356147
Thermal correction to Gibbs Free Energy=	0.282356
Sum of electronic and zero-point Energies=	-1028.763913
Sum of electronic and thermal Energies=	-1028.742543
Sum of electronic and thermal Enthalpies=	-1028.741599
Sum of electronic and thermal Free Energies=	-1028.815390

C	-4.160704000	-1.956285000	-0.555374000
C	-3.407848000	-0.787203000	-0.609599000
C	-2.052934000	-0.782796000	-0.239874000
C	-1.441919000	-2.008958000	0.139251000
C	-2.223145000	-3.175670000	0.226189000
C	-3.569181000	-3.149044000	-0.115368000
H	-5.204202000	-1.939231000	-0.854263000
H	-3.873227000	0.122644000	-0.962673000
H	-1.737767000	-4.093520000	0.542302000
H	-4.159039000	-4.059357000	-0.057455000
N	-0.082804000	-2.108008000	0.406629000
C	0.649510000	-1.095466000	0.069933000

O	0.182663000	0.078057000	-0.404432000
C	2.104881000	-1.158513000	0.135695000
C	3.103147000	-0.073964000	-0.014403000
C	2.783111000	1.265369000	0.277908000
C	4.415182000	-0.378748000	-0.425701000
C	3.751623000	2.262108000	0.154215000
H	1.780847000	1.531173000	0.588880000
C	5.378822000	0.623045000	-0.536365000
H	4.687906000	-1.401585000	-0.670910000
C	5.052644000	1.950863000	-0.249052000
H	3.482798000	3.289844000	0.381445000
H	6.383791000	0.362981000	-0.856472000
H	5.801503000	2.732146000	-0.339889000
N	2.564251000	-2.371982000	0.366724000
N	2.978063000	-3.412912000	0.563776000
C	-1.201850000	0.423911000	-0.219501000
N	-1.340677000	1.666113000	-0.090412000
C	-2.488244000	2.545856000	0.173123000
C	-3.224733000	2.850879000	-1.146936000
C	-3.443263000	2.010734000	1.258643000
C	-1.866315000	3.861489000	0.690743000
H	-2.523183000	3.240693000	-1.891599000
H	-3.708563000	1.968371000	-1.573103000
H	-3.997348000	3.608439000	-0.976115000
H	-2.884291000	1.761733000	2.167319000
H	-4.172221000	2.786569000	1.516902000
H	-3.999708000	1.124379000	0.951572000
H	-2.642483000	4.609963000	0.884485000
H	-1.316525000	3.685855000	1.621539000
H	-1.164110000	4.266322000	-0.044684000

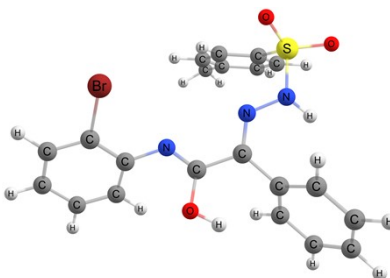
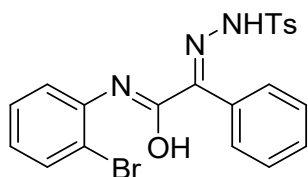
12.



Zero-point correction=	0.336900 (Hartree/Particle)
Thermal correction to Energy=	0.356967
Thermal correction to Enthalpy=	0.357911
Thermal correction to Gibbs Free Energy=	0.287859
Sum of electronic and zero-point Energies=	-1028.774808
Sum of electronic and thermal Energies=	-1028.754741
Sum of electronic and thermal Enthalpies=	-1028.753797
Sum of electronic and thermal Free Energies=	-1028.823849

C	-3.893203000	-2.172390000	-0.673325000
C	-3.284549000	-0.919524000	-0.692000000
C	-1.944720000	-0.761597000	-0.306494000
C	-1.226067000	-1.928841000	0.034535000
C	-1.826820000	-3.187599000	0.076931000
C	-3.171391000	-3.300009000	-0.266859000
H	-4.929851000	-2.269136000	-0.979838000
H	-3.848260000	-0.060450000	-1.027582000
H	-1.236276000	-4.052420000	0.355837000
H	-3.649591000	-4.274226000	-0.241800000
N	0.143666000	-1.761359000	0.272712000
C	0.808191000	-0.628793000	-0.066512000
O	0.159001000	0.441027000	-0.546233000
C	2.150505000	-0.892068000	0.173695000
C	3.344385000	-0.058327000	-0.001146000
C	3.250268000	1.260600000	-0.481661000
C	4.614224000	-0.576075000	0.314251000
C	4.398451000	2.038695000	-0.639084000
H	2.281222000	1.679985000	-0.730075000
C	5.756586000	0.206717000	0.153476000
H	4.695223000	-1.592438000	0.684827000
C	5.656020000	1.517781000	-0.323582000
H	4.306900000	3.055669000	-1.010392000
H	6.729163000	-0.209279000	0.401788000
H	6.547799000	2.125505000	-0.447918000
N	2.204421000	-2.179130000	0.650299000
N	1.020600000	-2.714414000	0.713324000
C	-1.256886000	0.558943000	-0.263142000
N	-1.588573000	1.749034000	-0.070492000
C	-2.828275000	2.442692000	0.309174000
C	-3.635254000	2.770003000	-0.963177000
C	-3.675705000	1.688790000	1.352442000
C	-2.355929000	3.770716000	0.940272000
H	-3.012157000	3.312115000	-1.681518000
H	-4.019516000	1.874744000	-1.459844000
H	-4.489870000	3.404134000	-0.704757000
H	-3.061169000	1.409331000	2.215101000
H	-4.473973000	2.346933000	1.711553000
H	-4.145910000	0.785006000	0.963050000
H	-3.213176000	4.391173000	1.222832000
H	-1.757798000	3.578774000	1.837169000
H	-1.734558000	4.329175000	0.233752000

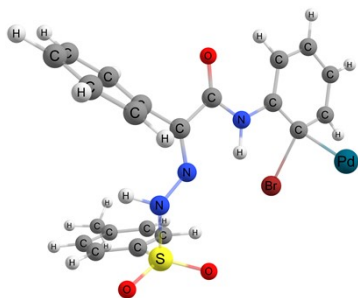
13.



Zero-point correction= 0.352984 (Hartree/Particle)
 Thermal correction to Energy= 0.379936
 Thermal correction to Enthalpy= 0.380880
 Thermal correction to Gibbs Free Energy= 0.289783
 Sum of electronic and zero-point Energies= -1612.171363
 Sum of electronic and thermal Energies= -1612.144412
 Sum of electronic and thermal Enthalpies= -1612.143467
 Sum of electronic and thermal Free Energies= -1612.234564

C	-5.585262000	-0.547744000	1.550377000
C	-5.174376000	-0.827396000	0.244956000
C	-3.870720000	-0.528185000	-0.144389000
C	-2.947868000	0.064951000	0.732039000
C	-3.387646000	0.339253000	2.042133000
C	-4.685280000	0.035406000	2.447333000
H	-6.598852000	-0.786673000	1.858114000
H	-5.861159000	-1.277097000	-0.464141000
H	-2.685496000	0.785524000	2.739694000
H	-4.993461000	0.255971000	3.465468000
Br	-3.327572000	-0.925462000	-1.977144000
N	-1.610917000	0.257157000	0.355308000
C	-1.076838000	1.410199000	0.289532000
O	-1.773849000	2.550805000	0.541155000
C	0.364113000	1.590813000	-0.082259000
C	1.061038000	2.858764000	0.304624000
C	1.224049000	3.196596000	1.661113000
C	1.568171000	3.723514000	-0.683217000
C	1.884309000	4.373645000	2.020121000
H	0.839657000	2.533751000	2.431987000
C	2.222303000	4.902262000	-0.318473000
H	1.443713000	3.472806000	-1.733048000
C	2.382989000	5.227755000	1.031756000
H	2.009206000	4.622074000	3.070074000
H	2.605035000	5.564845000	-1.089262000
H	2.894468000	6.143914000	1.312662000
N	0.908671000	0.622834000	-0.737023000
N	2.205933000	0.706966000	-1.097568000
H	2.842999000	1.327037000	-0.590675000

S	2.948673000	-0.755715000	-1.617505000
O	4.358252000	-0.360251000	-1.739411000
O	2.178675000	-1.235582000	-2.762937000
C	2.765523000	-1.914304000	-0.268622000
C	1.562704000	-2.613884000	-0.126264000
C	3.822019000	-2.090812000	0.628703000
C	1.426562000	-3.500758000	0.939922000
H	0.749942000	-2.462719000	-0.827548000
C	3.664884000	-2.989012000	1.684637000
H	4.750902000	-1.546484000	0.495886000
C	2.470624000	-3.706661000	1.857244000
H	0.491738000	-4.041954000	1.059386000
H	4.485850000	-3.136885000	2.381330000
C	2.317888000	-4.697257000	2.984371000
H	2.524975000	-5.717036000	2.634856000
H	3.010513000	-4.483571000	3.803935000
H	1.299015000	-4.692560000	3.384854000
H	-1.208340000	3.330341000	0.417280000

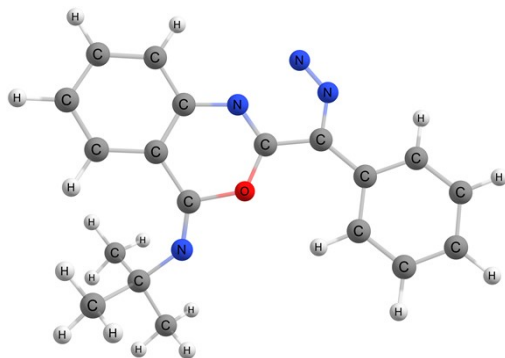


TS₃₋₄

Zero-point correction=	0.353802 (Hartree/Particle)
Thermal correction to Energy=	0.382112
Thermal correction to Enthalpy=	0.383056
Thermal correction to Gibbs Free Energy=	0.288377
Sum of electronic and zero-point Energies=	-1740.118715
Sum of electronic and thermal Energies=	-1740.090406
Sum of electronic and thermal Enthalpies=	-1740.089461
Sum of electronic and thermal Free Energies=	-1740.184141

C	-5.134635000	0.804045000	1.773065000
C	-4.572577000	-0.210041000	0.984194000
C	-3.240491000	-0.081813000	0.521527000
C	-2.420966000	1.022307000	0.931361000
C	-3.016594000	2.005174000	1.734578000
C	-4.352598000	1.894700000	2.144037000
H	-6.161425000	0.711211000	2.114429000
H	-5.117575000	-1.128470000	0.796277000
H	-2.421638000	2.857070000	2.032356000
H	-4.770056000	2.674863000	2.773704000
Br	-2.217881000	-1.984025000	0.231486000

N	-1.083950000	1.065961000	0.510159000
H	-0.763746000	0.293071000	-0.065843000
C	-0.161492000	2.057350000	0.711092000
O	-0.353129000	3.075050000	1.376566000
C	1.166612000	1.838527000	0.016661000
C	2.218369000	2.883155000	0.168740000
C	2.718884000	3.212066000	1.439422000
C	2.724401000	3.548492000	-0.961360000
C	3.716021000	4.179115000	1.573582000
H	2.324273000	2.714368000	2.319345000
C	3.714746000	4.523806000	-0.821257000
H	2.331770000	3.315227000	-1.947305000
C	4.214709000	4.838009000	0.445221000
H	4.097375000	4.424170000	2.560766000
H	4.091125000	5.037691000	-1.701132000
H	4.985836000	5.595605000	0.553540000
N	1.278949000	0.762288000	-0.688303000
N	2.416982000	0.519352000	-1.379680000
H	3.275781000	1.011099000	-1.116191000
S	2.688217000	-1.090880000	-1.912630000
O	3.958056000	-0.968461000	-2.637660000
O	1.455941000	-1.526676000	-2.566528000
C	2.949541000	-2.075239000	-0.442407000
C	1.852262000	-2.665993000	0.191836000
C	4.244884000	-2.222418000	0.060280000
C	2.065967000	-3.412052000	1.348988000
H	0.855082000	-2.550599000	-0.217741000
C	4.436005000	-2.975579000	1.219245000
H	5.087865000	-1.770558000	-0.451737000
C	3.355925000	-3.580393000	1.880817000
H	1.216380000	-3.874818000	1.844523000
H	5.442278000	-3.099518000	1.610312000
C	3.568520000	-4.410375000	3.122036000
H	2.870928000	-4.122680000	3.916345000
H	3.399037000	-5.474088000	2.913250000
H	4.586640000	-4.304073000	3.506901000
Pd	-3.690681000	-0.076612000	-1.427520000



TS₁₁₋₁₂

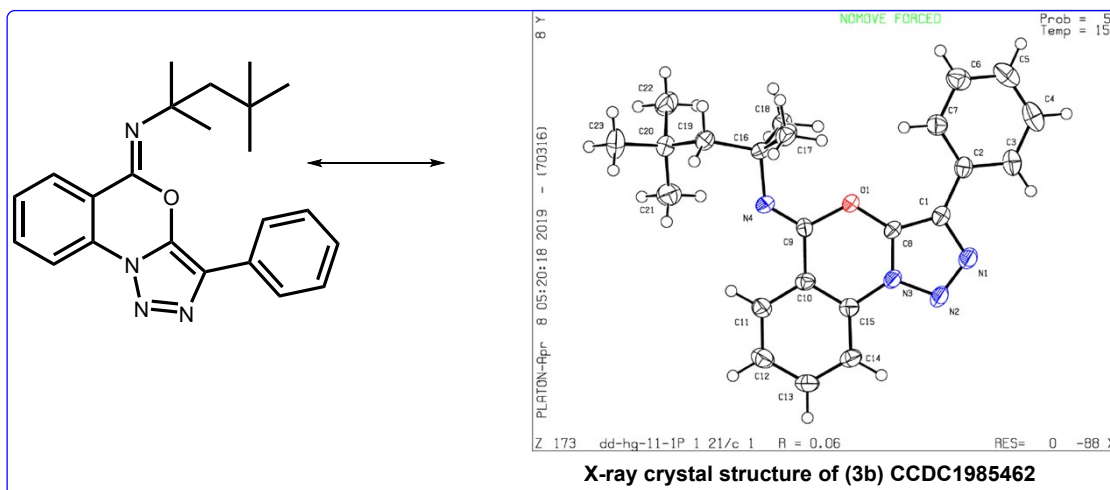
Zero-point correction=	0.333616 (Hartree/Particle)
Thermal correction to Energy=	0.354024
Thermal correction to Enthalpy=	0.354969
Thermal correction to Gibbs Free Energy=	0.282885
Sum of electronic and zero-point Energies=	-1028.745273
Sum of electronic and thermal Energies=	-1028.724864
Sum of electronic and thermal Enthalpies=	-1028.723920
Sum of electronic and thermal Free Energies=	-1028.796004

C	-4.061123000	-2.007797000	-0.631036000
C	-3.363172000	-0.804004000	-0.616396000
C	-2.007476000	-0.756018000	-0.252246000
C	-1.347187000	-1.978319000	0.043504000
C	-2.063210000	-3.186185000	0.056530000
C	-3.412731000	-3.197751000	-0.272614000
H	-5.106702000	-2.019743000	-0.922182000
H	-3.872923000	0.102481000	-0.910063000
H	-1.532513000	-4.099295000	0.305523000
H	-3.959696000	-4.136013000	-0.270178000
N	0.015181000	-1.995421000	0.286695000
C	0.723567000	-0.924004000	0.043841000
O	0.196240000	0.252765000	-0.325539000
C	2.156773000	-1.042732000	0.160913000
C	3.246383000	-0.081258000	-0.019542000
C	3.016346000	1.282327000	-0.287111000
C	4.581776000	-0.525986000	0.081166000
C	4.089439000	2.161827000	-0.446263000
H	2.004236000	1.656791000	-0.367978000
C	5.644681000	0.359141000	-0.078552000
H	4.784257000	-1.573567000	0.285877000
C	5.407104000	1.711935000	-0.344397000
H	3.886056000	3.209416000	-0.650721000
H	6.662931000	-0.010867000	0.004205000
H	6.236424000	2.401932000	-0.469417000
N	2.393432000	-2.322263000	0.501167000
N	1.668314000	-3.228982000	0.685259000
C	-1.224664000	0.495922000	-0.165972000
N	-1.441198000	1.719697000	-0.006492000
C	-2.624167000	2.547193000	0.265140000
C	-3.352875000	2.863036000	-1.056656000
C	-3.570937000	1.941650000	1.320228000
C	-2.059964000	3.869130000	0.830735000
H	-2.656179000	3.299909000	-1.779306000
H	-3.800110000	1.977806000	-1.516368000
H	-4.153919000	3.587442000	-0.874164000
H	-3.014046000	1.684744000	2.227839000
H	-4.331339000	2.681362000	1.593002000
H	-4.090723000	1.046027000	0.977734000

H	-2.867478000	4.579662000	1.038368000
H	-1.512951000	3.685677000	1.761420000
H	-1.366715000	4.324253000	0.116669000

X-ray crystal data of compound 3b:

X-ray data for compound 3b was collected at 150 K using Rigaku Oxford Diffraction, 2017 system. Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) was used for the experiments. The structures were solved by direct methods using SHELXT and refined using SHELXL.¹ **CCDC 1985462** contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk.



References:

- (a) Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3-8; <https://doi.org/10.1107/S2053273314026370>.
 (b) Sheldrick, G. M. *Acta Cryst.* **2015**, *C71*, 3-8; [doi:10.1107/S2053229614024218](https://doi.org/10.1107/S2053229614024218).

Crystal Data and Structure Refinement:

Identification code	3b (dd-hg-11)
Empirical formula	C ₂₃ H ₂₆ N ₄ O
Formula weight	374.48
Temperature/K	150°
Crystal system	monoclinic
Space group	P 1
<i>a</i> /Å	15.2432(13)
<i>b</i> /Å	6.8557(4)
<i>c</i> /Å	19.6543(15)
α /°	90
β /°	99.415(7)
γ /°	90
Volume/Å ³	2026.3(3)
<i>Z</i>	4
ρ_{calc} /cm ³	1.228
μ /mm ⁻¹	0.077
F(000)	800
Crystal size/mm ³	0.15 x 0.28 x 0.4
Radiation MoK α	0.71073
2 θ range for data collection/°	2.679- 25.999
Index ranges	-18 \leq h \leq 14, -6 \leq k \leq 8, -24 \leq l \leq 20
Reflections collected	3991
Independent reflections	2822
parameters	258
Goodness-of-fit on F ²	1.080
Final R indexes [<i>I</i> \geq 2 σ (<i>I</i>)]	0.0559
Final R indexes [all data]	0.0831
Largest diff. peak/hole / e Å ⁻³	0.299/ -0.311

CCDC Number	1985462
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