

Supporting Information for

Synthesis of *N*-fused polycyclic indoles via Pd-catalyzed multicomponent cascade reaction consisting of amide-directed [3+1+1] annulation reaction of 3-diazo oxindole and isocyanides

Pooja Soam,^a Debasish Mandal^a and Vikas Tyagi^{a*}

^aSchool of Chemistry and Biochemistry

^bCentre of Excellence for Emerging Materials

Thapar Institute of Engineering and Technology

Patiala-147004, Punjab, India

Email: vikas.tyagi@thapar.edu

Index

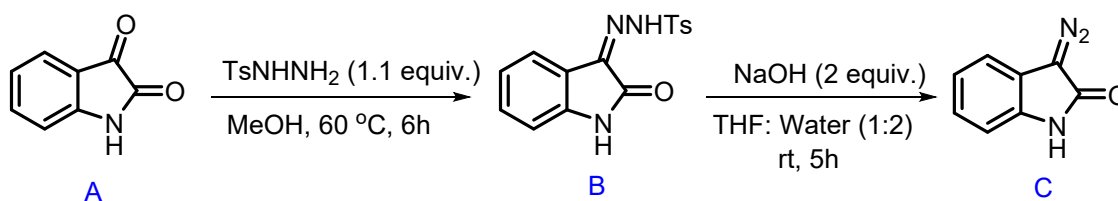
Table of Contents

General information.....	S2
General method for the synthesis of 3-diazo oxindole (1a-1p).....	S2
Method for crystallization.....	S2-S3
X-ray crystal data of compound 3a	S3- S4
Optimization of the reaction conditions.....	S4- S5
Copies of H ¹ NMR and C ¹³ NMR data of compounds (3a-3q, 4).....	S6-S25
Computational details, Optimized Cartesian Coordinates and electronic energies.....	S26-S71
References.....	S72

General Information: All the reagents and solvents involved in this synthesis were obtained directly from commercial sources and used without any additional purification. The ^1H NMR and $^{13}\text{C}\{^1\text{H}\}$ NMR were recorded using JEOL spectrometers at 400 MHz and 100 MHz respectively in CDCl_3 and d_6 -DMSO using tetramethylsilane (TMS) as an internal reference. The following terms are used in NMR follow-up experiments: b, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; td or dd, doublet of triplet and double doublet. The HRMS data were carried out using the Water QTOF mass spectrometer (XEVO G2 XS) in ESI(+ve) mode. Silica gel (GF-254) containing glass plates was used for Thin Layer Chromatography (TLC) for monitoring the progress of the reaction. The column chromatography was performed using silica gel (60-120 mesh) as the stationary phase and ethyl acetate in hexane as the mobile phase. All the compounds were characterized using ^1H NMR, ^{13}C NMR & HRMS data.

General method for the synthesis of 3-diazo oxindoles (1a-1p)¹⁻³

A mixture of isatin (1.0 equiv., 1g, 6.80mmol) and *para*-tosyl hydrazones (1.1 equiv., 1.39 gm, 7.48 mmol) were added in methanol as solvent (~ 20 mL) at 60 °C and stirred the resulting mixture for 5 to 6 h, a highly yellow colored solid 3-(2-(*p*-tolyl) hydrazono) indolin-2-one intermediates was filtered. The filtered solid and NaOH (2.0 equiv., 13.6mmol) were dissolved in a mixture of THF and water in a ratio of 1:2 and stirred the mixture at room temperature for 5 h. Upon complete conversion of the starting materials, work-up of the reaction with ethyl acetate and distilled water in a 2:1 ratio was done and the volatiles were removed using a high vacuum. The 3-diazo oxindole (83%, 900 mg) was obtained as an orange-red solid and used for the next step without further purification. (*Substrates 5 and 7 were synthesized using previously reported methods*)^{5,6}



Scheme S1: Synthesis of 3-diazo oxindole

Method for Crystallization

Single crystal growth was done by vapor diffusion method. The experimental set up consists of an inner container made up of glass and having compound 3a (6 mg) dissolved in 0.5 ml of dichloromethane and an outer container filled with hexane (2.5 ml). Next, the outer container

was closed and the two solvents started to equilibrate which resulted in a single crystal formation.⁴

Crystallographic Data

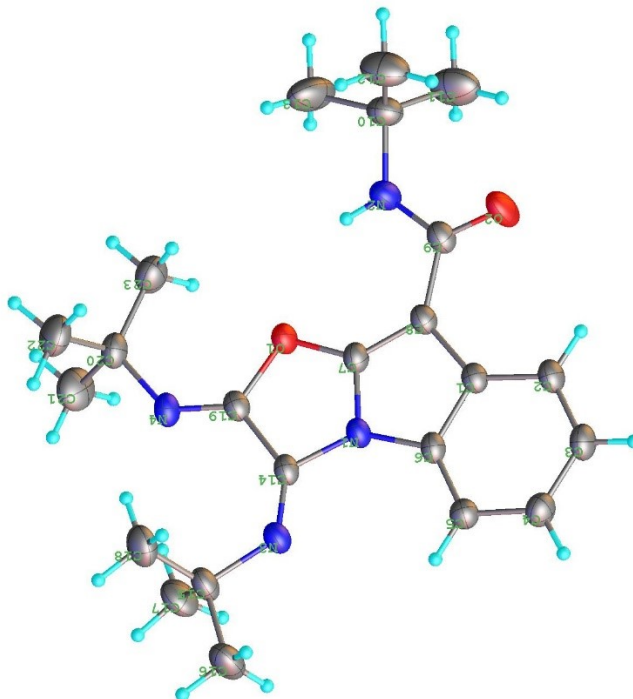


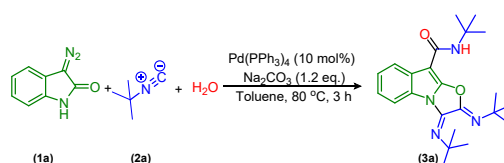
Figure S1: ORTEP diagram for the crystal structure of 3a (Ellipsoid = 50%)

Table S1:

Identification code	Ex-Thapar-pooja
Empirical formula	C ₂₃ H ₃₂ N ₄ O ₂
Formula weight	396.52
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.59358(18)
b/Å	10.5593(2)
c/Å	11.9248(3)
α /°	103.8143(19)
β /°	97.5949(17)
γ /°	98.8737(17)
Volume/Å ³	1140.89(4)
Z	2

$\rho_{\text{calc}}/\text{cm}^3$	1.154
μ/mm^{-1}	0.075
F(000)	428.0
Crystal size/ mm^3	$0.05 \times 0.04 \times 0.03$
Radiation	MoK α ($\lambda = 0.71073$)
2Θ range for data collection/ $^\circ$	6.474 to 52.74
Index ranges	$-11 \leq h \leq 11, -13 \leq k \leq 12, -14 \leq l \leq 14$
Reflections collected	15515
Independent reflections	4625 [Rint = 0.0351, Rsigma = 0.0350]
Data/restraints/parameters	4625/0/275
Goodness-of-fit on F^2	1.066
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0497, wR_2 = 0.1260$
Final R indexes [all data]	$R_1 = 0.0698, wR_2 = 0.1399$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.16/-0.23

Table S2: Optimization of the reaction conditions^a



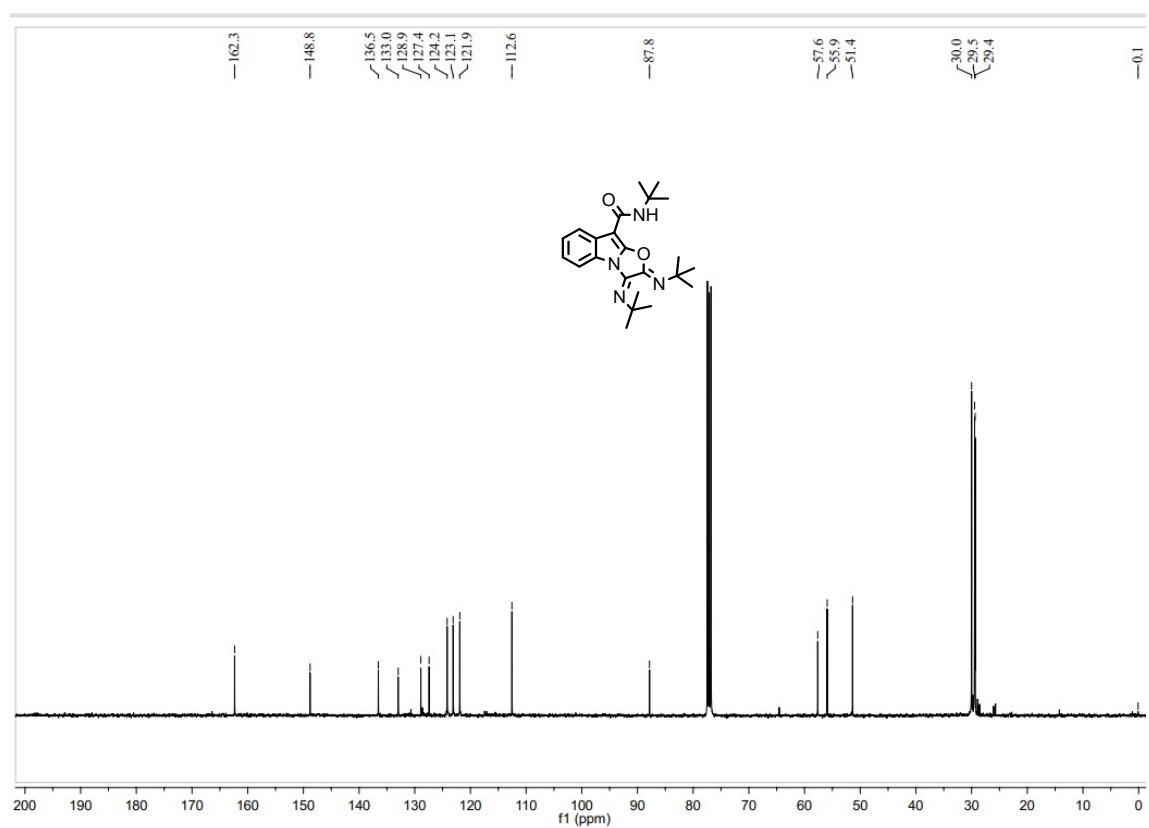
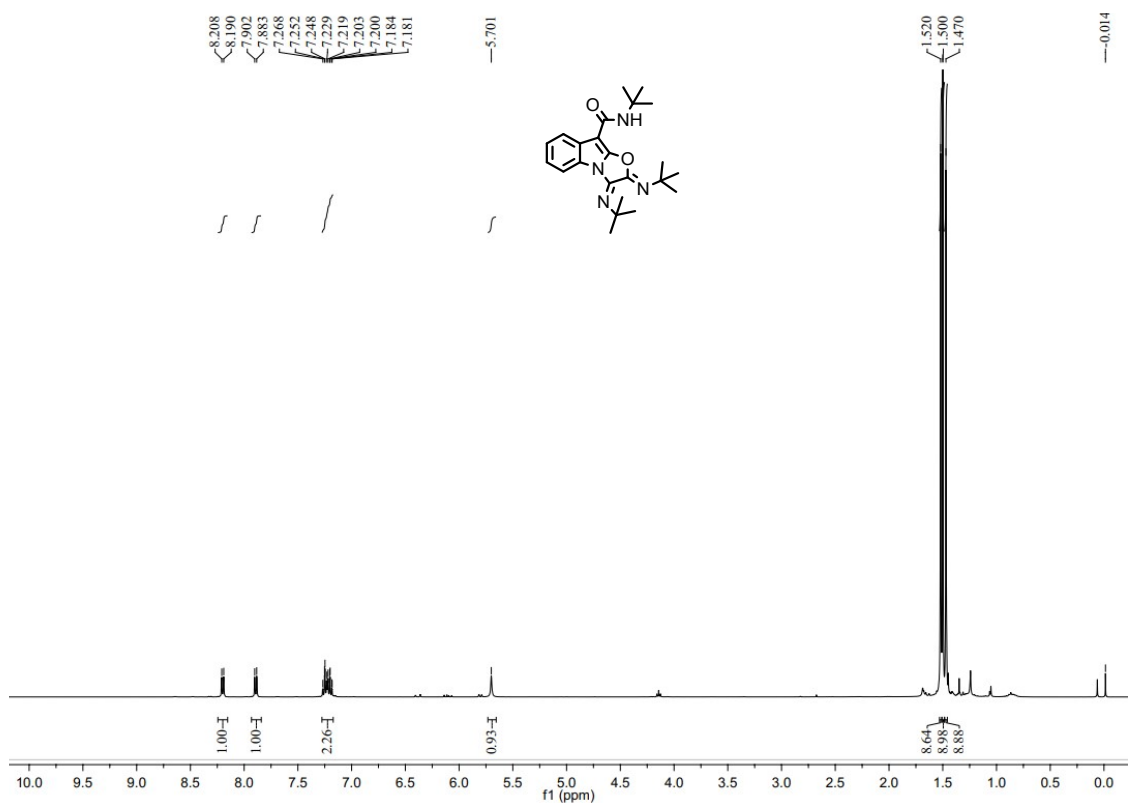
entry	deviation from standard conditions	yield ^b (%)
1.	PdCl_2 instead of $\text{Pd}(\text{PPh}_3)_4$	44
2.	$\text{PdCl}_2(\text{NCC}_6\text{H}_5)_2$ instead of $\text{Pd}(\text{PPh}_3)_4$	37
3.	$\text{Pd}(\text{DPPF})\text{Cl}_2$ instead of $\text{Pd}(\text{PPh}_3)_4$	41
4.	$\text{Pd}(\text{dba})_3$ instead of $\text{Pd}(\text{PPh}_3)_4$	32
5.	$\text{Pd}(\text{OAc})_2$ (5 mol% instead of 10 mol%).	48
6.	In absence of base	27
7.	CH_3CN instead of toluene	53
8.	DMF instead of toluene	57
9.	DMSO instead of toluene	54
10.	THF instead of toluene	50

11.	Added AgOAc as an additive	58
12.	Added CsOAc as an additive	63
13.	<i>tert</i> -butyl isocyanide (1.5 equiv.)	31
14.	<i>tert</i> -butyl isocyanide (2.0 equiv.)	43
15.	<i>tert</i> -butyl isocyanide (3.5 equiv.)	62
16.	<i>tert</i> -butyl isocyanide (4.0 equiv.)	60

^aReaction conditions: 3-diazo oxindole 1a (1.0 equiv., 0.31 mmol, 50 mg), *tert*-butyl isocyanide 2a (3.2 equiv., 113 μ L, 0.99 mmol), H₂O (1.0 equiv., 5.6 μ L), Pd-catalyst (10 mol%), base (1.2 equiv.), solvent (2 ml), for 3 h.
^bisolated yield.

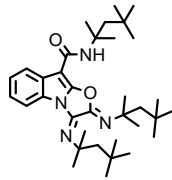
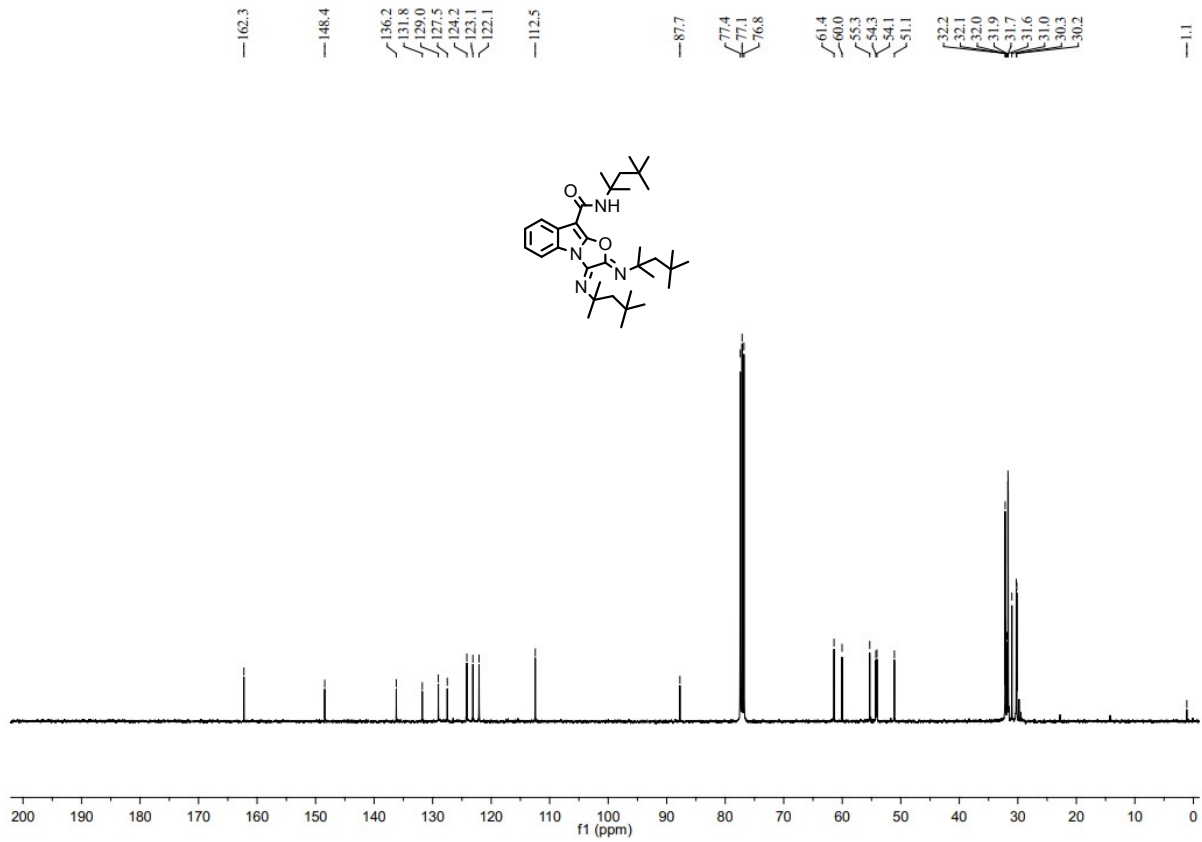
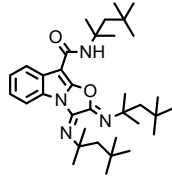
Copies of ¹H NMR and ¹³C{¹H} NMR data of compounds (3a-3q, 4)

¹H NMR (400 MHz, CDCl₃) and ¹³C{¹H} NMR (100 MHz, CDCl₃) spectra of 3a

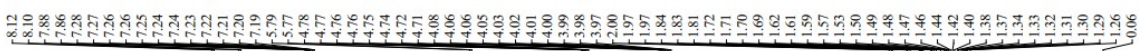


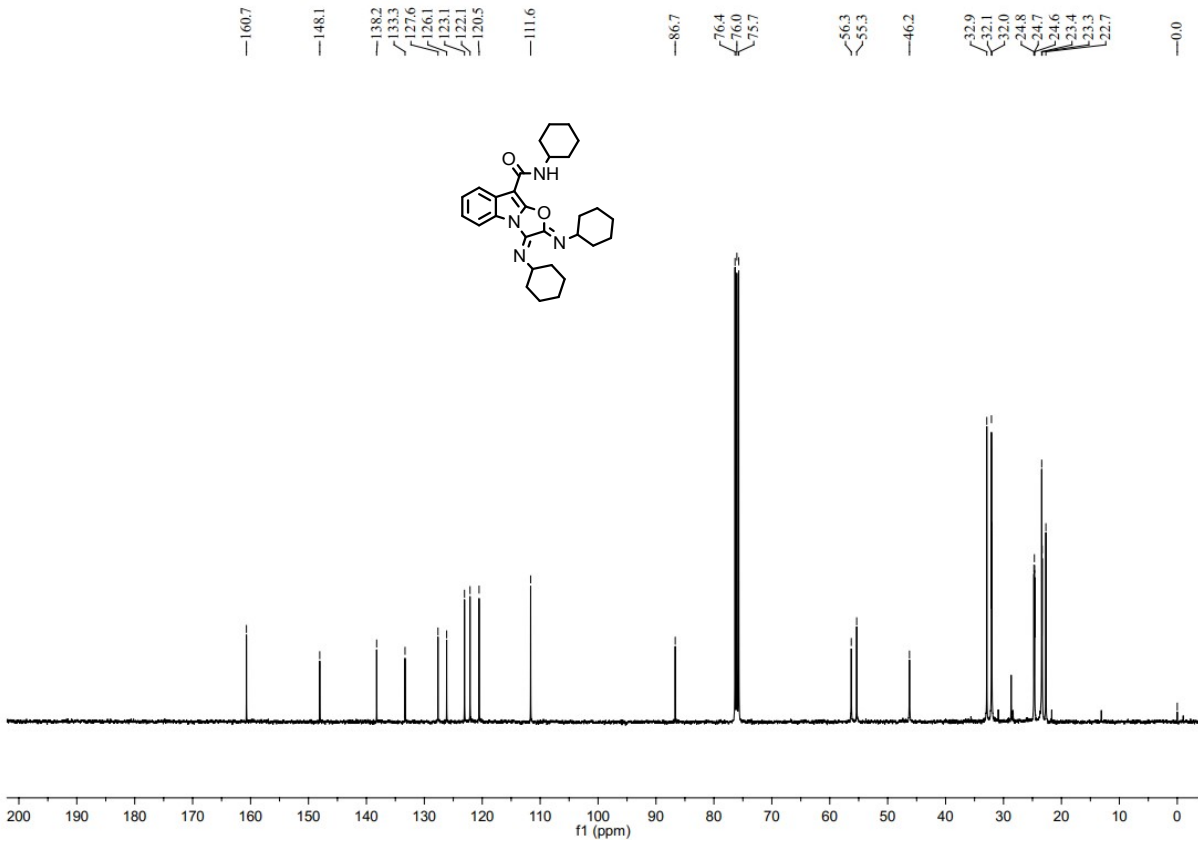
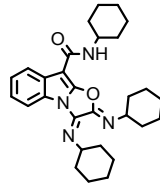
^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3b





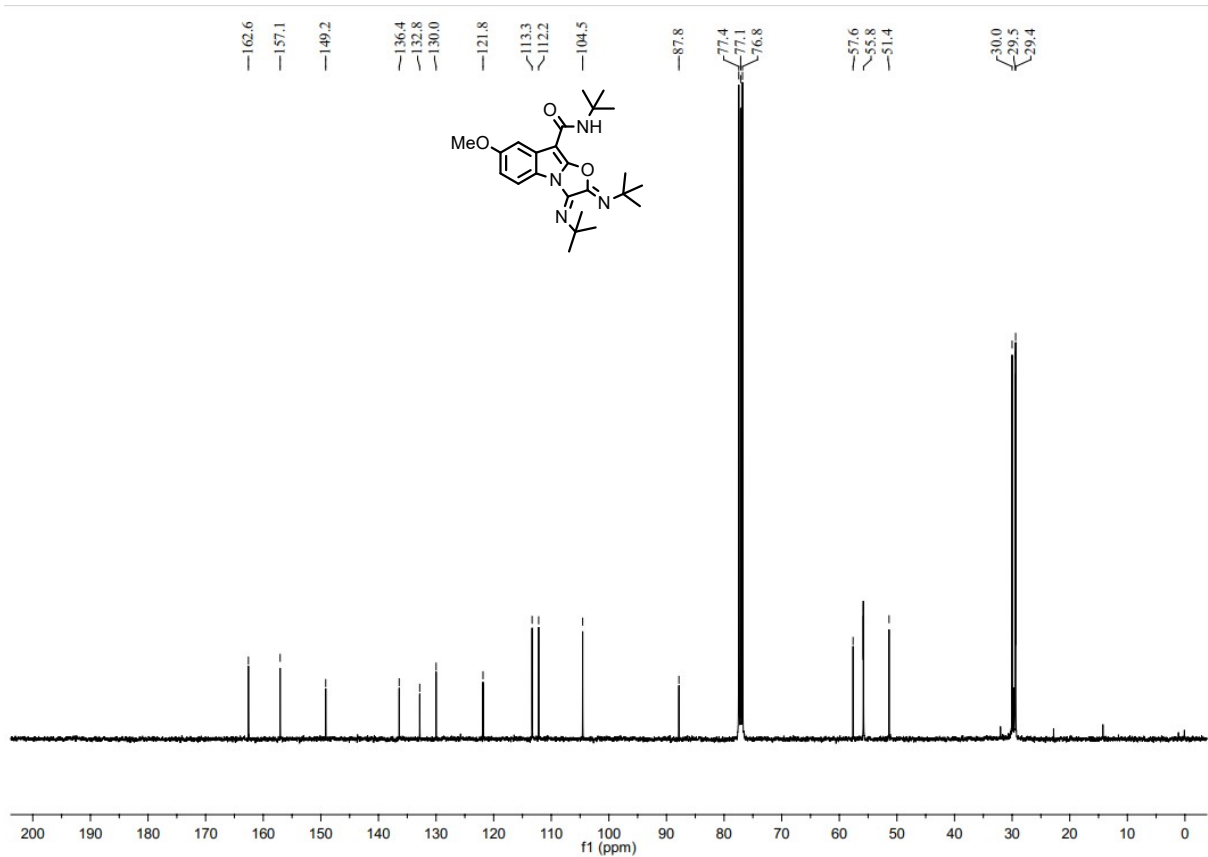
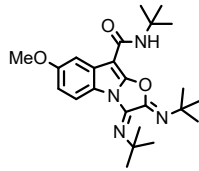
¹H NMR (400 MHz, CDCl₃) and ¹³C{¹H} NMR (100 MHz, CDCl₃) spectra of 3c



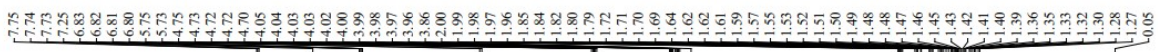


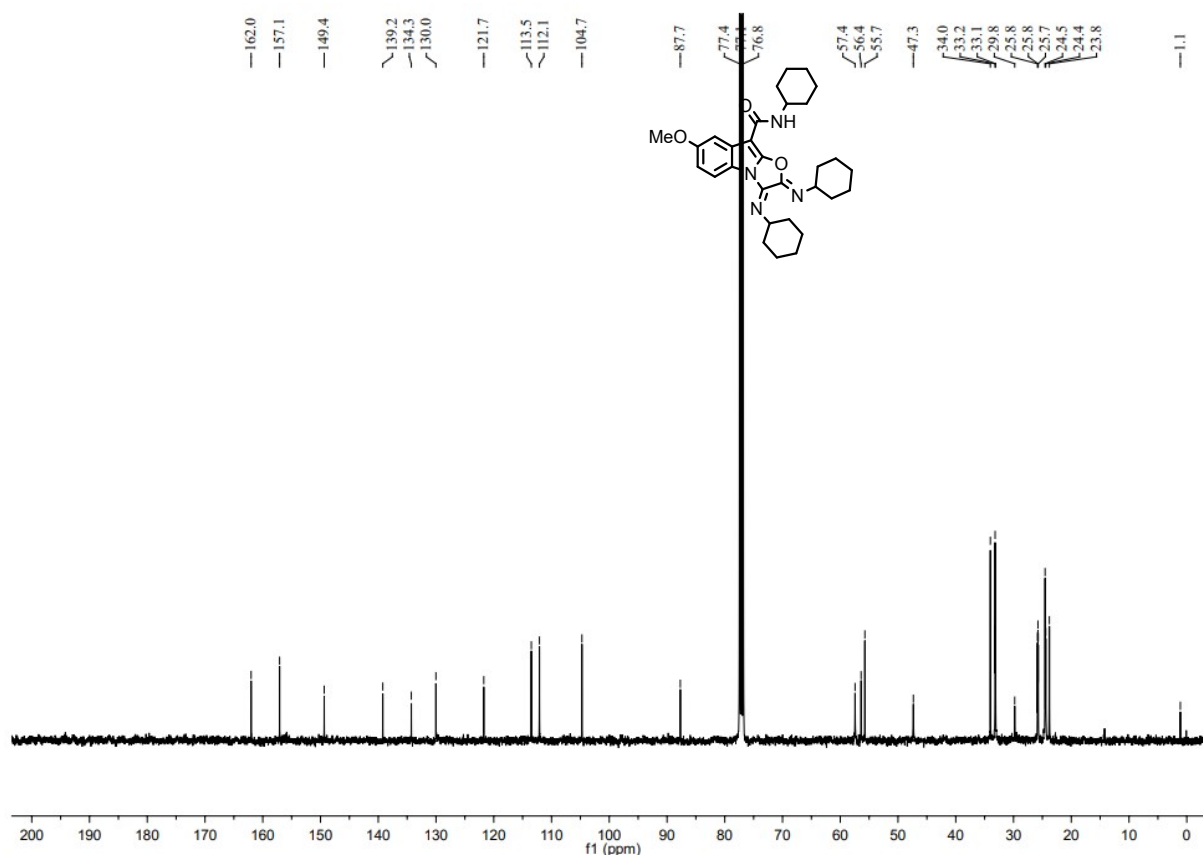
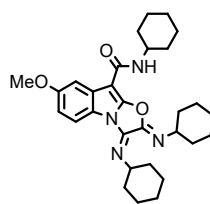
^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3d





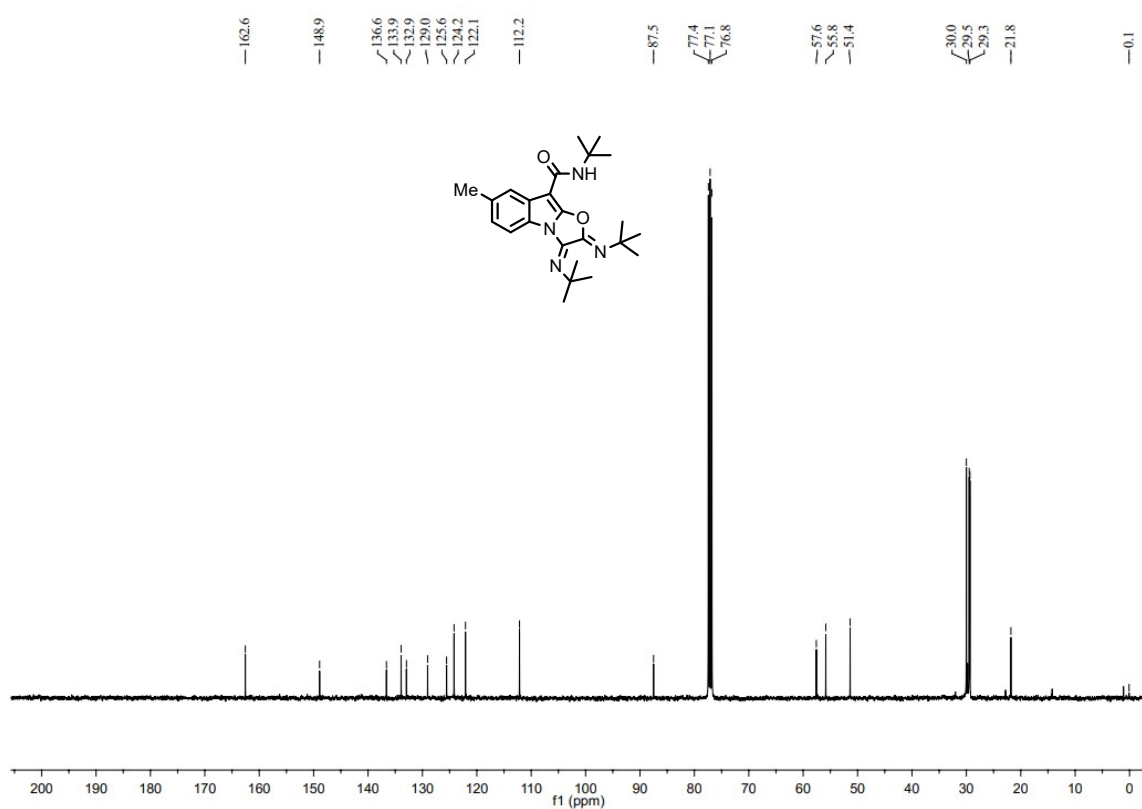
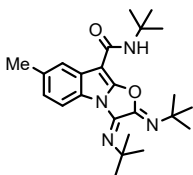
¹H NMR (400 MHz, CDCl₃) and ¹³C{¹H} NMR (100 MHz, CDCl₃) spectra of 3e





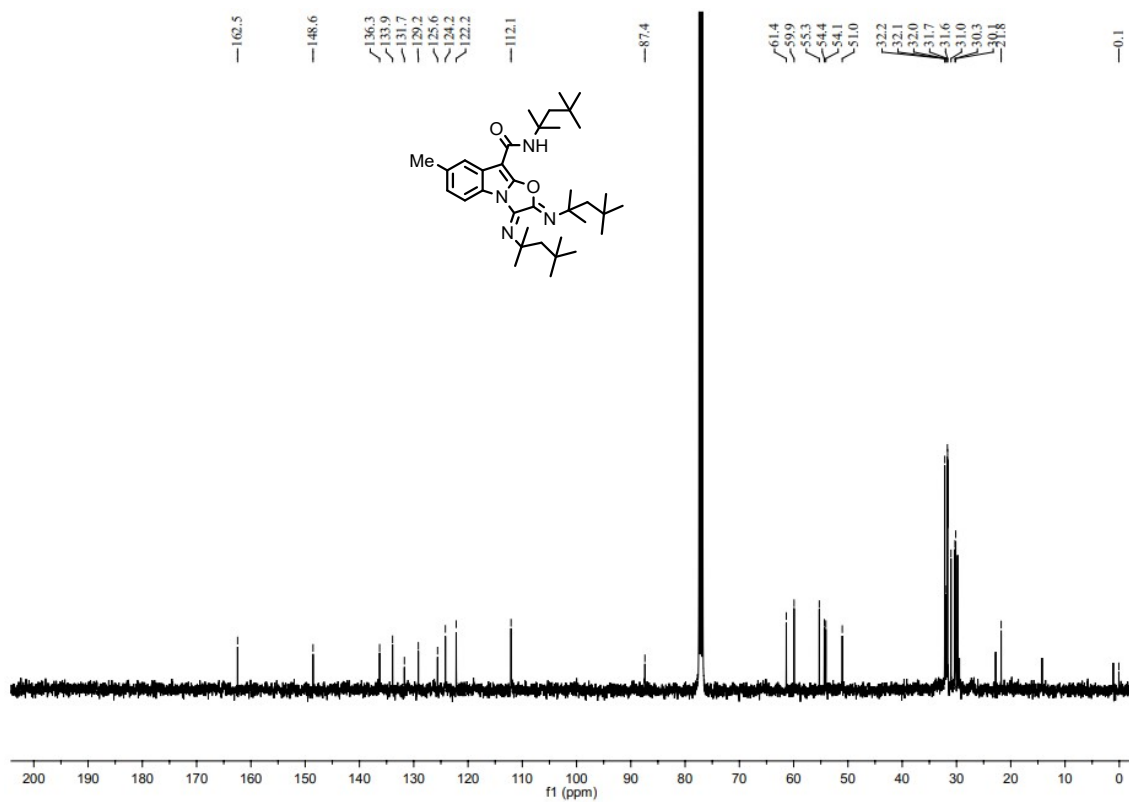
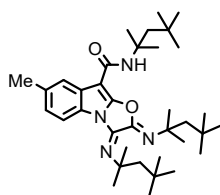
^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3f



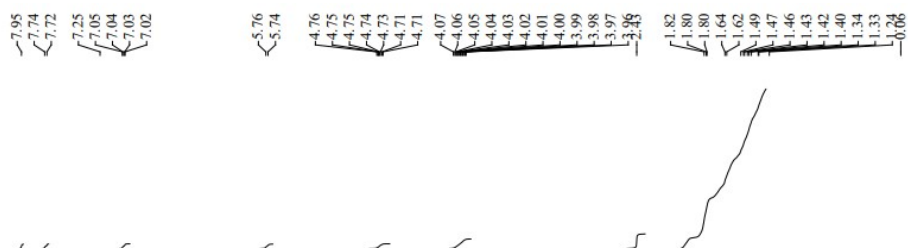


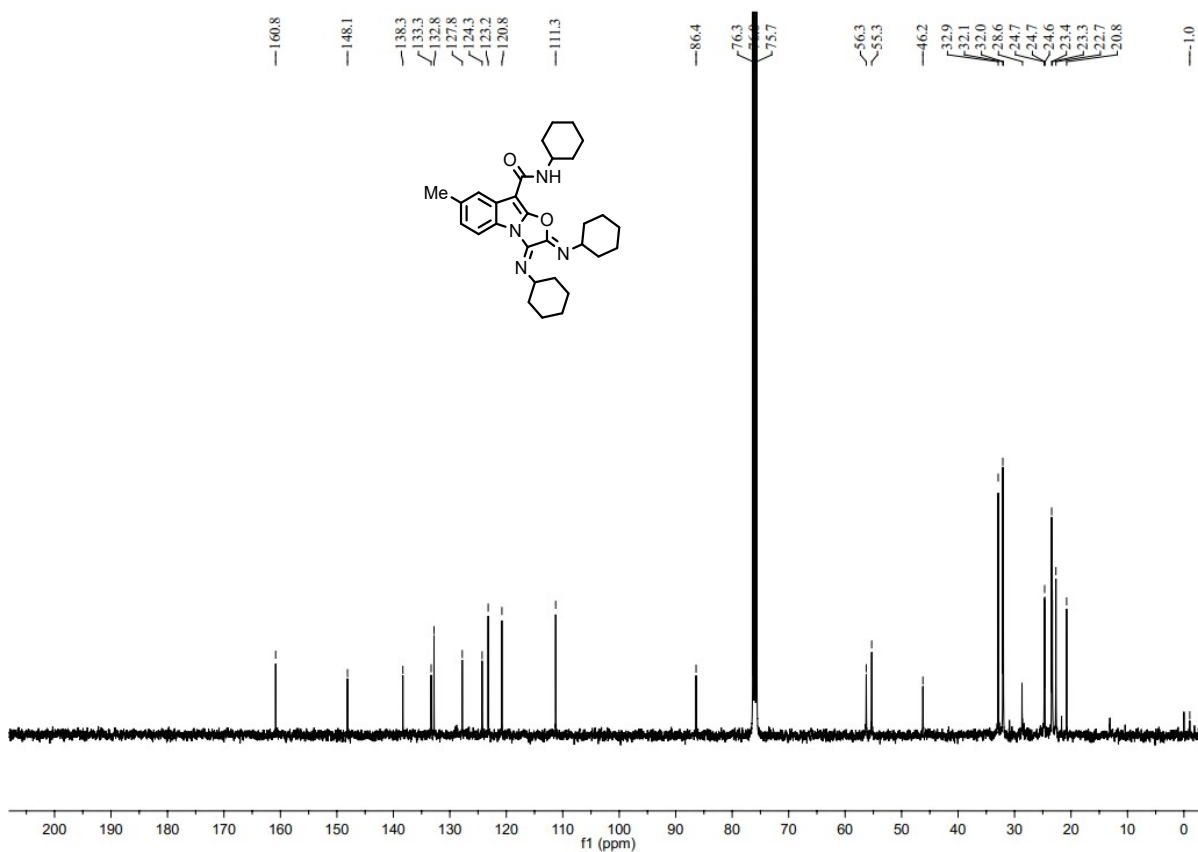
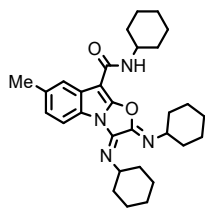
^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3g



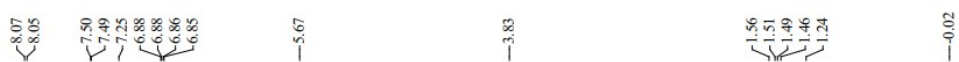


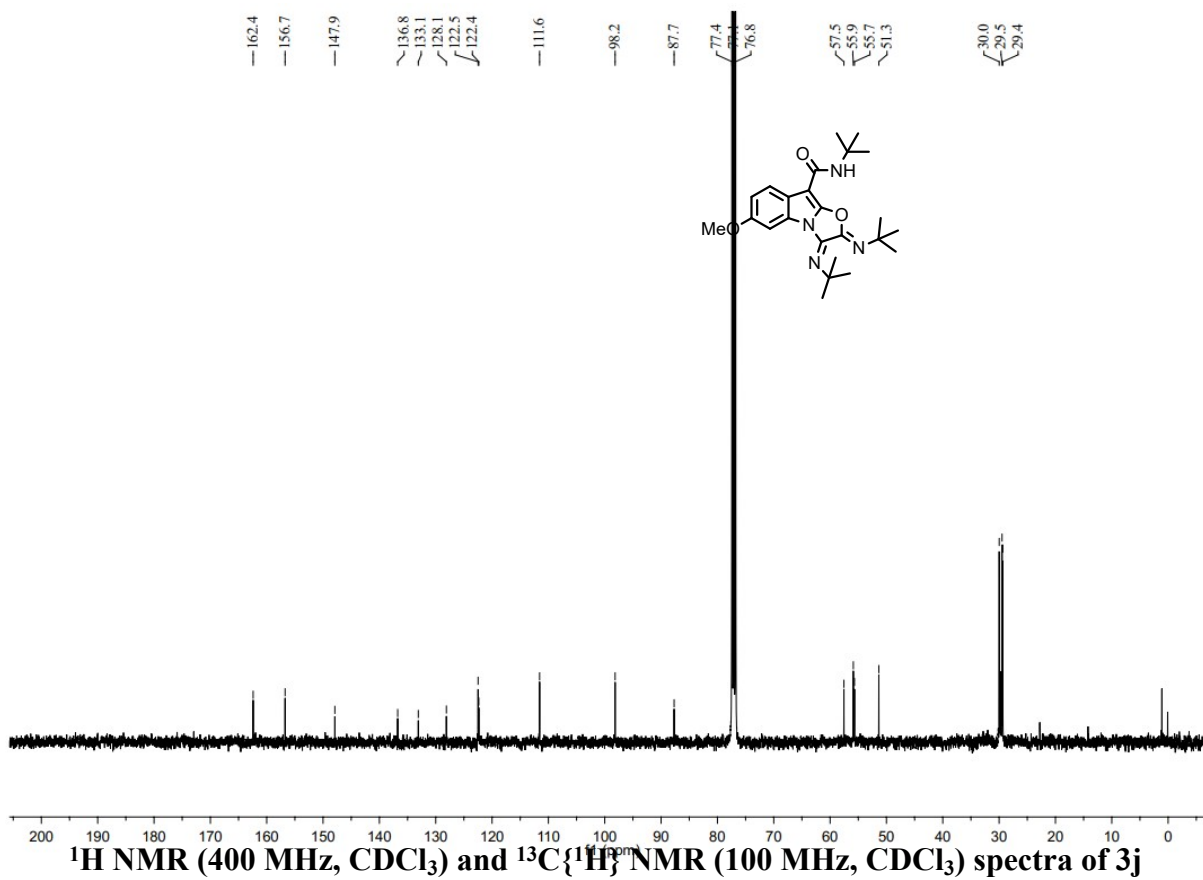
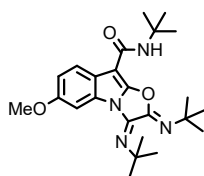
^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3h





^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3i

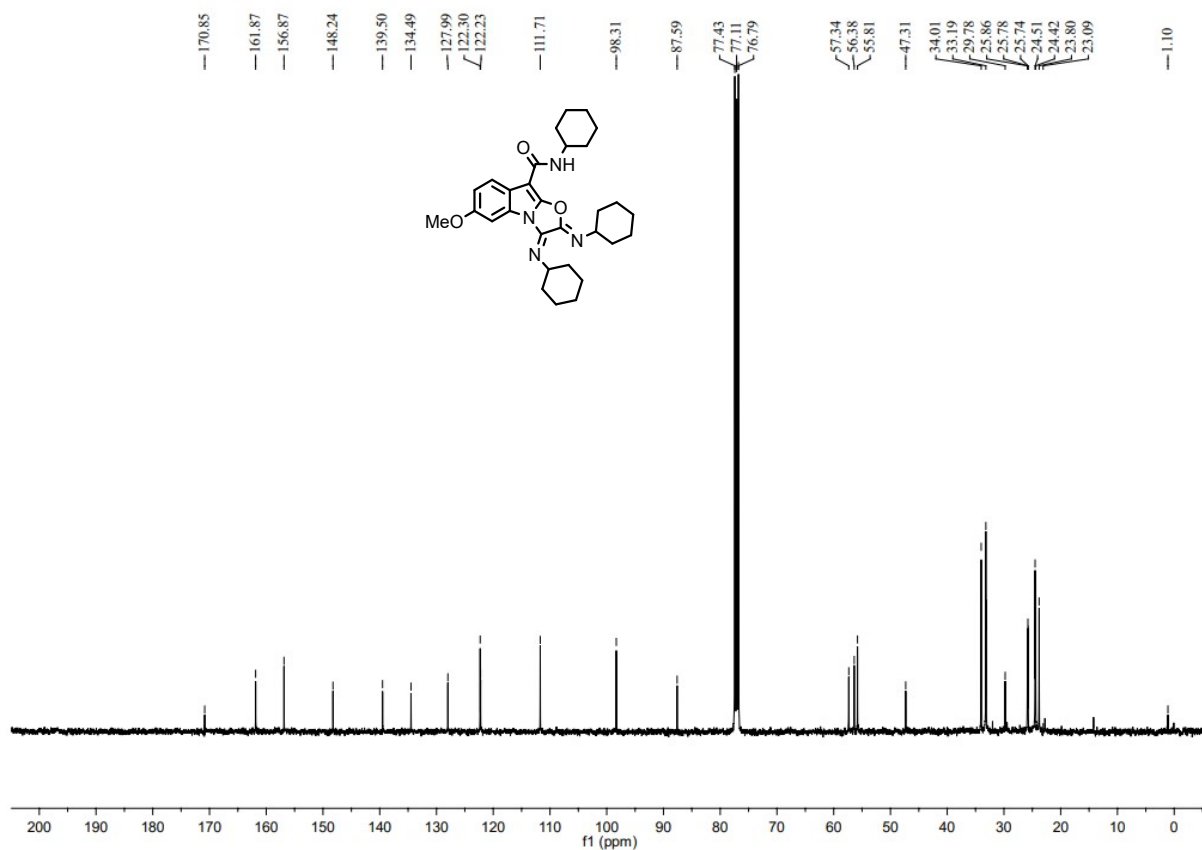
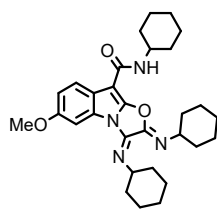




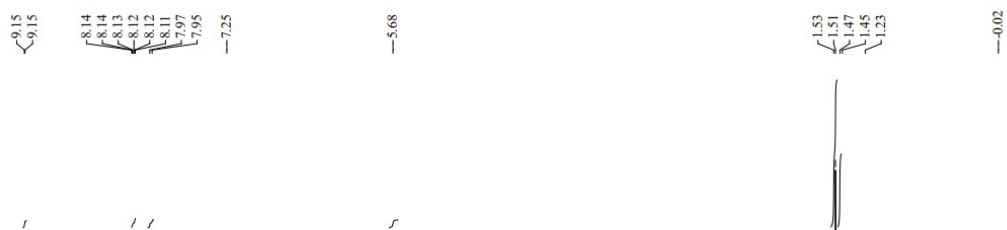
¹³C NMR peaks (ppm): 162.4, 156.7, 147.9, 136.8, 133.1, 128.1, 122.5, 122.4, 111.6, 98.2, 87.7, 77.4, 76.8, 57.5, 55.9, 55.7, 51.3, 30.0, 29.5, 29.4

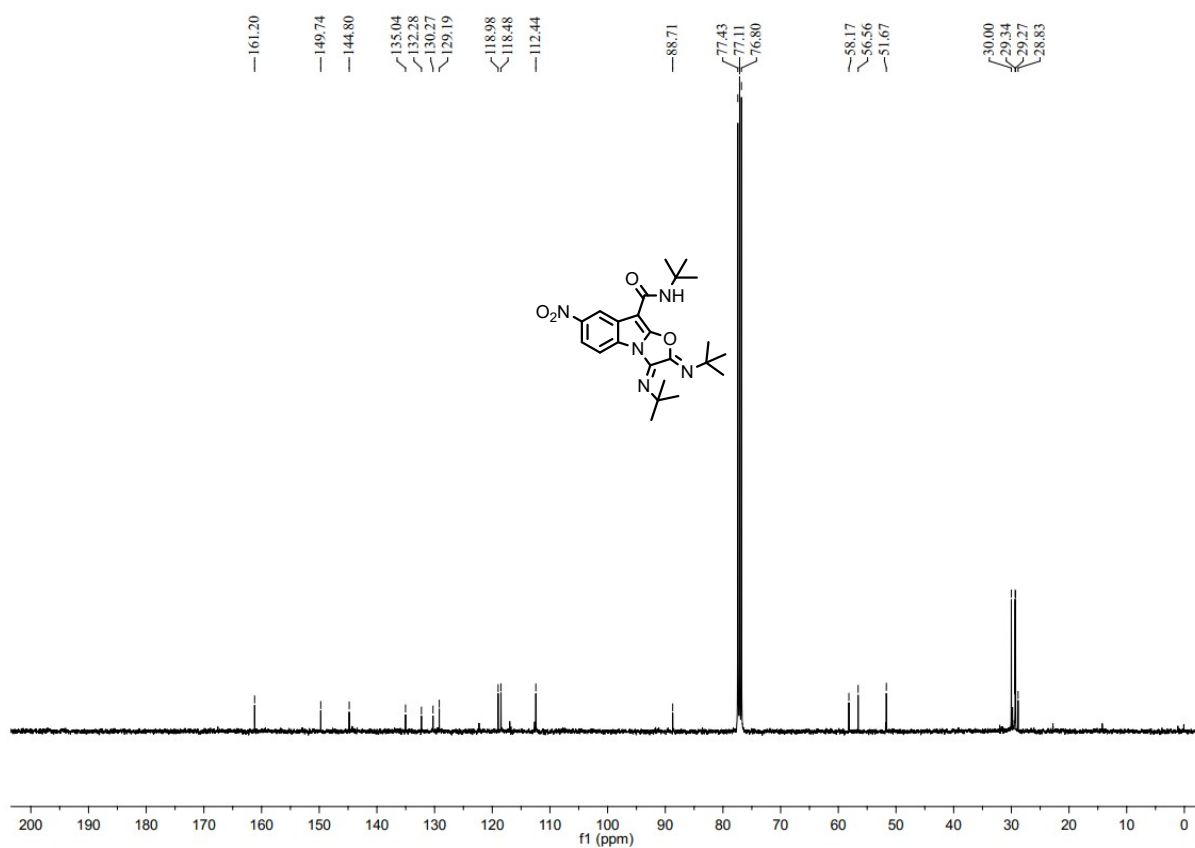
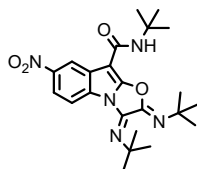
¹H NMR peaks (ppm): 8.01, 7.99, 7.46, 7.45, 7.25, 6.89, 6.88, 6.87, 5.73, 5.71, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.05, 4.04, 4.03, 4.01, 3.99, 3.99, 3.98, 3.96, 3.85, 1.82, 1.80, 1.80, 1.64, 1.62, 1.58, 1.50, 1.49, 1.47, 1.46, 1.45, 1.42, 1.40, 1.34, 1.32, 1.29, 1.29, 0.06, 0.02





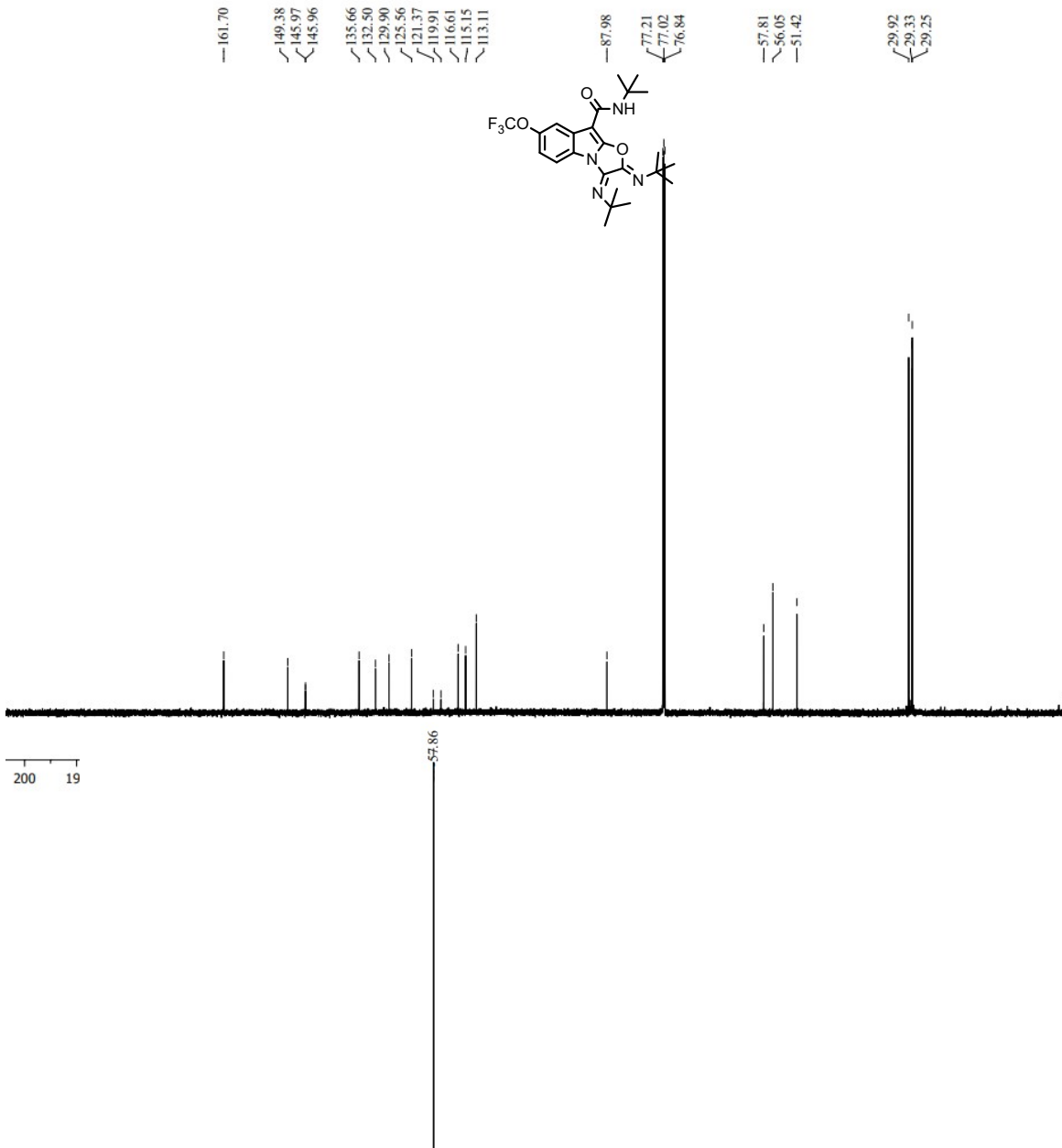
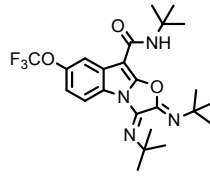
¹H NMR (400 MHz, CDCl₃) and ¹³C{¹H} NMR (100 MHz, CDCl₃) spectra of 31

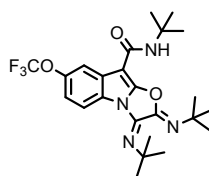




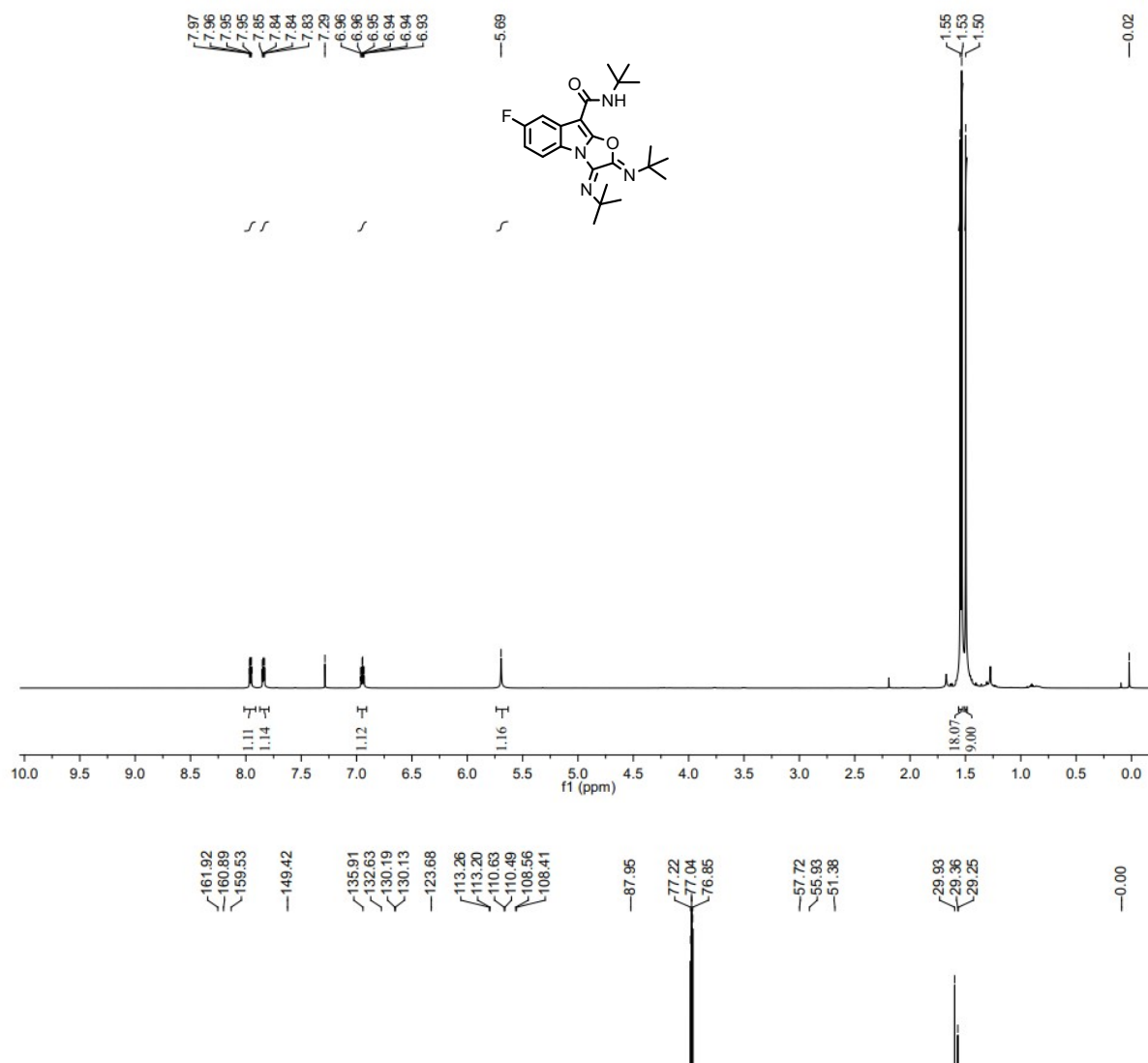
^1H NMR (700 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ NMR (175 MHz, CDCl_3), $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) spectra of 3m

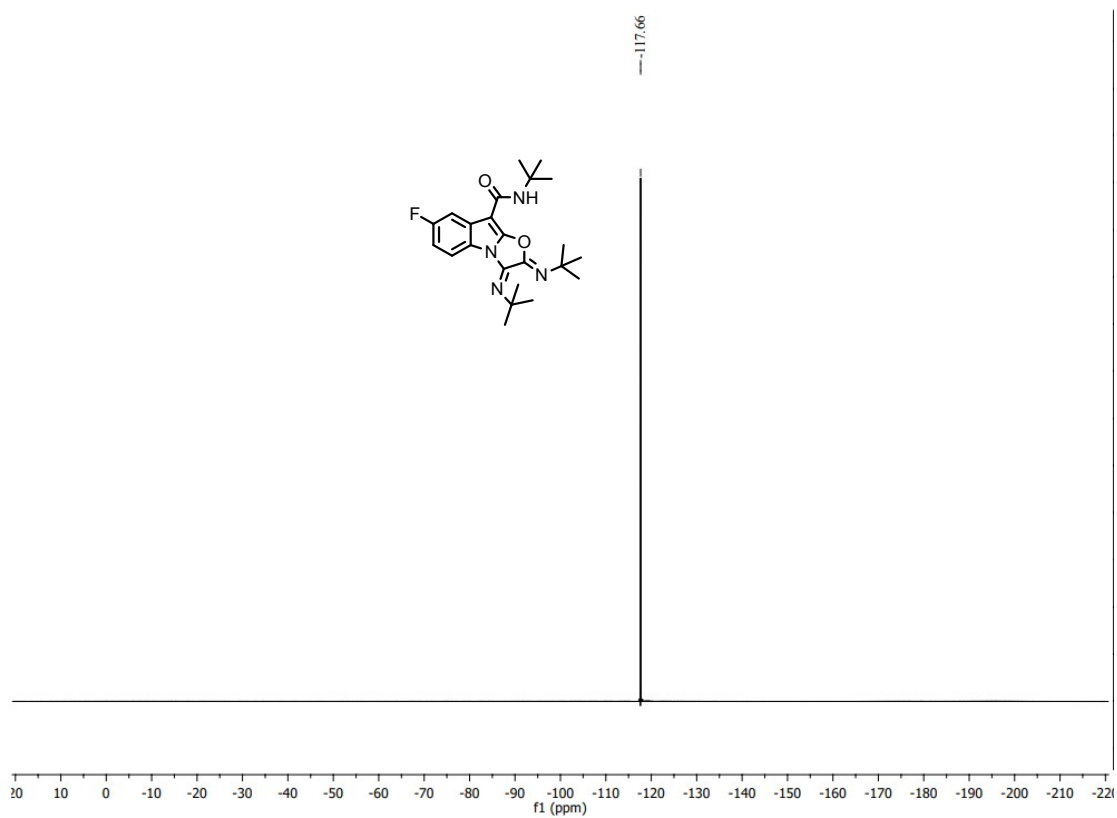
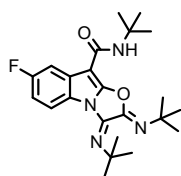




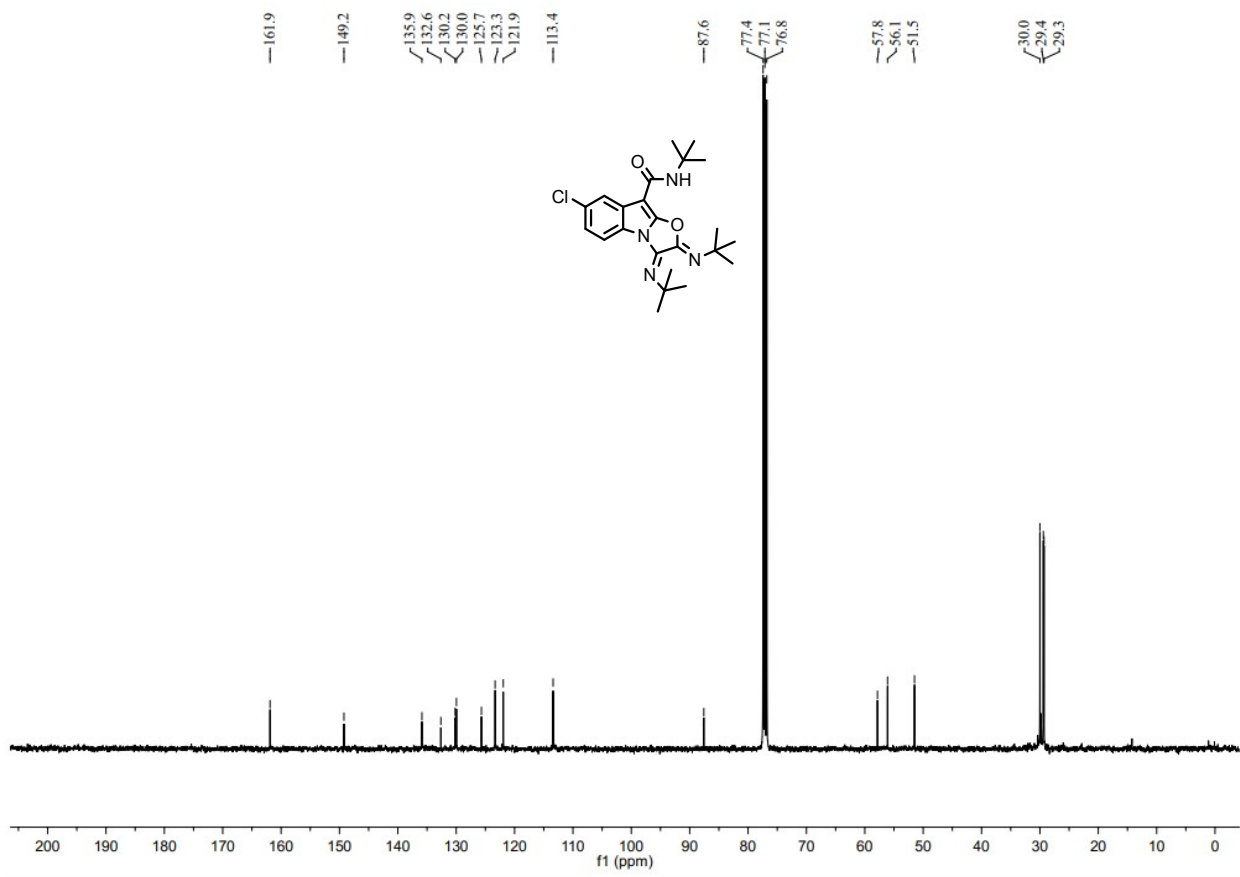
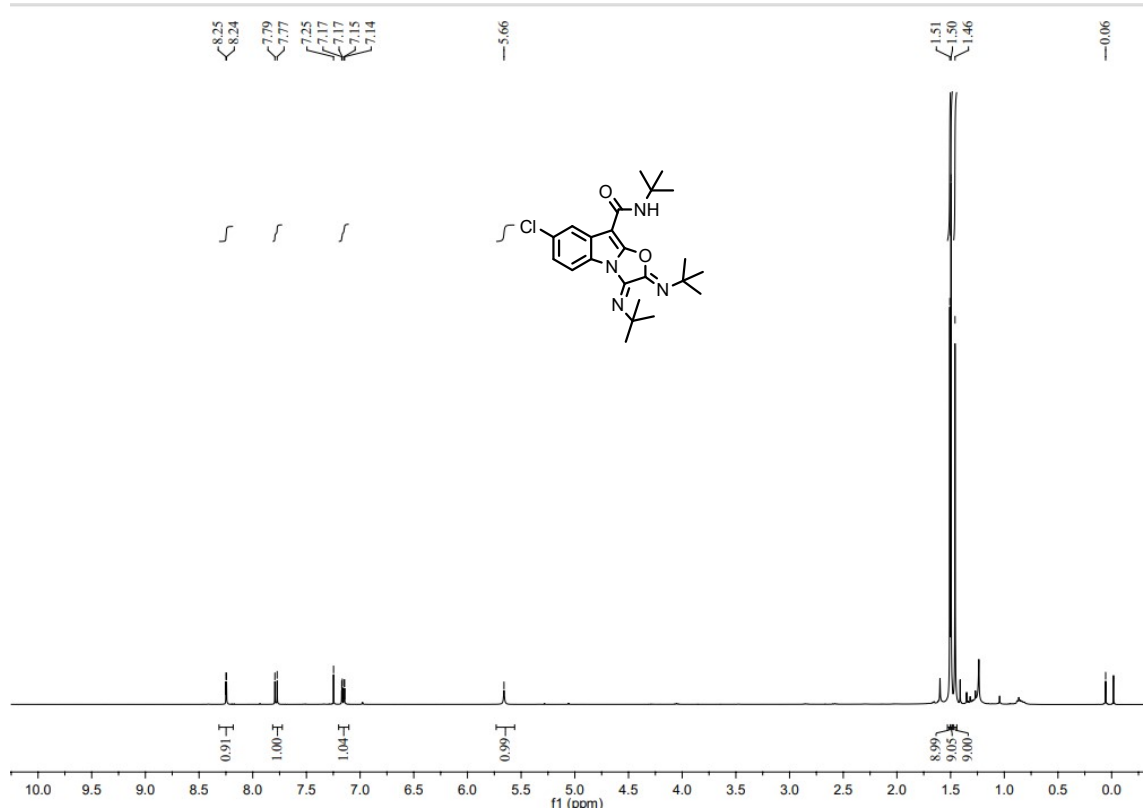


^1H NMR (700 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ NMR (175 MHz, CDCl_3) and $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) spectra of 3q



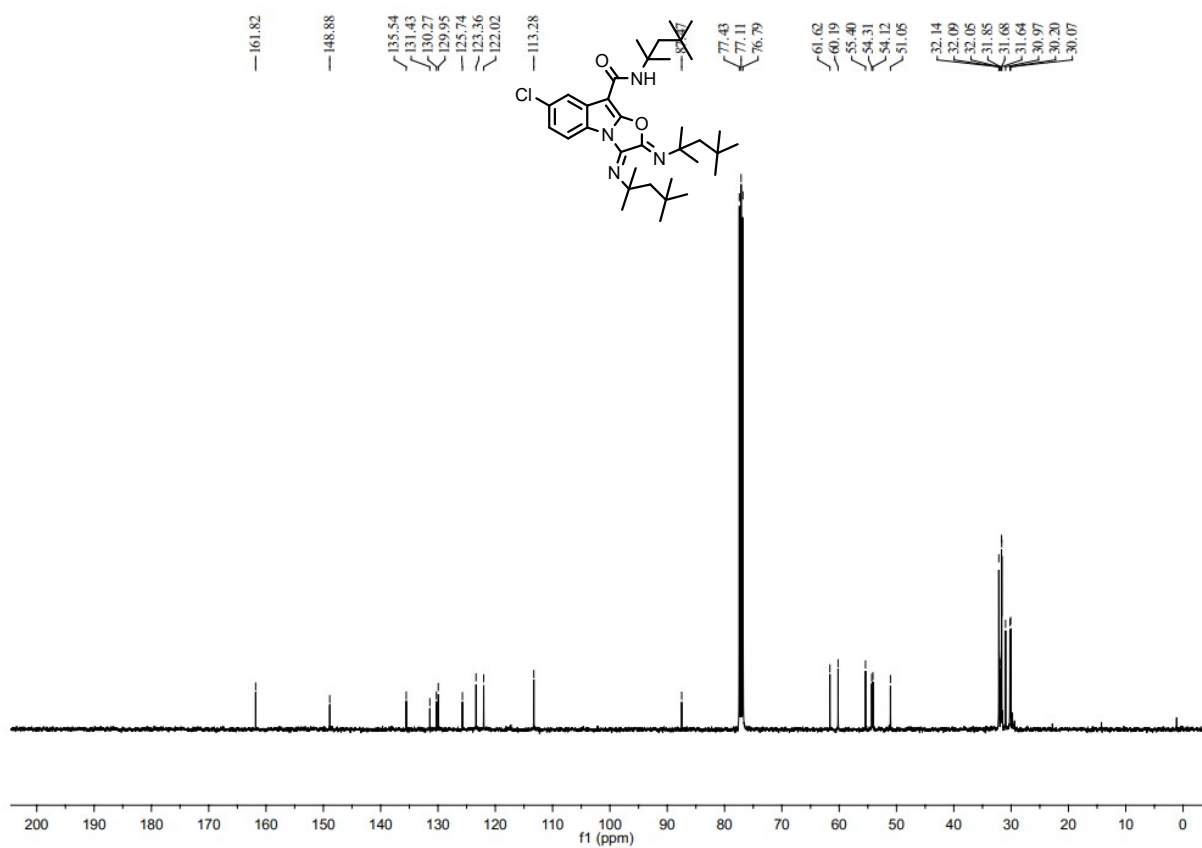
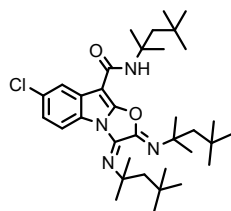


^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3r



¹H NMR (400 MHz, CDCl₃) and ¹³C{¹H} NMR (100 MHz, CDCl₃) spectra of 3s





^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3t

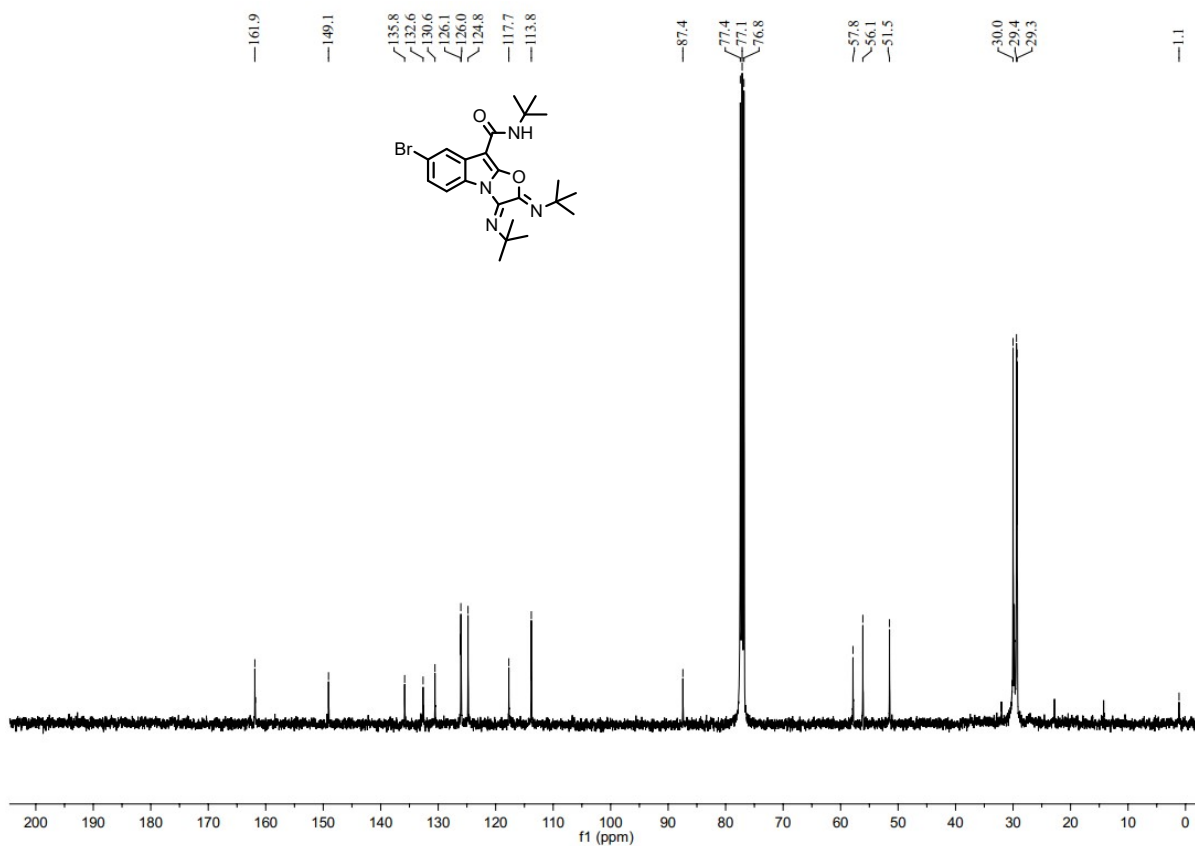
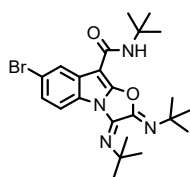
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8.41

7.74
7.72
7.31
7.31
7.29
7.29

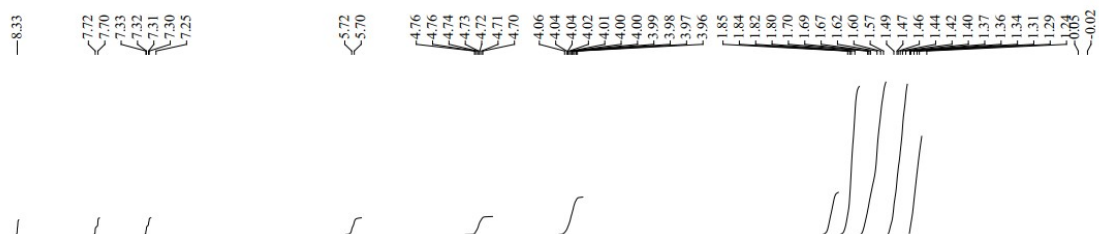
5.66

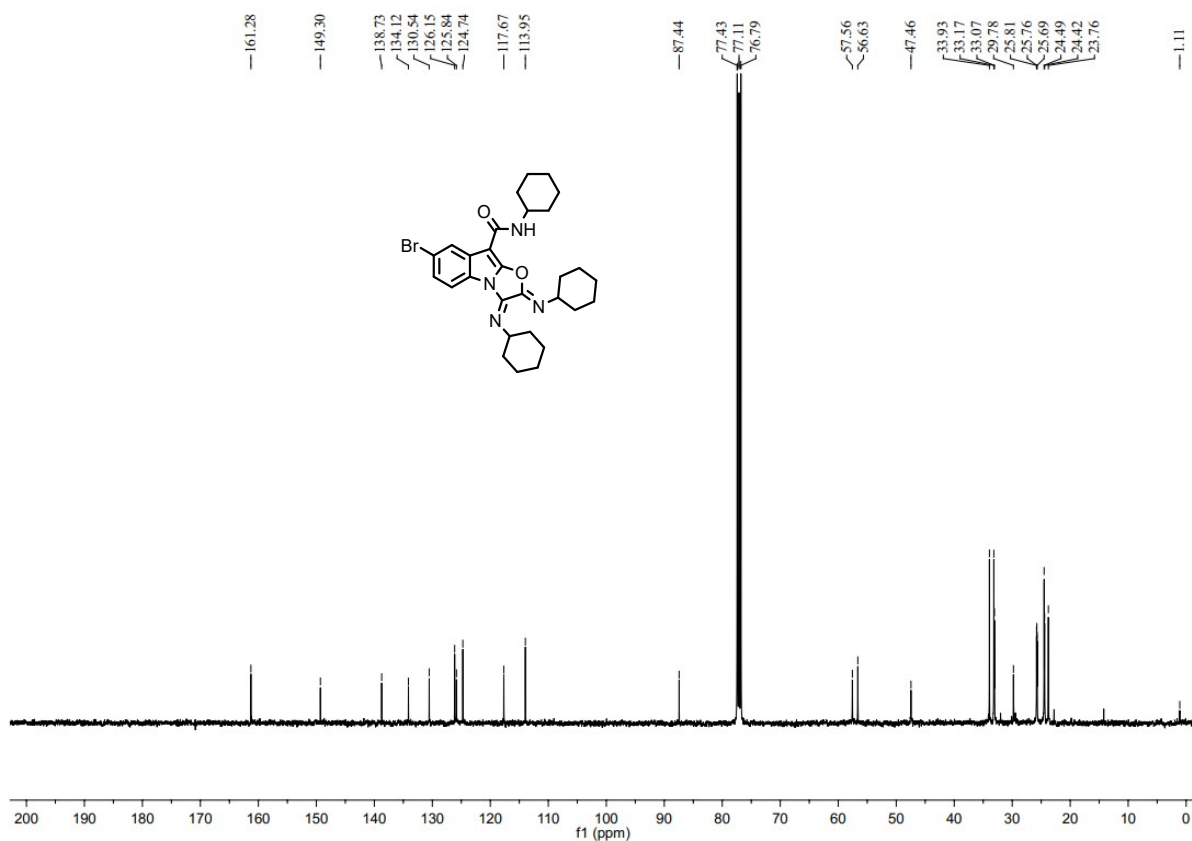
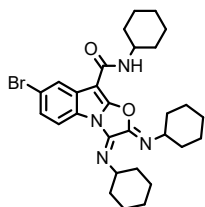
1.50
1.49
1.46

0.05

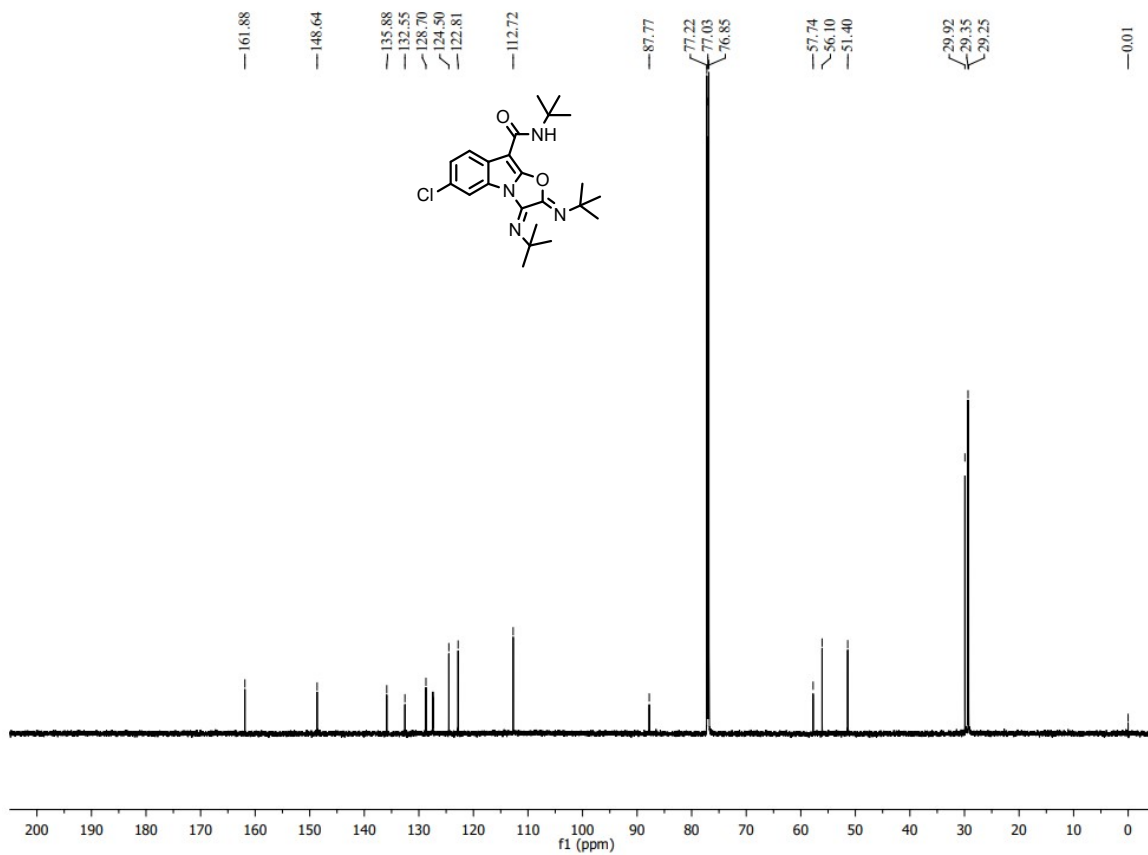
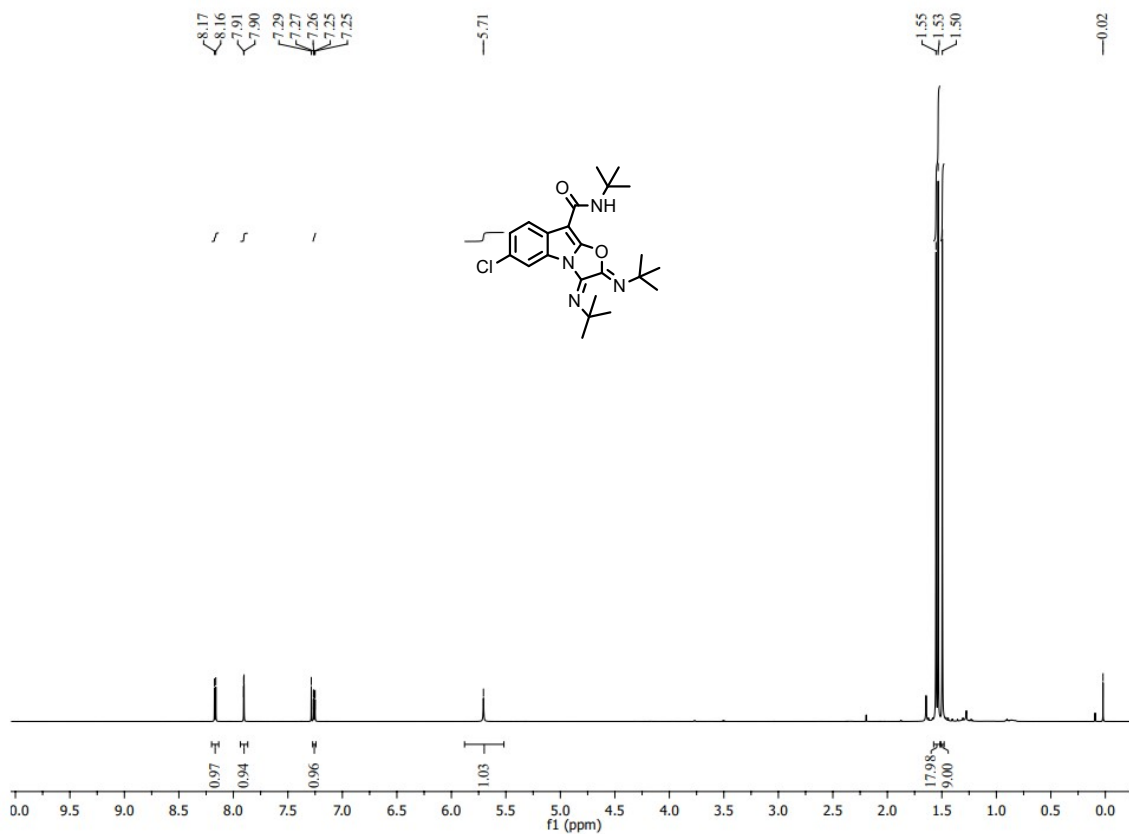


^1H NMR (400 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) spectra of 3u

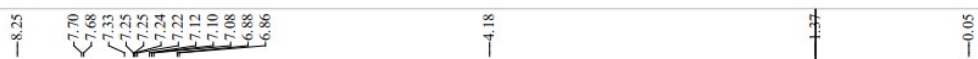


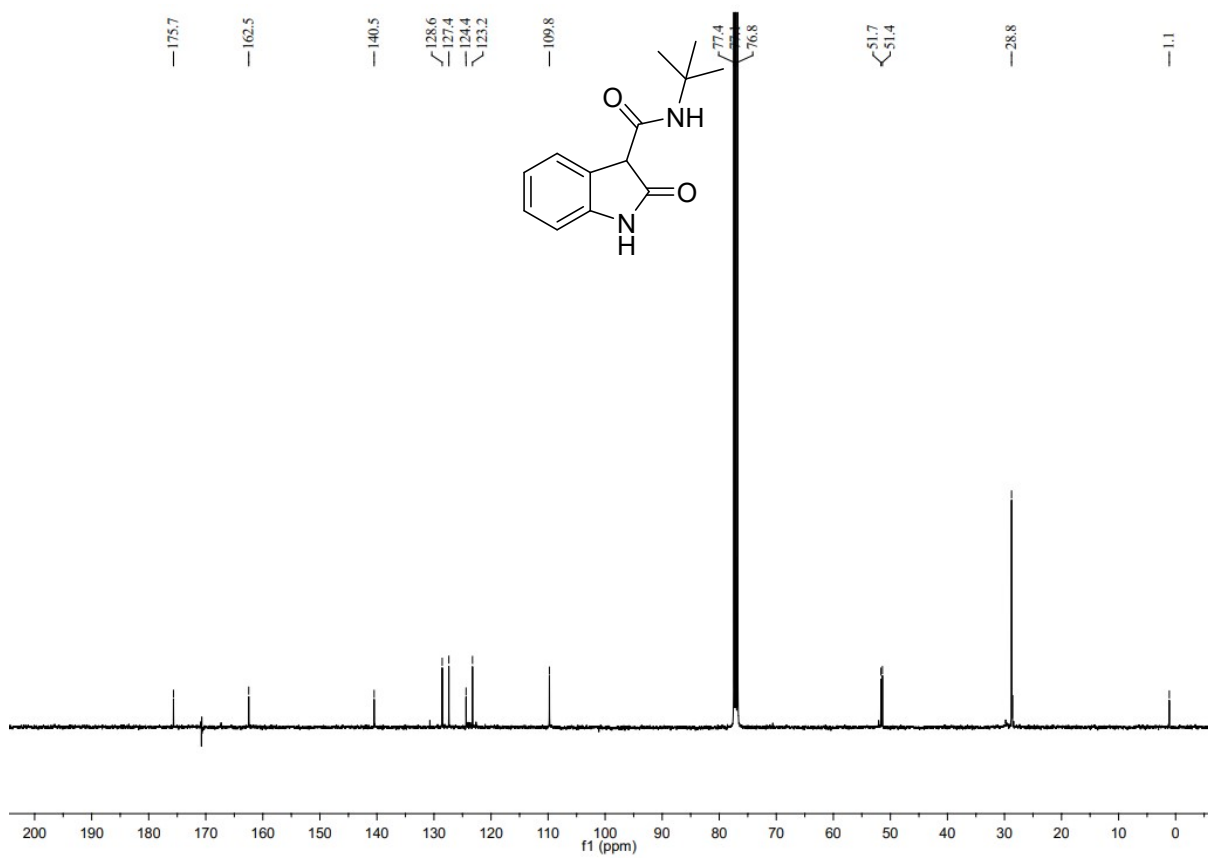
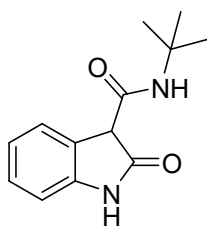


^1H NMR (700 MHz, CDCl_3) and $^{13}\text{C}\{^1\text{H}\}$ NMR (175 MHz, CDCl_3) spectra of 3v



¹H NMR (400 MHz, CDCl₃) and ¹³C{¹H} NMR (100 MHz, CDCl₃) spectra of 4

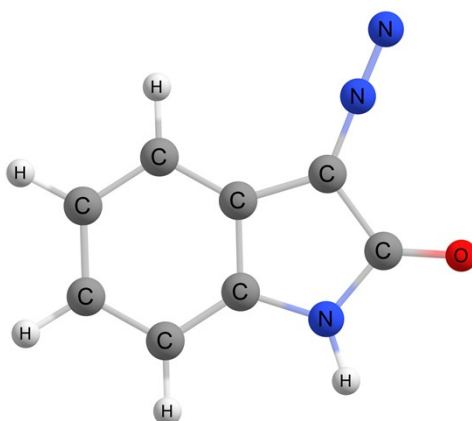




Computational details

All of the structures in the study were optimized using the DFT-B3LYP⁷ method with the 6-31+G(d,p)⁸ basis set for all atoms except for Pd, which uses the SDD method with its own electrostatic potential⁹. The optimization has been conducted in presence of solvent 1,4-Dioxane using solvation model density (SMD) approximation¹⁰. At the same level of theory, frequency studies were also done to make sure that the stationary points were either local minimums (with no imaginary frequencies) or transition states (with one imaginary frequency). Further energy refinement was also done using single-point calculations on the optimized geometries at the Minnesota density functional M06¹¹ with a larger basis set 6-31++G(2d,2p)¹² for all non-metal atoms. The previous level's basis for Pd and solvent corrections was maintained. The solvated Gibbs free energy, which was utilized for discussion, was determined by adding thermal correction to the Gibbs energy with the single-point electronic energy. The visualization and results analysis were carried out by using Chemcraft visualization Software.¹³ All the DFT calculations were performed using Gaussian 16 program.¹⁴

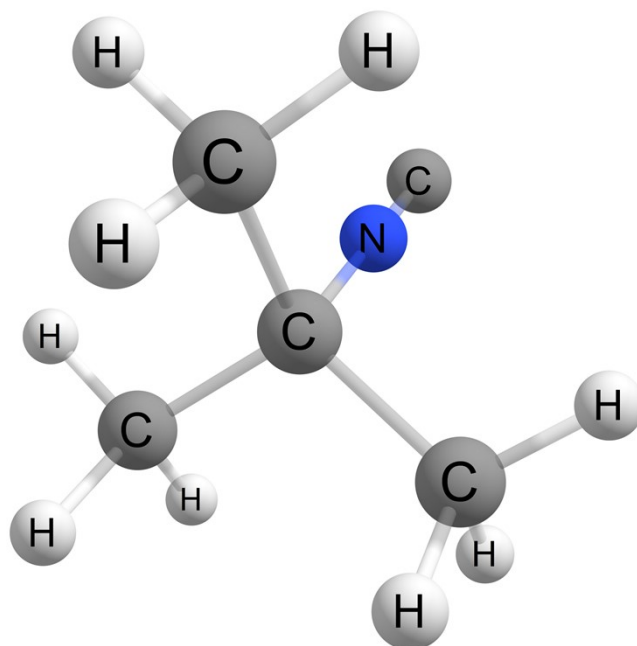
1. [1a] 3-diazo oxindole



Zero-point correction=	0.120545 (Hartree/Particle)
Thermal correction to Energy=	0.129484
Thermal correction to Enthalpy=	0.130428
Thermal correction to Gibbs Free Energy=	0.086195
Sum of electronic and zero-point Energies=	-547.226124
Sum of electronic and thermal Energies=	-547.217185
Sum of electronic and thermal Enthalpies=	-547.216241
Sum of electronic and thermal Free Energies=	-547.260474

C	0.333776000	-0.454081000	0.000000000
C	0.817770000	0.875940000	0.000000000
C	2.180394000	1.149056000	0.000000000
C	3.065993000	0.062263000	0.000000000
C	2.595946000	-1.256750000	0.000000000
C	1.221738000	-1.527766000	0.000000000
C	-1.115192000	-0.329748000	0.000000000
C	-1.489863000	1.105651000	0.000001000
H	2.547864000	2.170778000	0.000000000
H	4.135232000	0.251388000	0.000000000
H	3.302857000	-2.080656000	0.000000000
H	0.859172000	-2.551540000	0.000000000
N	-2.005555000	-1.279255000	0.000000000
N	-2.800354000	-2.093690000	0.000000000
O	-2.600427000	1.624262000	0.000000000
N	-0.266186000	1.758810000	0.000000000
H	-0.200423000	2.767499000	-0.000001000

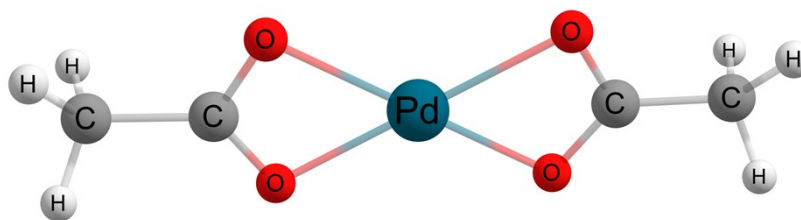
2. [2a] *tert*-butyl isocyanide



Zero-point correction=	0.129804 (Hartree/Particle)
Thermal correction to Energy=	0.137123
Thermal correction to Enthalpy=	0.138067
Thermal correction to Gibbs Free Energy=	0.099622
Sum of electronic and zero-point Energies=	-250.563278
Sum of electronic and thermal Energies=	-250.555959
Sum of electronic and thermal Enthalpies=	-250.555015
Sum of electronic and thermal Free Energies=	-250.593461

C	0.261415000	-0.000017000	-0.000075000
C	0.733521000	1.172140000	-0.877687000
H	0.371282000	2.125679000	-0.481890000
H	1.827615000	1.196609000	-0.896764000
H	0.370334000	1.061744000	-1.903860000
C	0.734078000	0.173999000	1.453659000
H	0.371346000	1.118112000	1.871007000
H	0.371803000	-0.645256000	2.081926000
H	1.828187000	0.177960000	1.483997000
C	0.733438000	-1.346236000	-0.576309000
H	0.370425000	-2.179457000	0.032820000
H	0.371086000	-1.480666000	-1.599885000
H	1.827519000	-1.374960000	-0.588158000
N	-1.188281000	0.000110000	0.000200000
C	-2.361057000	0.000025000	0.000313000

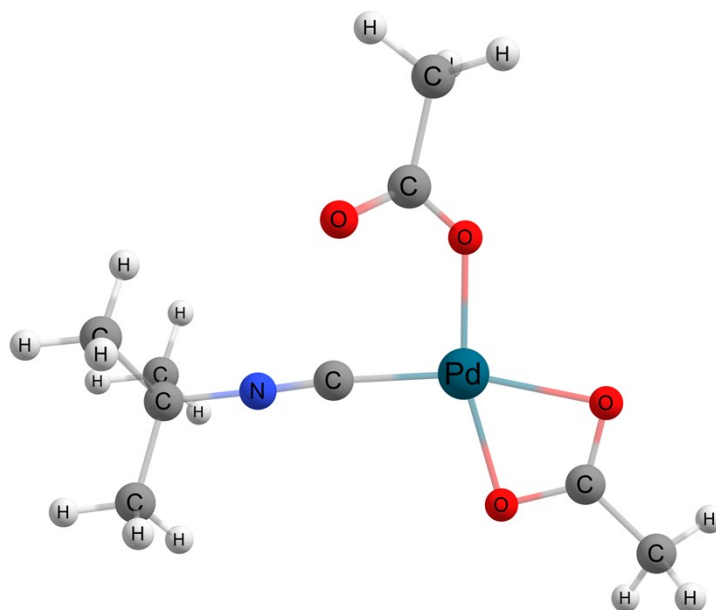
3. [Pd(OAc)₂]



Zero-point correction=	0.102793 (Hartree/Particle)
Thermal correction to Energy=	0.111825
Thermal correction to Enthalpy=	0.112769
Thermal correction to Gibbs Free Energy=	0.067170
Sum of electronic and zero-point Energies=	-584.850767
Sum of electronic and thermal Energies=	-584.841736
Sum of electronic and thermal Enthalpies=	-584.840792
Sum of electronic and thermal Free Energies=	-584.886391

Pd	-0.000029000	-0.001028000	-0.008675000
O	1.766433000	1.086931000	-0.010472000
C	2.446751000	0.000245000	-0.005206000
O	-1.768465000	-1.087042000	-0.010156000
C	-2.446727000	0.000784000	-0.005109000
O	-1.766155000	1.087247000	-0.010225000
O	1.768311000	-1.087416000	-0.010290000
C	-3.937388000	0.002259000	0.034555000
H	-4.330941000	-0.889997000	-0.457739000
H	-4.261973000	-0.009911000	1.081928000
H	-4.329053000	0.906168000	-0.437357000
C	3.937411000	0.002116000	0.034709000
H	4.329190000	0.889877000	-0.467117000
H	4.261653000	0.026955000	1.081988000
H	4.331179000	-0.905977000	-0.427200000

4. [I]

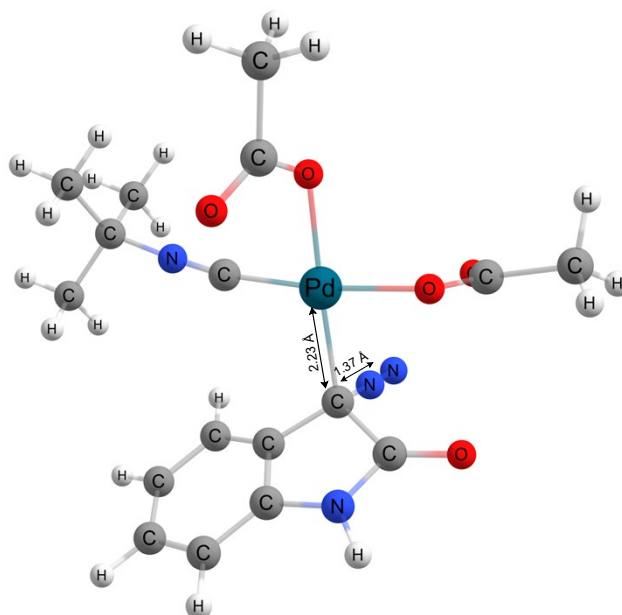


Zero-point correction=	0.234610 (Hartree/Particle)
Thermal correction to Energy=	0.254387
Thermal correction to Enthalpy=	0.255331
Thermal correction to Gibbs Free Energy=	0.181893
Sum of electronic and zero-point Energies=	-835.445454
Sum of electronic and thermal Energies=	-835.425677
Sum of electronic and thermal Enthalpies=	-835.424733
Sum of electronic and thermal Free Energies=	-835.498171

Pd	-1.031426000	0.029409000	0.114308000
O	-0.755962000	1.984504000	0.459467000
C	0.135705000	2.705767000	-0.179671000
O	-1.897257000	-1.855250000	-0.135272000
C	-3.077873000	-1.346587000	-0.078932000
O	-3.166936000	-0.086280000	0.096084000
O	0.963936000	2.278091000	-0.984277000
C	-4.289484000	-2.207165000	-0.245829000
H	-4.557597000	-2.234072000	-1.308876000
H	-4.084319000	-3.228437000	0.083002000
H	-5.131902000	-1.786996000	0.308460000
C	0.028314000	4.184911000	0.161346000
H	-0.830348000	4.610173000	-0.370794000
H	-0.139773000	4.332624000	1.231455000
H	0.933333000	4.706107000	-0.156308000
C	0.859155000	-0.358863000	0.067552000
N	1.968738000	-0.705314000	0.067957000
C	3.371497000	-1.080921000	0.029552000
C	3.840475000	-1.261511000	1.483533000
H	3.268528000	-2.047879000	1.985390000
H	4.897338000	-1.544769000	1.487247000

H	3.728705000	-0.331224000	2.048336000
C	4.140628000	0.051753000	-0.671016000
H	5.201274000	-0.214100000	-0.717427000
H	3.772331000	0.204221000	-1.689179000
H	4.039156000	0.992384000	-0.123118000
C	3.473874000	-2.398761000	-0.757503000
H	3.106989000	-2.272108000	-1.780362000
H	4.521742000	-2.710790000	-0.800624000
H	2.894968000	-3.190989000	-0.273254000

5. [II]



Zero-point correction=	0.355387 (Hartree/Particle)
Thermal correction to Energy=	0.386062
Thermal correction to Enthalpy=	0.387006
Thermal correction to Gibbs Free Energy=	0.289401
Sum of electronic and zero-point Energies=	-1382.639299
Sum of electronic and thermal Energies=	-1382.608624
Sum of electronic and thermal Enthalpies=	-1382.607680
Sum of electronic and thermal Free Energies=	-1382.705284

Pd	-0.542834000	-0.709348000	-0.060311000
O	-0.096509000	-2.679217000	0.315751000
C	0.440075000	-2.945968000	1.477634000
O	-2.899759000	-1.172661000	-1.838134000
C	-3.238721000	-1.391972000	-0.665927000
O	-2.467397000	-1.207920000	0.370017000
O	0.811419000	-2.111739000	2.309061000
C	-4.611705000	-1.941299000	-0.324635000
H	-5.330851000	-1.656987000	-1.096126000
H	-4.552461000	-3.036085000	-0.293406000
H	-4.948368000	-1.592390000	0.654411000
C	0.547711000	-4.441507000	1.748589000

H	-0.396634000	-4.781165000	2.190025000
H	0.710240000	-5.009088000	0.828947000
H	1.350633000	-4.634399000	2.463770000
C	1.374217000	-0.473544000	-0.371944000
N	2.523281000	-0.508802000	-0.557083000
C	3.958654000	-0.676646000	-0.718476000
C	4.203522000	-1.230374000	-2.132748000
H	3.838071000	-0.535728000	-2.895454000
H	5.277927000	-1.374094000	-2.282210000
H	3.702020000	-2.193110000	-2.267748000
C	4.424347000	-1.670273000	0.360202000
H	5.503451000	-1.824508000	0.263266000
H	4.212307000	-1.287832000	1.362429000
H	3.922060000	-2.634832000	0.244457000
C	4.624175000	0.696667000	-0.534042000
H	4.397484000	1.112309000	0.451795000
H	5.708758000	0.582798000	-0.622473000
H	4.290765000	1.402385000	-1.300656000
C	-0.064791000	2.386541000	-0.039132000
C	-0.521026000	2.953764000	1.165179000
C	0.256850000	3.853935000	1.885241000
C	1.498389000	4.216425000	1.347151000
C	1.940800000	3.692623000	0.127094000
C	1.161615000	2.761782000	-0.573857000
C	-1.118149000	1.408156000	-0.473659000
C	-2.351148000	1.771153000	0.396432000
H	-0.096027000	4.276910000	2.820713000
H	2.120952000	4.925829000	1.884237000
H	2.897639000	4.005507000	-0.278786000
H	1.510961000	2.346532000	-1.514281000
N	-1.414701000	1.388364000	-1.813900000
N	-1.647149000	1.337617000	-2.906046000
O	-3.520578000	1.520092000	0.200366000
N	-1.818771000	2.505840000	1.434079000
H	-2.413486000	2.871607000	2.166969000

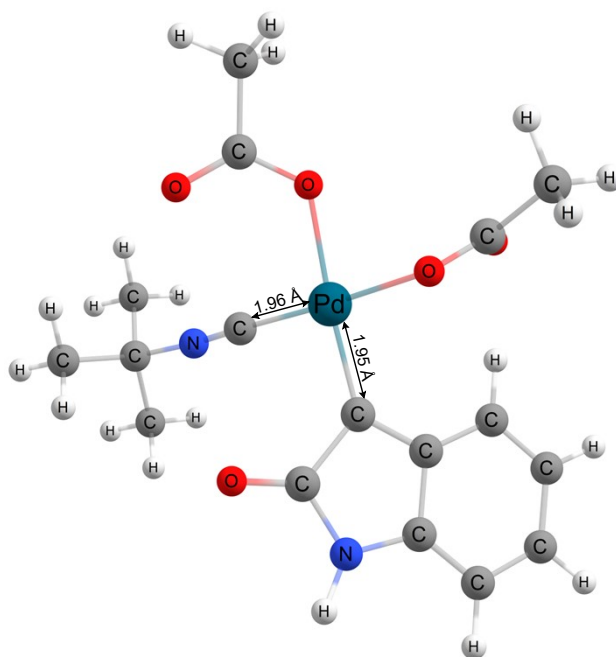
6. [TS1]

Zero-point correction=	0.355559 (Hartree/Particle)
Thermal correction to Energy=	0.386180
Thermal correction to Enthalpy=	0.387124
Thermal correction to Gibbs Free Energy=	0.290050
Sum of electronic and zero-point Energies=	-1382.646369
Sum of electronic and thermal Energies=	-1382.615748
Sum of electronic and thermal Enthalpies=	-1382.614804
Sum of electronic and thermal Free Energies=	-1382.711878

C	2.060535000	-1.574728000	-0.212259000
C	1.535713000	-2.869458000	-0.376758000
C	2.025481000	-3.736832000	-1.346065000

C	3.084803000	-3.284095000	-2.144173000
C	3.622470000	-2.002717000	-1.977638000
C	3.107215000	-1.127971000	-1.011592000
C	1.231112000	-0.910307000	0.850459000
C	0.348419000	-2.041735000	1.431478000
H	1.611612000	-4.732713000	-1.471745000
H	3.492508000	-3.943482000	-2.904667000
H	4.440091000	-1.674438000	-2.611692000
H	3.487440000	-0.118670000	-0.901769000
N	1.909964000	-0.276354000	1.870924000
N	2.408271000	0.257770000	2.715263000
O	-0.334519000	-2.014086000	2.438562000
N	0.515557000	-3.089664000	0.561346000
Pd	0.140018000	0.728868000	-0.087676000
O	1.965860000	1.684012000	-0.188124000
C	2.139467000	2.721473000	0.596073000
O	-0.598094000	2.286953000	-1.182712000
C	-1.744069000	2.854219000	-0.909987000
O	-2.564418000	2.473659000	-0.071215000
O	1.423401000	2.996698000	1.562838000
C	-1.982788000	4.110031000	-1.740541000
H	-1.474209000	4.949737000	-1.252576000
H	-1.572219000	4.009335000	-2.748416000
H	-3.051555000	4.330554000	-1.784576000
C	3.326613000	3.587274000	0.206094000
H	4.175375000	2.978624000	-0.119685000
H	3.033875000	4.221066000	-0.639482000
H	3.620262000	4.228341000	1.039879000
C	-1.582944000	-0.181418000	-0.067428000
N	-2.592710000	-0.759390000	-0.052488000
C	-3.925379000	-1.334222000	0.007252000
C	-3.784199000	-2.863304000	-0.078319000
H	-3.207655000	-3.249840000	0.767583000
H	-4.778510000	-3.319193000	-0.053436000
H	-3.291928000	-3.159691000	-1.010046000
C	-4.721175000	-0.781527000	-1.187658000
H	-5.734309000	-1.194858000	-1.165582000
H	-4.786668000	0.308533000	-1.140097000
H	-4.251482000	-1.064026000	-2.134960000
C	-4.552936000	-0.906990000	1.345666000
H	-4.625062000	0.181680000	1.411811000
H	-5.559202000	-1.331110000	1.420644000
H	-3.957288000	-1.269460000	2.188591000
H	0.032642000	-3.968911000	0.695591000

7. [III]



Zero-point correction=	0.346140 (Hartree/Particle)
Thermal correction to Energy=	0.374650
Thermal correction to Enthalpy=	0.375594
Thermal correction to Gibbs Free Energy=	0.282888
Sum of electronic and zero-point Energies=	-1273.158928
Sum of electronic and thermal Energies=	-1273.130418
Sum of electronic and thermal Enthalpies=	-1273.129474
Sum of electronic and thermal Free Energies=	-1273.222180

C	-2.414642000	-0.991584000	0.113873000
C	-2.959310000	-2.207269000	-0.439071000
C	-4.213770000	-2.671997000	-0.071574000
C	-4.923868000	-1.912072000	0.867544000
C	-4.415037000	-0.723002000	1.436278000
C	-3.167376000	-0.251949000	1.067212000
C	-1.139914000	-0.761363000	-0.420677000
C	-0.896152000	-1.964970000	-1.361342000
H	-4.632137000	-3.582876000	-0.486990000
H	-5.909275000	-2.256392000	1.170654000
H	-5.012305000	-0.180416000	2.161303000
H	-2.748170000	0.665031000	1.476484000
O	0.090482000	-2.207984000	-2.024689000
N	-2.046662000	-2.752099000	-1.317513000
Pd	0.107225000	0.714557000	-0.182565000
O	-1.354586000	2.075901000	-0.697195000
C	-1.875596000	2.831247000	0.227197000
O	1.314611000	2.367197000	0.109120000
C	2.538028000	2.460716000	-0.330337000

O	3.163904000	1.574576000	-0.926443000
O	-1.845703000	2.601785000	1.445331000
C	3.168065000	3.820294000	-0.051561000
H	2.633943000	4.591658000	-0.617718000
H	3.073477000	4.073807000	1.009235000
H	4.219967000	3.822790000	-0.343941000
C	-2.557126000	4.077323000	-0.319339000
H	-1.791274000	4.843938000	-0.487843000
H	-3.042171000	3.878106000	-1.278871000
H	-3.281919000	4.463843000	0.400757000
C	1.582206000	-0.529178000	0.165648000
N	2.419421000	-1.289510000	0.434168000
C	3.550838000	-2.164480000	0.682846000
C	2.999173000	-3.504713000	1.198026000
H	2.342770000	-3.968306000	0.455201000
H	3.831795000	-4.186341000	1.396645000
H	2.437424000	-3.365843000	2.127127000
C	4.439719000	-1.485445000	1.738937000
H	5.300260000	-2.127899000	1.949940000
H	4.804760000	-0.520241000	1.377928000
H	3.888925000	-1.326073000	2.671054000
C	4.300095000	-2.341914000	-0.649211000
H	4.653940000	-1.379282000	-1.027153000
H	5.162291000	-2.997144000	-0.489714000
H	3.651085000	-2.794956000	-1.404333000
H	-2.166708000	-3.601442000	-1.854038000

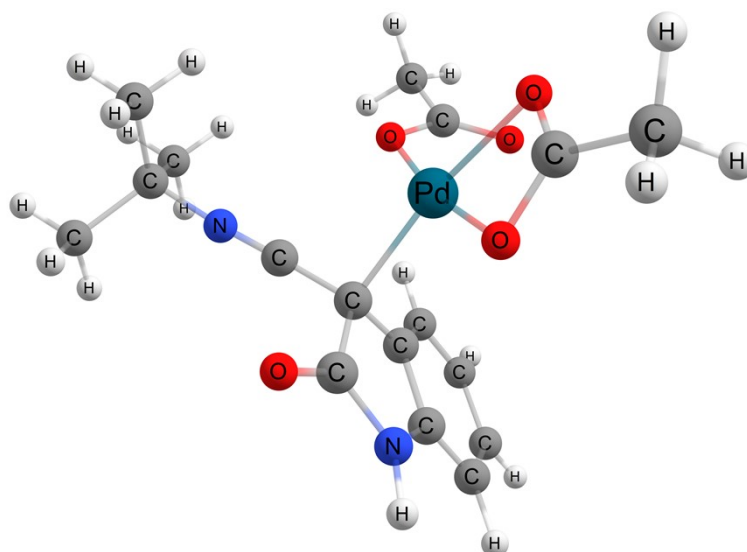
8. [TS2]

Zero-point correction=	0.343794 (Hartree/Particle)
Thermal correction to Energy=	0.372249
Thermal correction to Enthalpy=	0.373193
Thermal correction to Gibbs Free Energy=	0.280084
Sum of electronic and zero-point Energies=	-1273.116842
Sum of electronic and thermal Energies=	-1273.088387
Sum of electronic and thermal Enthalpies=	-1273.087442
Sum of electronic and thermal Free Energies=	-1273.180552

C	-2.215799000	0.238385000	-0.240526000
C	-3.348186000	0.636793000	0.537157000
C	-4.613063000	0.749393000	-0.025032000
C	-4.735075000	0.463844000	-1.391153000
C	-3.634293000	0.068255000	-2.178641000
C	-2.372750000	-0.053615000	-1.612072000
C	-1.082759000	0.163683000	0.623253000
C	-1.585674000	0.627186000	1.992499000
H	-5.475537000	1.041047000	0.565674000
H	-5.713958000	0.544364000	-1.855398000
H	-3.781789000	-0.153767000	-3.230429000
H	-1.518174000	-0.385880000	-2.191334000

O	-0.940039000	0.772702000	3.014629000
N	-2.947766000	0.848369000	1.849295000
Pd	0.603853000	-0.897467000	0.452045000
O	-0.005156000	-3.010464000	0.798415000
C	-0.243937000	-3.295263000	-0.419357000
O	2.579445000	-1.542956000	0.318727000
C	3.498268000	-0.787581000	-0.199556000
O	3.316505000	0.349931000	-0.666581000
O	-0.150739000	-2.438618000	-1.346290000
C	4.879330000	-1.429014000	-0.225440000
H	4.915298000	-2.161257000	-1.040931000
H	5.649639000	-0.674193000	-0.398664000
H	5.079000000	-1.965963000	0.706401000
C	-0.621275000	-4.724582000	-0.764720000
H	-1.156338000	-5.193678000	0.064330000
H	-1.221514000	-4.761248000	-1.676415000
H	0.301692000	-5.290335000	-0.938110000
C	0.446281000	1.012353000	0.142829000
N	0.698868000	2.135751000	-0.099935000
C	1.328542000	3.382469000	-0.497522000
C	0.277976000	4.500243000	-0.365090000
H	-0.074414000	4.588769000	0.667196000
H	0.732044000	5.451501000	-0.658101000
H	-0.580797000	4.312647000	-1.017160000
C	1.801144000	3.216445000	-1.952800000
H	2.296325000	4.139431000	-2.270617000
H	2.506891000	2.385915000	-2.028834000
H	0.954298000	3.030696000	-2.620958000
C	2.516995000	3.610750000	0.455306000
H	3.233455000	2.790425000	0.368179000
H	3.010405000	4.549249000	0.183425000
H	2.178339000	3.683582000	1.493276000
H	-3.544264000	1.140093000	2.612864000

9. [IV]

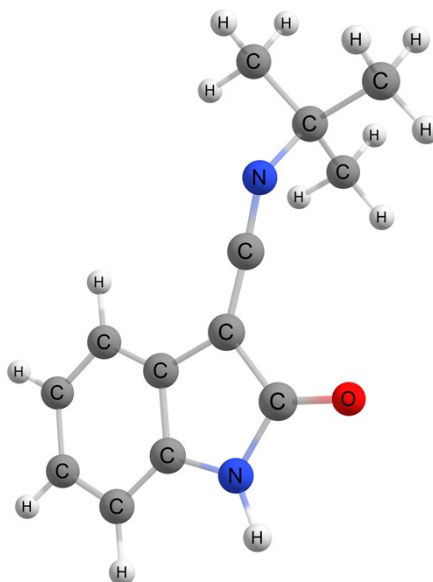


Zero-point correction=	0.347741 (Hartree/Particle)
Thermal correction to Energy=	0.374908
Thermal correction to Enthalpy=	0.375852
Thermal correction to Gibbs Free Energy=	0.286384
Sum of electronic and zero-point Energies=	-1273.191433
Sum of electronic and thermal Energies =	-1273.164266
Sum of electronic and thermal Enthalpies=	-1273.163322
Sum of electronic and thermal Free Energies=	-1273.252790

C	-0.364353000	-1.999809000	0.217926000
C	-1.242118000	-2.761029000	-0.579915000
C	-1.925362000	-3.861006000	-0.073714000
C	-1.696063000	-4.209739000	1.264562000
C	-0.810419000	-3.475607000	2.061157000
C	-0.140307000	-2.358883000	1.542915000
C	0.129954000	-0.869004000	-0.632722000
C	-0.386624000	-1.187902000	-2.043756000
H	-2.605970000	-4.435373000	-0.695131000
H	-2.216485000	-5.064818000	1.686129000
H	-0.650943000	-3.761583000	3.096249000
H	0.522708000	-1.774577000	2.171954000
O	-0.084954000	-0.649124000	-3.097832000
N	-1.258572000	-2.239562000	-1.879182000
Pd	-0.812702000	0.948450000	-0.004832000
O	-0.974452000	0.923388000	3.045355000
C	0.179179000	1.155826000	2.686508000
O	-2.113101000	2.681773000	0.147960000
C	-2.756050000	2.239992000	-0.856495000
O	-2.346372000	1.148646000	-1.400723000
O	0.607514000	1.127184000	1.442872000
C	-3.972662000	2.938999000	-1.381723000
H	-3.886338000	4.017312000	-1.227652000
H	-4.118771000	2.714031000	-2.440708000
H	-4.849672000	2.584394000	-0.827064000
C	1.273948000	1.522962000	3.679603000
H	0.894884000	1.446859000	4.700428000
H	2.142680000	0.866818000	3.560482000
H	1.609646000	2.549528000	3.495133000
C	1.488613000	-0.498980000	-0.625028000
N	2.604341000	-0.190602000	-0.678905000
C	3.967678000	0.318954000	-0.749724000
C	4.697784000	-0.480045000	-1.842288000
H	4.209061000	-0.353356000	-2.812670000
H	5.726013000	-0.115078000	-1.921524000
H	4.725904000	-1.546104000	-1.597852000
C	4.607417000	0.099031000	0.631201000
H	5.637857000	0.464940000	0.602006000
H	4.065226000	0.647110000	1.405996000
H	4.624804000	-0.963264000	0.892479000

C	3.882300000	1.813310000	-1.103770000
H	3.334475000	2.367509000	-0.337218000
H	4.896918000	2.217388000	-1.171396000
H	3.385391000	1.959418000	-2.067157000
H	-1.790041000	-2.616067000	-2.653082000

10. [V]



Zero-point correction=	0.244172 (Hartree/Particle)
Thermal correction to Energy=	0.259043
Thermal correction to Enthalpy=	0.259987
Thermal correction to Gibbs Free Energy=	0.201721
Sum of electronic and zero-point Energies=	-688.355566
Sum of electronic and thermal Energies=	-688.340695
Sum of electronic and thermal Enthalpies=	-688.339751
Sum of electronic and thermal Free Energies=	-688.398017

C	1.516460000	-0.347970000	0.135455000
C	2.616073000	0.519519000	-0.066469000
C	3.913087000	0.037670000	-0.203670000
C	4.106960000	-1.349283000	-0.135864000
C	3.028915000	-2.219706000	0.064876000
C	1.724990000	-1.724438000	0.202061000
C	0.331456000	0.505695000	0.237357000
C	0.775291000	1.917596000	0.082479000
H	4.749581000	0.713146000	-0.357323000
H	5.110897000	-1.750304000	-0.240076000
H	3.203315000	-3.290332000	0.115591000
H	0.892731000	-2.404699000	0.359679000
O	0.119626000	2.956902000	0.093865000
N	2.151448000	1.835808000	-0.092013000
C	-0.948301000	0.165506000	0.431684000
N	-2.080526000	-0.115502000	0.722940000
C	-3.298047000	-0.419310000	-0.079212000

C	-4.324953000	0.665162000	0.280186000
H	-3.966375000	1.656406000	-0.013758000
H	-5.265844000	0.467640000	-0.243585000
H	-4.521310000	0.674184000	1.356495000
C	-3.783158000	-1.802239000	0.379184000
H	-4.712615000	-2.057491000	-0.139668000
H	-3.041157000	-2.574813000	0.152615000
H	-3.973239000	-1.810833000	1.456694000
C	-2.980365000	-0.407892000	-1.579613000
H	-2.228691000	-1.163526000	-1.831200000
H	-3.886947000	-0.628324000	-2.152464000
H	-2.607790000	0.571534000	-1.896414000
H	2.723536000	2.658187000	-0.224723000

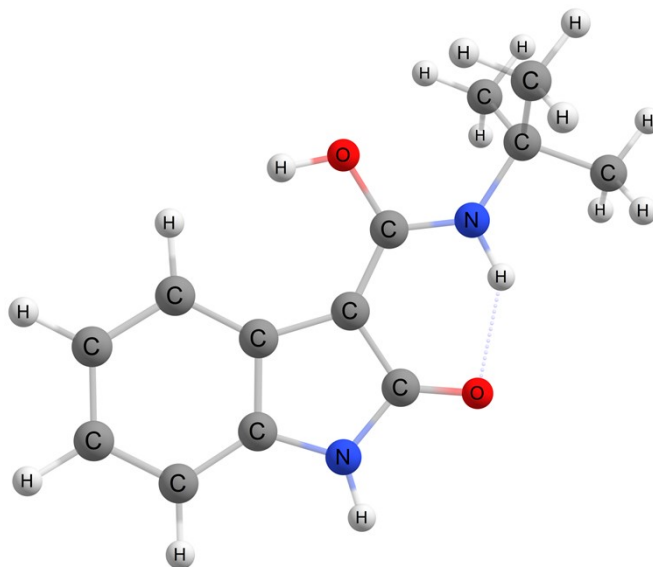
11. [TS3]

Zero-point correction=	0.266622 (Hartree/Particle)
Thermal correction to Energy=	0.282597
Thermal correction to Enthalpy=	0.283542
Thermal correction to Gibbs Free Energy=	0.224086
Sum of electronic and zero-point Energies=	-764.705025
Sum of electronic and thermal Energies=	-764.689049
Sum of electronic and thermal Enthalpies=	-764.688105
Sum of electronic and thermal Free Energies=	-764.747560

C	1.715172000	-0.318932000	-0.014396000
C	2.475410000	0.879762000	0.012245000
C	3.854439000	0.882281000	0.190446000
C	4.499612000	-0.351722000	0.350389000
C	3.768917000	-1.545593000	0.340131000
C	2.378234000	-1.538222000	0.163963000
C	0.320042000	0.074934000	-0.206118000
C	0.281144000	1.542720000	-0.290869000
H	4.414345000	1.813079000	0.207374000
H	5.576408000	-0.376886000	0.490082000
H	4.282743000	-2.492638000	0.478133000
H	1.828681000	-2.473733000	0.183202000
O	-0.663409000	2.320770000	-0.472690000
N	1.606223000	1.951994000	-0.154502000
C	-0.785031000	-0.734565000	-0.377667000
N	-2.064803000	-0.874072000	-0.383257000
C	-3.149602000	-0.103965000	0.263754000
C	-2.670261000	0.565041000	1.561709000
H	-1.928067000	1.339505000	1.358297000
H	-3.521861000	1.037324000	2.063378000
H	-2.241837000	-0.173458000	2.248588000
C	-4.249203000	-1.133900000	0.578580000
H	-5.117957000	-0.636158000	1.021496000
H	-4.576183000	-1.645226000	-0.333403000
H	-3.889157000	-1.888737000	1.286468000

C	-3.680554000	0.941533000	-0.734080000
H	-4.013948000	0.455920000	-1.658041000
H	-4.536328000	1.470832000	-0.299671000
H	-2.901237000	1.668372000	-0.973734000
H	1.869838000	2.926605000	-0.188644000
O	-0.460707000	-2.212611000	-0.846517000
H	-0.002662000	-2.232649000	-1.711659000
H	-1.589705000	-2.159102000	-0.882422000

12. [VI]



Zero-point correction=	0.273171 (Hartree/Particle)
Thermal correction to Energy=	0.289313
Thermal correction to Enthalpy=	0.290257
Thermal correction to Gibbs Free Energy=	0.228706
Sum of electronic and zero-point Energies=	-764.804465
Sum of electronic and thermal Energies=	-764.788323
Sum of electronic and thermal Enthalpies=	-764.787379
Sum of electronic and thermal Free Energies=	-764.848930

C	-1.808196000	-0.341175000	-0.000930000
C	-2.695773000	0.773264000	0.000841000
C	-4.078078000	0.630727000	0.001879000
C	-4.608778000	-0.666067000	0.001000000
C	-3.762357000	-1.780011000	-0.001125000
C	-2.369592000	-1.625921000	-0.002253000
C	-0.460422000	0.209885000	-0.001528000
C	-0.577747000	1.659920000	-0.000947000
H	-4.727963000	1.501348000	0.003258000
H	-5.685807000	-0.804425000	0.001781000
H	-4.185799000	-2.780022000	-0.002177000
H	-1.763842000	-2.530757000	-0.004825000
O	0.322500000	2.526561000	-0.001673000
N	-1.936073000	1.939202000	0.000934000
C	0.791151000	-0.413735000	-0.001181000

N	1.928693000	0.286133000	-0.003540000
C	3.337176000	-0.190366000	0.000294000
C	3.630480000	-1.005288000	1.273557000
H	3.046494000	-1.927919000	1.306292000
H	4.691913000	-1.274157000	1.304012000
H	3.401315000	-0.417581000	2.168745000
C	4.195102000	1.085472000	-0.003874000
H	5.256477000	0.821507000	-0.001345000
H	3.998181000	1.691620000	-0.895090000
H	3.995834000	1.699047000	0.881731000
C	3.634071000	-1.015846000	-1.265291000
H	3.406679000	-0.435881000	-2.165967000
H	4.695778000	-1.284114000	-1.290873000
H	3.050829000	-1.939130000	-1.291712000
H	-2.299715000	2.881601000	0.001592000
O	0.927231000	-1.754902000	0.001346000
H	0.055583000	-2.174329000	0.007440000
H	1.755633000	1.297411000	-0.004651000

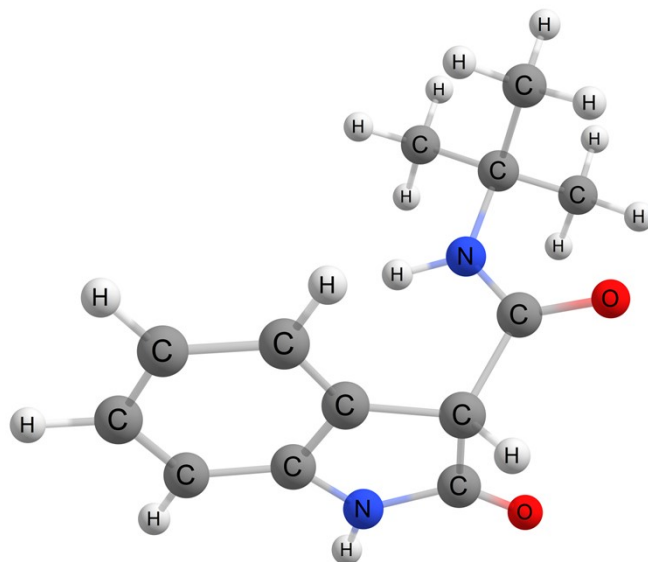
13. [TS4]

Zero-point correction=	0.268028 (Hartree/Particle)
Thermal correction to Energy=	0.283972
Thermal correction to Enthalpy=	0.284916
Thermal correction to Gibbs Free Energy=	0.224175
Sum of electronic and zero-point Energies=	-764.741930
Sum of electronic and thermal Energies=	-764.725986
Sum of electronic and thermal Enthalpies=	-764.725042
Sum of electronic and thermal Free Energies=	-764.785783

C	1.605657000	-0.308937000	0.251571000
C	2.710995000	0.433628000	-0.234045000
C	3.943047000	-0.159885000	-0.489008000
C	4.063239000	-1.540427000	-0.271829000
C	2.977833000	-2.293225000	0.191492000
C	1.745213000	-1.681092000	0.462671000
C	0.515848000	0.649435000	0.489150000
C	0.964520000	1.943216000	-0.084247000
H	4.783930000	0.423613000	-0.853066000
H	5.013376000	-2.028733000	-0.468417000
H	3.092312000	-3.361496000	0.351182000
H	0.913558000	-2.271219000	0.839233000
O	0.341433000	2.992096000	-0.263201000
N	2.314096000	1.761403000	-0.386651000
C	-0.927822000	0.340851000	0.553127000
N	-1.682281000	-0.186201000	-0.390271000
C	-3.142929000	-0.519321000	-0.332760000
C	-3.396332000	-1.526214000	0.800147000
H	-3.149210000	-1.102234000	1.776171000

H	-4.454977000	-1.804654000	0.808976000
H	-2.805553000	-2.436598000	0.653256000
C	-3.478001000	-1.149313000	-1.691499000
H	-4.538173000	-1.414645000	-1.725013000
H	-3.282269000	-0.450332000	-2.513025000
H	-2.897105000	-2.063140000	-1.861549000
C	-3.950848000	0.771632000	-0.125035000
H	-3.750811000	1.489881000	-0.926701000
H	-5.020884000	0.539522000	-0.130129000
H	-3.707872000	1.244076000	0.829793000
H	2.881980000	2.505259000	-0.768358000
O	-1.336376000	0.677718000	1.732878000
H	-0.110089000	0.932839000	1.824386000
H	-1.213899000	-0.349165000	-1.274119000

14. [4]

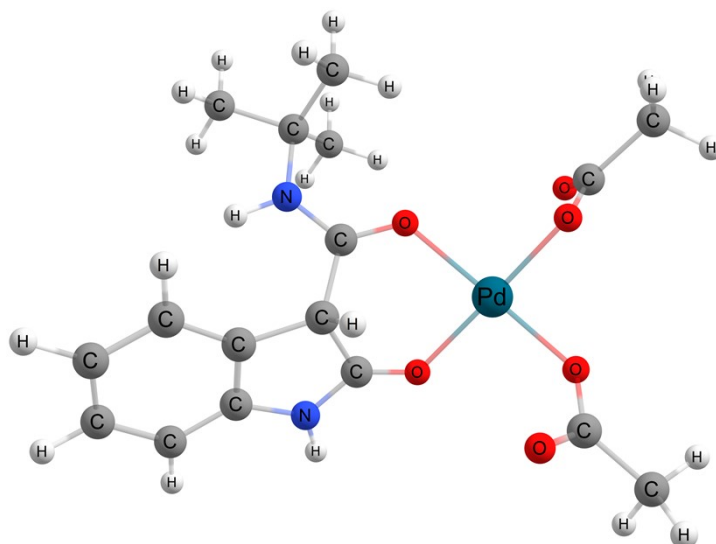


Zero-point correction=	0.272821 (Hartree/Particle)
Thermal correction to Energy=	0.289001
Thermal correction to Enthalpy=	0.289945
Thermal correction to Gibbs Free Energy=	0.228356
Sum of electronic and zero-point Energies=	-764.812423
Sum of electronic and thermal Energies=	-764.796243
Sum of electronic and thermal Enthalpies=	-764.795299
Sum of electronic and thermal Free Energies=	-764.856889

C	-1.532114000	-0.091387000	-0.600799000
C	-2.326708000	0.344651000	0.474143000
C	-3.361730000	-0.429572000	0.989222000
C	-3.593600000	-1.678200000	0.395699000
C	-2.814518000	-2.127293000	-0.675532000
C	-1.775518000	-1.330538000	-1.181063000
C	-0.518252000	0.984146000	-0.925874000
C	-0.840139000	2.084151000	0.120314000
H	-3.971419000	-0.081331000	1.817467000

H	-4.395688000	-2.303870000	0.776385000
H	-3.015412000	-3.096733000	-1.120984000
H	-1.171438000	-1.678395000	-2.014579000
O	-0.288467000	3.161615000	0.264565000
N	-1.895827000	1.615975000	0.876763000
C	0.977730000	0.584615000	-0.893055000
N	1.333991000	-0.204681000	0.150897000
C	2.696001000	-0.717920000	0.453640000
C	3.187742000	-1.620004000	-0.692563000
H	3.267552000	-1.058128000	-1.625949000
H	4.174989000	-2.028813000	-0.450634000
H	2.500204000	-2.459107000	-0.847541000
C	2.560998000	-1.538789000	1.745517000
H	3.532613000	-1.953598000	2.029359000
H	2.205946000	-0.916546000	2.575389000
H	1.865038000	-2.376253000	1.614436000
C	3.662295000	0.457831000	0.678366000
H	3.306791000	1.101095000	1.490474000
H	4.653442000	0.078228000	0.949995000
H	3.759967000	1.064952000	-0.224077000
H	-2.305696000	2.163508000	1.622474000
O	1.748904000	0.995338000	-1.757475000
H	-0.678127000	1.415438000	-1.918944000
H	0.587467000	-0.535281000	0.748292000

15. [VII]



Zero-point correction=	0.378225 (Hartree/Particle)
Thermal correction to Energy=	0.406616
Thermal correction to Enthalpy=	0.407560
Thermal correction to Gibbs Free Energy=	0.315617
Sum of electronic and zero-point Energies=	-1349.650414
Sum of electronic and thermal Energies=	-1349.622022
Sum of electronic and thermal Enthalpies=	-1349.621078

Sum of electronic and thermal Free Energies=

-1349.713022

C	2.887213000	-1.039655000	-0.517760000
C	3.114795000	-2.014754000	0.467922000
C	4.344259000	-2.638873000	0.629962000
C	5.375265000	-2.262054000	-0.242402000
C	5.165758000	-1.307837000	-1.242845000
C	3.912098000	-0.694262000	-1.392959000
C	1.441441000	-0.605768000	-0.431536000
C	0.902336000	-1.478651000	0.713083000
H	4.501398000	-3.394200000	1.393618000
H	6.349599000	-2.730779000	-0.142397000
H	5.975018000	-1.046429000	-1.917292000
H	3.747408000	0.026474000	-2.189578000
O	-0.255854000	-1.490651000	1.155545000
N	1.920070000	-2.234710000	1.183188000
Pd	-1.654225000	-0.238202000	0.166489000
O	-2.050259000	-2.932314000	-1.134499000
C	-2.979134000	-2.690110000	-0.355047000
O	-3.399571000	2.092038000	1.038587000
C	-3.548419000	1.860296000	-0.163198000
O	-2.915695000	0.940074000	-0.849398000
O	-3.112724000	-1.601625000	0.356883000
C	-4.550776000	2.634443000	-1.009047000
H	-4.207157000	2.747514000	-2.040625000
H	-5.494557000	2.076576000	-1.029369000
H	-4.738213000	3.613337000	-0.561811000
C	-4.093596000	-3.698038000	-0.110797000
H	-4.225265000	-4.326216000	-0.994961000
H	-3.807988000	-4.342219000	0.729662000
H	-5.033691000	-3.204398000	0.147072000
C	1.094097000	0.867001000	-0.139953000
N	2.091812000	1.748052000	-0.088816000
C	1.988799000	3.216556000	0.190821000
C	1.134757000	3.893898000	-0.893353000
H	0.106388000	3.527107000	-0.879939000
H	1.113414000	4.974132000	-0.716489000
H	1.557653000	3.720139000	-1.888972000
C	3.430158000	3.744737000	0.138970000
H	3.436198000	4.819910000	0.337917000
H	4.060844000	3.261964000	0.894939000
H	3.879790000	3.585333000	-0.848224000
C	1.390232000	3.437734000	1.590078000
H	1.994239000	2.938409000	2.355767000
H	1.375967000	4.509244000	1.814474000
H	0.365566000	3.065195000	1.652623000
H	1.795419000	-2.919378000	1.919931000
O	-0.102912000	1.193318000	0.033539000
H	0.874059000	-0.869987000	-1.335573000
H	3.025523000	1.377458000	-0.216748000

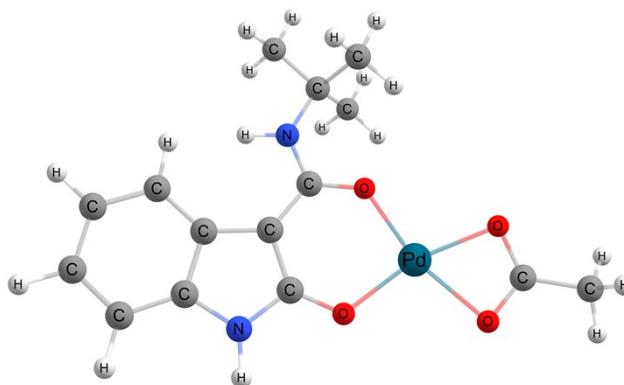
16. [TS-5]

Zero-point correction=	0.372934 (Hartree/Particle)
Thermal correction to Energy=	0.400691
Thermal correction to Enthalpy=	0.401636
Thermal correction to Gibbs Free Energy=	0.312470
Sum of electronic and zero-point Energies=	-1349.627904
Sum of electronic and thermal Energies=	-1349.600146
Sum of electronic and thermal Enthalpies=	-1349.599202
Sum of electronic and thermal Free Energies=	-1349.688368

C	-2.737928000	-0.350462000	0.182539000
C	-3.277022000	-1.212033000	-0.798265000
C	-4.615893000	-1.581626000	-0.827378000
C	-5.450110000	-1.062086000	0.171151000
C	-4.940402000	-0.218228000	1.164578000
C	-3.583142000	0.134277000	1.183358000
C	-1.271877000	-0.231050000	-0.070063000
C	-1.056356000	-1.072470000	-1.265696000
H	-5.001948000	-2.250183000	-1.591244000
H	-6.502722000	-1.328767000	0.177325000
H	-5.600207000	0.157351000	1.941044000
H	-3.197691000	0.751896000	1.990466000
O	0.054294000	-1.349046000	-1.800284000
N	-2.237765000	-1.611564000	-1.656993000
Pd	1.596779000	-0.671295000	-0.577703000
O	-0.096063000	-2.021065000	1.512344000
C	0.893678000	-2.785003000	1.201415000
O	4.139748000	0.642693000	-1.179061000
C	4.039960000	0.531540000	0.045437000
O	3.016060000	-0.015226000	0.659254000
O	1.756843000	-2.573853000	0.299972000
C	5.132115000	0.992525000	0.994384000
H	4.720623000	1.334291000	1.947565000
H	5.799860000	0.147054000	1.198746000
H	5.717306000	1.787517000	0.526713000
C	1.025832000	-4.050041000	2.014811000
H	0.096640000	-4.625229000	1.955731000
H	1.863765000	-4.653558000	1.664520000
H	1.180322000	-3.781920000	3.065375000
C	-0.571965000	1.094915000	-0.152093000
N	-1.231814000	2.184109000	0.267507000
C	-0.738101000	3.592926000	0.295701000
C	0.513982000	3.696420000	1.182616000
H	1.345599000	3.123041000	0.769146000
H	0.822783000	4.744556000	1.257419000
H	0.305871000	3.328595000	2.193264000
C	-1.882396000	4.415253000	0.909159000
H	-1.596700000	5.469696000	0.960174000

H	-2.794101000	4.345921000	0.303464000
H	-2.112239000	4.080085000	1.927335000
C	-0.447107000	4.081479000	-1.134230000
H	-1.341605000	4.000668000	-1.762017000
H	-0.141848000	5.133150000	-1.110760000
H	0.356163000	3.502493000	-1.595016000
H	-2.312873000	-2.308760000	-2.387481000
O	0.602835000	1.205017000	-0.620538000
H	-0.555694000	-1.102282000	0.804808000
H	-2.205428000	2.049972000	0.506128000

17. [VII]

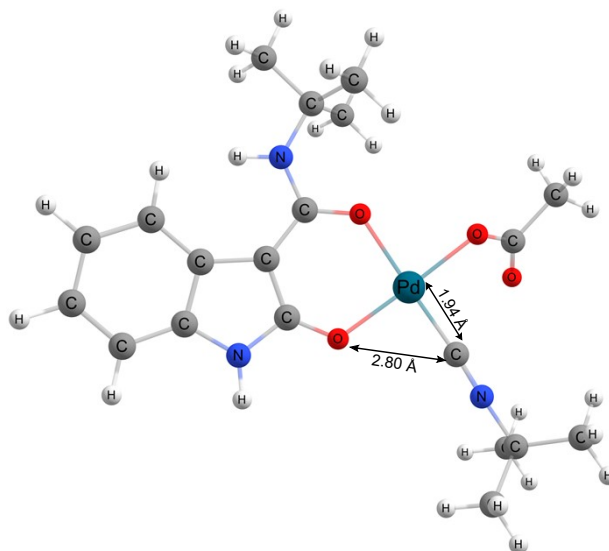


Zero-point correction=	0.315147 (Hartree/Particle)
Thermal correction to Energy=	0.337559
Thermal correction to Enthalpy=	0.338503
Thermal correction to Gibbs Free Energy=	0.261744
Sum of electronic and zero-point Energies=	-1120.617402
Sum of electronic and thermal Energies=	-1120.594990
Sum of electronic and thermal Enthalpies=	-1120.594046
Sum of electronic and thermal Free Energies=	-1120.670805

C	2.834479000	-0.716441000	-0.066132000
C	2.968147000	-2.127507000	0.063606000
C	4.193078000	-2.785161000	0.025818000
C	5.343434000	-2.011279000	-0.159148000
C	5.246114000	-0.621349000	-0.311646000
C	4.007525000	0.029096000	-0.271625000
C	1.406974000	-0.422817000	0.023288000
C	0.746777000	-1.671734000	0.177508000
H	4.251669000	-3.864928000	0.131229000
H	6.315689000	-2.493788000	-0.193756000
H	6.146405000	-0.034887000	-0.471700000
H	3.988597000	1.102744000	-0.431307000
O	-0.497657000	-1.988480000	0.292478000
N	1.693793000	-2.663697000	0.209186000
Pd	-1.914044000	-0.590413000	0.037012000
O	-3.661845000	-1.729483000	0.033942000
C	-4.359138000	-0.667111000	-0.131062000

O	-3.717551000	0.440079000	-0.195674000
C	-5.845475000	-0.721314000	-0.272702000
H	-6.295772000	0.209364000	0.080012000
H	-6.094696000	-0.844794000	-1.333504000
H	-6.249276000	-1.575056000	0.276347000
C	0.704352000	0.824768000	0.024152000
N	1.402077000	1.983418000	0.057230000
C	0.871354000	3.374272000	0.066102000
C	0.054155000	3.643652000	-1.209769000
H	-0.839459000	3.018013000	-1.251047000
H	-0.260121000	4.692874000	-1.231152000
H	0.657580000	3.449200000	-2.103200000
C	2.110732000	4.284040000	0.084565000
H	1.803934000	5.333813000	0.094207000
H	2.721809000	4.107531000	0.978245000
H	2.734337000	4.123919000	-0.802736000
C	0.025254000	3.625985000	1.328012000
H	0.610552000	3.426550000	2.232643000
H	-0.299157000	4.672165000	1.355893000
H	-0.863112000	2.991284000	1.342305000
H	1.462210000	-3.642617000	0.304048000
O	-0.579988000	0.919434000	-0.004625000
H	2.393486000	1.894596000	0.221217000

18. [VIII]

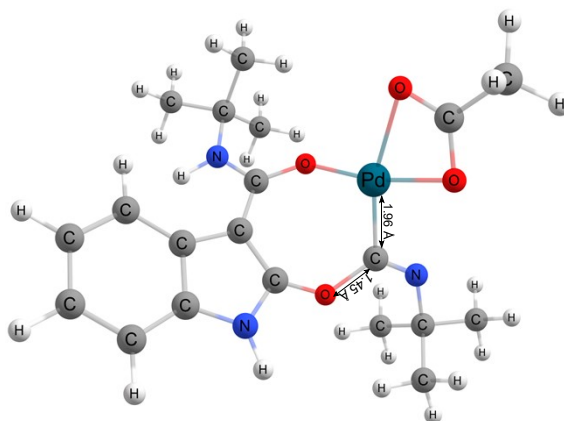


Zero-point correction=	0.446774 (Hartree/Particle)
Thermal correction to Energy=	0.478187
Thermal correction to Enthalpy=	0.479131
Thermal correction to Gibbs Free Energy=	0.380149
Sum of electronic and zero-point Energies=	-1371.210963
Sum of electronic and thermal Energies=	-1371.179549
Sum of electronic and thermal Enthalpies=	-1371.178605
Sum of electronic and thermal Free Energies=	-1371.277588

C	3.417133000	-1.535342000	-0.030595000
C	3.046567000	-2.903304000	0.104956000
C	3.965901000	-3.947185000	0.102970000
C	5.318774000	-3.625605000	-0.050202000
C	5.716477000	-2.290600000	-0.207293000
C	4.782142000	-1.248474000	-0.203447000
C	2.181970000	-0.760037000	0.016272000
C	1.121183000	-1.694590000	0.154179000
H	3.641378000	-4.978558000	0.211174000
H	6.062185000	-4.417315000	-0.056161000
H	6.768788000	-2.056747000	-0.342337000
H	5.141837000	-0.237240000	-0.365925000
O	-0.158643000	-1.564109000	0.240822000
N	1.662878000	-2.957205000	0.213307000
Pd	-1.011747000	0.259112000	-0.096769000
O	-1.783123000	2.078117000	-0.515227000
C	-2.814811000	2.562390000	0.127759000
O	-3.472062000	1.976562000	0.992409000
C	-3.134653000	3.995019000	-0.279877000
H	-4.171687000	4.230782000	-0.031695000
H	-2.480870000	4.673973000	0.280232000
H	-2.951517000	4.158735000	-1.344899000
C	1.969523000	0.659848000	-0.003901000
N	3.042471000	1.483788000	0.072721000
C	3.050925000	2.971334000	0.071824000
C	2.443232000	3.508050000	-1.236307000
H	1.388326000	3.241765000	-1.322800000
H	2.526862000	4.600247000	-1.260526000
H	2.977901000	3.105160000	-2.103665000
C	4.532681000	3.373826000	0.153527000
H	4.624703000	4.463827000	0.158985000
H	4.999265000	2.996052000	1.071697000
H	5.095628000	2.992751000	-0.706548000
C	2.295182000	3.520695000	1.296301000
H	2.728680000	3.132696000	2.225032000
H	2.365297000	4.614069000	1.318627000
H	1.239538000	3.243918000	1.263202000
H	1.102357000	-3.791280000	0.314414000
O	0.812089000	1.203077000	-0.093482000
H	3.920035000	1.041705000	0.301617000
C	-2.753734000	-0.584402000	-0.083098000
N	-3.760773000	-1.165394000	-0.093974000
C	-5.057249000	-1.816351000	-0.046992000
C	-4.895954000	-3.221153000	-0.651619000
H	-5.860227000	-3.737813000	-0.628350000
H	-4.558113000	-3.163270000	-1.690814000
H	-4.172081000	-3.811295000	-0.081451000
C	-6.034691000	-0.961435000	-0.871913000
H	-7.024502000	-1.427810000	-0.853256000

H	-6.115738000	0.046870000	-0.456602000
H	-5.705705000	-0.886847000	-1.912867000
C	-5.485367000	-1.886987000	1.429157000
H	-4.768334000	-2.469231000	2.015716000
H	-5.558429000	-0.885064000	1.861129000
H	-6.464719000	-2.370905000	1.496699000

19. [IX]

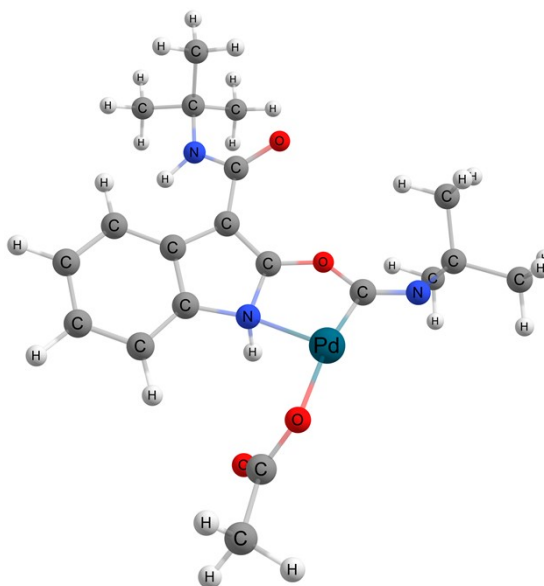


Zero-point correction=	0.447625 (Hartree/Particle)
Thermal correction to Energy=	0.478034
Thermal correction to Enthalpy=	0.478979
Thermal correction to Gibbs Free Energy=	0.384428
Sum of electronic and zero-point Energies=	-1371.170337
Sum of electronic and thermal Energies=	-1371.139928
Sum of electronic and thermal Enthalpies=	-1371.138984
Sum of electronic and thermal Free Energies=	-1371.233534

C	2.596674000	-1.404311000	-0.614180000
C	2.145998000	-2.679772000	-1.048755000
C	2.956647000	-3.571623000	-1.752439000
C	4.260864000	-3.168403000	-2.036100000
C	4.728078000	-1.902660000	-1.634225000
C	3.910643000	-1.016681000	-0.933486000
C	1.476596000	-0.767166000	0.059028000
C	0.417577000	-1.673411000	-0.008941000
H	2.581980000	-4.539431000	-2.073225000
H	4.920307000	-3.835994000	-2.582647000
H	5.743533000	-1.606828000	-1.881682000
H	4.288502000	-0.036350000	-0.659903000
O	-0.809980000	-1.698624000	0.528693000
N	0.820688000	-2.804547000	-0.661945000
Pd	-1.208941000	0.983159000	-0.595422000
O	-2.684399000	1.071271000	-2.069497000
C	-2.212629000	2.153519000	-2.582672000
O	-1.176814000	2.676566000	-2.071263000
C	-2.883597000	2.748694000	-3.789038000
H	-2.704987000	3.825537000	-3.830590000

H	-2.457302000	2.294023000	-4.691395000
H	-3.956075000	2.539939000	-3.777561000
C	1.419152000	0.536821000	0.708211000
N	2.537528000	0.995452000	1.299214000
C	2.740184000	2.310816000	1.972990000
C	2.485062000	3.457953000	0.980424000
H	1.447049000	3.475075000	0.642853000
H	2.702797000	4.415549000	1.465309000
H	3.134097000	3.364718000	0.103025000
C	4.210664000	2.324269000	2.419199000
H	4.435078000	3.263387000	2.932820000
H	4.424117000	1.504384000	3.115748000
H	4.888741000	2.240377000	1.561952000
C	1.820141000	2.425768000	3.201917000
H	2.000318000	1.600683000	3.900105000
H	2.019923000	3.365925000	3.727288000
H	0.767572000	2.411624000	2.911397000
H	0.221202000	-3.603373000	-0.817620000
O	0.359756000	1.237680000	0.735898000
H	3.294661000	0.329824000	1.383514000
C	-1.762825000	-0.608995000	0.403598000
N	-2.884729000	-0.704076000	0.941717000
C	-3.459040000	-1.804750000	1.749360000
C	-3.579074000	-3.086577000	0.902250000
H	-4.113604000	-3.860257000	1.465852000
H	-4.140216000	-2.886906000	-0.017042000
H	-2.597193000	-3.481581000	0.629034000
C	-4.865430000	-1.336945000	2.163229000
H	-5.370141000	-2.100878000	2.765736000
H	-4.805524000	-0.414637000	2.750847000
H	-5.476421000	-1.130770000	1.278197000
C	-2.612167000	-2.054868000	3.012485000
H	-1.617833000	-2.435396000	2.765135000
H	-2.494223000	-1.127753000	3.584201000
H	-3.109102000	-2.789210000	3.657380000

20. [X]

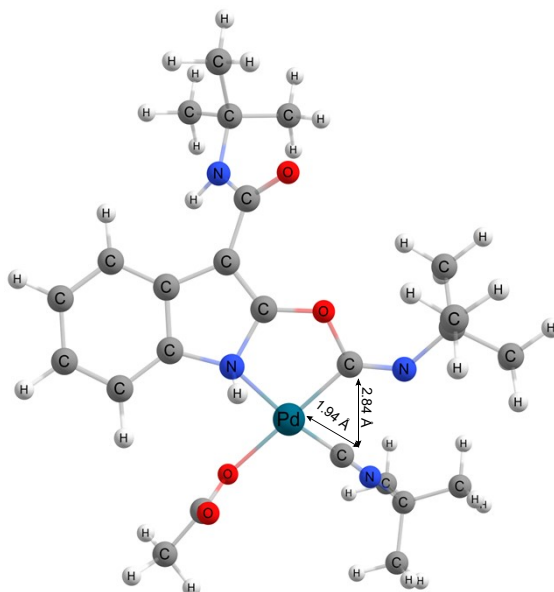


Zero-point correction=	0.447055 (Hartree/Particle)
Thermal correction to Energy=	0.477988
Thermal correction to Enthalpy=	0.478932
Thermal correction to Gibbs Free Energy=	0.381745
Sum of electronic and zero-point Energies=	-1371.130225
Sum of electronic and thermal Energies=	-1371.099292
Sum of electronic and thermal Enthalpies=	-1371.098348
Sum of electronic and thermal Free Energies=	-1371.195535

C	1.194996000	-2.005208000	0.037712000
C	-0.176222000	-2.137159000	0.339572000
C	-0.835659000	-3.355191000	0.383889000
C	-0.082936000	-4.495558000	0.075777000
C	1.272570000	-4.392441000	-0.264755000
C	1.925133000	-3.154606000	-0.287385000
C	1.533799000	-0.575732000	0.098399000
C	0.391036000	0.072505000	0.435334000
H	-1.887942000	-3.406781000	0.642259000
H	-0.562560000	-5.469421000	0.091702000
H	1.829715000	-5.290112000	-0.517084000
H	2.972773000	-3.095142000	-0.563593000
O	0.123964000	1.390390000	0.544855000
N	-0.714284000	-0.826639000	0.607578000
Pd	-2.353722000	0.227394000	-0.339172000
O	-3.709373000	-1.975073000	1.255300000
C	-4.254711000	-1.927135000	0.134563000
O	-3.872010000	-1.147616000	-0.827850000
C	-5.441670000	-2.817279000	-0.196623000
H	-5.204964000	-3.448282000	-1.060431000
H	-5.707046000	-3.446004000	0.655491000
H	-6.301837000	-2.199261000	-0.476471000
C	2.830361000	0.097105000	-0.237245000

N	3.933764000	-0.575868000	0.190896000
C	5.348901000	-0.148905000	0.030971000
C	5.694865000	-0.027499000	-1.463706000
H	5.091373000	0.743817000	-1.946813000
H	6.751791000	0.236664000	-1.579233000
H	5.522650000	-0.978434000	-1.979972000
C	6.200811000	-1.253907000	0.675315000
H	7.262686000	-1.002995000	0.595654000
H	5.964944000	-1.369744000	1.740293000
H	6.045616000	-2.218016000	0.176901000
C	5.586293000	1.187680000	0.757864000
H	5.343534000	1.098195000	1.822787000
H	6.638920000	1.479320000	0.671982000
H	4.972342000	1.981950000	0.327117000
H	-1.153906000	-0.777686000	1.534077000
O	2.861373000	1.163710000	-0.855080000
H	3.772308000	-1.376109000	0.788525000
C	-1.170853000	1.717700000	0.065215000
N	-1.625314000	2.864222000	-0.080560000
C	-1.001399000	4.200104000	0.107605000
C	-0.552630000	4.353699000	1.572804000
H	-0.173414000	5.368493000	1.738144000
H	-1.393665000	4.190917000	2.255558000
H	0.244283000	3.649013000	1.825836000
C	-2.080371000	5.240721000	-0.224457000
H	-1.682451000	6.255064000	-0.112667000
H	-2.430719000	5.118608000	-1.254746000
H	-2.942720000	5.132080000	0.442027000
C	0.191448000	4.341404000	-0.854829000
H	0.972918000	3.607287000	-0.641082000
H	-0.132302000	4.207951000	-1.892564000
H	0.625527000	5.343421000	-0.761069000

21. [XI]

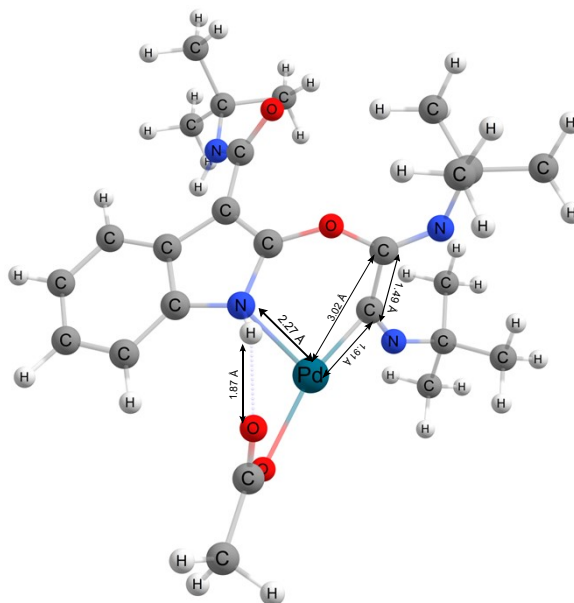


Zero-point correction=	0.578967 (Hartree/Particle)
Thermal correction to Energy=	0.617512
Thermal correction to Enthalpy=	0.618456
Thermal correction to Gibbs Free Energy=	0.504775
Sum of electronic and zero-point Energies=	-1621.745550
Sum of electronic and thermal Energies=	-1621.707005
Sum of electronic and thermal Enthalpies=	-1621.706061
Sum of electronic and thermal Free Energies=	-1621.819742

C	-2.663853000	1.734074000	-0.324740000
C	-1.426615000	2.305667000	-0.687489000
C	-1.206587000	3.673765000	-0.723744000
C	-2.269159000	4.505042000	-0.346451000
C	-3.503634000	3.963536000	0.035724000
C	-3.717070000	2.581095000	0.044004000
C	-2.548564000	0.279834000	-0.474878000
C	-1.291079000	0.037411000	-0.937334000
H	-0.253144000	4.077007000	-1.043591000
H	-2.131467000	5.582023000	-0.357354000
H	-4.315526000	4.628366000	0.316849000
H	-4.691235000	2.179852000	0.304327000
O	-0.663164000	-1.113353000	-1.181786000
N	-0.520667000	1.245887000	-1.057191000
Pd	1.368589000	0.646665000	-0.133454000
O	2.010980000	2.554413000	0.529181000
C	2.229790000	3.396888000	-0.431951000
O	1.981791000	3.181091000	-1.633417000
C	2.849473000	4.715633000	0.009108000
H	2.685374000	5.488719000	-0.744975000
H	2.449948000	5.036177000	0.975288000
H	3.930865000	4.575309000	0.127799000
C	-3.552995000	-0.781860000	-0.167757000
N	-4.325650000	-0.532003000	0.929257000

C	-5.382749000	-1.417671000	1.480974000
C	-6.488620000	-1.633137000	0.432268000
H	-6.100085000	-2.146338000	-0.449785000
H	-7.293589000	-2.240480000	0.860843000
H	-6.915137000	-0.674209000	0.117266000
C	-5.960067000	-0.681454000	2.700133000
H	-6.749711000	-1.281373000	3.162368000
H	-5.188943000	-0.503269000	3.459764000
H	-6.394705000	0.283263000	2.413082000
C	-4.778330000	-2.764299000	1.920979000
H	-3.994690000	-2.610284000	2.671547000
H	-5.554608000	-3.398354000	2.364091000
H	-4.343959000	-3.293552000	1.069873000
H	-0.122139000	1.389357000	-1.991698000
O	-3.661545000	-1.791008000	-0.870166000
H	-4.050070000	0.248848000	1.510543000
C	0.750365000	-1.148151000	-0.798874000
N	1.406919000	-2.202245000	-0.967867000
C	0.933307000	-3.487532000	-1.543522000
C	-0.174729000	-4.099839000	-0.664589000
H	-0.428348000	-5.101674000	-1.030478000
H	0.168118000	-4.196393000	0.372030000
H	-1.082664000	-3.493217000	-0.677290000
C	2.157440000	-4.420338000	-1.544418000
H	1.898928000	-5.402019000	-1.957071000
H	2.966878000	-3.994065000	-2.147347000
H	2.534443000	-4.562471000	-0.525680000
C	0.443386000	-3.295298000	-2.992514000
H	-0.468695000	-2.696163000	-3.036120000
H	1.214679000	-2.804012000	-3.596686000
H	0.230928000	-4.270697000	-3.445300000
C	2.988421000	-0.116941000	0.617875000
N	3.974021000	-0.528761000	1.076787000
C	5.212327000	-1.042659000	1.634568000
C	5.094741000	-0.970595000	3.166841000
H	4.258398000	-1.579246000	3.523353000
H	6.017169000	-1.350543000	3.616470000
H	4.944385000	0.060773000	3.499454000
C	5.374370000	-2.493820000	1.152601000
H	5.417292000	-2.540315000	0.060747000
H	6.304386000	-2.904585000	1.557482000
H	4.540590000	-3.114153000	1.493306000
C	6.354833000	-0.150271000	1.119727000
H	6.409560000	-0.177748000	0.027421000
H	6.213594000	0.887153000	1.437063000
H	7.304810000	-0.512019000	1.524636000

22. [XII]



Zero-point correction=	0.579673 (Hartree/Particle)
Thermal correction to Energy=	0.618400
Thermal correction to Enthalpy=	0.619344
Thermal correction to Gibbs Free Energy=	0.506056
Sum of electronic and zero-point Energies=	-1621.720294
Sum of electronic and thermal Energies=	-1621.681567
Sum of electronic and thermal Enthalpies=	-1621.680623
Sum of electronic and thermal Free Energies=	-1621.793910

C	1.195976000	-2.577599000	-0.293817000
C	-0.192686000	-2.703303000	-0.528532000
C	-0.872958000	-3.912055000	-0.390219000
C	-0.131415000	-5.023052000	0.011473000
C	1.249446000	-4.922421000	0.259034000
C	1.923260000	-3.711439000	0.106997000
C	1.564997000	-1.202469000	-0.603276000
C	0.416571000	-0.585309000	-1.023504000
H	-1.935296000	-3.984395000	-0.588535000
H	-0.630162000	-5.980294000	0.130309000
H	1.802930000	-5.806498000	0.562513000
H	2.995296000	-3.659253000	0.268257000
O	0.259526000	0.686242000	-1.480158000
N	-0.699213000	-1.443961000	-0.930649000
Pd	-2.067465000	-0.376765000	0.537783000
O	-3.682223000	-1.833696000	0.502182000
C	-3.994604000	-2.167929000	-0.698764000
O	-3.335665000	-1.859833000	-1.728074000
C	-5.275656000	-2.971831000	-0.859691000
H	-5.219187000	-3.619346000	-1.738334000
H	-5.489457000	-3.560330000	0.036024000
H	-6.108546000	-2.273803000	-1.010576000
C	2.903844000	-0.550032000	-0.492698000
N	3.646795000	-0.963244000	0.573468000

C	5.012640000	-0.502442000	0.932903000
C	5.994903000	-0.826388000	-0.207055000
H	5.726717000	-0.292821000	-1.121326000
H	7.009904000	-0.531571000	0.081638000
H	5.999407000	-1.901119000	-0.420165000
C	5.406558000	-1.283618000	2.196740000
H	6.408534000	-0.989086000	2.522884000
H	4.713409000	-1.081218000	3.022530000
H	5.418223000	-2.363804000	2.009597000
C	5.005740000	1.007878000	1.234242000
H	4.309214000	1.236673000	2.048968000
H	6.006086000	1.334271000	1.540147000
H	4.710144000	1.580485000	0.352322000
H	-1.516593000	-1.431672000	-1.575908000
O	3.291895000	0.287283000	-1.314032000
H	3.185040000	-1.562138000	1.244809000
C	-0.235653000	1.704136000	-0.662192000
N	-0.177629000	2.928475000	-0.941766000
C	0.423024000	3.539647000	-2.153295000
C	1.950220000	3.339369000	-2.126088000
H	2.397374000	3.847163000	-2.988118000
H	2.379564000	3.777952000	-1.218231000
H	2.226960000	2.283555000	-2.161882000
C	0.090197000	5.039481000	-2.074917000
H	0.529636000	5.573941000	-2.923820000
H	-0.993170000	5.201351000	-2.091943000
H	0.485486000	5.476908000	-1.151987000
C	-0.191135000	2.945468000	-3.436565000
H	0.098627000	1.903652000	-3.586554000
H	-1.284940000	3.004465000	-3.408185000
H	0.153821000	3.521830000	-4.301776000
C	-1.041770000	1.235144000	0.504587000
N	-1.569474000	1.695575000	1.526227000
C	-1.664058000	2.942621000	2.319483000
C	-2.280031000	2.567198000	3.673878000
H	-1.645492000	1.851527000	4.206970000
H	-2.389056000	3.461333000	4.295925000
H	-3.267882000	2.115338000	3.539596000
C	-0.255403000	3.530823000	2.504119000
H	0.189575000	3.799122000	1.543008000
H	-0.317810000	4.433786000	3.121096000
H	0.400599000	2.816475000	3.012832000
C	-2.582763000	3.909736000	1.551926000
H	-2.153909000	4.165709000	0.579721000
H	-3.571478000	3.465634000	1.397944000
H	-2.707223000	4.829824000	2.133279000

23. [TS-6]

Zero-point correction=

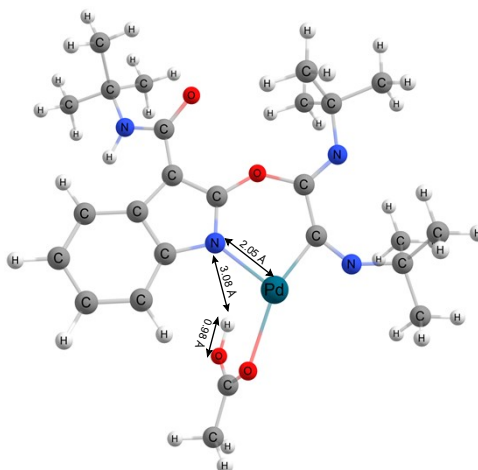
0.575548 (Hartree/Particle)

Thermal correction to Energy=	0.613689
Thermal correction to Enthalpy=	0.614634
Thermal correction to Gibbs Free Energy=	0.502960
Sum of electronic and zero-point Energies=	-1621.722959
Sum of electronic and thermal Energies=	-1621.684818
Sum of electronic and thermal Enthalpies=	-1621.683873
Sum of electronic and thermal Free Energies=	-1621.795547

C	1.546781000	-2.389429000	-0.087947000
C	0.167473000	-2.689462000	-0.205034000
C	-0.345961000	-3.952830000	0.095006000
C	0.549118000	-4.933187000	0.522978000
C	1.924126000	-4.658293000	0.635443000
C	2.433566000	-3.396908000	0.330325000
C	1.715407000	-1.007630000	-0.509193000
C	0.463306000	-0.576548000	-0.874809000
H	-1.405568000	-4.164427000	0.010358000
H	0.177292000	-5.923805000	0.768033000
H	2.601409000	-5.444263000	0.957729000
H	3.501223000	-3.211030000	0.392866000
O	0.127489000	0.656859000	-1.354962000
N	-0.524454000	-1.556046000	-0.696196000
Pd	-2.041949000	-0.669582000	0.606473000
O	-3.471886000	-2.317042000	0.127210000
C	-3.481455000	-2.640122000	-1.099910000
O	-2.565256000	-2.337305000	-1.944024000
C	-4.647288000	-3.449370000	-1.626249000
H	-5.384404000	-3.633526000	-0.843152000
H	-5.116824000	-2.914124000	-2.458327000
H	-4.282045000	-4.403092000	-2.022265000
C	2.960621000	-0.188703000	-0.534768000
N	3.830055000	-0.450111000	0.485276000
C	5.146821000	0.196425000	0.713813000
C	6.073053000	-0.050617000	-0.490629000
H	5.667849000	0.402820000	-1.397574000
H	7.060229000	0.383475000	-0.296415000
H	6.200933000	-1.124537000	-0.666361000
C	5.736822000	-0.469812000	1.967210000
H	6.712522000	-0.033391000	2.201056000
H	5.087891000	-0.322931000	2.839454000
H	5.877686000	-1.546544000	1.816613000
C	4.966802000	1.706051000	0.961579000
H	4.312734000	1.881513000	1.823436000
H	5.936521000	2.172175000	1.169849000
H	4.529034000	2.194233000	0.088012000
H	-1.445818000	-1.823130000	-1.397997000
O	3.180458000	0.648640000	-1.417356000
H	3.497499000	-1.060298000	1.219962000
C	-0.511375000	1.606980000	-0.567683000
N	-0.630499000	2.821280000	-0.879084000

C	-0.116341000	3.475196000	-2.108180000
C	1.423294000	3.504510000	-2.068798000
H	1.798359000	4.049542000	-2.942513000
H	1.774839000	4.026510000	-1.171479000
H	1.852771000	2.500334000	-2.076073000
C	-0.667261000	4.911405000	-2.080341000
H	-0.303323000	5.477892000	-2.944159000
H	-1.762531000	4.911460000	-2.108596000
H	-0.349900000	5.431679000	-1.170357000
C	-0.623608000	2.758758000	-3.375755000
H	-0.183441000	1.766603000	-3.491186000
H	-1.714647000	2.657663000	-3.355291000
H	-0.358170000	3.353140000	-4.256813000
C	-1.263349000	1.072039000	0.614107000
N	-1.884165000	1.498165000	1.597988000
C	-2.172515000	2.762461000	2.314144000
C	-2.788761000	2.377989000	3.666202000
H	-2.089186000	1.779067000	4.258626000
H	-3.038329000	3.279372000	4.235097000
H	-3.703903000	1.794312000	3.523758000
C	-0.862326000	3.541823000	2.515009000
H	-0.417719000	3.818944000	1.556369000
H	-1.068386000	4.457550000	3.079887000
H	-0.139706000	2.947048000	3.083828000
C	-3.178598000	3.560798000	1.466492000
H	-2.748014000	3.823880000	0.497265000
H	-4.093990000	2.982482000	1.303650000
H	-3.446325000	4.482806000	1.994027000

24. [XIII]



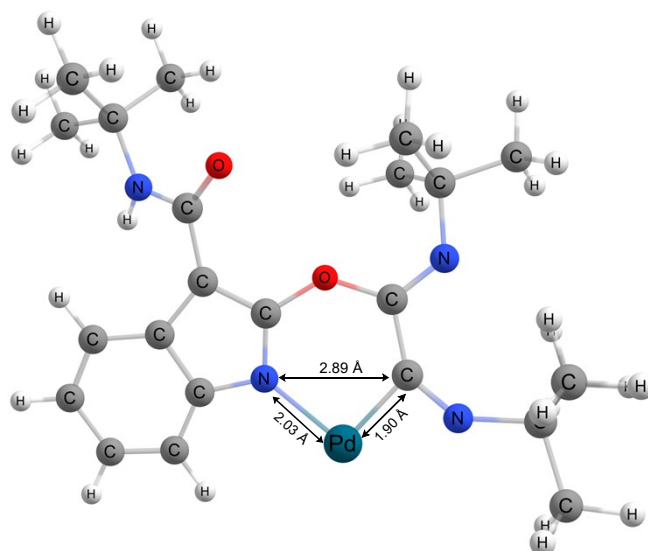
Zero-point correction=	0.580018 (Hartree/Particle)
Thermal correction to Energy=	0.618908
Thermal correction to Enthalpy=	0.619852
Thermal correction to Gibbs Free Energy=	0.505718
Sum of electronic and zero-point Energies=	-1621.731495

Sum of electronic and thermal Energies=	-1621.692605
Sum of electronic and thermal Enthalpies=	-1621.691661
Sum of electronic and thermal Free Energies=	-1621.805795

C	2.082662000	-1.888289000	-0.612254000
C	0.698052000	-2.222414000	-0.734125000
C	0.279236000	-3.511868000	-1.083299000
C	1.250057000	-4.488660000	-1.300079000
C	2.620038000	-4.177431000	-1.189899000
C	3.042619000	-2.891139000	-0.859513000
C	2.134316000	-0.476290000	-0.311966000
C	0.791527000	-0.078282000	-0.288684000
H	-0.775750000	-3.734559000	-1.208544000
H	0.947626000	-5.495333000	-1.575927000
H	3.360799000	-4.949044000	-1.382631000
H	4.104876000	-2.668386000	-0.825725000
O	0.426592000	1.222693000	-0.033068000
N	-0.077879000	-1.093303000	-0.507148000
Pd	-2.104559000	-0.926932000	-0.225889000
O	-2.087691000	-3.340193000	1.954991000
C	-2.843076000	-3.714565000	0.922773000
O	-2.986326000	-3.011715000	-0.080051000
C	-3.481581000	-5.055751000	1.099599000
H	-4.157290000	-5.260267000	0.269748000
H	-2.700837000	-5.823378000	1.139263000
H	-4.024524000	-5.090025000	2.049055000
C	3.307446000	0.390110000	-0.080748000
N	4.406221000	-0.258267000	0.426590000
C	5.711801000	0.353295000	0.765890000
C	6.347913000	0.977710000	-0.489583000
H	5.726268000	1.785303000	-0.881486000
H	7.336496000	1.384003000	-0.246391000
H	6.471416000	0.223254000	-1.274607000
C	6.600635000	-0.792636000	1.277257000
H	7.587733000	-0.409965000	1.554983000
H	6.165514000	-1.268257000	2.165114000
H	6.741125000	-1.560109000	0.507146000
C	5.545001000	1.412773000	1.872920000
H	5.102431000	0.966092000	2.770965000
H	6.519654000	1.833603000	2.146657000
H	4.897609000	2.225093000	1.535251000
H	-1.672589000	-2.475686000	1.741730000
O	3.313517000	1.606306000	-0.327130000
H	4.254084000	-1.197158000	0.767950000
C	-0.795717000	1.828574000	-0.144306000
N	-0.951231000	3.086313000	-0.227280000
C	0.136833000	4.088267000	-0.311407000
C	0.993474000	4.063676000	0.971144000
H	1.698452000	4.902309000	0.952882000
H	0.361801000	4.174241000	1.860371000

H	1.570364000	3.140703000	1.048796000
C	-0.563429000	5.452944000	-0.436852000
H	0.175413000	6.258903000	-0.502002000
H	-1.188107000	5.488871000	-1.336243000
H	-1.204928000	5.645847000	0.430293000
C	1.008212000	3.835647000	-1.558720000
H	1.597239000	2.921936000	-1.459722000
H	0.383578000	3.777313000	-2.457749000
H	1.705145000	4.671610000	-1.688106000
C	-1.996406000	0.968204000	-0.104789000
N	-3.231883000	1.047264000	0.021761000
C	-4.288208000	2.066020000	0.236594000
C	-4.352825000	2.961008000	-1.013270000
H	-5.155927000	3.696265000	-0.891771000
H	-3.409420000	3.492194000	-1.159084000
H	-4.567501000	2.365214000	-1.906562000
C	-3.947019000	2.881553000	1.495106000
H	-4.743916000	3.609300000	1.683359000
H	-3.868138000	2.229134000	2.371370000
H	-3.006078000	3.421628000	1.368010000
C	-5.606652000	1.304292000	0.426005000
H	-5.834814000	0.694945000	-0.454625000
H	-5.553578000	0.642181000	1.296831000
H	-6.429322000	2.009854000	0.580123000

25. [XIV]



Zero-point correction=	0.516944 (Hartree/Particle)
Thermal correction to Energy=	0.549715
Thermal correction to Enthalpy=	0.550659
Thermal correction to Gibbs Free Energy=	0.451914
Sum of electronic and zero-point Energies=	-1392.666856
Sum of electronic and thermal Energies=	-1392.634085
Sum of electronic and thermal Enthalpies=	-1392.633141

Sum of electronic and thermal Free Energies=

-1392.731886

C	2.296241000	-1.897364000	-0.046308000
C	1.062811000	-2.581609000	0.185403000
C	1.001831000	-3.971159000	0.339610000
C	2.187324000	-4.698645000	0.253469000
C	3.411992000	-4.045706000	0.005205000
C	3.476832000	-2.661716000	-0.147849000
C	1.964803000	-0.495795000	-0.170880000
C	0.574242000	-0.454974000	-0.011885000
H	0.052102000	-4.469425000	0.521997000
H	2.167119000	-5.778462000	0.371721000
H	4.322729000	-4.633346000	-0.074410000
H	4.430870000	-2.191909000	-0.367687000
O	-0.126442000	0.728048000	-0.010173000
N	0.022235000	-1.667913000	0.216669000
Pd	-1.981187000	-1.990663000	0.132847000
C	2.843945000	0.664395000	-0.419223000
N	4.131855000	0.517370000	0.031544000
C	5.222233000	1.514440000	-0.074879000
C	5.504854000	1.837061000	-1.553581000
H	4.633341000	2.293364000	-2.027337000
H	6.348549000	2.532591000	-1.630278000
H	5.761600000	0.925333000	-2.104529000
C	6.463135000	0.860273000	0.554863000
H	7.313079000	1.548812000	0.517234000
H	6.287977000	0.604621000	1.607365000
H	6.745423000	-0.053376000	0.018821000
C	4.862819000	2.797108000	0.700551000
H	4.674061000	2.569927000	1.756263000
H	5.688617000	3.516393000	0.649300000
H	3.968620000	3.263733000	0.281288000
O	2.458377000	1.690501000	-1.000986000
H	4.302575000	-0.262978000	0.650669000
C	-1.464820000	0.976435000	0.072469000
N	-1.951616000	2.138256000	0.236247000
C	-1.163814000	3.382644000	0.401098000
C	-0.228056000	3.284831000	1.623808000
H	0.238622000	4.259767000	1.802444000
H	-0.793081000	3.012406000	2.522700000
H	0.567097000	2.553329000	1.470752000
C	-2.193788000	4.500968000	0.638950000
H	-1.690910000	5.466460000	0.759693000
H	-2.885819000	4.579384000	-0.206515000
H	-2.781572000	4.306295000	1.542992000
C	-0.363803000	3.674902000	-0.884972000
H	0.420314000	2.933615000	-1.054323000
H	-1.031725000	3.698822000	-1.753974000
H	0.109350000	4.660013000	-0.800218000
C	-2.423151000	-0.152409000	-0.027524000

N	-3.634802000	-0.380222000	-0.154765000
C	-4.919085000	0.336304000	-0.352521000
C	-5.988585000	-0.733761000	-0.608921000
H	-6.061978000	-1.423034000	0.238819000
H	-6.965044000	-0.260753000	-0.753174000
H	-5.752679000	-1.314866000	-1.506607000
C	-4.785759000	1.273424000	-1.564226000
H	-5.743707000	1.774656000	-1.740292000
H	-4.022034000	2.034406000	-1.389040000
H	-4.525569000	0.709228000	-2.465961000
C	-5.229697000	1.119451000	0.934771000
H	-4.459072000	1.869286000	1.127834000
H	-6.194713000	1.626132000	0.825542000
H	-5.293733000	0.444651000	1.794795000

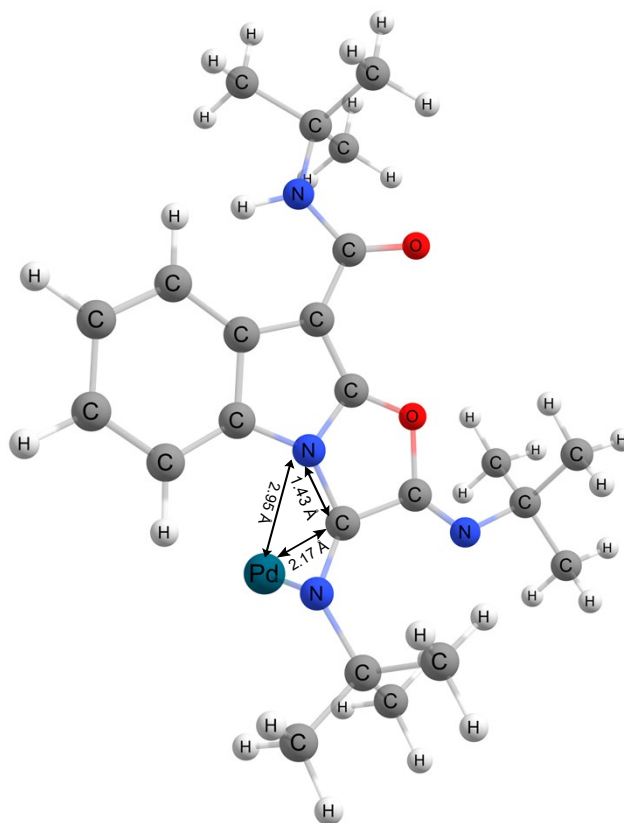
26. [TS-7]

Zero-point correction=	0.515909 (Hartree/Particle)
Thermal correction to Energy=	0.548227
Thermal correction to Enthalpy=	0.549171
Thermal correction to Gibbs Free Energy=	0.451565
Sum of electronic and zero-point Energies=	-1392.625707
Sum of electronic and thermal Energies=	-1392.593389
Sum of electronic and thermal Enthalpies=	-1392.592445
Sum of electronic and thermal Free Energies=	-1392.690050

C	-1.841126000	-1.759625000	0.121320000
C	-0.506309000	-2.193794000	-0.141706000
C	-0.130237000	-3.535455000	-0.117142000
C	-1.109071000	-4.480564000	0.195894000
C	-2.429265000	-4.080321000	0.468279000
C	-2.804358000	-2.735560000	0.432935000
C	-1.843757000	-0.301453000	0.039937000
C	-0.534582000	0.016084000	-0.265145000
H	0.895602000	-3.825904000	-0.323804000
H	-0.846499000	-5.533808000	0.234526000
H	-3.173385000	-4.831608000	0.718282000
H	-3.826181000	-2.460909000	0.675746000
O	0.108138000	1.216799000	-0.304439000
N	0.272365000	-1.069639000	-0.431560000
Pd	1.974297000	-1.106392000	-1.833878000
C	-2.916736000	0.689557000	0.282258000
N	-4.191348000	0.220039000	0.105230000
C	-5.442349000	1.003954000	0.245815000
C	-5.567898000	1.544731000	1.681563000
H	-4.755175000	2.236365000	1.912200000
H	-6.520407000	2.073929000	1.798678000
H	-5.541197000	0.723420000	2.406417000
C	-6.593213000	0.024897000	-0.037938000
H	-7.555297000	0.539607000	0.046063000

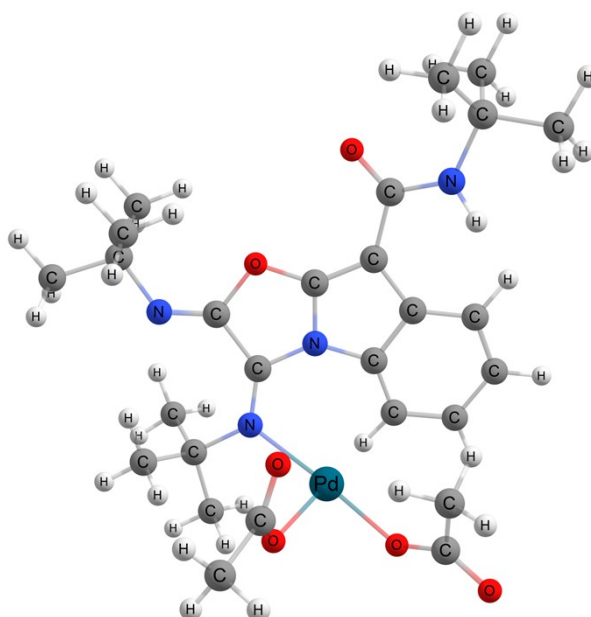
H	-6.524284000	-0.388285000	-1.052024000
H	-6.592098000	-0.806490000	0.676648000
C	-5.476204000	2.157570000	-0.775260000
H	-5.396947000	1.771081000	-1.798003000
H	-6.419476000	2.709711000	-0.692209000
H	-4.651168000	2.852345000	-0.602447000
O	-2.668268000	1.854423000	0.621938000
H	-4.279916000	-0.673511000	-0.358688000
C	1.471747000	1.077902000	-0.078497000
N	2.297532000	2.029782000	-0.034905000
C	1.953440000	3.459705000	-0.232243000
C	1.387327000	3.684737000	-1.649070000
H	1.252668000	4.757499000	-1.825964000
H	2.080781000	3.302843000	-2.407002000
H	0.418880000	3.196621000	-1.782028000
C	3.275138000	4.232282000	-0.081667000
H	3.112760000	5.307162000	-0.216315000
H	3.706304000	4.071694000	0.912387000
H	4.006864000	3.897734000	-0.825262000
C	0.951497000	3.935553000	0.839504000
H	-0.015094000	3.434857000	0.748616000
H	1.345960000	3.752647000	1.845277000
H	0.789828000	5.014358000	0.735551000
C	1.898975000	-0.368800000	0.052188000
N	2.682498000	-1.039515000	0.760297000
C	3.607197000	-0.685630000	1.861352000
C	4.026548000	-2.014626000	2.511123000
H	4.506870000	-2.668317000	1.775278000
H	4.732985000	-1.836698000	3.329250000
H	3.155081000	-2.540949000	2.914732000
C	2.896286000	0.200128000	2.902077000
H	3.561283000	0.363492000	3.757590000
H	2.632431000	1.176164000	2.488993000
H	1.986208000	-0.286003000	3.269608000
C	4.842051000	0.029311000	1.283001000
H	4.559303000	0.974773000	0.813301000
H	5.562859000	0.233551000	2.082925000
H	5.335884000	-0.601267000	0.535205000

27. [XV]



Zero-point correction=	0.517941 (Hartree/Particle)
Thermal correction to Energy=	0.550374
Thermal correction to Enthalpy=	0.551318
Thermal correction to Gibbs Free Energy=	0.453554
Sum of electronic and zero-point Energies=	-1392.661423
Sum of electronic and thermal Energies=	-1392.628990
Sum of electronic and thermal Enthalpies=	-1392.628046
Sum of electronic and thermal Free Energies=	-1392.725809

28. [XVI]



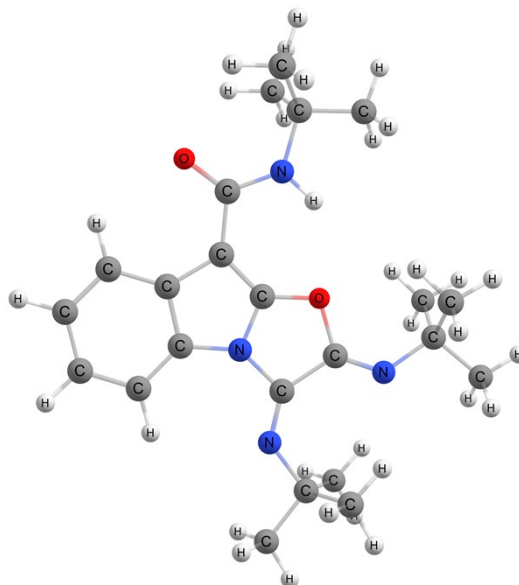
Zero-point correction=	0.622010 (Hartree/Particle)
Thermal correction to Energy=	0.664952
Thermal correction to Enthalpy=	0.665896
Thermal correction to Gibbs Free Energy=	0.544155
Sum of electronic and zero-point Energies=	-1849.571250
Sum of electronic and thermal Energies=	-1849.528309
Sum of electronic and thermal Enthalpies=	-1849.527365
Sum of electronic and thermal Free Energies=	-1849.649105

C	1.840702000	-1.364749000	-1.016395000
C	0.474395000	-1.027645000	-1.207744000
C	-0.478069000	-1.897179000	-1.731412000
C	-0.059396000	-3.202284000	-2.032133000
C	1.279707000	-3.568310000	-1.848368000
C	2.234959000	-2.664336000	-1.362729000
C	2.545536000	-0.165560000	-0.531367000
C	1.574281000	0.795490000	-0.465177000
H	-1.455885000	-1.546350000	-2.125260000
H	-0.773210000	-3.916009000	-2.428595000
H	1.590772000	-4.576148000	-2.105383000
H	3.270600000	-2.976310000	-1.276264000
O	1.467675000	2.101701000	-0.150875000
N	0.337125000	0.298542000	-0.813244000
Pd	-2.327260000	-1.183972000	-0.341346000
C	3.977742000	0.060858000	-0.197712000
N	4.643246000	-1.036892000	0.261576000
C	6.060873000	-1.079429000	0.708813000
C	6.988420000	-0.679276000	-0.451839000
H	6.808855000	0.351565000	-0.763855000
H	8.033864000	-0.769077000	-0.137026000
H	6.834448000	-1.336592000	-1.314858000
C	6.333857000	-2.536912000	1.112441000

H	7.365586000	-2.642967000	1.460507000
H	5.673638000	-2.855394000	1.928739000
H	6.192829000	-3.217561000	0.264697000
C	6.267706000	-0.151764000	1.920679000
H	5.608351000	-0.440487000	2.747072000
H	7.303167000	-0.218664000	2.272767000
H	6.059417000	0.887784000	1.657293000
O	4.490374000	1.175716000	-0.341089000
H	4.074036000	-1.831059000	0.525360000
C	0.109446000	2.492707000	-0.314589000
N	-0.327147000	3.646213000	-0.117960000
C	0.467094000	4.822664000	0.315724000
C	1.082824000	4.558533000	1.704600000
H	1.559500000	5.475079000	2.067712000
H	0.308628000	4.271571000	2.423995000
H	1.840529000	3.772203000	1.673582000
C	-0.523759000	5.995240000	0.402112000
H	-0.006588000	6.908710000	0.712996000
H	-0.994090000	6.180919000	-0.569299000
H	-1.314933000	5.785250000	1.129325000
C	1.559311000	5.139757000	-0.725637000
H	2.315684000	4.353435000	-0.780275000
H	1.119442000	5.275375000	-1.719763000
H	2.060330000	6.073515000	-0.449753000
C	-0.668917000	1.230842000	-0.683944000
N	-1.914916000	0.901683000	-0.769964000
C	-3.062951000	1.861803000	-1.009457000
C	-4.269517000	1.022909000	-1.467505000
H	-4.615670000	0.343579000	-0.686595000
H	-5.093539000	1.699852000	-1.715575000
H	-4.033564000	0.444276000	-2.367303000
C	-2.697786000	2.824927000	-2.156260000
H	-3.576967000	3.429117000	-2.401732000
H	-1.891196000	3.506715000	-1.887115000
H	-2.416040000	2.267009000	-3.056290000
C	-3.427712000	2.625237000	0.275710000
H	-2.592802000	3.223221000	0.641863000
H	-4.261124000	3.301697000	0.056245000
H	-3.750386000	1.935616000	1.057383000
O	-3.564701000	-0.682171000	1.196582000
O	-2.865192000	-3.087406000	-0.110008000
C	-2.991805000	-0.336342000	2.322999000
C	-2.352359000	-3.994951000	0.699313000
O	-1.775655000	-0.223310000	2.502116000
O	-2.755763000	-5.156611000	0.642135000
C	-3.988609000	-0.110832000	3.450413000
H	-4.973656000	0.177162000	3.076944000
H	-4.097572000	-1.051324000	4.003417000
H	-3.603066000	0.645949000	4.137762000
C	-1.243925000	-3.591366000	1.652930000

H	-1.201564000	-4.304887000	2.479022000
H	-0.287664000	-3.638135000	1.117395000
H	-1.360580000	-2.576259000	2.038274000

29. [3a]

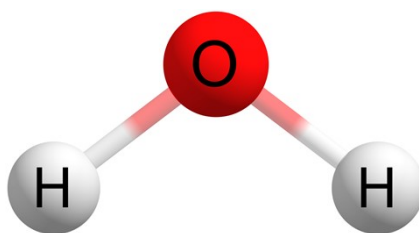


Zero-point correction=	0.517784 (Hartree/Particle)
Thermal correction to Energy=	0.548295
Thermal correction to Enthalpy=	0.549239
Thermal correction to Gibbs Free Energy=	0.456675
Sum of electronic and zero-point Energies=	-1264.774898
Sum of electronic and thermal Energies=	-1264.744386
Sum of electronic and thermal Enthalpies=	-1264.743442
Sum of electronic and thermal Free Energies=	-1264.836006

C	1.097192000	2.580359000	0.000173000
C	-0.326006000	2.580005000	0.000391000
C	-1.091777000	3.742010000	0.000461000
C	-0.397416000	4.954921000	0.000265000
C	1.007150000	4.985904000	0.000053000
C	1.764730000	3.811993000	0.000020000
C	1.565411000	1.190278000	0.000161000
C	0.407756000	0.456586000	0.000444000
H	-2.174012000	3.696834000	0.000644000
H	-0.955819000	5.886384000	0.000283000
H	1.517330000	5.944998000	-0.000088000
H	2.847539000	3.837888000	-0.000143000
O	0.082001000	-0.863860000	0.000327000
N	-0.716208000	1.235450000	0.000659000
C	2.975315000	0.740760000	-0.000131000
N	3.176288000	-0.611320000	-0.000170000
C	4.489449000	-1.303367000	-0.000262000

C	5.284634000	-0.939113000	-1.267381000
H	5.502427000	0.130447000	-1.297648000
H	6.233128000	-1.487626000	-1.285476000
H	4.719277000	-1.204649000	-2.167705000
C	4.176734000	-2.807995000	-0.000053000
H	5.106509000	-3.384579000	-0.000195000
H	3.604987000	-3.095441000	0.890455000
H	3.604629000	-3.095611000	-0.890278000
C	5.284981000	-0.938854000	1.266562000
H	4.719776000	-1.204011000	2.167098000
H	6.233365000	-1.487556000	1.284606000
H	5.502985000	0.130674000	1.296505000
O	3.901574000	1.562240000	-0.000344000
H	2.359421000	-1.206629000	0.000102000
C	-1.341365000	-0.959125000	0.000267000
N	-1.986257000	-2.030654000	0.000217000
C	-1.420211000	-3.400452000	0.000264000
C	-0.580796000	-3.631996000	-1.271674000
H	-0.262524000	-4.678930000	-1.315630000
H	-1.172662000	-3.421309000	-2.168668000
H	0.313096000	-3.004084000	-1.292689000
C	-2.623178000	-4.358931000	0.000157000
H	-2.284347000	-5.400115000	0.000151000
H	-3.246590000	-4.200601000	0.886141000
H	-3.246473000	-4.200565000	-0.885904000
C	-0.581075000	-3.631923000	1.272404000
H	0.312884000	-3.004108000	1.293521000
H	-1.173101000	-3.421057000	2.169250000
H	-0.262928000	-4.678887000	1.316554000
C	-1.891612000	0.469375000	0.000220000
N	-3.034926000	1.012747000	0.000008000
C	-4.377725000	0.400350000	-0.000472000
C	-5.360972000	1.586860000	-0.000949000
H	-5.209816000	2.212821000	-0.886903000
H	-6.397160000	1.231867000	-0.001271000
H	-5.210427000	2.213035000	0.884956000
C	-4.604782000	-0.437582000	1.272931000
H	-5.646605000	-0.774914000	1.310175000
H	-3.959043000	-1.317121000	1.294915000
H	-4.414569000	0.166105000	2.167229000
C	-4.603940000	-0.437875000	-1.273822000
H	-3.958278000	-1.317478000	-1.295165000
H	-5.645774000	-0.775103000	-1.311713000
H	-4.413061000	0.165582000	-2.168137000

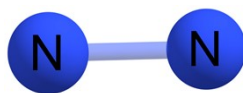
30. [H₂O]



Zero-point correction=	0.021166 (Hartree/Particle)
Thermal correction to Energy=	0.024002
Thermal correction to Enthalpy=	0.024946
Thermal correction to Gibbs Free Energy=	0.003512
Sum of electronic and zero-point Energies=	-76.417578
Sum of electronic and thermal Energies=	-76.414742
Sum of electronic and thermal Enthalpies=	-76.413798
Sum of electronic and thermal Free Energies=	-76.435232

O	0.000000000	0.000000000	0.117148000
H	0.000000000	0.768628000	-0.468593000
H	0.000000000	-0.768628000	-0.468593000

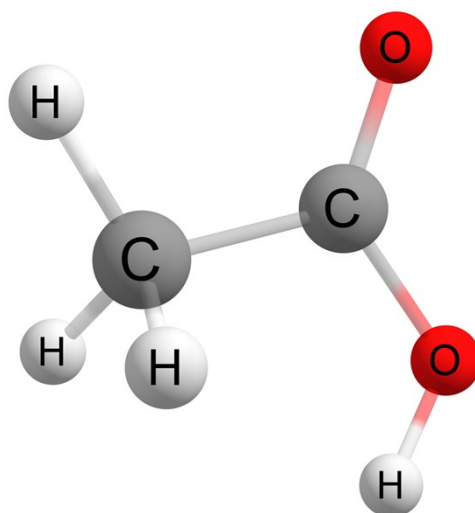
31. [N₂]



Zero-point correction=	0.005598 (Hartree/Particle)
Thermal correction to Energy=	0.007958
Thermal correction to Enthalpy=	0.008902
Thermal correction to Gibbs Free Energy=	-0.012851
Sum of electronic and zero-point Energies=	-109.518274
Sum of electronic and thermal Energies=	-109.515913
Sum of electronic and thermal Enthalpies=	-109.514969
Sum of electronic and thermal Free Energies=	-109.536722

N	0.000000000	0.000000000	0.552392000
N	0.000000000	0.000000000	-0.552392000

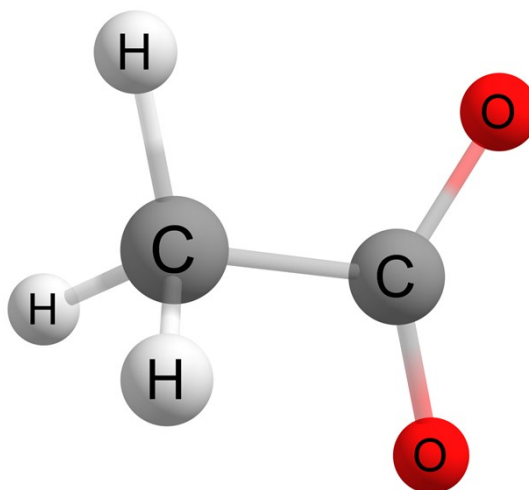
32. [CH₃COOH]



Zero-point correction=	0.061548 (Hartree/Particle)
Thermal correction to Energy=	0.066053
Thermal correction to Enthalpy=	0.066997
Thermal correction to Gibbs Free Energy=	0.034786
Sum of electronic and zero-point Energies=	-229.043131
Sum of electronic and thermal Energies=	-229.038625
Sum of electronic and thermal Enthalpies=	-229.037681
Sum of electronic and thermal Free Energies=	-229.069892

C	1.374843000	0.040662000	-0.000077000
H	1.857066000	-0.936849000	-0.000221000
H	1.695616000	0.599438000	-0.886895000
H	1.695681000	0.599207000	0.886864000
C	-0.126413000	-0.135111000	-0.000032000
O	-0.857174000	1.013820000	0.000217000
O	-0.700313000	-1.199785000	-0.000141000
H	-0.279046000	1.792621000	0.000295000

33. [CH₃COO⁻]



Zero-point correction=	0.048340 (Hartree/Particle)
Thermal correction to Energy=	0.052713
Thermal correction to Enthalpy=	0.053657
Thermal correction to Gibbs Free Energy=	0.021131
Sum of electronic and zero-point Energies=	-228.548194
Sum of electronic and thermal Energies=	-228.543821
Sum of electronic and thermal Enthalpies=	-228.542877
Sum of electronic and thermal Free Energies=	-228.575404

C	1.350740000	-0.049290000	-0.000026000
H	1.729110000	-1.076350000	-0.000659000
H	1.739639000	0.476086000	-0.881632000
H	1.740039000	0.475147000	0.881978000
C	-0.200598000	0.000662000	0.000226000
O	-0.705993000	1.158980000	-0.000057000
O	-0.807712000	-1.106869000	-0.000054000

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