– Supporting Information –

Iodine-Catalyzed Nazarov Cyclizations

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1 Details of the GC-FID Analysis

1.1 Linear Behavior of the Absorption

A stock solution of Ph_2O (0.19 g, 1.1 mmol) in *i*-PrOH (2 mL) was prepared in a volumetric flask. This stock solution was distributed to five samples to give Ph_2O concentrations between 0.02 and 0.07 mmol L^{-1}. The samples were analyzed by GC-FID. Table S1 summarizes the determined integrals and Figure S1 shows a linear correlation between the determined integrals and the employed standard concentrations. This indicates that the GC-FID integral correlates linearly with the standard concentration within the concentration range.

Table S1: Solutions and GC-FID Integrals for Ph_2O at Different Concentrations.

V [mL]	*n* [mmol]	Area
0.020	0.11	11899.9
0.030	0.16	17485.8
0.040	0.22	23191.6
0.050	0.27	29358.4
0.060	0.33	33975.6
0.070	0.38	39629.8

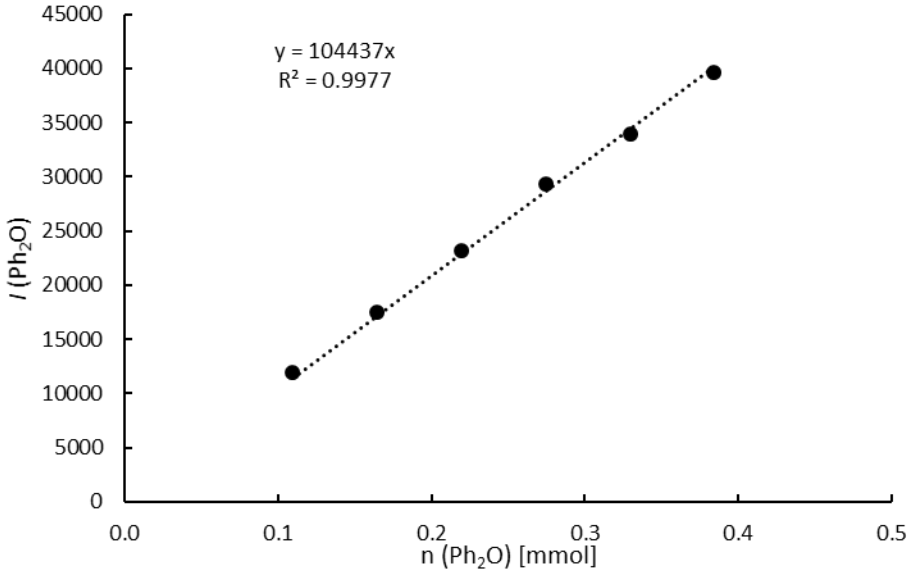


Figure S1: Correlation between the employed concentration and the GC-FID integral *I* for Ph_2O.

1.2 Determination of Calibration Curves

To interconvert the observed GC-FID integrals to concentrations, we have determined calibration lines for the 6-methyl-3,4,5,6-tetrahydrocyclopenta[*b*]pyran-7(2*H*)-one (**2a**). Therefore, a stock solution of **2a** was prepared (0.23 g, 1.5 mmol) in *i*-PrOH (2 mL) a volumetric flask. The stock solution was then filled into 5 GC vials according to Table S2 and filled to the top with *i*-PrOH. The resulting linear correlation between the ratio of Ph_2O and **2a** is shown in Figure S2.

Table S2: Calibration Solutions and GC-FID Integrals (*I*) for **2a**.

V (Ph_2O) [µL]	*n* [**2a**] [mmol]	*I* (Ph_2O)	*I* (**2a**)
50	0.076	41093.5	310948
50	0.062	34429.5	292887
50	0.048	26678.9	293956
50	0.033	19090.8	305391
50	0.019	10865.2	310914

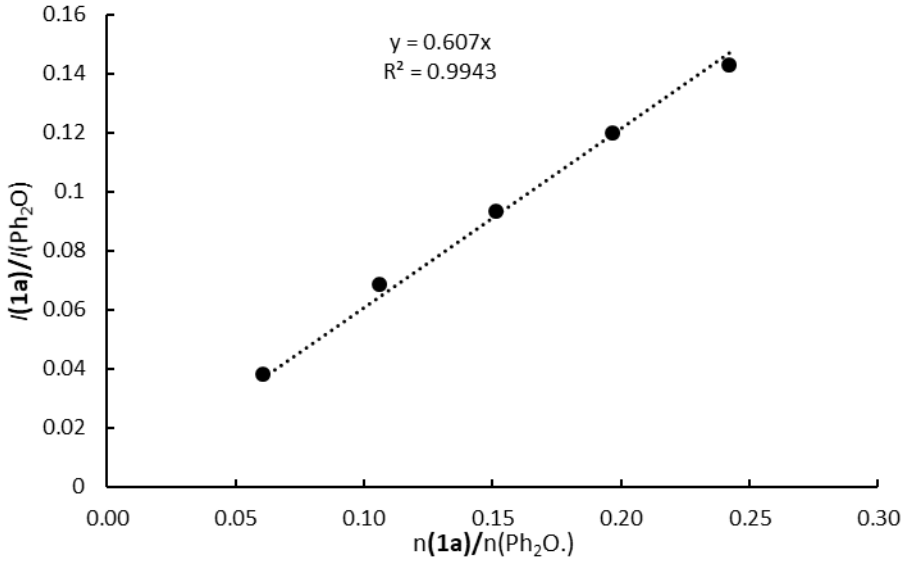
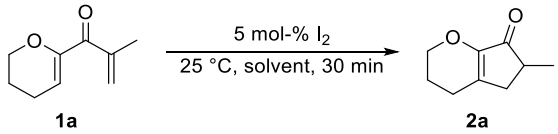


Figure S2: Correlation between the concentrations and GC-FID integrals *I*.

1.3 Solvent Effects on the Iodine-Catalyzed Nazarov Cyclization



1a **2a**

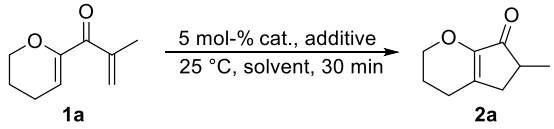
1a (50 mg, 0.33 mmol) was dissolved in the corresponding solvent (0.33 mL) and tempered to 25 °C with a cryostat. Molecular iodine (21 mg, 8.1 µmol) was dissolved in the corresponding solvent (2.5 mL) and 0.33 mL of this solution was added. A sample was taken after 5 and after 30 minutes and deactivated through filtering over a mixture of 1:1 (wt%) of Na_2CO_3 and $Na_2S_2O_4$. The samples were investigated via GC-FID and the obtained yields are listed below (Table S3).

Table S3: Experimental Data for the Iodine-Catalyzed Nazarov Cyclization of **1a** in various solvents (25 °C, Ph_2O as internal standard; isolated yields are shown in parenthesis).

Entry	Solvent	Water content	Yield (5 min)	Yield (30 min)
1	MeCN	10.5 ppm	62 %	87 % (80 %)
2	EtOAc	178.5 ppm	91 % (86 %)	97 %
3	DCM	18.6 ppm	51 %	74 % (66 %)
4	DCE	93.7 ppm	68 %	76 %
5	CCl_4	39.2 ppm	37 %	44 %
6	$CHCl_3$	1.6 ppm	0 %	0 %
7	$CHCl_3$ [a]	1.4 ppm	68 %	85 % (78 %)
8	THF	78.3 ppm	68 %	64 % (50 %)
9	1,4-Dioxan	39.2 ppm	82 %	82 % (60 %)
10	Toluene	37.0 ppm	44 %	71 %
11	Benzene	7.8 ppm	57 %	79 %
12	Et_2O	89.6 ppm	78 %	85 (82 %)
13	MeOAc	<3000 ppm	62 %	65 % (58 %)
14	MTBE	13.4 ppm	49 %	55 %
15	DMSO	12.5 ppm	<1 %	<1 %
16	MeOH	59.6 ppm	<1 %	<1 %
17	EtOH	<6000 ppm	<1 %	<1 %
18	DMF	13.4 ppm	<1 %	<1 %

[a]: $CHCl_3$ was stirred over Na_2CO_3 prior to use.

1.4 Details for the Additive Screening



1a (50 mg, 0.33 mmol) was placed under Argon in a flame-dried flask. Solvent, additive, Ph_2O as internal standard, and the catalyst were added consecutively. A sample was taken after 5 and after 30 minutes and deactivated through filtering over a mixture of 1:1 wt% of Na_2CO_3 and $Na_2S_2O_4$. The samples were investigated via GC-FID and the obtained yields are listed below.

Table S4: Experimental Data for the Iodine-Catalyzed Nazarov Cyclization of **1a** with Various Additives (CH_3CN, 25 °C, Ph_2O as internal standard).

Entry	Additive / Condition	Yield (5 min)	Yield (30 min)
1	I_2	62 %	87 %
2	dark with I_2	44 %	84 %
3	NaI	2 %	2 %
4	I_2 + NaI	4 %	4 %
5	aq. HI	30 %	67 %
6	aq. HI + NaI	16 %	55 %
7	*N*-iodosuccinimide	3 %	3 %
8	I_2 in MeOH	<1 %	<1 %
9	aq. HI in MeOH	13 %	98 %

2 Kinetic Investigations

2.1 Determination of the Reaction Order

Kinetics were recorded on a Bruker in situ IR. Two stock solutions were prepared: **1a** (0.304 g, 2.00 mmol in 2 mL MeCN, volumetric flask) and I_2 (76 mg 0.30 mmol, in 2 mL MeCN, volumetric flask). The Schlenk flasks used were flame dried and under argon. The temperature was controlled with a cryostat.

Table S5: Concentrations and Initial Rates (for 10 % and 15 % Conversion) for the I_2-Catalyzed Nazarov Cyclization of **1a** (MeCN, 25 °C).

1a [mmol L^{-1}]	I_2 [mmol L^{-1}]	mol%	10 % initial rate [mmol L^{-1} s^{-1}]	15 % initial rate [mmol L^{-1} s^{-1}]
500	75	3	0.716	0.635
500	60	6	1.38	1.29
500	45	9	1.80	1.80
500	30	12	2.25	2.20
500	15	15	2.78	2.86

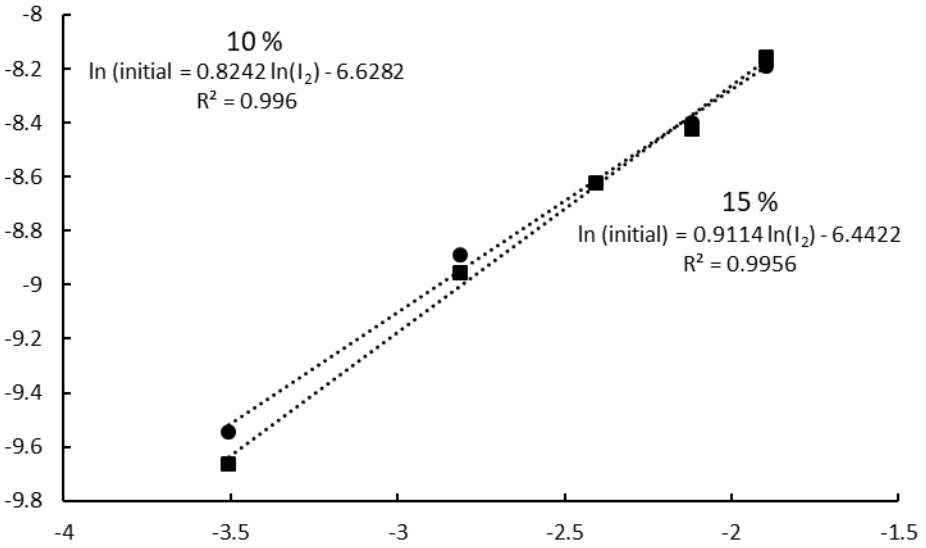


Figure S3: Double-logarithmic plots of the initial rates vs. the iodine concentrations for the molecular iodine catalyzed cyclization of **1a** (MeCN, 25 °C) considering up to 10 % yield (round dots) or up to 15 % yield (squares).

2.2 Determination of the Activation Parameters

Kinetics were recorded on a Bruker in situ IR. Two stock solutions were prepared: **1a** (0.304 g, 2.00 mol in 2 mL MeCN, volumetric flask) and I_2 (761 mg 0.30 mmol, in 2 mL MeCN, volumetric flask). The Schlenk flasks used were flame dried and under argon. The temperature was controlled with a cryostat.

Table S6: Temperatures and Initial Rates (for 10 %, 15 %, and 2 0% Conversion) for the I_2-Catalyzed Nazarov Cyclization of **1a** (MeCN).

1a [mmol L^{-1}]	I_2 [mmol L^{-1}]	*T* [°C]	10 % initial rate [mmol L^{-1} s^{-1}]	15 % initial rate [mmol L^{-1} s^{-1}]	20 % initial rate [mmol L^{-1} s^{-1}]
500	60	15	2.04	2.05	2.05
500	60	20	2.80	2.69	2.64
500	60	25	3.39	3.55	3.51
500	60	30	4.85	5.07	5.14
500	60	35	7.78	7.66	7.62
500	60	40	9.85	10.3	10.5

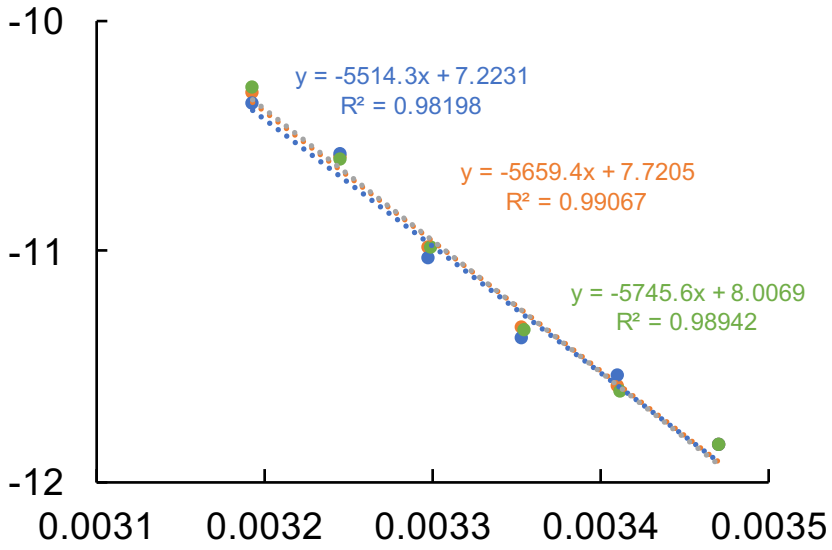


Figure S4: Eyring plots of the initial rates vs. the reciprocal temperature for the molecular iodine catalyzed cyclization of **1a** (MeCN, 25 °C) considering up to 10% yield (blue), up to 15% yield (orange), or up to 20 % (green).

3 Crystallographic Data

3.1 General Information

Crystals suitable for X-ray crystallography were obtained by the slow evaporation of the solvents used for the recrystallization. The measurements were carried out using a Bruker D8 venture equipped with a copper micro focus source. Structure solution was performed with SHELXT[1] and structure refinement with SHELXL.[2] All H atoms bonded to carbon were placed with idealized geometry and refined using a riding model with C–H = 0.95 Å, $U_{iso}(H) = 1.2U_{eq}(C)$ for CH, C–H = 0.99 Å, $U_{iso}(H) = 1.2U_{eq}(C)$ for CH_2, C–H = 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3.

3.2 Crystal data and structure refinement for 3e

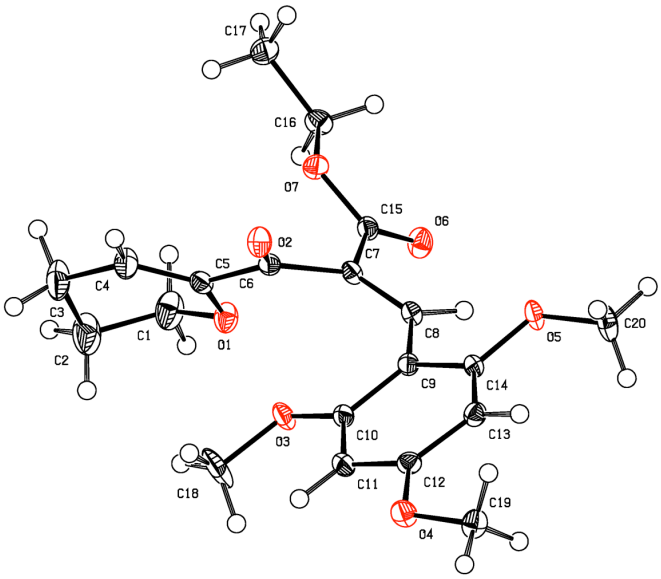


Figure S5: The molecular structure of **3e** (Displacement ellipsoids are drawn at the 50% probability level).

Identification code	3e	
Empirical formula	C20 H24 O7	
Moiety formula	C20 H24 O7	
Formula weight	376.39	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7751(4) Å	α = 99.719(2)°
	b = 10.6282(5) Å	β = 100.404(2)°
	c = 10.8238(5) Å	γ = 98.862(2)°
Volume	960.72(8) Å^3	
Z	2	
Density (calculated)	1.301 Mg/m^3	
Absorption coefficient	0.821 mm^{-1}	
F(000)	400	
Crystal size	0.400 × 0.400 × 0.050 mm^3	
Theta range for data collection	4.240 to 72.183°	
Index ranges	–9≤h≤10, –13≤k≤13, –13≤l≤13	
Reflections collected	19454	
Independent reflections	3779 [R(int) = 0.0562]	
Completeness to theta = 67.679°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7535 and 0.3695	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3779 / 0 / 252	
Goodness-of-fit on F^2	1.128	
Final R indices [I>2sigma(I)]	R_1 = 0.0510, wR_2 = 0.1218	
R indices (all data)	R_1 = 0.0587, wR_2 = 0.1269	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.339 and -0.326 e Å^{-3}	

3.3 Crystal data and structure refinement for 2c.

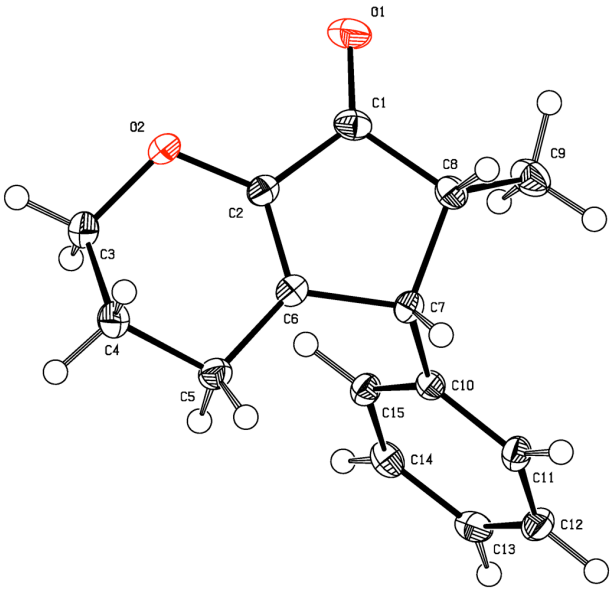


Figure S6: The molecular structure of **2c** (Displacement ellipsoids are drawn at the 50% probability level).

Identification code	2c	
Empirical formula	C15 H16 O2	
Moiety formula	C15 H16 O2	
Formula weight	228.28	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 6.4612(2) Å	α = 90°
	b = 11.7915(4) Å	β = 100.808(2)°
	c = 15.9166(5) Å	γ = 90°
Volume	1191.13(7) Å^3	
Z	4	
Density (calculated)	1.273 Mg/m^3	
Absorption coefficient	0.661 mm^{-1}	
F(000)	488	
Crystal size	0.300 × 0.200 × 0.200 mm^3	
Theta range for data collection	4.697 to 72.062°	
Index ranges	–7≤h≤7, –13≤k≤14,–16≤l≤19	
Reflections collected	6421	
Independent reflections	2261 [R(int) = 0.0335]	
Completeness to theta = 67.679°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7535 and 0.6160	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2261 / 0 / 155	
Goodness-of-fit on F^2	1.115	
Final R indices [I>2sigma(I)]	R_1 = 0.0381, wR_2 = 0.0949	
R indices (all data)	R_1 = 0.0458, wR_2 = 0.0993	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.211 and -0.234 e Å^{-3}	

3.4 Crystal data and structure refinement for 4a

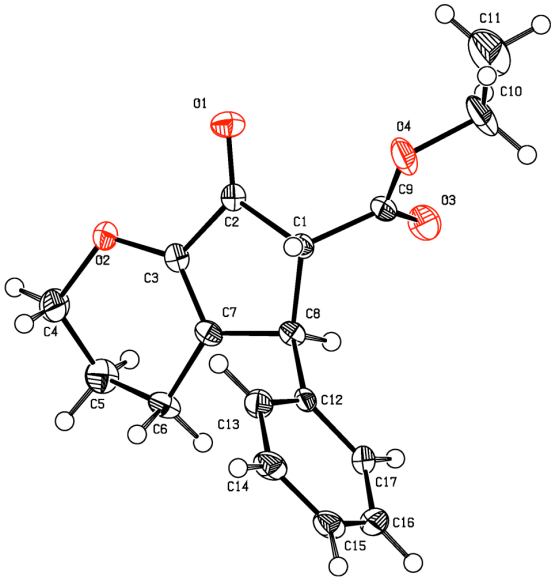


Figure S7: The molecular structure of **4a** (Displacement ellipsoids are drawn at the 50% probability level).

Identification code	4a	
Empirical formula	C17 H18 O4	
Moiety formula	C17 H18 O4	
Formula weight	286.31	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.5833(4) Å	α = 103.165(2)°
	b = 12.0583(5) Å	β = 101.617(2)°
	c = 13.2284(6) Å	γ = 90.070(2)°
Volume	1456.21(11) $Å^3$	
Z	4	
Density (calculated)	1.306 Mg/m^3	
Absorption coefficient	0.757 mm^{-1}	
F(000)	608	
Crystal size	0.150 × 0.150 × 0.020 mm^3	
Theta range for data collection	3.507 to 72.480°	
Index ranges	$-11 \le h \le 11$, $-14 \le k \le 14$, $-15 \le l \le 16$	
Reflections collected	11710	
Independent reflections	3554 [R(int) = 0.0642]	
Completeness to theta = 67.679°	61.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.4337	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3554 / 0 / 381	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R_1 = 0.0964, wR_2 = 0.2553	
R indices (all data)	R_1 = 0.1579, wR_2 = 0.2765	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.662 and -0.347 e $Å^{-3}$	

3.5 Crystal data and structure refinement for 4e

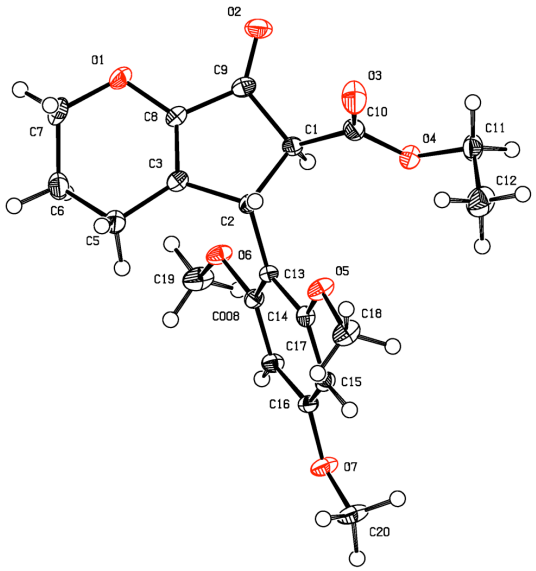


Figure S8: The molecular structure of **4e** (Displacement ellipsoids are drawn at the 50% probability level).

Identification code	4e	
Empirical formula	C20 H24 O7	
Moiety formula	C20 H24 O7	
Formula weight	376.39	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.8437(2) Å	α = 90°
	b = 11.9146(3) Å	β = 90°
	c = 20.1565(6) Å	γ = 90°
Volume	1883.72(9) Å^3	
Z	4	
Density (calculated)	1.327 Mg/m^3	
Absorption coefficient	0.837 mm^{-1}	
F(000)	800	
Crystal size	0.300 × 0.200 × 0.100 mm^3	
Theta range for data collection	4.310 to 72.054°	
Index ranges	–9≤h≤9, –14≤k≤14, –23≤l≤24	
Reflections collected	14487	
Independent reflections	3710 [R(int) = 0.0504]	
Completeness to theta = 67.679°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.5191	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3710 / 0 / 248	
Goodness-of-fit on F^2	1.105	
Final R indices [I>2sigma(I)]	R_1 = 0.0326, wR_2 = 0.0781	
R indices (all data)	R_1 = 0.0366, wR_2 = 0.0807	
Absolute structure parameter	0.39(8)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.189 and -0.229 e Å^{-3}	

4 Stability of Iodine in Ethyl Acetate

To test the stability of molecular iodine in ethyl acetate and to rule out the formation of HI through an α-iodination reaction, we prepared a NMR sample containing 15 µL ethyl acetate and 25 mg molecular iodine in 0.6 mL CD_3CN. For a better solubility, the sample was sonicated. The sample was measured initially, after 19, and 82 minutes (Figure S9).

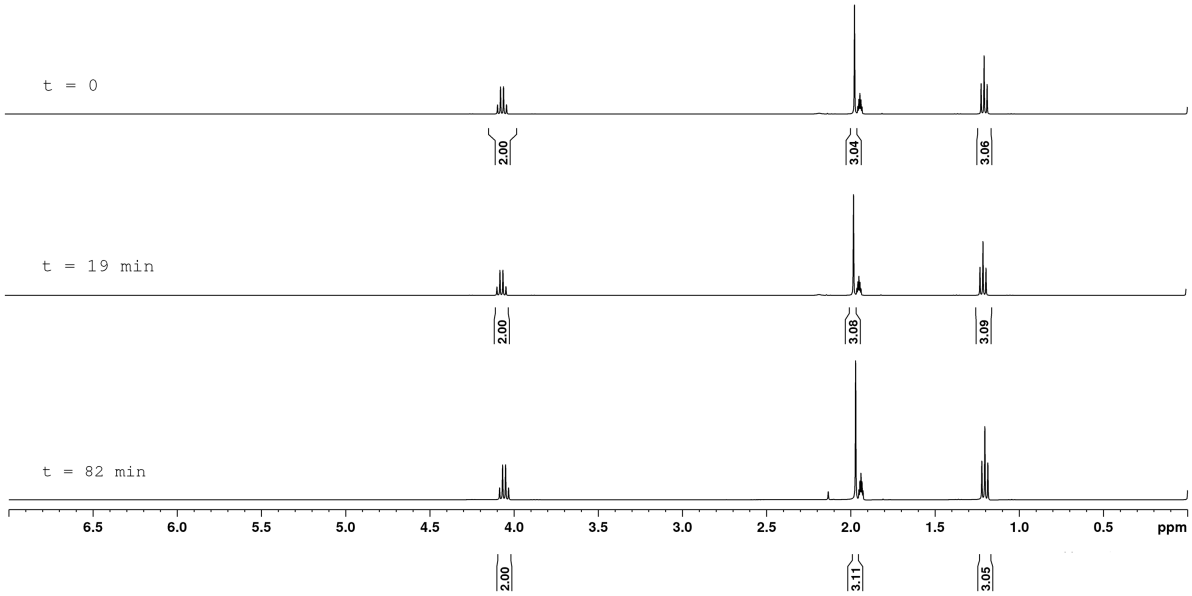


Figure S9: ^1H NMR measurements of 25 mg I_2 and 15 µL ethyl acetate in 0.6 mL CD_3CN over time.

5 *cis*/*trans* Isomerization

cis-Stilbene (45 mg, 0.25 mmol, 1 eq.) was dissolved in 0.25 mL CD_3CN. After an initial measurement, 0.25 mL (0.025 mmol, 0.1 eq.) of a molecular iodine solution (0.032 g in 1.25 mL) was added and the reaction was followed via NMR-spectroscopy (see Figure S10).

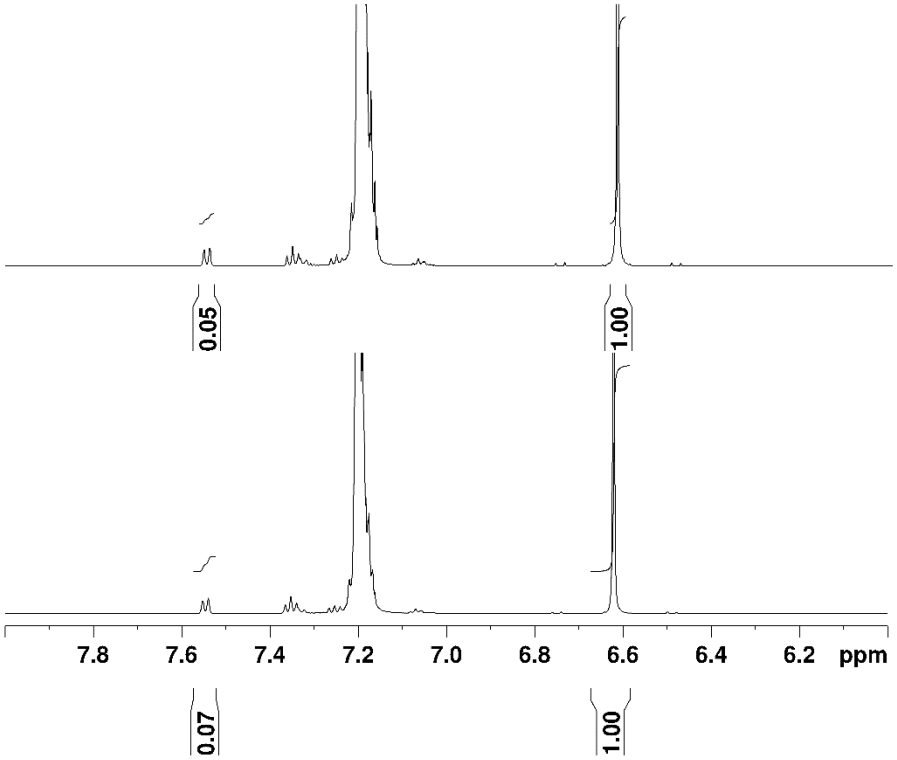


Figure S10: ^{1}H-NMR Spectra before the addition of molecular iodine and after 15 h reaction time.

6 Computational Investigations

6.1 Computational Details

The conformational space for all intermediates of the Nazarov cyclizations was explored using the OPLS3 force field[3] and a modified Monte Carlo search routine implemented in MacroModel.[4] An energy cutoff of 20 kcal mol^{-1} was chosen for the conformational analysis, and structures with heavy-atom root-mean-square deviations (RMSD) less than 1 Å after the initial force field optimizations were considered to be the same conformer. The remaining structures were subsequently optimized with the meta-hybrid M06-2X functional,[5] the triple-ζ basis set 6-311+G(d,p) for all atoms except I, and the aug-cc-pVTZ basis set with the corresponding pseudopotential (commonly called aug-cc-pVTZ-PP) for I.[6] Solvation by dichloromethane was accounted for by the SMD solvation model[7] with refined SMD parameters for iodine.[8] Vibrational analysis verified that each structure was a minimum or transition state. Following the intrinsic reaction coordinates (IRC) confirmed that all transition states connected the corresponding minima on the potential energy surface. Thermal corrections were calculated rom unscaled harmonic vibrational frequencies at the same level of theory and refer to a standard state of 298.15 K and 1 mol L^{-1}. Entropic contributions to free energies were obtained from partition functions evaluated with Grimme's quasi-harmonic approximation.[9] This method employs the free-rotor approximation for all frequencies below 100 cm^{-1}, the rigid-rotor-harmonic-oscillator (RRHO) approximation for all frequencies above 100 cm^{-1}, and a damping function to interpolate between the two expressions. Similar results were obtained from partition functions evaluated with Cramer's and Truhlar's quasiharmonic approximation.[10] This method uses the same approximations as the usual harmonic oscillator approximation, except that all vibrational frequencies lower than 100 cm^{-1} are set equal to 100 cm^{-1}. Energies were subsequently calculated with single-point calculations employing the double-hybrid B2PLYP functional,[11] Grimme's D3 correction (zero damping),[12] the large triple-ζ basis set aug-cc-pVTZ for all atoms, the aug-cc-pVTZ-PP pseudopotential for I,[6] and, the modified SMD solvation model for dichloromethane.[7-8]An ultrafine grid corresponding to 99 radial shells and 590 angular points was

used throughout this investigation for the numerical integration of the density. All DFT calculations were performed with Gaussian 16.[13]

6.2 Nazarov Cyclization 1a → 2a

6.2.1 Divinylketone **1a**

SCF energy:	–500.394997
Zero-point correction:	+0.194427
Enthalpy correction:	+0.206088
Free energy correction:	+0.157812
Truhlar's Delta G correction:	+0.158702
Grimme's Delta G correction:	+0.158813

Cartesian Coordinates

C	-2.52896	1.01718	-0.01864
H	-3.09366	1.77463	0.52298
H	-2.58150	1.23158	-1.09294
C	-3.02856	-0.38822	0.26514
O	-1.17038	1.17891	0.40169
H	-2.93854	-0.58344	1.33776
C	-2.18369	-1.38585	-0.52599
H	-4.08427	-0.46254	-0.00214
H	-2.30229	-2.39860	-0.13052
C	-0.73434	-0.99837	-0.46642
H	-2.51029	-1.42411	-1.57132
C	-0.32881	0.19062	0.00343
C	1.10357	0.62757	0.03604
C	2.20460	-0.38489	0.12865
O	1.37594	1.81008	-0.02212
C	2.07222	-1.47866	0.88140
C	3.48533	0.00026	-0.55556
H	3.87441	0.93128	-0.13714
H	3.31710	0.17333	-1.62213
H	4.23466	-0.78262	-0.43688
H	0.01355	-1.69945	-0.81182
H	1.15227	-1.70846	1.40545
H	2.90588	-2.16135	1.01382

6.2.2 Molecular Iodine

SCF energy:	–590.937090
Zero-point correction:	+0.000532
Enthalpy correction:	+0.004347
Free energy correction:	–0.025150
Truhlar's Delta G correction:	–0.025150
Grimme's Delta G correction:	–0.025152

Cartesian Coordinates

I	0.00000	0.00000	1.33036
I	0.00000	0.00000	-1.33036

6.2.3 Iodine-Complex **1a–I_2**

SCF energy:	–1091.347487
Zero-point correction:	+0.195532
Enthalpy correction:	+0.211869
Free energy correction:	+0.146130
Truhlar's Delta G correction:	+0.152179
Grimme's Delta G correction:	+0.150814

Cartesian Coordinates

C	1.41666	2.45318	-0.42633
H	0.77102	2.83947	-1.21363
H	0.84303	2.38452	0.50609
C	2.66103	3.30030	-0.22664
O	1.76422	1.12455	-0.83307
H	3.22239	3.32599	-1.16504
C	3.51430	2.68603	0.88322
H	2.37171	4.32356	0.01917
H	4.53821	3.06859	0.84659
C	3.54144	1.19107	0.75737
H	3.12052	2.95803	1.86902
C	2.72309	0.53166	-0.07543
C	2.66162	-0.95519	-0.17548
C	3.86522	-1.79637	0.08663
O	1.60431	-1.49370	-0.46754
C	5.08285	-1.36691	-0.25358
C	3.58593	-3.17533	0.61245
H	2.97888	-3.73829	-0.10017
H	3.02166	-3.12640	1.54753
H	4.51779	-3.71333	0.78684
H	4.23410	0.62068	1.36210
H	5.24901	-0.38669	-0.68346
H	5.94632	-2.01399	-0.13492
I	-0.98970	-0.49549	-0.21197
I	-3.57777	0.10305	0.20577

6.2.4 Transition State $\mathbf{TS_{uncat}}$

SCF energy:	–500.351104
Zero-point correction:	+0.193522
Enthalpy correction:	+0.204276
Free energy correction:	+0.158484
Truhlar's Delta G correction:	+0.158666
Grimme's Delta G correction:	+0.158836
Imaginary Frequency:	558.3 *i*cm^{-1}

Cartesian Coordinates

C	2.50202	0.95705	0.11180
H	3.10347	1.72730	-0.36644
H	2.67867	0.97580	1.19285
C	2.75099	-0.42701	-0.45749
O	1.13575	1.34356	-0.12823
H	2.48971	-0.41877	-1.52005
C	1.88978	-1.43121	0.30910
H	3.80982	-0.67821	-0.37461

H	1.81479	-2.37844	-0.23328
C	0.50359	-0.88271	0.54625
H	2.34857	-1.66100	1.27555
C	0.20999	0.43740	0.17652
C	-1.19132	0.81920	-0.02243
C	-1.92946	-0.39858	-0.17352
O	-1.62200	1.98612	-0.01434
C	-1.16305	-1.53036	-0.48749
C	-3.39359	-0.44869	0.12657
H	-3.65419	0.24521	0.92931
H	-3.69923	-1.46125	0.40109
H	-3.97951	-0.15899	-0.75279
H	-0.03987	-1.32732	1.36844
H	-0.49669	-1.56228	-1.34109
H	-1.55920	-2.50998	-0.21425

6.2.5 Transition State Iodine Catalysis $\mathbf{TS_{cat}–I_2}$

SCF energy:	–1091.315098
Zero-point correction:	+0.194932
Enthalpy correction:	+0.210254
Free energy correction:	+0.148846
Truhlar's Delta G correction:	+0.152120
Grimme's Delta G correction:	+0.151812
Imaginary Frequency:	470.7 *i*cm^{-1}

Cartesian Coordinates

C	2.09687	2.62026	-0.57889
H	1.73223	3.17629	-1.43965
H	1.47431	2.84673	0.29342
C	3.56498	2.87204	-0.29024
O	1.90173	1.23235	-0.91872
H	4.14902	2.56957	-1.16440
C	3.97218	2.06561	0.94396
H	3.73242	3.93799	-0.12803
H	5.06008	1.97388	1.01504
C	3.36098	0.69122	0.91863
H	3.64416	2.57267	1.85671
C	2.45710	0.35133	-0.09242
C	2.20003	-1.05257	-0.34832
C	3.26068	-1.82374	0.19117
O	1.17037	-1.50499	-0.93511
C	4.43374	-1.11220	0.46253
C	3.06514	-3.26517	0.53826
H	2.04082	-3.45456	0.86484
H	3.76677	-3.57207	1.31642
H	3.25119	-3.89339	-0.33891
H	3.30707	0.16859	1.86331
H	4.90115	-0.46733	-0.26997
H	5.11613	-1.50087	1.21807
I	-0.99266	-0.57400	-0.36764
I	-3.48323	0.38047	0.35398

6.2.6 Intermediate **11a**

SCF energy:	–500.389923
Zero-point correction:	+0.195973
Enthalpy correction:	+0.206958
Free energy correction:	+0.159988
Truhlar's Delta G correction:	+0.160702
Grimme's Delta G correction:	+0.160962

Cartesian Coordinates

C	2.49913	0.79225	0.35704
H	3.19125	1.60169	0.14095
H	2.57579	0.52051	1.41231
C	2.69545	-0.40242	-0.56344
O	1.17554	1.36377	0.15016
H	2.75223	-0.03418	-1.58958
C	1.55185	-1.43597	-0.43200
H	3.66285	-0.84663	-0.32336
H	1.11229	-1.62457	-1.41349
C	0.43921	-0.91267	0.50126
H	1.91797	-2.38835	-0.04725
C	0.20040	0.51724	0.21619
C	-1.17377	0.88317	-0.03818
C	-1.83873	-0.34840	0.03007
O	-1.60083	2.04842	-0.28338
C	-0.95833	-1.51743	0.33834
C	-3.29779	-0.50336	-0.18998
H	-3.75933	0.46057	-0.40747
H	-3.77733	-0.93612	0.69579
H	-3.49611	-1.19023	-1.02060
H	0.78424	-1.00123	1.53940
H	-0.97475	-2.25012	-0.47678
H	-1.29127	-2.04331	1.24000

6.2.7 Iodine Complex Intermediate **11a–I_2**

SCF energy:	–1091.359948
Zero-point correction:	+0.197957
Enthalpy correction:	+0.213314
Free energy correction:	+0.150400
Truhlar's Delta G correction:	+0.155057
Grimme's Delta G correction:	+0.154287

Cartesian Coordinates

C	-3.18306	2.56959	0.08723
H	-2.92559	3.41690	0.71615
H	-2.87889	2.77007	-0.94208
C	-4.64742	2.17749	0.19994
O	-2.34361	1.47506	0.57570
H	-4.90629	2.13311	1.25930
C	-4.94904	0.81999	-0.47828
H	-5.23423	2.98212	-0.24563
H	-5.43278	0.15107	0.23560
C	-3.64960	0.14504	-0.96733
H	-5.62215	0.93907	-1.32709

C	-2.59725	0.33080	0.05325
C	-1.93982	-0.87764	0.43667
C	-2.54716	-1.87839	-0.29433
O	-0.98134	-0.96653	1.32140
C	-3.65879	-1.37596	-1.16137
C	-2.16821	-3.30725	-0.22788
H	-1.31955	-3.45878	0.43873
H	-1.91756	-3.67296	-1.22901
H	-3.01627	-3.90515	0.12307
H	-3.31368	0.64933	-1.88208
H	-4.61306	-1.81051	-0.84507
H	-3.50317	-1.67036	-2.20313
I	1.05878	-0.32734	0.53768
I	3.60772	0.43651	-0.44641

6.2.8 Nazarov Product **2a**

SCF energy:	–500.432109
Zero-point correction:	+0.197026
Enthalpy correction:	+0.207714
Free energy correction:	+0.161735
Truhlar's Delta G correction:	+0.162455
Grimme's Delta G correction:	+0.162473

Cartesian Coordinates

C	-2.44376	0.88037	0.49273
H	-2.34214	0.70844	1.57081
H	-3.18764	1.65752	0.32503
C	-2.80748	-0.41590	-0.21789
O	-1.20179	1.42346	0.01311
H	-3.78638	-0.74836	0.13261
C	-1.73626	-1.48382	0.03826
H	-2.88641	-0.21866	-1.29096
H	-1.85771	-1.92943	1.03248
C	-0.38849	-0.84665	-0.06523
H	-1.81724	-2.30323	-0.68223
C	-0.23536	0.48776	-0.09422
C	1.18186	0.85517	-0.24433
C	1.97249	-0.44280	-0.36795
O	1.64367	1.97594	-0.25933
C	0.92914	-1.56172	-0.17158
C	3.13607	-0.47626	0.61836
H	2.76588	-0.42947	1.64661
H	3.80495	0.37086	0.45481
H	3.71049	-1.39794	0.50306
H	1.12957	-2.13530	0.74034
H	0.92068	-2.27487	-1.00083
H	2.36160	-0.47161	-1.39088

6.2.9 Iodine Complex **2a–I_2**

SCF energy:	–1091.384419
Zero-point correction:	+0.198274
Enthalpy correction:	+0.213581
Free energy correction:	+0.151199
Truhlar's Delta G correction:	+0.155934
Grimme's Delta G correction:	+0.155049

Cartesian Coordinates

C	5.39489	-1.64691	0.35630
H	5.71822	-1.23817	1.32062
H	5.63767	-2.70747	0.31934
C	6.03740	-0.87736	-0.78910
O	3.95795	-1.57884	0.30775
H	7.11914	-1.01511	-0.74313
C	5.66649	0.60897	-0.70964
H	5.68727	-1.29720	-1.73650
H	6.26224	1.12174	0.05458
C	4.21728	0.72494	-0.36891
H	5.86816	1.11887	-1.65615
C	3.50794	-0.33086	0.07060
C	2.10429	0.03268	0.26136
C	1.96064	1.51335	-0.04512
O	1.21021	-0.71960	0.61560
C	3.36646	1.95442	-0.50073
C	1.45607	2.26061	1.19109
H	2.17666	2.16902	2.00888
H	0.49823	1.86041	1.52909
H	1.32570	3.32053	0.96419
H	3.75578	2.76626	0.12259
H	3.37249	2.31405	-1.53376
H	1.23284	1.61458	-0.85631
I	-1.44173	-0.31490	0.20522
I	-4.07277	-0.00734	-0.28023

6.3 Nazarov Cyclization 1e → 2e

6.3.1 Divinylketone **1e** (*E* configuration)

SCF energy:	–500.399798
Zero-point correction:	+0.194156
Enthalpy correction:	+0.206104
Free energy correction:	+0.156242
Truhlar's Delta G correction:	+0.158018
Grimme's Delta G correction:	+0.157778

Cartesian Coordinates

C	2.05801	-1.50982	-0.35863
H	2.06160	-2.57318	-0.12352
H	2.19809	-1.38093	-1.43865
C	3.12278	-0.74473	0.40752
O	0.74482	-1.04679	-0.02261
H	2.93877	-0.86462	1.47922
C	3.05370	0.73332	0.02280

H	4.10447	-1.16763	0.18624
H	3.58536	1.35092	0.75189
C	1.62210	1.17496	-0.05503
H	3.54601	0.90324	-0.94153
C	0.60202	0.30910	-0.03929
C	-0.82578	0.77261	-0.03033
C	-1.87742	-0.27090	0.02485
O	-1.08176	1.96277	-0.06287
C	-3.17069	0.06627	0.02945
H	1.37689	2.22921	-0.09722
C	-4.30158	-0.90195	0.08519
H	-3.42438	1.12389	-0.01080
H	-4.94669	-0.77820	-0.79012
H	-4.92498	-0.70194	0.96214
H	-3.95091	-1.93388	0.12574
H	-1.56741	-1.30797	0.06130

6.3.2 Divinylketone **1e** (*Z* configuration)

SCF energy:	–500.395681
Zero-point correction:	+0.194397
Enthalpy correction:	+0.206240
Free energy correction:	+0.156473
Truhlar's Delta G correction:	+0.158453
Grimme's Delta G correction:	+0.158206

Cartesian Coordinates

C	-2.27640	-1.30763	0.42308
H	-2.49907	-2.35179	0.20820
H	-2.31848	-1.14773	1.50722
C	-3.22281	-0.35674	-0.28852
O	-0.92346	-1.10822	-0.00302
H	-3.13620	-0.51677	-1.36728
C	-2.84666	1.08289	0.06261
H	-4.25059	-0.58146	0.00253
H	-3.29849	1.78643	-0.64199
C	-1.35490	1.24121	0.03878
H	-3.23117	1.35011	1.05354
C	-0.52313	0.19502	-0.02327
C	0.96459	0.37503	-0.13148
C	1.77785	-0.84684	-0.30717
O	1.44804	1.49291	-0.08821
C	3.10624	-0.89191	-0.12848
H	-0.91035	2.22904	0.04233
H	3.58400	-1.85305	-0.30561
C	4.01583	0.21606	0.29644
H	1.24864	-1.75056	-0.58108
H	4.91333	-0.19191	0.76316
H	3.52654	0.91305	0.97582
H	4.33148	0.79457	-0.57893

6.3.3 Iodine Complex **1e–I_2** (*E* configuration)

SCF energy:	–1091.351449
Zero-point correction:	+0.195768
Enthalpy correction:	+0.212238
Free energy correction:	+0.146611
Truhlar's Delta G correction:	+0.152017
Grimme's Delta G correction:	+0.151028

Cartesian Coordinates

C	1.31414	2.73512	-0.21673
H	0.53435	3.10224	-0.88243
H	0.91093	2.66097	0.80058
C	2.55514	3.60997	-0.23758
O	1.61650	1.41237	-0.67332
H	2.94493	3.64067	-1.25908
C	3.60064	3.02042	0.70917
H	2.29078	4.62864	0.05156
H	4.59406	3.42527	0.49690
C	3.63897	1.52581	0.58200
H	3.37569	3.28826	1.74780
C	2.70148	0.84215	-0.09119
C	2.68618	-0.64242	-0.23266
C	3.92521	-1.40115	0.03917
O	1.65174	-1.19922	-0.57481
C	3.90241	-2.73574	0.11006
H	4.44609	0.98327	1.05640
C	5.09286	-3.59244	0.36779
H	2.94834	-3.24001	-0.02860
H	4.93565	-4.19290	1.26899
H	6.00155	-3.00132	0.48712
H	5.23148	-4.29866	-0.45660
H	4.85392	-0.85825	0.16783
I	-1.00142	-0.41475	-0.22693
I	-3.63473	-0.11381	0.23362

6.3.4 Iodine Complex **1e–I_2** (*Z* configuration)

SCF energy:	–1091.347915
Zero-point correction:	+0.195735
Enthalpy correction:	+0.212163
Free energy correction:	+0.146048
Truhlar's Delta G correction:	+0.152215
Grimme's Delta G correction:	+0.150948

Cartesian Coordinates

C	1.65695	2.62186	-0.19696
H	0.93903	3.08821	-0.87011
H	1.21236	2.54294	0.80265
C	2.97326	3.37721	-0.13866
O	1.85241	1.29697	-0.70299
H	3.40058	3.41350	-1.14487
C	3.92621	2.65469	0.81395
H	2.79327	4.40329	0.18680
H	4.95960	2.97244	0.64971

C	3.82888	1.16961	0.62376
H	3.69136	2.90116	1.85566
C	2.85812	0.60563	-0.10973
C	2.71686	-0.86482	-0.31407
C	3.86722	-1.73845	-0.00731
O	1.65929	-1.31159	-0.73785
C	3.74878	-3.03287	0.31955
H	4.56318	0.53015	1.09666
H	4.67653	-3.56972	0.50496
C	2.49816	-3.83427	0.48043
H	4.85415	-1.29398	-0.05082
H	1.63113	-3.21830	0.71380
H	2.63846	-4.58800	1.25734
H	2.27981	-4.36726	-0.45173
I	-0.91609	-0.32725	-0.29168
I	-3.50240	0.16784	0.25679

6.3.5 Transition State Uncatalyzed Conrotatory

SCF energy:	–500.351711
Zero-point correction:	+0.193638
Enthalpy correction:	+0.204290
Free energy correction:	+0.158812
Truhlar's Delta G correction:	+0.158914
Grimme's Delta G correction:	+0.159060
Imaginary Frequency:	484.3 *i*cm^{-1}

Cartesian Coordinates

C	-2.59577	0.29176	0.04992
H	-2.81188	0.26103	1.12292
H	-3.41235	0.78662	-0.47110
C	-2.30010	-1.09472	-0.49010
O	-1.45090	1.14761	-0.15015
H	-3.19845	-1.71173	-0.43424
C	-1.16229	-1.70670	0.32795
H	-2.01902	-1.00582	-1.54397
H	-1.54121	-2.07097	1.28740
C	-0.07831	-0.68754	0.57979
H	-0.73131	-2.57172	-0.18646
C	-0.27830	0.64471	0.19969
C	0.90746	1.51329	0.02911
C	2.00919	0.62991	-0.12162
O	0.86349	2.75568	0.04372
C	1.70361	-0.71466	-0.42473
H	1.11204	-0.93994	-1.30732
H	3.02207	0.93663	0.12093
H	0.57647	-0.88876	1.41692
C	2.63847	-1.82369	-0.03360
H	3.39174	-1.95574	-0.81727
H	2.10037	-2.77001	0.05749
H	3.14708	-1.61004	0.90783

6.3.6 Transition State Uncatalyzed Disrotatory

SCF energy:	–500.345893
Zero-point correction:	+0.194023
Enthalpy correction:	+0.204344
Free energy correction:	+0.159742
Truhlar's Delta G correction:	+0.159891
Grimme's Delta G correction:	+0.160006
Imaginary Frequency:	528.9 *i*cm^{-1}

Cartesian Coordinates

C	2.17478	-1.13454	0.18574
H	2.69934	-1.73902	0.92239
H	2.43796	-1.47506	-0.82078
C	2.42867	0.35180	0.34769
O	0.77456	-1.41718	0.39861
H	2.09391	0.65757	1.34351
C	1.65959	1.10227	-0.73996
H	3.49933	0.55146	0.27821
H	1.59110	2.16899	-0.50452
C	0.27237	0.53566	-0.90867
H	2.18932	1.02968	-1.69491
C	-0.08472	-0.62885	-0.22278
C	-1.52649	-0.95856	-0.08074
C	-2.21783	0.26009	-0.31005
O	-1.94694	-2.10605	0.13689
C	-1.45661	1.44325	-0.18307
H	-1.76256	2.27028	-0.82902
H	-3.21673	0.26978	-0.73270
H	-0.21522	0.75149	-1.84884
C	-0.86706	1.93918	1.11860
H	-1.64922	2.50054	1.64167
H	-0.03059	2.62328	0.95885
H	-0.55379	1.11501	1.76168

6.3.7 Transition State Iodine Catalysis Conrotatory

SCF energy:	–1091.316669
Zero-point correction:	+0.195329
Enthalpy correction:	+0.210398
Free energy correction:	+0.149962
Truhlar's Delta G correction:	+0.152652
Grimme's Delta G correction:	+0.152484
Imaginary Frequency:	389.8 *i*cm^{-1}

Cartesian Coordinates

C	-4.86753	-2.03354	0.25364
H	-5.24986	-2.19014	-0.76003
H	-4.87513	-2.97639	0.79543
C	-5.63031	-0.93366	0.96733
O	-3.47125	-1.67447	0.15123
H	-6.66269	-1.24784	1.12812
C	-5.57219	0.33739	0.11951
H	-5.17247	-0.76965	1.94740
H	-6.28334	0.27613	-0.70993

C	-4.19083	0.54119	-0.44004
H	-5.85493	1.21705	0.70659
C	-3.21895	-0.44514	-0.26778
C	-1.81872	-0.06512	-0.43703
C	-1.72079	1.32765	-0.29033
O	-0.92015	-0.92625	-0.69377
C	-2.81630	1.97420	0.31360
H	-3.17049	1.62240	1.27676
H	-0.90975	1.89639	-0.73432
H	-4.09893	1.21621	-1.27997
C	-3.13512	3.40590	0.01937
H	-2.58917	4.04292	0.72382
H	-4.19877	3.60170	0.17123
H	-2.85624	3.68549	-0.99703
I	1.35469	-0.41175	-0.26389
I	4.02036	0.14341	0.27602

6.3.8 Transition State Iodine Catalysis Disrotatory

SCF energy:	–1091.310064
Zero-point correction:	+0.195464
Enthalpy correction:	+0.210318
Free energy correction:	+0.149992
Truhlar's Delta G correction:	+0.153349
Grimme's Delta G correction:	+0.152882
Imaginary Frequency:	447.7 *i*cm^{-1}

Cartesian Coordinates

C	4.92699	-1.76808	0.52049
H	4.98142	-2.52379	1.30071
H	5.24702	-2.20164	-0.43217
C	5.71713	-0.51643	0.85085
O	3.52214	-1.44607	0.41157
H	5.32504	-0.08842	1.77814
C	5.57907	0.47369	-0.30580
H	6.76332	-0.77725	1.01808
H	5.88841	1.47947	-0.00302
C	4.16276	0.52219	-0.80494
H	6.23372	0.18803	-1.13529
C	3.22378	-0.37967	-0.31153
C	1.80128	-0.08725	-0.51917
C	1.67292	1.29072	-0.75789
O	0.92983	-1.00718	-0.52049
C	2.74884	2.10054	-0.34349
H	2.92904	2.99166	-0.94811
H	0.87289	1.68831	-1.37342
H	4.00094	0.96748	-1.77622
C	3.19421	2.27445	1.08573
H	2.60442	3.09872	1.50338
H	4.24462	2.56419	1.15770
H	3.00864	1.38348	1.68667
I	-1.36617	-0.43674	-0.19613
I	-4.02773	0.19891	0.22650

6.3.9 Zwitterionic Intermediate Conrotatory

SCF energy:	–500.381189
Zero-point correction:	+0.196199
Enthalpy correction:	+0.206777
Free energy correction:	+0.161441
Truhlar's Delta G correction:	+0.161653
Grimme's Delta G correction:	+0.161775

Cartesian Coordinates

C	2.56948	0.44002	0.06115
H	3.29653	0.90777	-0.59881
H	2.85180	0.62599	1.09864
C	2.39005	-1.03919	-0.21243
O	1.34511	1.23346	-0.12225
H	2.35543	-1.22077	-1.29031
C	1.10713	-1.55902	0.43835
H	3.27463	-1.54479	0.18046
H	0.98569	-2.62937	0.26634
C	-0.04440	-0.78149	-0.18814
H	1.12986	-1.38860	1.51970
C	0.19220	0.67849	-0.12357
C	-1.03387	1.47583	0.00188
C	-1.97557	0.50455	0.32835
O	-1.08603	2.73052	-0.09389
C	-1.47616	-0.90831	0.36584
H	-1.39440	-1.24980	1.40589
H	-3.00521	0.74710	0.57476
H	-0.08191	-1.02440	-1.26101
C	-2.35404	-1.89523	-0.40177
H	-3.35247	-1.94264	0.03921
H	-1.92549	-2.90085	-0.37813
H	-2.45599	-1.58541	-1.44565

6.3.10 Zwitterionic Intermediate Disrotatory

SCF energy:	–500.379608
Zero-point correction:	+0.196498
Enthalpy correction:	+0.206946
Free energy correction:	+0.161930
Truhlar's Delta G correction:	+0.162185
Grimme's Delta G correction:	+0.162292

Cartesian Coordinates

C	2.33998	0.82982	-0.41963
H	2.42338	0.73868	-1.50394
H	3.03815	1.58561	-0.06735
C	2.52145	-0.50591	0.27025
O	1.01496	1.43048	-0.20934
H	3.43725	-0.94798	-0.12772
C	1.31140	-1.41063	0.02865
H	2.66480	-0.35674	1.34409
H	1.17418	-1.57783	-1.04346
C	0.10645	-0.68775	0.62120
H	1.44779	-2.38114	0.50793

C	0.01703	0.71148	0.14211
C	-1.35364	1.23190	0.08184
C	-2.11032	0.07494	0.23578
O	-1.65350	2.43655	-0.13418
C	-1.33910	-1.19581	0.42299
H	-1.67910	-1.73040	1.31718
H	-3.19460	0.07395	0.17424
H	0.27630	-0.59748	1.70467
C	-1.47892	-2.14677	-0.77305
H	-2.52816	-2.41665	-0.91210
H	-0.90895	-3.06609	-0.61505
H	-1.12874	-1.66780	-1.69121

6.3.11 Zwitterionic Intermediate Iodine Complex Conrotatory

SCF energy:	–1091.350544
Zero-point correction:	+0.198296
Enthalpy correction:	+0.213224
Free energy correction:	+0.152832
Truhlar's Delta G correction:	+0.155977
Grimme's Delta G correction:	+0.155506

Cartesian Coordinates

C	4.89869	-2.02200	-0.29457
H	5.15333	-2.86075	0.34870
H	4.78203	-2.37201	-1.32082
C	5.88354	-0.87571	-0.19468
O	3.52353	-1.66284	0.10728
H	6.17466	-0.72056	0.84764
C	5.28590	0.41485	-0.75886
H	6.77586	-1.17810	-0.74650
H	6.00404	1.23365	-0.70595
C	4.05793	0.72803	0.08658
H	4.99685	0.28169	-1.80600
C	3.16106	-0.44571	0.17596
C	1.76491	-0.07264	0.29726
C	1.74053	1.26489	-0.00371
O	0.84707	-0.94981	0.56267
C	3.08590	1.86074	-0.29531
H	3.17476	2.02698	-1.37586
H	0.83324	1.85648	-0.06064
H	4.38413	0.91299	1.12182
C	3.34062	3.17710	0.43365
H	2.62566	3.93723	0.11204
H	4.34741	3.54539	0.22257
H	3.23867	3.04371	1.51390
I	-1.33985	-0.41515	0.21526
I	-4.07090	0.17019	-0.21881

6.3.12 Zwitterionic Intermediate Iodine Complex Disrotatory

SCF energy:	–1091.349184
Zero-point correction:	+0.198554
Enthalpy correction:	+0.213370
Free energy correction:	+0.153109
Truhlar's Delta G correction:	+0.156414
Grimme's Delta G correction:	+0.155873

Cartesian Coordinates

C	4.92534	-1.78584	0.67803
H	4.83636	-1.76845	1.76501
H	5.17263	-2.79244	0.34995
C	5.89465	-0.74019	0.16960
O	3.53898	-1.58511	0.21019
H	6.81120	-0.85013	0.75274
C	5.30994	0.66750	0.30886
H	6.14179	-0.93626	-0.87719
H	5.07695	0.88199	1.35539
C	4.04476	0.69278	-0.54114
H	6.01773	1.41889	-0.04263
C	3.16000	-0.45227	-0.22595
C	1.75947	-0.14976	-0.44751
C	1.72386	1.20858	-0.62734
O	0.84739	-1.07174	-0.39242
C	3.05968	1.88266	-0.53495
H	3.22317	2.52366	-1.40626
H	0.81075	1.77580	-0.77054
H	4.33998	0.52109	-1.58741
C	3.17016	2.74651	0.72813
H	2.40443	3.52465	0.71586
H	4.14862	3.22911	0.78139
H	3.02561	2.13987	1.62572
I	-1.33030	-0.46281	-0.15251
I	-4.05437	0.22068	0.18552

6.3.13 Nazarov Product **2f**

SCF energy:	–500.432349
Zero-point correction:	+0.196879
Enthalpy correction:	+0.207548
Free energy correction:	+0.161715
Truhlar's Delta G correction:	+0.162175
Grimme's Delta G correction:	+0.162341

Cartesian Coordinates

C	-2.42584	0.53516	0.50760
H	-2.31747	0.22364	1.55321
H	-3.30964	1.16407	0.41357
C	-2.49808	-0.68360	-0.40203
O	-1.31120	1.38334	0.18177
H	-3.39615	-1.25352	-0.15656
C	-1.23664	-1.54233	-0.24381
H	-2.58953	-0.34532	-1.43834
H	-1.28484	-2.13829	0.67499

C	-0.04772	-0.63723	-0.19782
H	-1.13469	-2.25183	-1.07092
C	-0.17275	0.68784	-0.01813
C	1.13798	1.35716	-0.07208
C	2.17514	0.26673	-0.27414
O	1.34754	2.54690	0.02508
C	1.39034	-1.05732	-0.37215
H	1.50793	-1.49392	-1.37015
H	2.86129	0.27713	0.57759
H	2.75964	0.48621	-1.17020
C	1.81671	-2.09844	0.66438
H	1.69954	-1.69788	1.67581
H	2.86463	-2.37384	0.52318
H	1.21379	-3.00627	0.58218

6.3.14 Iodine Complex Nazarov Product **2f–I_2**

SCF energy:	–1091.385117
Zero-point correction:	+0.198106
Enthalpy correction:	+0.213371
Free energy correction:	+0.151282
Truhlar's Delta G correction:	+0.155586
Grimme's Delta G correction:	+0.154892

Cartesian Coordinates

C	5.28176	-1.74560	0.49427
H	5.38751	-1.43238	1.53941
H	5.60146	-2.78180	0.39846
C	6.07225	-0.82034	-0.42006
O	3.87833	-1.74422	0.17380
H	7.13311	-0.90930	-0.17933
C	5.59008	0.62731	-0.26125
H	5.93594	-1.14606	-1.45532
H	5.99138	1.07339	0.65625
C	4.09748	0.63062	-0.20652
H	5.93415	1.25440	-1.08941
C	3.39527	-0.50181	-0.02091
C	1.95746	-0.23273	-0.05992
C	1.78239	1.25468	-0.26814
O	1.07127	-1.06543	0.05503
C	3.20774	1.83516	-0.36788
H	3.37304	2.26059	-1.36354
H	1.22394	1.66593	0.57840
H	1.18655	1.42693	-1.16815
C	3.50207	2.91329	0.67700
H	3.35886	2.51473	1.68568
H	2.83242	3.76625	0.54535
H	4.53048	3.27224	0.59089
I	-1.52963	-0.42079	0.01376
I	-4.15725	0.18964	-0.01317

6.4 Nazarov Cyclization 1g → 2g

6.4.1 Divinylketone **1g** (*E* configuration)

SCF energy:	–692.061734
Zero-point correction:	+0.248336
Enthalpy correction:	+0.263151
Free energy correction:	+0.205413
Truhlar's Delta G correction:	+0.208483
Grimme's Delta G correction:	+0.208060

Cartesian Coordinates

C	-3.43213	-1.70832	0.39127
H	-3.21902	-2.75626	0.18548
H	-3.61296	-1.58306	1.46566
C	-4.61526	-1.19124	-0.40806
O	-2.23250	-1.00020	0.05728
H	-4.39378	-1.29952	-1.47386
C	-4.84906	0.28016	-0.06497
H	-5.49633	-1.79584	-0.18518
H	-5.48079	0.76023	-0.81737
C	-3.53631	1.00139	0.01690
H	-5.38161	0.37332	0.88840
C	-2.36382	0.35682	0.03728
C	-1.05849	1.09598	0.03067
C	0.17880	0.28103	0.01892
O	-1.04362	2.31399	0.02948
C	1.37350	0.88957	0.00800
H	-3.50771	2.08412	0.03186
C	2.69293	0.25103	-0.00873
H	1.38135	1.97766	0.01316
H	0.07020	-0.79519	0.01887
C	3.82685	1.07319	0.00580
C	5.10538	0.52605	-0.00779
C	5.26760	-0.85526	-0.03738
C	4.14603	-1.68564	-0.05388
C	2.87032	-1.14042	-0.04001
H	3.69680	2.15026	0.02844
H	5.97196	1.17689	0.00415
H	6.26204	-1.28651	-0.04835
H	4.27025	-2.76212	-0.07833
H	2.01061	-1.80027	-0.05518

6.4.2 Iodine Complex **1g–I_2** (*E* configuration)

SCF energy:	–1283.013339
Zero-point correction:	+0.249661
Enthalpy correction:	+0.269106
Free energy correction:	+0.195215
Truhlar's Delta G correction:	+0.202929
Grimme's Delta G correction:	+0.201292

Cartesian Coordinates

C	-1.03529	3.29356	-0.16615
H	-1.91102	3.34850	-0.81122

H	-1.35196	3.00909	0.84466
C	-0.25341	4.59475	-0.13571
O	-0.23500	2.23157	-0.69701
H	0.06673	4.83507	-1.15355
C	0.96245	4.42809	0.77555
H	-0.89919	5.40258	0.21289
H	1.70285	5.21075	0.58831
C	1.59803	3.08557	0.56282
H	0.67225	4.52599	1.82786
C	1.00040	2.11732	-0.14819
C	1.57698	0.76061	-0.37445
C	3.02155	0.55294	-0.15231
O	0.84338	-0.14622	-0.74532
C	3.53259	-0.68579	-0.20861
H	2.56558	2.89289	1.00722
C	4.93598	-1.06575	-0.02675
H	2.84523	-1.50529	-0.40686
H	3.64285	1.41746	0.03966
C	5.26734	-2.42588	-0.06879
C	6.58302	-2.84403	0.09906
C	7.58749	-1.90476	0.30910
C	7.27063	-0.54625	0.35073
C	5.95836	-0.12856	0.18470
H	4.48149	-3.15567	-0.23359
H	6.82273	-3.90039	0.06455
H	8.61455	-2.22613	0.43883
H	8.05231	0.18716	0.51144
H	5.72906	0.93032	0.21630
I	-1.89686	-0.48244	-0.26089
I	-4.40384	-1.27315	0.30592

6.4.3 Transition State Uncatalyzed Conrotatory

SCF energy:	–692.014921
Zero-point correction:	+0.247363
Enthalpy correction:	+0.260972
Free energy correction:	+0.207481
Truhlar's Delta G correction:	+0.208878
Grimme's Delta G correction:	+0.208942
Imaginary Frequency:	469.7 *i*cm^{-1}

Cartesian Coordinates

C	-3.60897	-1.21883	0.29311
H	-3.71890	-1.25254	1.38174
H	-4.57888	-1.37181	-0.17466
C	-2.55719	-2.20167	-0.18499
O	-3.22614	0.12539	-0.07395
H	-2.89497	-3.22201	0.00359
C	-1.24729	-1.91286	0.54856
H	-2.43420	-2.08309	-1.26595
H	-1.28915	-2.30955	1.56726
C	-0.98764	-0.42921	0.60956
H	-0.40161	-2.40500	0.05684
C	-1.97504	0.46727	0.17558
C	-1.56206	1.84139	-0.18616
C	-0.16884	1.76559	-0.44213

O	-2.33986	2.81008	-0.23710
C	0.36708	0.46391	-0.62517
H	-0.02699	-0.17097	-1.41396
H	0.46690	2.64418	-0.42076
H	-0.30395	-0.09592	1.37794
C	1.78007	0.16703	-0.30556
C	2.44913	0.85778	0.71147
C	3.77751	0.56991	0.99943
C	4.44937	-0.41916	0.28216
C	3.78759	-1.12222	-0.72135
C	2.45802	-0.83348	-1.00961
H	1.91886	1.61448	1.28139
H	4.28911	1.11011	1.78765
H	5.48494	-0.64463	0.50986
H	4.30689	-1.89365	-1.27814
H	1.93948	-1.37615	-1.79383

6.4.4 Transition State Uncatalyzed Disrotatory

SCF energy:	–692.008583
Zero-point correction:	+0.247243
Enthalpy correction:	+0.260668
Free energy correction:	+0.208203
Truhlar's Delta G correction:	+0.209256
Grimme's Delta G correction:	+0.209389
Imaginary Frequency:	512.8 *i*cm^{-1}

Cartesian Coordinates

C	-1.44922	2.31236	-0.78417
H	-1.38383	2.74240	-1.78092
H	-2.27960	2.77345	-0.24100
C	-0.15207	2.41660	-0.00556
O	-1.78584	0.92127	-1.00377
H	0.63889	1.90274	-0.56160
C	-0.34830	1.77469	1.36691
H	0.12955	3.46665	0.08958
H	0.61454	1.60954	1.86011
C	-1.07666	0.46408	1.24417
H	-0.92535	2.43742	2.01985
C	-1.66141	0.10846	0.02201
C	-2.04293	-1.31591	-0.19199
C	-1.23481	-2.05589	0.70512
O	-2.92638	-1.67183	-0.98825
C	-0.10684	-1.37411	1.22973
H	0.18388	-1.64015	2.24863
H	-1.53196	-3.02867	1.08034
H	-1.51329	0.06942	2.15071
C	1.07258	-0.91728	0.43663
C	1.11932	-1.01093	-0.96066
C	2.22985	-0.55212	-1.65880
C	3.31294	0.00248	-0.97842
C	3.28575	0.07708	0.41110
C	2.17667	-0.38681	1.11237
H	0.29353	-1.45873	-1.50170
H	2.25411	-0.63755	-2.73930
H	4.17765	0.35731	-1.52726

H	4.12975	0.49093	0.95121
H	2.16071	-0.33651	2.19684

6.4.5 Transition State Iodine Catalysis Conrotatory

SCF energy:	–1282.980202
Zero-point correction:	+0.249132
Enthalpy correction:	+0.267194
Free energy correction:	+0.198600
Truhlar's Delta G correction:	+0.203464
Grimme's Delta G correction:	+0.202771
Imaginary Frequency:	374.8 *i*cm^{-1}

Cartesian Coordinates

C	-3.28953	-3.93974	0.17347
H	-3.63931	-4.18033	-0.83523
H	-2.99163	-4.85266	0.68377
C	-4.32498	-3.14075	0.94170
O	-2.07048	-3.17054	0.04776
H	-5.20769	-3.75770	1.11617
C	-4.68186	-1.89194	0.13540
H	-3.90656	-2.86990	1.91569
H	-5.35994	-2.14707	-0.68468
C	-3.44514	-1.26015	-0.43965
H	-5.20603	-1.15495	0.75275
C	-2.21361	-1.91239	-0.32673
C	-1.00072	-1.11568	-0.49547
C	-1.32208	0.22781	-0.26034
O	0.11176	-1.64938	-0.80334
C	-2.55759	0.47016	0.39104
H	-2.75318	-0.01301	1.34321
H	-0.70376	1.04257	-0.62079
H	-3.58295	-0.56553	-1.25636
C	-3.31223	1.71606	0.18954
C	-3.19993	2.44464	-1.00135
C	-3.91793	3.62093	-1.17103
C	-4.76305	4.07515	-0.15898
C	-4.89255	3.34903	1.02248
C	-4.17379	2.17184	1.19392
H	-2.55736	2.07976	-1.79630
H	-3.82623	4.18185	-2.09372
H	-5.32442	4.99241	-0.29499
H	-5.55136	3.70065	1.80777
H	-4.26604	1.60310	2.11362
I	2.13746	-0.52258	-0.29180
I	4.52511	0.74164	0.34330

6.4.6 Transition State Iodine Catalysis Disrotatory

SCF energy:	–1282.973451
Zero-point correction:	+0.248827
Enthalpy correction:	+0.266736
Free energy correction:	+0.199009
Truhlar's Delta G correction:	+0.203644
Grimme's Delta G correction:	+0.202955
Imaginary Frequency:	428.4 *i*cm^{-1}

Cartesian Coordinates

C	-4.01755	-2.17615	-1.47139
H	-4.03279	-2.17132	-2.55869
H	-4.21940	-3.18760	-1.10648
C	-4.96726	-1.16481	-0.85919
O	-2.65116	-1.84673	-1.12060
H	-4.69746	-0.16418	-1.21250
C	-4.85897	-1.24270	0.66282
H	-5.98518	-1.37678	-1.18983
H	-5.32205	-0.36887	1.13271
C	-3.42407	-1.32504	1.09012
H	-5.39053	-2.12017	1.04551
C	-2.42614	-1.52421	0.13593
C	-1.03644	-1.22326	0.51245
C	-1.07038	-0.29642	1.56206
O	-0.05687	-1.78872	-0.05965
C	-2.28952	0.40200	1.73382
H	-2.55835	0.65980	2.75963
H	-0.26463	-0.20501	2.28194
H	-3.22353	-1.60419	2.11485
C	-2.90526	1.32417	0.74624
C	-4.07983	1.99827	1.09967
C	-4.70292	2.85641	0.19928
C	-4.14999	3.06453	-1.06094
C	-2.96307	2.42118	-1.40976
C	-2.34153	1.55886	-0.51591
H	-4.50434	1.84404	2.08675
H	-5.61506	3.36734	0.48544
H	-4.62925	3.73839	-1.76161
H	-2.51259	2.60111	-2.37912
H	-1.40606	1.08468	-0.79151
I	2.06248	-0.66943	-0.03833
I	4.49267	0.64961	-0.07519

6.4.7 Intermediate Uncatalyzed Conrotatory

SCF energy:	–692.039270
Zero-point correction:	+0.249575
Enthalpy correction:	+0.263306
Free energy correction:	+0.208978
Truhlar's Delta G correction:	+0.211174
Grimme's Delta G correction:	+0.210897

Cartesian Coordinates

C	-3.55337	-1.23000	0.35726
H	-4.27966	-1.26652	1.16610
H	-4.06708	-1.36330	-0.59602
C	-2.42565	-2.22634	0.53059
O	-3.10954	0.17258	0.32887
H	-2.09332	-2.24173	1.57217
C	-1.24851	-1.87505	-0.38064
H	-2.83358	-3.21221	0.29822
H	-0.44222	-2.60327	-0.28219
C	-0.77279	-0.49190	0.04304
H	-1.56724	-1.85721	-1.42795
C	-1.89011	0.47658	0.09799
C	-1.49750	1.85903	-0.20919
C	-0.23200	1.68559	-0.76011
O	-2.23887	2.86332	-0.05436
C	0.27304	0.27293	-0.80532
H	0.20622	-0.12214	-1.82628
H	0.34574	2.50333	-1.17903
H	-0.38460	-0.55376	1.06974
C	1.70026	0.08932	-0.33167
C	2.15669	0.73979	0.81794
C	3.45891	0.55206	1.26815
C	4.32546	-0.28927	0.57186
C	3.88051	-0.93943	-0.57483
C	2.57452	-0.74928	-1.02278
H	1.48416	1.39933	1.35939
H	3.80022	1.06433	2.16074
H	5.34177	-0.43294	0.92052
H	4.54960	-1.59192	-1.12454
H	2.23043	-1.25330	-1.92083

6.4.8 Intermediate Uncatalyzed Disrotatory

SCF energy:	–692.037650
Zero-point correction:	+0.249727
Enthalpy correction:	+0.263412
Free energy correction:	+0.209275
Truhlar's Delta G correction:	+0.211513
Grimme's Delta G correction:	+0.211271

Cartesian Coordinates

C	-2.68305	-1.70340	0.88414
H	-2.25472	-1.81092	1.88190
H	-3.73078	-1.99428	0.90811
C	-1.88271	-2.46016	-0.15516
O	-2.71489	-0.24815	0.66499
H	-1.73814	-3.47161	0.23012
C	-0.54493	-1.76667	-0.42168
H	-2.45291	-2.53697	-1.08511
H	0.03882	-1.69764	0.50079
C	-0.88242	-0.37696	-0.94953
H	0.04621	-2.31909	-1.15366
C	-1.83980	0.32603	-0.06521
C	-1.69667	1.78896	-0.07288
C	-0.48427	1.96299	-0.73052

O	-2.50610	2.58418	0.47129
C	0.20113	0.71028	-1.18452
H	0.45116	0.75985	-2.24955
H	-0.02253	2.93603	-0.86386
H	-1.41958	-0.50442	-1.90094
C	1.49236	0.39513	-0.44026
C	1.63742	0.65725	0.92404
C	2.80582	0.30221	1.59302
C	3.84824	-0.31591	0.90679
C	3.71501	-0.57480	-0.45444
C	2.54481	-0.21971	-1.12078
H	0.83453	1.14493	1.46674
H	2.90374	0.51502	2.65175
H	4.75934	-0.58727	1.42772
H	4.52247	-1.05080	-0.99952
H	2.44480	-0.42247	-2.18279

6.4.9 Intermediate Iodine Catalysis Conrotatory

SCF energy:	–1283.007900
Zero-point correction:	+0.251557
Enthalpy correction:	+0.269652
Free energy correction:	+0.200583
Truhlar's Delta G correction:	+0.205975
Grimme's Delta G correction:	+0.204963

Cartesian Coordinates

C	3.43486	-3.84155	-0.00193
H	3.47912	-4.60194	0.77395
H	3.18410	-4.30763	-0.95537
C	4.69519	-3.00697	-0.09036
O	2.22567	-3.05944	0.32920
H	5.05868	-2.76686	0.91234
C	4.44458	-1.71464	-0.87036
H	5.45012	-3.62744	-0.57730
H	5.35693	-1.12326	-0.95366
C	3.38342	-0.94544	-0.09589
H	4.08560	-1.93639	-1.88022
C	2.20960	-1.79568	0.19948
C	0.97273	-1.03839	0.26987
C	1.28952	0.18799	-0.25535
O	-0.12852	-1.57476	0.68898
C	2.72214	0.32463	-0.68656
H	2.77726	0.24318	-1.77853
H	0.57622	0.99151	-0.40001
H	3.79207	-0.67104	0.88768
C	3.38878	1.61770	-0.27131
C	3.17520	2.15150	1.00192
C	3.81374	3.32406	1.39160
C	4.67583	3.97615	0.51196
C	4.89372	3.45038	-0.75785
C	4.25119	2.27717	-1.14664
H	2.50286	1.64653	1.69004
H	3.63725	3.73092	2.38083
H	5.17188	4.89111	0.81486
H	5.56003	3.95442	-1.44867

H	4.41565	1.87088	-2.13972
I	-2.11481	-0.52622	0.25884
I	-4.60082	0.69562	-0.27135

6.4.10 Intermediate Iodine Catalysis Disrotatory

SCF energy:	–1283.006612
Zero-point correction:	+0.251725
Enthalpy correction:	+0.269768
Free energy correction:	+0.200916
Truhlar's Delta G correction:	+0.206414
Grimme's Delta G correction:	+0.205387

Cartesian Coordinates

C	3.86079	-2.92906	1.22785
H	3.82653	-2.49474	2.22772
H	3.89093	-4.01332	1.30271
C	4.99010	-2.35852	0.39664
O	2.51765	-2.64392	0.67963
H	5.89099	-2.41386	1.01102
C	4.69258	-0.91725	-0.02308
H	5.15429	-2.97738	-0.48943
H	4.54567	-0.28384	0.85636
C	3.42150	-0.97032	-0.86178
H	5.51454	-0.50062	-0.60628
C	2.34527	-1.70926	-0.16219
C	1.01877	-1.23747	-0.51960
C	1.23776	-0.07094	-1.20474
O	-0.05041	-1.86571	-0.14580
C	2.68226	0.30628	-1.34424
H	2.92501	0.50821	-2.39103
H	0.44776	0.57185	-1.57618
H	3.63208	-1.57521	-1.75624
C	3.06901	1.54101	-0.54100
C	2.52312	1.80178	0.71783
C	2.94231	2.90741	1.45299
C	3.90956	3.76670	0.93866
C	4.45418	3.51586	-0.31769
C	4.03377	2.41031	-1.05206
H	1.76420	1.14321	1.12757
H	2.50642	3.10017	2.42677
H	4.23106	4.62980	1.51012
H	5.20336	4.18276	-0.72921
H	4.45742	2.21891	-2.03304
I	-2.02665	-0.71195	-0.05962
I	-4.47927	0.66746	0.10873

6.4.11 Nazarov Product **2g**

SCF energy:	–692.090229
Zero-point correction:	+0.250209
Enthalpy correction:	+0.264032
Free energy correction:	+0.209078
Truhlar's Delta G correction:	+0.211840
Grimme's Delta G correction:	+0.211370

Cartesian Coordinates

C	-3.20502	-1.56502	0.13823
H	-3.99582	-1.94738	0.78146
H	-3.55524	-1.56810	-0.90046
C	-1.92409	-2.37652	0.26873
O	-3.01493	-0.19443	0.53433
H	-1.58994	-2.34384	1.30997
C	-0.83189	-1.80420	-0.64378
H	-2.13941	-3.41728	0.01998
H	0.15487	-2.18193	-0.35920
C	-0.85870	-0.31402	-0.53688
H	-0.99444	-2.10312	-1.68597
C	-1.88250	0.33870	0.03634
C	-1.64059	1.79201	0.06826
C	-0.28795	2.02465	-0.57995
O	-2.37947	2.63843	0.52014
C	0.23629	0.62752	-0.98981
H	0.33907	0.56431	-2.07743
H	0.37086	2.52210	0.13519
H	-0.41173	2.69272	-1.43490
C	1.57637	0.26452	-0.37634
C	2.66424	-0.07029	-1.18043
C	3.89029	-0.41446	-0.61177
C	4.03763	-0.43048	0.77074
C	2.95300	-0.10094	1.58339
C	1.73261	0.24143	1.01304
H	2.55220	-0.05993	-2.26003
H	4.72783	-0.66985	-1.25124
H	4.98941	-0.69790	1.21531
H	3.06000	-0.11287	2.66227
H	0.88946	0.49379	1.65064

6.4.12 Iodine Complex Nazarov Product **2g–I_2**

SCF energy:	–1283.042706
Zero-point correction:	+0.251348
Enthalpy correction:	+0.269816
Free energy correction:	+0.198822
Truhlar's Delta G correction:	+0.205739
Grimme's Delta G correction:	+0.204284

Cartesian Coordinates

C	4.08680	-3.23068	0.79789
H	4.36666	-2.66797	1.69586
H	4.15505	-4.29643	1.00848
C	4.96438	-2.82626	-0.37822
O	2.69218	-2.97877	0.53832
H	5.99800	-3.09586	-0.15444
C	4.83480	-1.32200	-0.65071
H	4.65480	-3.39242	-1.26134
H	5.41864	-0.73952	0.07186
C	3.39528	-0.94231	-0.54557
H	5.21729	-1.06197	-1.64247
C	2.48073	-1.76524	-0.00314
C	1.14175	-1.17597	-0.07385

C	1.27944	0.18614	-0.71726
O	0.10980	-1.69925	0.31249
C	2.78520	0.35069	-1.03051
H	2.94056	0.43088	-2.11056
H	0.90607	0.94816	-0.02831
H	0.66156	0.22493	-1.61787
C	3.43790	1.55538	-0.37614
C	4.11118	2.50462	-1.14254
C	4.72496	3.60085	-0.53726
C	4.67200	3.75473	0.84353
C	4.00283	2.80742	1.61829
C	3.39338	1.71538	1.01197
H	4.15304	2.38701	-2.22069
H	5.24288	4.33263	-1.14699
H	5.14801	4.60615	1.31625
H	3.95854	2.92084	2.69562
H	2.87771	0.97710	1.62051
I	-2.30999	-0.52499	0.11453
I	-4.74620	0.61129	-0.07550

6.5 Nazarov Cyclization 12 → 13

6.5.1 Divinylketone **12** (*E* configuration)

SCF energy:	–919.876319
Zero-point correction:	+0.291542
Enthalpy correction:	+0.310743
Free energy correction:	+0.242790
Truhlar's Delta G correction:	+0.247374
Grimme's Delta G correction:	+0.246676

Cartesian Coordinates

C	0.24575	1.42136	0.18249
O	-0.08217	2.44645	1.00611
C	-0.40844	3.67035	0.33657
C	-1.37412	3.42822	-0.80985
H	0.52286	4.11474	-0.03417
H	-0.83057	4.31753	1.10386
C	-0.71035	2.51267	-1.83793
H	-1.65967	4.38299	-1.25488
H	-2.27833	2.95589	-0.41436
C	0.01777	1.40320	-1.13944
H	-0.00921	3.07693	-2.46333
H	-1.45154	2.08254	-2.51714
C	0.90831	0.30226	0.90773
O	1.26385	0.41579	2.05919
C	1.12105	-0.99635	0.17322
C	2.52667	-1.35743	-0.17106
O	2.88110	-2.42859	-0.59883
O	3.35383	-0.32932	0.02027
C	4.73367	-0.56454	-0.29023
H	5.24763	0.36615	-0.06423
H	4.84550	-0.81558	-1.34534
H	5.12465	-1.37463	0.32577
C	0.14939	-1.85209	-0.17488
C	-1.29780	-1.71266	0.02513
H	0.46646	-2.75012	-0.70105
C	-1.86696	-0.97562	1.07317
C	-2.14528	-2.35615	-0.88645
C	-3.52533	-2.22927	-0.78419
C	-4.07909	-1.47725	0.24837
C	-3.24706	-0.86101	1.18112
H	-1.23983	-0.51828	1.82928
H	-1.71093	-2.94907	-1.68458
H	-4.16761	-2.72291	-1.50418
H	-5.15539	-1.38329	0.33604
H	-3.67442	-0.29567	2.00108
H	0.34837	0.54393	-1.70929

6.5.2 Divinylketone **12** (*Z* configuration)

SCF energy:	–919.875155
Zero-point correction:	+0.291603
Enthalpy correction:	+0.310622
Free energy correction:	+0.243702
Truhlar's Delta G correction:	+0.247615
Grimme's Delta G correction:	+0.247154

Cartesian Coordinates

C	-2.42549	-0.79123	-0.02891
O	-2.26702	0.35245	-0.75241
C	-3.32969	1.29871	-0.58042
C	-4.67810	0.63027	-0.79185
H	-3.14244	2.08757	-1.30746
H	-3.25184	1.71118	0.43289
C	-4.87298	-0.47823	0.24524
H	-4.70228	0.21070	-1.80158
H	-5.47032	1.37792	-0.72149
C	-3.58903	-1.22033	0.46911
H	-5.64738	-1.17966	-0.07784
H	-5.21645	-0.06031	1.19817
C	-1.14258	-1.51512	0.21235
O	-1.11987	-2.70938	0.42374
C	0.11382	-0.69865	0.17759
C	-0.00590	0.76339	0.47070
O	-0.53290	1.19463	1.46799
O	0.54418	1.52422	-0.46933
C	0.51889	2.93500	-0.22220
H	0.99907	3.39314	-1.08317
H	1.07100	3.16919	0.68948
H	-0.51020	3.28433	-0.12908
C	1.27746	-1.32624	-0.05435
C	2.63138	-0.75995	-0.04638
H	1.21284	-2.38932	-0.27710
C	3.59266	-1.32323	-0.89437
C	3.00635	0.29164	0.80044
C	4.30340	0.78646	0.77245
C	5.24305	0.24189	-0.10151
C	4.88618	-0.81592	-0.93317
H	3.31462	-2.15605	-1.53174
H	2.29524	0.70229	1.50932
H	4.58530	1.59268	1.43967
H	6.25413	0.63202	-0.12208
H	5.61677	-1.25198	-1.60445
H	-3.57962	-2.12979	1.05816

6.5.3 Iodine Complex with **12** to CO Group (*E* configuration)

SCF energy:	–1510.830120
Zero-point correction:	+0.292825
Enthalpy correction:	+0.316612
Free energy correction:	+0.233294
Truhlar's Delta G correction:	+0.242290
Grimme's Delta G correction:	+0.240499

Cartesian Coordinates

C	2.83937	1.26988	-0.46197
O	3.03444	1.59657	-1.76172
C	4.22659	2.35125	-2.01592
C	5.42435	1.73585	-1.31475
H	4.06125	3.37672	-1.66526
H	4.33895	2.35863	-3.09882
C	5.18657	1.75697	0.19467
H	6.32688	2.28854	-1.58120
H	5.54439	0.70524	-1.66179
C	3.77476	1.35564	0.49697
H	5.37939	2.75486	0.60479
H	5.86849	1.07506	0.71037
C	1.45308	0.81546	-0.19262
O	0.57966	0.95217	-1.03025
C	1.14502	0.17464	1.13089
C	0.19525	0.89441	2.03064
O	-0.27998	0.43520	3.03912
O	-0.05002	2.12794	1.58940
C	-1.00937	2.88525	2.33903
H	-1.10810	3.83291	1.81597
H	-0.65326	3.04580	3.35686
H	-1.96524	2.35994	2.35968
C	1.63062	-1.00749	1.53866
C	2.55001	-1.89613	0.81976
H	1.32168	-1.33915	2.52790
C	2.57496	-1.99881	-0.57778
C	3.43751	-2.67415	1.57391
C	4.36464	-3.49702	0.94582
C	4.39623	-3.57510	-0.44414
C	3.49230	-2.83388	-1.20266
H	1.85568	-1.45631	-1.18114
H	3.40378	-2.61850	2.65690
H	5.05530	-4.08360	1.54030
H	5.11215	-4.22403	-0.93533
H	3.49601	-2.91239	-2.28353
H	3.50099	1.09973	1.51260
I	-2.04364	0.17324	-0.63986
I	-4.59603	-0.58265	-0.27587

6.5.4 Iodine Complex with **12** to CO Group (*Z* configuration)

SCF energy:	–1510.826026
Zero-point correction:	+0.292917
Enthalpy correction:	+0.316572
Free energy correction:	+0.233684
Truhlar's Delta G correction:	+0.242266
Grimme's Delta G correction:	+0.240570

Cartesian Coordinates

C	0.62483	1.84387	0.20783
O	1.39701	2.37718	-0.77808
C	1.42310	3.81141	-0.78097
C	0.01040	4.36995	-0.74297
H	1.95414	4.09315	-1.68887

H	1.99740	4.13805	0.09436
C	-0.68717	3.92310	0.54383
H	-0.53370	3.99765	-1.61555
H	0.04752	5.45864	-0.81129
C	-0.33402	2.50288	0.86724
H	-1.77322	4.01265	0.44908
H	-0.39887	4.56351	1.38487
C	0.99328	0.44360	0.54679
O	0.16958	-0.33968	0.99238
C	2.40694	0.03126	0.31730
C	3.43964	1.11369	0.26671
O	3.58283	1.93013	1.14434
O	4.18271	1.06170	-0.83258
C	5.23307	2.03256	-0.92063
H	5.93860	1.90137	-0.09861
H	4.81843	3.04096	-0.89281
H	5.72373	1.84910	-1.87308
C	2.68262	-1.28081	0.21917
C	3.99226	-1.92440	0.08273
H	1.82764	-1.95351	0.24086
C	4.06404	-3.13911	-0.61060
C	5.16052	-1.39400	0.64718
C	6.37424	-2.04913	0.49031
C	6.44060	-3.23857	-0.23397
C	5.28293	-3.78422	-0.78186
H	3.15756	-3.56757	-1.02490
H	5.11756	-0.48833	1.24266
H	7.26944	-1.63671	0.94092
H	7.39068	-3.74572	-0.35682
H	5.32751	-4.71605	-1.33326
H	-0.84888	1.98409	1.66755
I	-2.53328	-0.55203	0.33853
I	-5.09533	-0.93361	-0.36196

6.5.5 Iodine Complex with **12** to CO_2Me Group (*E* configuration)

SCF energy:	–1510.826012
Zero-point correction:	+0.292423
Enthalpy correction:	+0.316339
Free energy correction:	+0.231640
Truhlar's Delta G correction:	+0.241912
Grimme's Delta G correction:	+0.239501

Cartesian Coordinates

C	2.81141	-1.28472	0.79919
O	1.51932	-1.71291	0.71139
C	1.31710	-3.04625	1.19509
C	1.93100	-3.21643	2.57462
H	1.77765	-3.73936	0.47985
H	0.23851	-3.19664	1.19902
C	3.44138	-2.98439	2.49544
H	1.70533	-4.21495	2.95326
H	1.47221	-2.48993	3.25134
C	3.74597	-1.83735	1.57875
H	3.95209	-3.88266	2.13029
H	3.85629	-2.77873	3.48608

C	3.09432	-0.12546	-0.09838
O	4.14521	0.47277	-0.07766
C	1.98398	0.24325	-1.04555
C	1.46127	-0.84966	-1.90577
O	0.36142	-0.86881	-2.41884
O	2.35594	-1.81692	-2.06898
C	1.92111	-2.96859	-2.80761
H	1.03305	-3.39700	-2.34207
H	2.75041	-3.67018	-2.77030
H	1.70203	-2.69210	-3.83892
C	1.45347	1.46741	-1.17704
C	1.73470	2.66388	-0.37411
H	0.71962	1.59738	-1.97047
C	2.04204	2.59843	0.99037
C	1.64319	3.91652	-0.99197
C	1.90359	5.07817	-0.27448
C	2.22738	5.00196	1.07725
C	2.28494	3.76094	1.70962
H	2.06408	1.64049	1.49848
H	1.37723	3.97251	-2.04232
H	1.84360	6.04150	-0.76728
H	2.42115	5.90709	1.64132
H	2.51291	3.70032	2.76741
H	4.74633	-1.42291	1.53310
I	-1.86329	-0.31595	-0.76243
I	-4.00857	0.11833	0.78415

6.5.6 Iodine Complex with **12** to CO_2Me Group (*Z* configuration)

SCF energy:	–1510.827955
Zero-point correction:	+0.292714
Enthalpy correction:	+0.316397
Free energy correction:	+0.233076
Truhlar's Delta G correction:	+0.242415
Grimme's Delta G correction:	+0.240353

Cartesian Coordinates

C	0.34090	2.61531	-0.98638
O	1.19806	3.14295	-0.06677
C	0.55719	3.98212	0.90393
C	-0.31126	5.02373	0.21824
H	1.36301	4.43311	1.48116
H	-0.04485	3.33899	1.55792
C	-1.40951	4.32966	-0.59044
H	0.32189	5.62329	-0.44188
H	-0.73855	5.69164	0.96844
C	-0.87145	3.10356	-1.26448
H	-1.82618	5.00656	-1.34158
H	-2.24451	4.04084	0.05830
C	0.85000	1.36320	-1.61695
O	0.49850	1.02097	-2.72568
C	1.80843	0.53872	-0.80912
C	1.83739	0.74353	0.67049
O	0.85467	0.64225	1.37896
O	3.04114	1.02031	1.13544
C	3.15238	1.15534	2.56046

H	4.19997	1.37248	2.75120
H	2.86000	0.22462	3.04860
H	2.52127	1.97242	2.91091
C	2.55552	-0.38145	-1.44035
C	3.47268	-1.35901	-0.84512
H	2.46741	-0.40926	-2.52448
C	4.60126	-1.74830	-1.57666
C	3.24076	-1.94069	0.40847
C	4.13700	-2.86415	0.92968
C	5.27694	-3.21704	0.20930
C	5.50631	-2.65962	-1.04585
H	4.76943	-1.32123	-2.55968
H	2.33815	-1.70359	0.96239
H	3.94177	-3.31762	1.89449
H	5.97602	-3.93663	0.61968
H	6.38410	-2.94206	-1.61519
H	-1.47613	2.56714	-1.98649
I	-1.53259	-0.53152	0.57155
I	-3.82626	-1.72059	-0.15477

6.5.7 Transition State Uncatalyzed Conrotatory

SCF energy:	–919.836727
Zero-point correction:	+0.290809
Enthalpy correction:	+0.308810
Free energy correction:	+0.245595
Truhlar's Delta G correction:	+0.247626
Grimme's Delta G correction:	+0.247829
Imaginary Frequency:	394.4 *i*cm^{-1}

Cartesian Coordinates

C	0.10095	1.54499	0.02972
O	0.92096	2.19320	0.81955
C	2.13268	2.71972	0.22110
C	2.76372	1.67442	-0.67723
H	2.76120	2.99260	1.06536
H	1.85776	3.61860	-0.33801
C	1.79191	1.33585	-1.80685
H	2.98750	0.78310	-0.08190
H	3.70448	2.06053	-1.07266
C	0.39805	1.16464	-1.27414
H	2.09497	0.41664	-2.31819
H	1.78788	2.12771	-2.56300
C	-1.17541	1.05294	0.66218
O	-1.73908	1.67347	1.55516
C	-1.48569	-0.17080	-0.02431
C	-2.82466	-0.66792	-0.31648
O	-3.06659	-1.56689	-1.10074
O	-3.78734	-0.02182	0.35434
C	-5.12384	-0.46271	0.10232
H	-5.23597	-1.51614	0.36234
H	-5.38604	-0.31750	-0.94648
H	-5.75930	0.15094	0.73677
C	-0.38415	-0.74104	-0.72368
C	0.85678	-1.26631	-0.10539
C	1.79199	-1.90906	-0.92490

C	1.12767	-1.14086	1.26433
C	2.32045	-1.62251	1.78848
C	3.25857	-2.23612	0.95917
C	2.98817	-2.38490	-0.39825
H	1.57460	-2.03300	-1.98113
H	0.39862	-0.68441	1.92465
H	2.51553	-1.52670	2.85042
H	4.18746	-2.61072	1.37349
H	3.70458	-2.87671	-1.04619
H	-0.40960	1.09771	-1.99051
H	-0.63047	-1.24820	-1.65801

6.5.8 Transition State Uncatalyzed Disrotatory

SCF energy:	–919.836941
Zero-point correction:	+0.290707
Enthalpy correction:	+0.308923
Free energy correction:	+0.244531
Truhlar's Delta G correction:	+0.247352
Grimme's Delta G correction:	+0.247281
Imaginary Frequency:	364.6 *i*cm^{-1}

Cartesian Coordinates

C	-2.24105	0.46987	0.21545
O	-3.49090	0.55241	-0.18576
C	-4.31402	-0.61894	0.03280
C	-3.56758	-1.86397	-0.40640
H	-5.21697	-0.43694	-0.54503
H	-4.56065	-0.65629	1.09812
C	-2.31923	-2.02597	0.46110
H	-3.29675	-1.75638	-1.46107
H	-4.22321	-2.73139	-0.31637
C	-1.62917	-0.70300	0.64244
H	-1.61483	-2.73612	0.01466
H	-2.58519	-2.42788	1.44358
C	-1.40030	1.69070	0.02820
O	-1.86718	2.82721	0.04943
C	-0.06358	1.22317	-0.19939
C	1.09031	2.11284	-0.02098
O	1.10288	3.11824	0.65284
O	2.16502	1.70602	-0.72362
C	3.37166	2.43625	-0.49602
H	3.65240	2.38952	0.55796
H	3.25471	3.47848	-0.79523
H	4.12985	1.95231	-1.10771
C	0.02793	-0.16051	-0.54893
C	1.18390	-1.00878	-0.21190
C	1.51684	-2.07528	-1.05133
C	1.93310	-0.79264	0.95200
C	3.01307	-1.60988	1.25013
C	3.35353	-2.65865	0.39330
C	2.60408	-2.89213	-0.75522
H	0.92741	-2.25249	-1.94524
H	1.65771	0.01370	1.62614
H	3.58879	-1.43775	2.15213
H	4.19757	-3.29664	0.62935

H	2.86293	-3.70991	-1.41756
H	-0.87801	-0.63525	1.41637
H	-0.53134	-0.52641	-1.40470

6.5.9 Transition State Catalyzed Conrotatory (I_2 to CO)

SCF energy:	–1510.796222
Zero-point correction:	+0.292049
Enthalpy correction:	+0.314690
Free energy correction:	+0.235847
Truhlar's Delta G correction:	+0.242429
Grimme's Delta G correction:	+0.241414
Imaginary Frequency:	369.5 *i*cm^{-1}

Cartesian Coordinates

C	2.58057	0.77547	1.27654
O	2.70687	-0.08631	2.25703
C	4.04967	-0.31971	2.75415
C	5.01032	-0.48302	1.59255
H	3.96518	-1.21385	3.36686
H	4.31944	0.53334	3.38314
C	5.03231	0.80968	0.77830
H	4.67886	-1.32240	0.97247
H	6.00337	-0.71936	1.97760
C	3.64118	1.32909	0.56930
H	5.50292	0.64972	-0.19714
H	5.62297	1.57904	1.28655
C	1.19114	1.03681	0.80229
O	0.21872	0.98613	1.57256
C	1.28661	1.31366	-0.59137
C	0.41173	2.22079	-1.33740
O	0.54975	2.48632	-2.51374
O	-0.54844	2.75289	-0.57583
C	-1.51883	3.55565	-1.25373
H	-2.01102	2.97451	-2.03518
H	-1.04993	4.43734	-1.69192
H	-2.23879	3.84885	-0.49313
C	2.48635	0.85577	-1.20358
C	2.92652	-0.55272	-1.30517
C	4.09901	-0.83419	-2.01653
C	2.21450	-1.60980	-0.72041
C	2.68722	-2.91130	-0.82413
C	3.87176	-3.17865	-1.50966
C	4.57302	-2.13798	-2.11215
H	4.63779	-0.02167	-2.49362
H	1.27991	-1.42090	-0.20339
H	2.12417	-3.72195	-0.37638
H	4.23562	-4.19664	-1.58772
H	5.48449	-2.34156	-2.66222
H	3.52793	2.31988	0.15080
H	2.87351	1.47824	-2.01173
I	-2.05038	0.08575	0.68791
I	-4.35774	-1.05164	-0.17280

6.5.10 Transition State Catalyzed Conrotatory (I_2 to CO_2Me)

SCF energy:	–1510.790520
Zero-point correction:	+0.291828
Enthalpy correction:	+0.314560
Free energy correction:	+0.234787
Truhlar's Delta G correction:	+0.242238
Grimme's Delta G correction:	+0.240824
Imaginary Frequency:	370.4 *i*cm^{-1}

Cartesian Coordinates

C	3.77952	0.27910	0.06674
O	4.58989	-0.40964	0.83193
C	5.37808	-1.44417	0.18898
C	4.50474	-2.25362	-0.74901
H	5.78308	-2.03253	1.00881
H	6.19312	-0.94861	-0.34595
C	3.95552	-1.33435	-1.83935
H	3.68674	-2.70038	-0.17467
H	5.09533	-3.06317	-1.18051
C	3.47790	-0.03927	-1.24952
H	3.12492	-1.81224	-2.36880
H	4.72404	-1.12165	-2.58964
C	3.01693	1.38827	0.74746
O	3.49964	2.04701	1.65675
C	1.74036	1.43621	0.08346
C	0.95107	2.63103	-0.13534
O	-0.07629	2.66514	-0.80885
O	1.44134	3.72342	0.44739
C	0.68152	4.92547	0.27632
H	-0.33077	4.79463	0.66008
H	0.64081	5.20516	-0.77680
H	1.20764	5.68540	0.84893
C	1.42219	0.25728	-0.65201
C	1.21153	-1.09407	-0.08757
C	0.77778	-2.11302	-0.94341
C	1.41266	-1.38286	1.26895
C	1.21241	-2.67225	1.74485
C	0.80790	-3.68811	0.87954
C	0.58364	-3.40413	-0.46485
H	0.58971	-1.88481	-1.98806
H	1.70400	-0.59664	1.95678
H	1.36261	-2.88369	2.79725
H	0.65141	-4.69213	1.25679
H	0.24972	-4.18477	-1.13857
H	3.20361	0.75768	-1.92759
H	0.87497	0.41071	-1.58405
I	-2.10374	0.87147	-0.32011
I	-4.00720	-0.94862	0.20156

6.5.11 Transition State Catalyzed Disrotatory (I_2 to CO)

SCF energy:	–1510.797815
Zero-point correction:	+0.292198
Enthalpy correction:	+0.314945
Free energy correction:	+0.235420
Truhlar's Delta G correction:	+0.242281
Grimme's Delta G correction:	+0.241242
Imaginary Frequency:	327.6 *i*cm^{-1}

Cartesian Coordinates

C	2.07162	2.19313	-0.41783
O	1.76550	3.42738	-0.07743
C	2.88134	4.31649	0.17291
C	3.90183	3.62538	1.05667
H	2.43857	5.19337	0.63892
H	3.31046	4.59136	-0.79523
C	4.45948	2.41061	0.31494
H	3.41188	3.32233	1.98678
H	4.69784	4.32686	1.31034
C	3.35650	1.65892	-0.37298
H	4.98038	1.73084	0.99761
H	5.19458	2.72141	-0.43384
C	0.94886	1.28609	-0.71609
O	-0.15126	1.70694	-1.14093
C	1.35845	-0.03025	-0.38777
C	0.67525	-1.20538	-0.97929
O	0.19212	-1.23117	-2.08559
O	0.63955	-2.24413	-0.13788
C	0.05356	-3.44383	-0.65582
H	0.60789	-3.78783	-1.53058
H	-0.98891	-3.27007	-0.92558
H	0.12089	-4.17450	0.14650
C	2.50140	-0.11490	0.46054
C	3.43810	-1.24628	0.43834
C	4.11644	-1.59296	1.61151
C	3.68355	-1.96904	-0.73691
C	4.56821	-3.03716	-0.72763
C	5.22362	-3.39045	0.45297
C	4.99969	-2.66708	1.62074
H	3.93512	-1.02467	2.51820
H	3.19209	-1.68148	-1.66199
H	4.75562	-3.59209	-1.63939
H	5.91523	-4.22517	0.45731
H	5.51334	-2.93769	2.53574
H	3.63844	0.93612	-1.12534
H	2.49542	0.42831	1.39935
I	-2.27339	0.62176	-0.34124
I	-4.56083	-0.48193	0.65917

6.5.12 Transition State Catalyzed Disrotatory (I_2 to CO_2Me)

SCF energy:	–1510.790996
Zero-point correction:	+0.292150
Enthalpy correction:	+0.314961
Free energy correction:	+0.234716
Truhlar's Delta G correction:	+0.242412
Grimme's Delta G correction:	+0.240973
Imaginary Frequency:	335.4 *i*cm^{-1}

Cartesian Coordinates

C	-3.82775	-0.05721	-1.06069
O	-4.41050	-0.38357	-2.19254
C	-5.19323	-1.60281	-2.18478
C	-4.41380	-2.71315	-1.50713
H	-5.40161	-1.80641	-3.23237
H	-6.12838	-1.39108	-1.65790
C	-4.16304	-2.32697	-0.04948
H	-3.46808	-2.85326	-2.03933
H	-4.97710	-3.64500	-1.57479
C	-3.74956	-0.88627	0.04933
H	-3.38177	-2.95092	0.39816
H	-5.06567	-2.48172	0.54973
C	-3.05929	1.22866	-1.05870
O	-3.36779	2.17730	-1.77137
C	-1.96692	1.03967	-0.14075
C	-1.21094	2.14024	0.44784
O	-0.09128	2.05170	0.93713
O	-1.85376	3.30520	0.40026
C	-1.12956	4.44811	0.86985
H	-0.20498	4.57130	0.30492
H	-0.89983	4.34525	1.93088
H	-1.78897	5.29691	0.70590
C	-1.69554	-0.33479	0.15735
C	-1.14279	-0.80853	1.43512
C	-0.37002	-1.97439	1.44923
C	-1.40399	-0.14405	2.63949
C	-0.86917	-0.61756	3.82817
C	-0.07627	-1.76657	3.82906
C	0.16931	-2.44747	2.64036
H	-0.17752	-2.49517	0.51638
H	-2.03468	0.73989	2.64026
H	-1.07174	-0.09813	4.75749
H	0.34030	-2.13414	4.75992
H	0.77878	-3.34352	2.64111
H	-3.73902	-0.43262	1.02999
H	-1.51371	-1.02098	-0.66423
I	1.97974	0.60864	-0.04071
I	4.07943	-0.73255	-1.05588

6.5.13 Zwitterionic Intermediate Conrotatory

SCF energy:	–919.864848
Zero-point correction:	+0.293400
Enthalpy correction:	+0.311530
Free energy correction:	+0.247156
Truhlar's Delta G correction:	+0.250331
Grimme's Delta G correction:	+0.250090

Cartesian Coordinates

C	-0.92984	-1.73083	0.03576
O	-1.75969	-2.41606	0.69610
C	-3.21256	-2.14172	0.61671
C	-3.60116	-1.31641	-0.59039
H	-3.42775	-1.63029	1.55548
H	-3.66533	-3.13011	0.62671
C	-2.65184	-0.12945	-0.76817
H	-4.62791	-0.98297	-0.42703
H	-3.59319	-1.93971	-1.48855
C	-1.26035	-0.71439	-0.97799
H	-2.66845	0.50812	0.12010
H	-2.94029	0.47955	-1.62566
C	0.54235	-1.87711	0.27002
O	1.01349	-2.81981	0.92311
C	1.05854	-0.73810	-0.36742
C	2.45243	-0.32634	-0.43535
O	2.83563	0.66312	-1.03270
O	3.29294	-1.13946	0.22048
C	4.67342	-0.77411	0.16935
H	5.19931	-1.53117	0.74675
H	4.82781	0.21157	0.61082
H	5.03263	-0.76970	-0.86086
C	0.02575	0.15991	-0.99918
C	-0.18872	1.48055	-0.27204
C	-0.47259	2.63043	-1.00940
C	-0.16238	1.56500	1.12147
C	-0.42383	2.77305	1.76240
C	-0.71065	3.91513	1.01854
C	-0.73212	3.84077	-0.37121
H	-0.48518	2.57712	-2.09376
H	0.07080	0.68468	1.71196
H	-0.39598	2.82346	2.84522
H	-0.90763	4.85668	1.51829
H	-0.94636	4.72555	-0.96030
H	-1.26404	-1.28159	-1.92228
H	0.29379	0.39833	-2.03145

6.5.14 Zwitterionic Intermediate Disrotatory

SCF energy:	–919.865039
Zero-point correction:	+0.292914
Enthalpy correction:	+0.311228
Free energy correction:	+0.245930
Truhlar's Delta G correction:	+0.249574
Grimme's Delta G correction:	+0.249197

Cartesian Coordinates

C	-2.06304	0.41595	0.29014
O	-3.31622	0.56437	0.36391
C	-4.24200	-0.53252	0.00429
C	-3.57480	-1.88984	-0.05446
H	-4.63730	-0.22377	-0.96383
H	-5.02629	-0.47050	0.75484
C	-2.23828	-1.80880	-0.79400
H	-4.27104	-2.56261	-0.55914
H	-3.41617	-2.27411	0.95663
C	-1.36136	-0.84363	-0.00670
H	-2.38390	-1.43334	-1.81162
H	-1.76267	-2.78804	-0.85676
C	-1.14950	1.59171	0.41530
O	-1.53553	2.68600	0.85215
C	0.03602	1.10139	-0.15627
C	1.22602	1.88152	-0.47606
O	2.11501	1.49070	-1.20874
O	1.25588	3.08599	0.11132
C	2.39195	3.89672	-0.19588
H	2.44493	4.09469	-1.26744
H	3.31215	3.40846	0.12828
H	2.24643	4.82569	0.35080
C	-0.01585	-0.34683	-0.58936
C	1.15341	-1.20152	-0.14028
C	1.71296	-2.14019	-1.00555
C	1.66068	-1.09109	1.15610
C	2.70952	-1.90159	1.57705
C	3.26443	-2.83736	0.70544
C	2.76299	-2.95512	-0.58704
H	1.33088	-2.22477	-2.01833
H	1.23496	-0.35855	1.83636
H	3.09743	-1.80164	2.58466
H	4.08479	-3.46635	1.03179
H	3.19227	-3.67637	-1.27347
H	-1.15218	-1.28090	0.98237
H	-0.08627	-0.41705	-1.68047

6.5.15 Zwitterionic Intermediate Conrotatory I_2-Complex

SCF energy:	–1510.827184
Zero-point correction:	+0.294779
Enthalpy correction:	+0.317492
Free energy correction:	+0.237747
Truhlar's Delta G correction:	+0.245263
Grimme's Delta G correction:	+0.243876

Cartesian Coordinates

C	2.31153	-1.78361	0.25412
O	2.19351	-2.78952	-0.49756
C	3.31463	-3.22975	-1.36258
C	4.65041	-2.65325	-0.94802
H	3.01017	-2.90296	-2.35724
H	3.27613	-4.31471	-1.30526
C	4.53413	-1.15521	-0.65605

H	5.34347	-2.84428	-1.76963
H	5.02735	-3.17809	-0.06624
C	3.54849	-1.01747	0.49705
H	4.16965	-0.62046	-1.53737
H	5.50069	-0.73274	-0.38009
C	1.14554	-1.22632	0.97558
O	0.04164	-1.84796	1.02895
C	1.59710	0.00460	1.42274
C	0.83988	0.98004	2.21800
O	1.21961	2.11173	2.42758
O	-0.29586	0.48071	2.70551
C	-1.14185	1.40073	3.40198
H	-2.02240	0.83017	3.68756
H	-1.42242	2.22563	2.74518
H	-0.63752	1.79038	4.28701
C	2.99193	0.35390	0.97576
C	3.04966	1.39677	-0.13324
C	4.10476	2.30923	-0.14833
C	2.11511	1.42735	-1.16971
C	2.24048	2.34976	-2.20540
C	3.29926	3.25401	-2.21632
C	4.23082	3.23304	-1.18228
H	4.83036	2.29760	0.65899
H	1.27685	0.73759	-1.17038
H	1.50395	2.36569	-3.00091
H	3.39207	3.97513	-3.02026
H	5.05464	3.93791	-1.17721
H	3.98706	-1.49757	1.38558
H	3.58299	0.72914	1.81402
I	-1.97579	-0.76064	0.15894
I	-4.21544	0.37760	-0.95987

6.5.16 Zwitterionic Intermediate Disrotatory I_2-Complex

SCF energy:	–1510.828432
Zero-point correction:	+0.294691
Enthalpy correction:	+0.317421
Free energy correction:	+0.237966
Truhlar's Delta G correction:	+0.245007
Grimme's Delta G correction:	+0.243828

Cartesian Coordinates

C	-1.85140	1.99156	0.44403
O	-1.53559	3.20684	0.58448
C	-2.37599	4.28647	0.01581
C	-3.76559	3.82880	-0.37189
H	-1.79725	4.62855	-0.84245
H	-2.37420	5.05294	0.78693
C	-3.71863	2.48874	-1.10852
H	-4.19099	4.61385	-1.00006
H	-4.39356	3.73897	0.51832
C	-3.10718	1.48422	-0.14106
H	-3.10147	2.56333	-2.00898
H	-4.71784	2.16852	-1.40472
C	-0.91163	0.91549	0.79740
O	0.16101	1.14176	1.44634

C	-1.44182	-0.19719	0.17361
C	-0.81322	-1.53288	0.12681
O	-0.90652	-2.28179	-0.81806
O	-0.14709	-1.82129	1.24275
C	0.60451	-3.04107	1.22503
H	1.32541	-3.02515	0.40586
H	-0.06211	-3.89692	1.11368
H	1.12014	-3.08199	2.18123
C	-2.70098	0.06663	-0.61504
C	-3.79291	-0.96527	-0.43106
C	-4.55734	-1.38097	-1.52002
C	-4.06663	-1.49335	0.83262
C	-5.08864	-2.42136	1.00309
C	-5.85086	-2.83012	-0.08957
C	-5.58352	-2.30774	-1.35131
H	-4.34144	-0.98245	-2.50644
H	-3.47375	-1.17875	1.68753
H	-5.28867	-2.82809	1.98792
H	-6.64529	-3.55569	0.04239
H	-6.16829	-2.62581	-2.20697
H	-3.78471	1.35809	0.71747
H	-2.45839	0.13111	-1.68141
I	2.24438	0.39894	0.48056
I	4.62183	-0.36869	-0.69516

6.5.17 Nazarov Product **13** (*cis* configuration)

SCF energy:	–919.906238
Zero-point correction:	+0.293807
Enthalpy correction:	+0.312008
Free energy correction:	+0.247105
Truhlar's Delta G correction:	+0.250747
Grimme's Delta G correction:	+0.250299

Cartesian Coordinates

C	-2.17512	0.51552	-0.04116
O	-3.40747	0.51096	0.49655
C	-3.85856	-0.81405	0.83621
C	-3.57821	-1.80951	-0.28014
H	-3.34547	-1.11592	1.75648
H	-4.92392	-0.71601	1.03668
C	-2.06926	-1.91435	-0.53463
H	-4.08711	-1.47430	-1.18846
H	-3.99656	-2.77816	-0.00117
C	-1.48767	-0.53803	-0.51101
H	-1.58493	-2.53282	0.22970
H	-1.86057	-2.38918	-1.49816
C	-1.42545	1.76658	-0.21643
O	-1.79820	2.88662	0.03655
C	-0.07661	1.39366	-0.82913
C	1.05859	1.80105	0.08105
O	0.96206	1.99690	1.26507
O	2.20612	1.86747	-0.59226
C	3.38694	2.05374	0.20041
H	3.34528	3.00751	0.72677
H	3.48533	1.23778	0.91831
H	4.21714	2.04368	-0.50136

C	-0.13219	-0.15845	-1.05253
C	1.00606	-0.94723	-0.42759
C	2.06745	-1.38686	-1.22018
C	1.03126	-1.21528	0.94305
C	2.09821	-1.90758	1.50898
C	3.15387	-2.34030	0.71037
C	3.13616	-2.07836	-0.65716
H	2.05623	-1.18003	-2.28575
H	0.21300	-0.87698	1.57150
H	2.10396	-2.10932	2.57417
H	3.98380	-2.88083	1.15102
H	3.95283	-2.41390	-1.28639
H	-0.11232	-0.35302	-2.12879
H	0.04045	1.91260	-1.78237

6.5.18 Nazarov Product **13** (*trans* configuration)

SCF energy:	–919.907896
Zero-point correction:	+0.293682
Enthalpy correction:	+0.312049
Free energy correction:	+0.245722
Truhlar's Delta G correction:	+0.250359
Grimme's Delta G correction:	+0.249562

Cartesian Coordinates

C	-0.54109	-1.89832	-0.26416
O	-0.66470	-3.21404	-0.51624
C	0.21582	-4.01836	0.29234
C	1.62084	-3.43658	0.34819
H	0.20284	-5.00812	-0.16046
H	-0.21514	-4.07702	1.29817
C	1.59855	-2.03923	0.98028
H	2.01968	-3.37686	-0.66877
H	2.25985	-4.11354	0.91790
C	0.43347	-1.28634	0.42752
H	2.52657	-1.49825	0.77303
H	1.50813	-2.10146	2.07106
C	-1.55897	-0.94233	-0.71984
O	-2.59608	-1.18255	-1.28727
C	-1.04724	0.45418	-0.32311
C	-2.15815	1.21436	0.36038
O	-2.41589	1.13532	1.53565
O	-2.84975	1.95303	-0.50179
C	-3.98685	2.64582	0.03462
H	-4.69874	1.93281	0.45087
H	-3.67054	3.34721	0.80680
H	-4.42851	3.17756	-0.80411
C	0.19649	0.20090	0.56035
C	1.39851	1.03537	0.16504
C	1.90542	2.00394	1.02926
C	2.01647	0.84263	-1.07396
C	3.11708	1.60767	-1.44174
C	3.61690	2.57667	-0.57221
C	3.00899	2.77330	0.66296
H	1.43279	2.15649	1.99442
H	1.63169	0.08529	-1.75195

H	3.58811	1.44802	-2.40513
H	4.47648	3.17224	-0.85758
H	3.39247	3.52373	1.34503
H	-0.05362	0.42790	1.60121
H	-0.77806	0.96779	-1.24895

6.5.19 Iodine-Complex Nazarov Product **13–I_2** (*cis* configuration)

SCF energy:	–1510.859489
Zero-point correction:	+0.295022
Enthalpy correction:	+0.317854
Free energy correction:	+0.237138
Truhlar's Delta G correction:	+0.245375
Grimme's Delta G correction:	+0.243720

Cartesian Coordinates

C	2.45917	2.06404	0.01363
O	2.69353	3.28314	-0.49846
C	4.09814	3.54063	-0.69569
C	4.92373	3.11501	0.50945
H	4.41474	2.99410	-1.59120
H	4.17263	4.60994	-0.88408
C	4.78408	1.60605	0.74696
H	4.57596	3.66467	1.38866
H	5.96600	3.38776	0.33571
C	3.34962	1.22788	0.57664
H	5.39874	1.03850	0.03880
H	5.12384	1.32594	1.74861
C	1.11222	1.49849	0.04766
O	0.08848	2.03341	-0.32992
C	1.21193	0.11848	0.68354
C	0.71459	-0.94464	-0.27114
O	0.69823	-0.83508	-1.47008
O	0.33680	-2.03696	0.38604
C	-0.03727	-3.15727	-0.42897
H	-0.89550	-2.90006	-1.05071
H	0.80230	-3.45729	-1.05774
H	-0.29538	-3.95271	0.26543
C	2.72634	-0.05948	1.04967
C	3.38736	-1.30133	0.47616
C	3.53459	-2.43842	1.27195
C	3.81697	-1.34498	-0.85196
C	4.38187	-2.50518	-1.37377
C	4.52292	-3.63579	-0.57318
C	4.09768	-3.60033	0.75223
H	3.19967	-2.41231	2.30419
H	3.70281	-0.46913	-1.48326
H	4.71146	-2.52553	-2.40630
H	4.96409	-4.53868	-0.97972
H	4.20561	-4.47577	1.38251
H	2.81272	-0.11563	2.13863
H	0.59650	0.09508	1.58593
I	-2.37317	0.81379	-0.11263
I	-4.76826	-0.37839	0.14971

6.5.20 Iodine-Complex Nazarov Product **13–I_2** (*trans* configuration)

SCF energy:	–1510.859586
Zero-point correction:	+0.294797
Enthalpy correction:	+0.317776
Free energy correction:	+0.235505
Truhlar's Delta G correction:	+0.245047
Grimme's Delta G correction:	+0.242860

Cartesian Coordinates

C	2.46731	-1.86039	-0.19350
O	2.62715	-3.13734	-0.57866
C	4.01465	-3.50018	-0.72769
C	4.85645	-3.00822	0.44065
H	4.37271	-3.06746	-1.66862
H	4.02310	-4.58558	-0.80680
C	4.81073	-1.47730	0.52700
H	5.88049	-3.36161	0.30896
H	4.46798	-3.44475	1.36506
C	3.40472	-1.03191	0.29883
H	5.46437	-1.02018	-0.22507
H	5.15936	-1.12125	1.50114
C	1.16206	-1.20312	-0.25324
O	0.11249	-1.70954	-0.59709
C	1.36801	0.24701	0.17067
C	0.43760	0.71408	1.26691
O	0.06360	1.85067	1.39694
O	0.13262	-0.27327	2.10762
C	-0.74370	0.07092	3.19081
H	-0.27252	0.81300	3.83580
H	-0.91554	-0.85418	3.73482
H	-1.68363	0.46326	2.80002
C	2.85687	0.33240	0.62984
C	3.63069	1.46637	-0.01352
C	3.89993	1.44996	-1.38478
C	4.07731	2.54106	0.75257
C	4.77950	3.58906	0.15950
C	5.04227	3.56722	-1.20581
C	4.60027	2.49348	-1.97809
H	3.55800	0.61398	-1.98911
H	3.87159	2.55896	1.81818
H	5.11953	4.42064	0.76620
H	5.58847	4.38104	-1.66869
H	4.80324	2.47056	-3.04279
H	2.90243	0.46896	1.71632
H	1.19791	0.88507	-0.69982
I	-2.37933	-0.56299	-0.44159
I	-4.80959	0.56662	-0.24628

6.6 Nazarov Cyclization 14 → 15

6.6.1 Divinylketone **14** (*E* configuration)

SCF energy:	–883.972371
Zero-point correction:	+0.315103
Enthalpy correction:	+0.334656
Free energy correction:	+0.265731
Truhlar's Delta G correction:	+0.270752
Grimme's Delta G correction:	+0.269885

Cartesian Coordinates

C	0.20484	1.40397	0.24722
C	-0.25053	2.54425	1.12424
C	-1.23963	3.45064	0.39167
C	-0.71591	3.79885	-1.00071
H	-1.41776	4.35550	0.97709
H	-2.20024	2.93129	0.29368
C	-0.57990	2.53248	-1.84582
H	-1.37645	4.51104	-1.50017
H	0.26519	4.27714	-0.90440
C	0.03756	1.39933	-1.08393
H	0.01137	2.71983	-2.74724
H	-1.56547	2.20106	-2.19967
C	0.87855	0.27560	0.93115
O	1.22689	0.35852	2.09316
C	1.13568	-1.00837	0.17864
C	2.55295	-1.33365	-0.15199
O	2.94009	-2.39512	-0.57646
O	3.35238	-0.28470	0.04705
C	4.74007	-0.48567	-0.25112
H	5.22933	0.45707	-0.02012
H	4.86791	-0.73306	-1.30532
H	5.14552	-1.28656	0.36762
C	0.18874	-1.87696	-0.20216
C	-1.26419	-1.76065	-0.02235
H	0.52891	-2.75923	-0.74023
C	-1.85490	-1.07975	1.05104
C	-2.09247	-2.36333	-0.97786
C	-3.47501	-2.24897	-0.89207
C	-4.05037	-1.55130	0.16642
C	-3.23732	-0.97755	1.14210
H	-1.23986	-0.65729	1.83700
H	-1.64194	-2.91387	-1.79712
H	-4.10230	-2.71017	-1.64601
H	-5.12849	-1.46721	0.24032
H	-3.68199	-0.45623	1.98191
H	0.35961	0.53640	-1.66048
H	0.62294	3.11861	1.45385
H	-0.70007	2.13245	2.03245

6.6.2 Divinylketone **14** (*Z* configuration)

SCF energy:	–883.968234
Zero-point correction:	+0.315402
Enthalpy correction:	+0.334818
Free energy correction:	+0.266926
Truhlar's Delta G correction:	+0.270892
Grimme's Delta G correction:	+0.270487

Cartesian Coordinates

C	2.49483	0.12770	-0.11360
C	3.75349	0.43466	-0.89104
C	4.75657	-0.71539	-0.81321
C	4.92451	-1.17861	0.63270
H	5.71432	-0.39897	-1.23264
H	4.39739	-1.55427	-1.42049
C	3.59980	-1.71630	1.17397
H	5.24627	-0.32864	1.24465
H	5.69810	-1.94574	0.71074
C	2.43452	-0.84359	0.80977
H	3.63407	-1.82482	2.26193
H	3.40750	-2.72303	0.77983
C	1.35731	1.05668	-0.33157
O	1.55394	2.18706	-0.74466
C	-0.05636	0.63739	-0.06833
C	-0.93977	1.78021	0.33634
O	-0.79798	2.40468	1.35745
O	-1.88292	2.03240	-0.56610
C	-2.81223	3.07118	-0.22602
H	-3.50044	3.13464	-1.06489
H	-2.28869	4.01741	-0.08882
H	-3.34844	2.80904	0.68741
C	-0.50982	-0.60249	-0.30351
C	-1.88941	-1.08939	-0.15283
H	0.20251	-1.33625	-0.67089
C	-2.76642	-0.59007	0.81876
C	-2.32998	-2.11243	-1.00070
C	-3.63091	-2.59405	-0.91265
C	-4.50106	-2.07649	0.04298
C	-4.06226	-1.08108	0.91408
H	-2.42931	0.15962	1.52666
H	-1.64710	-2.52025	-1.73865
H	-3.96284	-3.37720	-1.58429
H	-5.51340	-2.45631	0.11907
H	-4.72875	-0.69294	1.67558
H	1.51080	-1.00804	1.35613
H	3.48769	0.65078	-1.92969
H	4.19897	1.35444	-0.49597

6.6.3 Iodine Complex with **14** to CO Group (*E* configuration)

SCF energy:	–1474.927177
Zero-point correction:	+0.316422
Enthalpy correction:	+0.340494
Free energy correction:	+0.256707
Truhlar's Delta G correction:	+0.265761
Grimme's Delta G correction:	+0.263946

Cartesian Coordinates

C	2.83085	1.21162	-0.50758
C	3.13731	1.53538	-1.94935
C	4.64428	1.61875	-2.19149
C	5.31223	2.47818	-1.11958
H	4.83680	2.02199	-3.18812
H	5.07110	0.60943	-2.15975
C	5.12843	1.84221	0.25803
H	6.37593	2.60880	-1.32974
H	4.85529	3.47397	-1.12254
C	3.73621	1.33712	0.47637
H	5.38094	2.54465	1.05798
H	5.81266	0.99174	0.38225
C	1.45666	0.76770	-0.20719
O	0.57185	0.88363	-1.04497
C	1.12968	0.16543	1.13359
C	0.19753	0.92618	2.01715
O	-0.29008	0.50119	3.03497
O	-0.01728	2.15629	1.54980
C	-0.95725	2.95217	2.28349
H	-1.03121	3.89199	1.74246
H	-0.59829	3.12322	3.29864
H	-1.92642	2.45219	2.31298
C	1.59595	-1.01277	1.57153
C	2.50602	-1.92572	0.86943
H	1.28441	-1.31786	2.56839
C	2.50557	-2.07523	-0.52387
C	3.41069	-2.67413	1.63243
C	4.32975	-3.51430	1.01482
C	4.33626	-3.63889	-0.37202
C	3.41506	-2.92700	-1.13795
H	1.77204	-1.55403	-1.12912
H	3.39724	-2.58187	2.71339
H	5.03427	-4.07761	1.61555
H	5.04605	-4.30100	-0.85440
H	3.39908	-3.04266	-2.21546
H	3.46530	1.06368	1.49225
H	2.65305	2.48080	-2.21911
H	2.68349	0.77081	-2.58649
I	-2.03505	0.16433	-0.63952
I	-4.60493	-0.53956	-0.26962

6.6.4 Iodine Complex with **14** to CO Group (*Z* configuration)

SCF energy:	–1474.920021
Zero-point correction:	+0.316197
Enthalpy correction:	+0.340438
Free energy correction:	+0.255362
Truhlar's Delta G correction:	+0.265315
Grimme's Delta G correction:	+0.263129

Cartesian Coordinates

C	-3.35735	-1.15871	0.46305
C	-3.56972	-2.65300	0.47041
C	-4.99665	-3.01482	0.05922
C	-6.00651	-2.15584	0.81855
H	-5.17570	-4.07656	0.24255
H	-5.11794	-2.84557	-1.01686
C	-5.81533	-0.67946	0.47142
H	-5.85775	-2.29598	1.89495
H	-7.02968	-2.46177	0.58999
C	-4.37094	-0.27885	0.45507
H	-6.35406	-0.03465	1.17184
H	-6.23624	-0.46077	-0.51907
C	-1.95961	-0.68302	0.54958
O	-1.07835	-1.43200	0.94852
C	-1.61797	0.72911	0.16572
C	-2.20662	1.25387	-1.10549
O	-2.72506	2.33114	-1.25009
O	-2.10280	0.34237	-2.07429
C	-2.70470	0.68775	-3.33078
H	-3.77395	0.85774	-3.19786
H	-2.53249	-0.16470	-3.98265
H	-2.23559	1.58224	-3.74085
C	-0.79319	1.42810	0.95868
C	-0.22068	2.76199	0.72955
H	-0.49891	0.95185	1.89231
C	0.17005	3.19934	-0.54140
C	-0.00888	3.59722	1.83249
C	0.53456	4.86526	1.66291
C	0.90260	5.29927	0.39232
C	0.72957	4.45952	-0.70654
H	0.06363	2.54361	-1.39867
H	-0.28312	3.24967	2.82305
H	0.68080	5.50915	2.52228
H	1.33687	6.28345	0.25907
H	1.03838	4.78532	-1.69301
H	-4.16371	0.78849	0.45953
H	-2.84086	-3.11885	-0.19854
H	-3.35283	-3.03976	1.47248
I	1.63487	-1.20188	0.33803
I	4.23930	-1.13645	-0.31241

6.6.5 Iodine Complex with **14** to CO_2Me Group (*E* configuration)

SCF energy:	–1474.923377
Zero-point correction:	+0.316381
Enthalpy correction:	+0.340585
Free energy correction:	+0.256068
Truhlar's Delta G correction:	+0.265568
Grimme's Delta G correction:	+0.263573

Cartesian Coordinates

C	-1.09753	-0.99907	-0.14871
C	-0.48284	-2.13459	-0.92674
C	-0.45151	-3.42550	-0.10927
C	0.07502	-3.15193	1.29844
H	0.16588	-4.16998	-0.61696
H	-1.46552	-3.83621	-0.03918
C	-0.86266	-2.19620	2.03594
H	1.07005	-2.69740	1.22618
H	0.18243	-4.08016	1.86395
C	-1.28378	-1.04110	1.17951
H	-0.39547	-1.80814	2.94629
H	-1.76691	-2.72487	2.36606
C	-1.41527	0.22460	-0.91688
O	-1.04550	0.36527	-2.06644
C	-2.17964	1.35063	-0.25841
C	-1.34891	2.54787	0.02503
O	-0.13536	2.54602	-0.03254
O	-2.04733	3.62189	0.37119
C	-1.28449	4.79042	0.71163
H	-0.68878	5.11130	-0.14266
H	-0.63352	4.58058	1.56030
H	-2.01751	5.54960	0.97142
C	-3.48045	1.31686	0.06734
C	-4.41660	0.19783	-0.10152
H	-3.89560	2.19946	0.54636
C	-4.30119	-0.75942	-1.11896
C	-5.47820	0.09488	0.80676
C	-6.37503	-0.96412	0.73275
C	-6.23837	-1.92136	-0.26895
C	-5.20685	-1.80963	-1.19942
H	-3.52642	-0.67004	-1.87141
H	-5.58830	0.84724	1.58098
H	-7.18384	-1.03778	1.45037
H	-6.94129	-2.74387	-0.33460
H	-5.11229	-2.53831	-1.99614
H	-1.74686	-0.19654	1.68253
H	0.53223	-1.84788	-1.22892
H	-1.04435	-2.27341	-1.85542
I	2.12568	0.84793	-0.06776
I	4.30549	-0.70925	-0.02918

6.6.6 Iodine Complex with **14** to CO_2Me Group (*Z* configuration)

SCF energy:	–1474.921978
Zero-point correction:	+0.316586
Enthalpy correction:	+0.340658
Free energy correction:	+0.256870
Truhlar's Delta G correction:	+0.265849
Grimme's Delta G correction:	+0.264036

Cartesian Coordinates

C	0.14928	2.51703	0.53289
C	0.73720	3.69164	1.27995
C	1.37118	4.70403	0.32707
C	2.27139	3.99424	-0.68278
H	1.93679	5.44385	0.89809
H	0.58242	5.24291	-0.21056
C	1.44764	3.03933	-1.54635
H	3.03476	3.42350	-0.14205
H	2.79283	4.71505	-1.31646
C	0.47352	2.23387	-0.73758
H	2.09444	2.35476	-2.10318
H	0.88318	3.59962	-2.30358
C	-0.69555	1.59922	1.33838
O	-0.57075	1.54704	2.55058
C	-1.73134	0.72269	0.70275
C	-2.04235	-0.49903	1.51592
O	-1.25474	-1.39876	1.72149
O	-3.26872	-0.48357	2.00482
C	-3.67165	-1.64552	2.75011
H	-4.69411	-1.44955	3.06129
H	-3.02458	-1.77856	3.61666
H	-3.62837	-2.52868	2.11152
C	-2.42792	1.06723	-0.39084
C	-3.50141	0.29766	-1.03484
H	-2.20083	2.02480	-0.85072
C	-3.51824	-1.10294	-1.04927
C	-4.52853	0.99591	-1.68080
C	-5.57557	0.31107	-2.28584
C	-5.59431	-1.08123	-2.27652
C	-4.55861	-1.78594	-1.66612
H	-2.69876	-1.66400	-0.61175
H	-4.50673	2.08061	-1.69348
H	-6.37210	0.86287	-2.77115
H	-6.40536	-1.61667	-2.75638
H	-4.55616	-2.86969	-1.67983
H	0.04727	1.35886	-1.21885
H	-0.04582	4.16072	1.88251
H	1.48390	3.32001	1.99058
I	1.22050	-1.39008	0.47651
I	3.57955	-1.22036	-0.79151

6.6.7 Transition State Uncatalyzed Conrotatory

SCF energy:	–883.918703
Zero-point correction:	+0.313614
Enthalpy correction:	+0.331925
Free energy correction:	+0.268130
Truhlar's Delta G correction:	+0.270288
Grimme's Delta G correction:	+0.270435
Imaginary Frequency:	368.3 *i*cm^{-1}

Cartesian Coordinates

C	0.12097	1.64615	0.00581
C	1.05845	2.41582	0.85552
C	2.37997	2.74909	0.16538
C	2.87037	1.54235	-0.63784
H	3.11588	3.04817	0.91377
H	2.23977	3.59843	-0.51131
C	1.87574	1.22743	-1.75479
H	2.96792	0.67542	0.02697
H	3.85492	1.73645	-1.06776
C	0.45513	1.14896	-1.25485
H	2.12853	0.28984	-2.25870
H	1.91602	2.00795	-2.52292
C	-1.18960	1.20609	0.55996
O	-1.79737	1.84724	1.42093
C	-1.47883	-0.02983	-0.10716
C	-2.79489	-0.61325	-0.34017
O	-3.00229	-1.54814	-1.09199
O	-3.77391	-0.00698	0.34132
C	-5.08737	-0.53764	0.14640
H	-5.12342	-1.58878	0.43580
H	-5.39196	-0.43704	-0.89622
H	-5.73941	0.05176	0.78688
C	-0.35203	-0.58576	-0.80626
C	0.80760	-1.24713	-0.13457
C	1.02133	-1.16617	1.24749
C	1.70547	-1.97832	-0.91657
C	2.81759	-2.58616	-0.34050
C	3.03604	-2.48090	1.02917
C	2.12804	-1.77858	1.82145
H	0.31352	-0.63915	1.87768
H	1.52860	-2.06944	-1.98358
H	3.50751	-3.14571	-0.96167
H	3.89826	-2.95666	1.48197
H	2.27882	-1.71597	2.89311
H	-0.30580	1.17292	-2.03021
H	-0.59425	-1.08017	-1.74879
H	0.52370	3.30679	1.20853
H	1.22610	1.81529	1.76360

6.6.8 Transition State Uncatalyzed Disrotatory

SCF energy:	–883.921299
Zero-point correction:	+0.313505
Enthalpy correction:	+0.332072
Free energy correction:	+0.266882
Truhlar's Delta G correction:	+0.269975
Grimme's Delta G correction:	+0.269872
Imaginary Frequency:	371.3 *i*cm^{-1}

Cartesian Coordinates

C	-2.24414	0.49658	0.30397
C	-3.67705	0.55077	-0.08665
C	-4.36298	-0.81517	-0.04677
C	-3.42019	-1.89203	-0.58872
H	-5.28857	-0.77584	-0.62374
H	-4.63244	-1.06472	0.98484
C	-2.21066	-2.02587	0.33610
H	-3.08962	-1.61078	-1.59616
H	-3.93095	-2.85328	-0.67104
C	-1.57446	-0.68840	0.62055
H	-1.45062	-2.69149	-0.08737
H	-2.51546	-2.47510	1.28731
C	-1.40029	1.69934	0.17431
O	-1.83648	2.85483	0.24227
C	-0.08159	1.21943	-0.12541
C	1.10087	2.09402	-0.04987
O	1.19276	3.08538	0.63624
O	2.09213	1.68010	-0.85904
C	3.32277	2.40033	-0.75655
H	3.71380	2.34032	0.26080
H	3.18075	3.44614	-1.03138
H	4.00650	1.91762	-1.45108
C	-0.02317	-0.18083	-0.45031
C	1.15997	-1.00949	-0.12876
C	1.91592	-0.77270	1.02532
C	1.51623	-2.06026	-0.97644
C	2.63183	-2.84420	-0.69549
C	3.38958	-2.58963	0.44321
C	3.02768	-1.55392	1.30635
H	1.62276	0.02236	1.70594
H	0.92338	-2.25198	-1.86524
H	2.90763	-3.65182	-1.36352
H	4.25664	-3.20089	0.66612
H	3.61027	-1.36379	2.20034
H	-0.88629	-0.67083	1.46011
H	-0.53929	-0.52519	-1.34337
H	-3.73328	0.99728	-1.08894
H	-4.16447	1.28155	0.57145

6.6.9 Transition State Catalyzed Conrotatory (I_2 to CO)

SCF energy:	–1474.884872
Zero-point correction:	+0.315194
Enthalpy correction:	+0.338254
Free energy correction:	+0.258032
Truhlar's Delta G correction:	+0.265082
Grimme's Delta G correction:	+0.263963
Imaginary Frequency:	348.9 *i*cm^{-1}

Cartesian Coordinates

C	2.00933	2.19108	-0.49004
C	1.73057	3.61632	-0.16086
C	2.97470	4.37106	0.31051
C	3.82436	3.47628	1.21578
H	2.67105	5.28137	0.82996
H	3.57435	4.67357	-0.55421
C	4.36496	2.29836	0.40625
H	3.20828	3.10810	2.04509
H	4.65424	4.03613	1.65056
C	3.27346	1.60077	-0.36147
H	4.86819	1.56351	1.04398
H	5.11745	2.64758	-0.30894
C	0.92487	1.27720	-0.79300
O	-0.19488	1.66489	-1.24014
C	1.33651	-0.02492	-0.41591
C	0.64651	-1.24174	-0.92641
O	0.22157	-1.35729	-2.04917
O	0.55148	-2.18998	0.00582
C	-0.07046	-3.41258	-0.41166
H	0.49501	-3.86182	-1.22937
H	-1.09602	-3.22227	-0.73090
H	-0.05805	-4.06143	0.46042
C	2.51428	-0.06436	0.39589
C	3.44342	-1.21010	0.37468
C	3.66274	-1.94345	-0.79780
C	4.12896	-1.55976	1.54152
C	4.99929	-2.64490	1.54550
C	5.19801	-3.37969	0.38025
C	4.53089	-3.02607	-0.79300
H	3.16382	-1.65455	-1.71872
H	3.96516	-0.98577	2.44808
H	5.52118	-2.91626	2.45563
H	5.87835	-4.22358	0.38135
H	4.69634	-3.59019	-1.70338
H	3.60821	0.94617	-1.16029
H	2.48091	0.44324	1.35580
H	0.93946	3.63519	0.60025
H	1.28050	4.07691	-1.04905
I	-2.22684	0.62902	-0.39187
I	-4.50048	-0.49275	0.68112

6.6.10 Transition State Catalyzed Conrotatory (I_2 to CO_2Me)

SCF energy:	–1474.874703
Zero-point correction:	+0.314806
Enthalpy correction:	+0.338008
Free energy correction:	+0.256965
Truhlar's Delta G correction:	+0.264823
Grimme's Delta G correction:	+0.263420
Imaginary Frequency:	361.8 *i*cm^{-1}

Cartesian Coordinates

C	1.53267	2.26034	0.56586
C	1.68374	3.68025	0.97277
C	2.40457	4.53087	-0.07310
C	3.56935	3.74349	-0.67766
H	2.75251	5.45725	0.38703
H	1.70712	4.80499	-0.87143
C	3.03046	2.53654	-1.44514
H	4.23489	3.40695	0.12654
H	4.16042	4.37221	-1.34614
C	2.05892	1.73536	-0.61604
H	3.83876	1.87389	-1.77307
H	2.51823	2.86870	-2.35433
C	0.97151	1.27398	1.51234
O	0.16034	1.55485	2.40021
C	1.62748	0.03340	1.21406
C	1.14566	-1.23838	1.75526
O	-0.00200	-1.45542	2.10623
O	2.10171	-2.16558	1.85562
C	1.67553	-3.47536	2.24953
H	0.93725	-3.85950	1.54380
H	1.24899	-3.45277	3.25251
H	2.57125	-4.09150	2.23243
C	2.74688	0.15831	0.31583
C	3.10941	-0.91907	-0.63112
C	2.12829	-1.72415	-1.22214
C	4.45174	-1.12838	-0.95533
C	4.81365	-2.14791	-1.83123
C	3.83343	-2.95576	-2.39878
C	2.48806	-2.73999	-2.09573
H	1.07894	-1.54390	-1.00246
H	5.21307	-0.49857	-0.50631
H	5.85833	-2.31024	-2.06967
H	4.11296	-3.74783	-3.08397
H	1.72325	-3.36017	-2.54861
H	1.44508	1.02808	-1.16588
H	3.61066	0.73079	0.64513
H	2.21127	3.69706	1.93657
H	0.67828	4.05808	1.19930
I	-2.08142	-0.47913	0.58101
I	-4.09989	0.20280	-1.05901

6.6.11 Transition State Catalyzed Disrotatory (I_2 to CO)

SCF energy:	–1474.880851
Zero-point correction:	+0.314889
Enthalpy correction:	+0.337818
Free energy correction:	+0.258573
Truhlar's Delta G correction:	+0.265085
Grimme's Delta G correction:	+0.264085
Imaginary Frequency:	353.1 *i*cm^{-1}

Cartesian Coordinates

C	2.49872	0.81633	1.34844
C	2.63736	-0.10301	2.50388
C	4.08885	-0.42720	2.85310
C	4.90060	-0.64477	1.57436
H	4.11815	-1.31122	3.49217
H	4.52664	0.40032	3.42078
C	4.94252	0.65035	0.76446
H	4.43837	-1.44043	0.97741
H	5.91808	-0.96201	1.81000
C	3.57678	1.25436	0.57678
H	5.40023	0.49320	-0.21680
H	5.56529	1.39421	1.27452
C	1.16391	1.16057	0.83841
O	0.14964	1.16547	1.57892
C	1.30718	1.40244	-0.55187
C	0.44135	2.24430	-1.38613
O	0.62372	2.43222	-2.57066
O	-0.55220	2.80616	-0.69709
C	-1.50533	3.55217	-1.46069
H	-1.95632	2.91726	-2.22485
H	-1.02930	4.41300	-1.93143
H	-2.25941	3.87861	-0.74850
C	2.54005	0.91700	-1.10135
C	2.86183	-0.52541	-1.29507
C	2.06366	-1.55012	-0.76960
C	3.99469	-0.86047	-2.04140
C	4.34974	-2.19326	-2.22876
C	3.56593	-3.20483	-1.68383
C	2.41609	-2.87866	-0.96449
H	1.15546	-1.31132	-0.22655
H	4.59819	-0.07068	-2.47717
H	5.23383	-2.43888	-2.80562
H	3.83666	-4.24372	-1.83264
H	1.78594	-3.66392	-0.56304
H	3.56823	2.27877	0.21538
H	2.97210	1.53567	-1.88921
H	2.08540	0.33498	3.34476
H	2.07817	-1.01643	2.24711
I	-1.97566	0.16363	0.71978
I	-4.22941	-1.10848	-0.15776

6.6.12 Transition State Catalyzed Disrotatory (I_2 to CO_2Me)

SCF energy:	–1474.872350
Zero-point correction:	+0.314581
Enthalpy correction:	+0.337620
Free energy correction:	+0.257404
Truhlar's Delta G correction:	+0.264826
Grimme's Delta G correction:	+0.263483
Imaginary Frequency:	346.7 *i*cm^{-1}

Cartesian Coordinates

C	3.85730	0.17325	-0.02582
C	4.81638	-0.63623	0.75866
C	5.36133	-1.84516	0.00094
C	4.23294	-2.52606	-0.77676
H	5.82521	-2.53726	0.70573
H	6.13876	-1.52226	-0.69914
C	3.68344	-1.57078	-1.83607
H	3.43202	-2.81053	-0.08367
H	4.58901	-3.43944	-1.25695
C	3.37054	-0.20764	-1.27420
H	2.78242	-1.97599	-2.30619
H	4.41614	-1.43974	-2.64027
C	3.21674	1.37147	0.59321
O	3.78963	2.07384	1.42564
C	1.90493	1.43464	0.01504
C	1.08256	2.61893	-0.12388
O	0.03495	2.66032	-0.76545
O	1.56714	3.69457	0.49286
C	0.77868	4.88627	0.39499
H	-0.21902	4.71827	0.80205
H	0.70063	5.20871	-0.64370
H	1.30660	5.63269	0.98348
C	1.53361	0.23641	-0.69577
C	1.14202	-1.04554	-0.03994
C	1.32243	-1.27057	1.32973
C	0.54236	-2.03831	-0.81908
C	0.15862	-3.24925	-0.25081
C	0.35926	-3.47408	1.10763
C	0.93344	-2.47775	1.89645
H	1.74432	-0.49326	1.95755
H	0.36798	-1.85364	-1.87456
H	-0.30538	-4.01081	-0.86698
H	0.05441	-4.41301	1.55523
H	1.06752	-2.63805	2.96013
H	3.19365	0.57040	-2.01210
H	0.96436	0.40032	-1.61341
H	5.60445	0.04155	1.11050
H	4.28827	-0.94702	1.67445
I	-2.04320	0.91809	-0.32158
I	-3.97312	-0.88409	0.16116

6.6.13 Zwitterionic Intermediate Conrotatory

SCF energy:	–883.940122
Zero-point correction:	+0.315085
Enthalpy correction:	+0.333810
Free energy correction:	+0.267143
Truhlar's Delta G correction:	+0.271653
Grimme's Delta G correction:	+0.270979

Cartesian Coordinates

C	-2.00569	0.32651	0.46840
C	-3.41191	0.33615	0.87231
C	-4.28998	-0.48872	-0.09520
C	-3.64958	-1.83437	-0.43106
H	-4.42982	0.08802	-1.01439
H	-5.27346	-0.62386	0.35729
C	-2.25804	-1.64146	-1.03212
H	-4.28265	-2.37450	-1.13921
H	-3.57803	-2.44767	0.47422
C	-1.35102	-0.87989	-0.04229
H	-2.33115	-1.05922	-1.95698
H	-1.78803	-2.59628	-1.27721
C	-1.13425	1.50161	0.49920
O	-1.46853	2.59925	0.98341
C	0.02417	1.05598	-0.18701
C	1.18034	1.87644	-0.58432
O	1.97457	1.53470	-1.43538
O	1.27174	3.02725	0.08120
C	2.37730	3.86415	-0.27562
H	2.31486	4.14919	-1.32656
H	3.32063	3.34794	-0.09274
H	2.29688	4.74249	0.35997
C	0.00191	-0.38533	-0.58895
C	1.19312	-1.19476	-0.10816
C	1.65868	-1.06510	1.20263
C	1.81671	-2.10532	-0.95965
C	2.88619	-2.87767	-0.51143
C	3.34440	-2.74342	0.79552
C	2.72750	-1.83344	1.65219
H	1.18314	-0.35468	1.87328
H	1.46723	-2.20283	-1.98274
H	3.36394	-3.57910	-1.18619
H	4.17948	-3.33992	1.14460
H	3.08143	-1.72082	2.67083
H	-1.18758	-1.53871	0.82598
H	-0.02984	-0.45945	-1.68291
H	-3.75822	1.36163	1.00953
H	-3.43014	-0.15023	1.86272

6.6.14 Zwitterionic Intermediate Disrotatory

SCF energy:	–883.938585
Zero-point correction:	+0.315663
Enthalpy correction:	+0.334188
Free energy correction:	+0.268711
Truhlar's Delta G correction:	+0.272377
Grimme's Delta G correction:	+0.272027

Cartesian Coordinates

C	-2.14966	-0.65882	-0.33639
C	-3.60605	-0.62831	-0.21735
C	-3.97795	0.67475	0.55363
C	-3.31987	1.89481	-0.08495
H	-3.64890	0.57464	1.59195
H	-5.06543	0.76364	0.55821
C	-1.80037	1.74802	-0.12984
H	-3.57717	2.78928	0.48836
H	-3.70870	2.03544	-1.09936
C	-1.41330	0.46154	-0.91790
H	-1.40231	1.67389	0.88624
H	-1.32352	2.60472	-0.61027
C	-1.29326	-1.71185	0.20783
O	-1.71910	-2.71177	0.81624
C	0.00621	-1.30562	-0.18627
C	1.21129	-2.11479	0.05310
O	1.30487	-3.01898	0.84954
O	2.22791	-1.72853	-0.73664
C	3.46137	-2.42920	-0.55151
H	3.81985	-2.30169	0.47093
H	3.33322	-3.49138	-0.76395
H	4.16179	-1.98521	-1.25482
C	0.06876	0.01274	-0.88918
C	1.02838	1.01923	-0.27489
C	1.30151	1.03214	1.09427
C	1.63266	1.97686	-1.09059
C	2.48619	2.93499	-0.55078
C	2.75163	2.94249	0.81603
C	2.15785	1.98683	1.63631
H	0.84322	0.29245	1.74385
H	1.43477	1.96866	-2.15820
H	2.94860	3.67099	-1.19894
H	3.42037	3.68393	1.23803
H	2.36203	1.98209	2.70114
H	-1.75654	0.61830	-1.94973
H	0.39261	-0.14054	-1.92578
H	-4.04118	-0.55592	-1.22187
H	-3.97455	-1.52391	0.28201

6.6.15 Zwitterionic Intermediate Conrotatory I_2-Complex to CO

SCF energy:	–1474.905064
Zero-point correction:	+0.316811
Enthalpy correction:	+0.340032
Free energy correction:	+0.258252
Truhlar's Delta G correction:	+0.266970
Grimme's Delta G correction:	+0.265096

Cartesian Coordinates

C	-1.90779	1.97258	0.57691
C	-1.76868	3.36208	1.01699
C	-2.17718	4.34017	-0.11047
C	-3.49754	3.93173	-0.76014
H	-1.38520	4.35203	-0.86497
H	-2.24061	5.34346	0.31287
C	-3.41365	2.51437	-1.32425
H	-3.74028	4.62986	-1.56469
H	-4.30724	3.98919	-0.02429
C	-3.06638	1.51333	-0.20185
H	-2.63135	2.46614	-2.08904
H	-4.35278	2.20732	-1.78903
C	-0.94421	0.93056	0.81154
O	0.12516	1.09270	1.49930
C	-1.42959	-0.17290	0.10645
C	-0.75890	-1.49739	0.00130
O	-0.70739	-2.12402	-1.02827
O	-0.25294	-1.89511	1.15916
C	0.50496	-3.11447	1.12411
H	1.33895	-3.01113	0.42801
H	-0.13187	-3.94618	0.82188
H	0.87070	-3.26017	2.13700
C	-2.69521	0.08283	-0.64092
C	-3.76580	-0.96665	-0.41256
C	-4.06624	-1.39794	0.88218
C	-4.47121	-1.50163	-1.48884
C	-5.46899	-2.45022	-1.27621
C	-5.76477	-2.87478	0.01534
C	-5.06015	-2.34689	1.09548
H	-3.51817	-0.98921	1.72704
H	-4.23351	-1.17846	-2.49727
H	-6.00990	-2.86092	-2.12110
H	-6.53791	-3.61627	0.18067
H	-5.28319	-2.67627	2.10390
H	-3.92208	1.47594	0.48968
H	-2.46254	0.10462	-1.71368
H	-0.76493	3.54338	1.40237
H	-2.47757	3.48302	1.85229
I	2.18129	0.38269	0.52188
I	4.55416	-0.39389	-0.67893

6.6.16 Zwitterionic Intermediate Conrotatory I_2-Complex to CO_2Me

SCF energy:	–1474.902503
Zero-point correction:	+0.316913
Enthalpy correction:	+0.340177
Free energy correction:	+0.257591
Truhlar's Delta G correction:	+0.267187
Grimme's Delta G correction:	+0.264961

Cartesian Coordinates

C	1.19176	1.96545	0.07139
C	0.45452	3.19970	-0.20178
C	1.43232	4.40556	-0.18804
C	2.66917	4.13062	-1.03977
H	1.73045	4.60139	0.84592
H	0.89213	5.28270	-0.54656
C	3.40151	2.87899	-0.56018
H	3.34514	4.98769	-0.98884
H	2.37721	4.00835	-2.08846
C	2.45621	1.65355	-0.60710
H	3.73819	3.01705	0.47284
H	4.27971	2.66373	-1.17205
C	0.82835	0.97916	1.05586
O	-0.23281	1.02460	1.77351
C	1.87481	0.05720	1.04879
C	1.90488	-1.15584	1.90721
O	0.92561	-1.75879	2.26167
O	3.15624	-1.49862	2.21150
C	3.30371	-2.68291	3.00975
H	2.88839	-3.54247	2.48310
H	2.79886	-2.55595	3.96769
H	4.37350	-2.80601	3.15629
C	2.97045	0.37744	0.08693
C	3.30218	-0.76787	-0.85367
C	2.28056	-1.46358	-1.50503
C	4.62838	-1.12332	-1.09296
C	4.93281	-2.15599	-1.97687
C	3.91148	-2.84487	-2.62404
C	2.58359	-2.49708	-2.38519
H	1.24290	-1.19775	-1.32088
H	5.42492	-0.59251	-0.58156
H	5.96801	-2.42382	-2.15543
H	4.14737	-3.65165	-3.30836
H	1.78280	-3.03226	-2.88258
H	2.22673	1.45276	-1.66351
H	3.87630	0.62502	0.65494
H	-0.37658	3.31771	0.49404
H	0.04787	3.10600	-1.22015
I	-2.15524	0.21988	0.60491
I	-4.37903	-0.69412	-0.77456

6.6.17 Zwitterionic Intermediate Disrotatory I_2-Complex to CO

SCF energy:	–1474.901620
Zero-point correction:	+0.317187
Enthalpy correction:	+0.340232
Free energy correction:	+0.259510
Truhlar's Delta G correction:	+0.267481
Grimme's Delta G correction:	+0.265904

Cartesian Coordinates

C	1.06148	1.70160	-1.48711
C	0.14266	2.79968	-1.78089
C	-0.16493	3.51575	-0.42818
C	1.12181	3.86155	0.31522
H	-0.78543	2.85599	0.18496
H	-0.75067	4.40865	-0.65103
C	1.97107	2.61872	0.57183
H	0.87289	4.32682	1.27246
H	1.69908	4.59208	-0.26155
C	2.32542	1.93114	-0.78253
H	1.41758	1.90984	1.19470
H	2.90272	2.85907	1.08762
C	0.78667	0.30418	-1.69936
O	-0.28370	-0.15381	-2.23843
C	1.91298	-0.36513	-1.22467
C	2.03776	-1.84675	-1.22566
O	1.11255	-2.60278	-1.08070
O	3.30476	-2.22425	-1.39042
C	3.54371	-3.63962	-1.35562
H	3.24445	-4.04354	-0.38792
H	2.98855	-4.13552	-2.15213
H	4.61339	-3.75991	-1.50451
C	2.98621	0.53204	-0.70648
C	3.54807	0.12842	0.64404
C	2.74638	-0.46610	1.62103
C	4.89183	0.37427	0.92779
C	5.42646	0.03931	2.16828
C	4.62199	-0.55385	3.13752
C	3.28151	-0.80734	2.86006
H	1.69646	-0.66145	1.42103
H	5.52324	0.82555	0.16883
H	6.47260	0.23512	2.37441
H	5.03820	-0.82100	4.10203
H	2.64882	-1.27108	3.60821
H	2.94052	2.64501	-1.34393
H	3.81932	0.51593	-1.42132
H	0.65516	3.52210	-2.42803
H	-0.76167	2.44035	-2.27182
I	-2.08000	-0.29232	-0.67620
I	-4.16057	-0.41268	1.15456

6.6.18 Zwitterionic Intermediate Disrotatory I_2-Complex to CO_2Me

SCF energy:	–1474.902639
Zero-point correction:	+0.317461
Enthalpy correction:	+0.340432
Free energy correction:	+0.260705
Truhlar's Delta G correction:	+0.267572
Grimme's Delta G correction:	+0.266506

Cartesian Coordinates

C	1.80465	2.08677	-0.39192
C	1.81689	3.54734	-0.33510
C	3.13343	3.94727	0.40364
C	4.34588	3.27841	-0.23763
H	3.05180	3.64845	1.45254
H	3.21446	5.03477	0.37322
C	4.21033	1.75712	-0.24229
H	5.24751	3.55408	0.31548
H	4.46940	3.64201	-1.26333
C	2.91332	1.34478	-1.00167
H	4.15145	1.38333	0.78415
H	5.06110	1.27348	-0.72614
C	0.85587	1.23235	0.26405
O	-0.16505	1.65481	0.91803
C	1.28990	-0.06568	-0.00509
C	0.64174	-1.28269	0.55877
O	0.36375	-1.40752	1.72332
O	0.44541	-2.20730	-0.37413
C	-0.18561	-3.41908	0.07346
H	0.43153	-3.90360	0.83028
H	-1.17159	-3.19489	0.48237
H	-0.27214	-4.04688	-0.80920
C	2.48965	-0.14069	-0.88824
C	3.55701	-1.11862	-0.43896
C	3.81685	-1.34618	0.91439
C	4.31694	-1.79090	-1.39730
C	5.32469	-2.66985	-1.01229
C	5.57818	-2.89204	0.33870
C	4.82081	-2.22980	1.30078
H	3.23822	-0.82889	1.67392
H	4.11338	-1.62647	-2.45085
H	5.90633	-3.18620	-1.76744
H	6.35891	-3.58078	0.64026
H	5.01007	-2.39974	2.35451
H	3.04280	1.65965	-2.04407
H	2.15274	-0.46257	-1.88284
H	1.87468	3.94388	-1.35533
H	0.93126	3.93396	0.16721
I	-2.24901	0.66055	0.35423
I	-4.66322	-0.48309	-0.39824

6.6.19 Nazarov Product **15** (*cis* configuration)

SCF energy:	–884.004398
Zero-point correction:	+0.317450
Enthalpy correction:	+0.335933
Free energy correction:	+0.270650
Truhlar's Delta G correction:	+0.274091
Grimme's Delta G correction:	+0.273768

Cartesian Coordinates

C	-2.11937	0.42779	-0.12154
C	-3.46081	0.35747	0.53961
C	-3.73147	-1.07099	1.02570
C	-3.36115	-2.09637	-0.04978
H	-4.78144	-1.17564	1.30727
H	-3.13342	-1.26435	1.92357
C	-1.86117	-2.04630	-0.36451
H	-3.92765	-1.87866	-0.96198
H	-3.63670	-3.10365	0.26961
C	-1.39399	-0.63329	-0.51209
H	-1.62460	-2.60284	-1.27758
H	-1.28548	-2.52441	0.43769
C	-1.41255	1.66740	-0.46237
O	-1.80124	2.80183	-0.29227
C	-0.07972	1.29532	-1.12573
C	1.10643	1.86931	-0.38911
O	2.11408	2.26277	-0.91908
O	0.92506	1.84605	0.93090
C	2.05800	2.21326	1.72863
H	2.32935	3.25310	1.54485
H	2.90354	1.56333	1.49772
H	1.74665	2.08040	2.76185
C	-0.07678	-0.26815	-1.15938
C	1.13105	-0.93215	-0.52045
C	1.19847	-1.15895	0.85682
C	2.22201	-1.28866	-1.31498
C	3.36068	-1.85488	-0.74807
C	3.41881	-2.07638	0.62472
C	2.33340	-1.72877	1.42573
H	0.36078	-0.88153	1.48892
H	2.17927	-1.11538	-2.38581
H	4.20003	-2.12379	-1.37929
H	4.30285	-2.52007	1.06832
H	2.36996	-1.90120	2.49557
H	-0.10636	-0.58932	-2.20499
H	-0.06005	1.70345	-2.13685
H	-3.49888	1.06979	1.36870
H	-4.23215	0.67178	-0.17317

6.6.20 Nazarov Product **15** (*trans* configuration)

SCF energy:	–884.006414
Zero-point correction:	+0.317143
Enthalpy correction:	+0.335849
Free energy correction:	+0.268482
Truhlar's Delta G correction:	+0.273613
Grimme's Delta G correction:	+0.272604

Cartesian Coordinates

C	-0.52335	-1.87889	-0.32431
C	-0.58146	-3.35564	-0.56896
C	0.36921	-4.08194	0.38979
C	1.72688	-3.37663	0.45658
H	0.49430	-5.11994	0.07412
H	-0.07456	-4.09772	1.39153
C	1.58704	-1.95336	1.00966
H	2.15447	-3.32721	-0.55115
H	2.42400	-3.94529	1.07561
C	0.42519	-1.24909	0.38881
H	2.50062	-1.37313	0.84533
H	1.43007	-1.97297	2.09636
C	-1.52984	-0.91372	-0.77689
O	-2.55370	-1.14457	-1.37852
C	-1.06424	0.49219	-0.33542
C	-2.19967	1.17772	0.38300
O	-2.45351	1.03285	1.55343
O	-2.92225	1.93079	-0.44173
C	-4.08307	2.55219	0.12902
H	-4.76712	1.79329	0.50931
H	-4.54641	3.10848	-0.68169
H	-3.79241	3.22549	0.93559
C	0.18285	0.24066	0.53505
C	1.38406	1.07851	0.14591
C	1.96146	0.93857	-1.11955
C	1.93748	1.99041	1.04295
C	3.04654	2.75500	0.68339
C	3.61389	2.61075	-0.57805
C	3.06751	1.69899	-1.48072
H	1.54041	0.22651	-1.82442
H	1.49673	2.10323	2.02831
H	3.46569	3.46142	1.39101
H	4.47734	3.20307	-0.85842
H	3.50603	1.58011	-2.46510
H	-0.05731	0.44581	1.58310
H	-0.82248	1.05116	-1.24181
H	-1.61017	-3.70584	-0.44524
H	-0.30638	-3.56329	-1.60947

6.6.21 Iodine-Complex Nazarov Product **15–I_2** (*cis* configuration, CO coordination)

SCF energy:	–1474.958574
Zero-point correction:	+0.318540
Enthalpy correction:	+0.341703
Free energy correction:	+0.260411
Truhlar's Delta G correction:	+0.268643
Grimme's Delta G correction:	+0.267041

Cartesian Coordinates

C	-2.42663	2.07607	-0.02246
C	-2.76191	3.43074	0.52006
C	-4.27735	3.55435	0.71620
C	-5.03589	3.01514	-0.50005
H	-4.54351	4.59728	0.89990
H	-4.57215	2.98246	1.60322
C	-4.76699	1.51855	-0.69777
H	-4.71389	3.55970	-1.39448
H	-6.10888	3.18323	-0.38751
C	-3.31144	1.21406	-0.55719
H	-5.11807	1.17078	-1.67502
H	-5.31524	0.92836	0.04758
C	-1.09000	1.49635	-0.07875
O	-0.05149	2.03607	0.26497
C	-1.18366	0.09310	-0.67246
C	-0.69954	-0.93522	0.32643
O	-0.68969	-0.77930	1.52081
O	-0.31553	-2.05340	-0.28268
C	0.08053	-3.12953	0.57997
H	-0.74954	-3.41417	1.22791
H	0.34699	-3.95171	-0.07922
H	0.93872	-2.83082	1.18312
C	-2.69264	-0.07755	-1.04227
C	-3.36976	-1.32030	-0.49426
C	-3.74752	-1.40260	0.84847
C	-3.59547	-2.41651	-1.32783
C	-4.18172	-3.57722	-0.83071
C	-4.55186	-3.65219	0.50916
C	-4.33450	-2.56137	1.34756
H	-3.57637	-0.55723	1.50794
H	-3.30464	-2.35997	-2.37208
H	-4.35084	-4.42072	-1.49041
H	-5.01020	-4.55429	0.89806
H	-4.62275	-2.61172	2.39141
H	-2.78042	-0.10940	-2.13231
H	-0.55595	0.03276	-1.56438
H	-2.22815	3.59176	1.46070
H	-2.40209	4.19691	-0.17629
I	2.37462	0.81870	0.07693
I	4.77252	-0.38503	-0.14707

6.6.22 Iodine-Complex Nazarov Product **15–I_2** (*cis* configuration, CO_2Me coordination)

SCF energy:	–1474.958061
Zero-point correction:	+0.318522
Enthalpy correction:	+0.341644
Free energy correction:	+0.261077
Truhlar's Delta G correction:	+0.268929
Grimme's Delta G correction:	+0.267460

Cartesian Coordinates

C	-0.49727	1.98594	-1.11914
C	0.81622	2.70345	-1.10182
C	1.06876	3.28014	0.29466
C	-0.17485	4.00831	0.81385
H	1.92597	3.95642	0.27157
H	1.31828	2.46060	0.98002
C	-1.35366	3.04112	0.97855
H	-0.44983	4.79456	0.10220
H	0.03532	4.49544	1.76831
C	-1.46152	2.11775	-0.19247
H	-2.29933	3.57890	1.10635
H	-1.22726	2.43676	1.88545
C	-0.91737	1.02399	-2.14245
O	-0.31614	0.70743	-3.14459
C	-2.28763	0.46555	-1.74199
C	-2.20125	-1.01552	-1.47152
O	-1.20160	-1.60644	-1.12641
O	-3.37867	-1.60629	-1.60909
C	-3.44943	-2.98263	-1.20192
H	-3.17729	-3.07016	-0.14915
H	-4.48398	-3.27891	-1.35440
H	-2.78295	-3.59172	-1.81222
C	-2.68886	1.27233	-0.46198
C	-3.14131	0.43498	0.72016
C	-2.21722	-0.19709	1.55580
C	-4.50373	0.24573	0.95898
C	-4.93605	-0.56024	2.00817
C	-4.00730	-1.18683	2.83517
C	-2.64606	-1.00252	2.60698
H	-1.15388	-0.05940	1.38345
H	-5.22945	0.72996	0.31306
H	-5.99765	-0.69669	2.18081
H	-4.34227	-1.81260	3.65453
H	-1.91600	-1.48427	3.24760
H	-3.51436	1.94083	-0.72438
H	-3.00339	0.62639	-2.54937
H	1.61248	2.01318	-1.39678
H	0.80607	3.50431	-1.85043
I	1.41450	-1.02453	-0.25034
I	3.88063	-0.45298	0.62676

6.6.23 Iodine-Complex Nazarov Product **15–I_2** (*trans* configuration, CO coordination)

SCF energy:	–1474.958633
Zero-point correction:	+0.318426
Enthalpy correction:	+0.341679
Free energy correction:	+0.259483
Truhlar's Delta G correction:	+0.268421
Grimme's Delta G correction:	+0.266560

Cartesian Coordinates

C	2.44927	-1.86705	-0.21054
C	2.69957	-3.29238	-0.59588
C	4.05380	-3.75293	-0.04420
C	5.13632	-2.69873	-0.29269
H	4.33630	-4.70358	-0.50114
H	3.96276	-3.92461	1.03413
C	4.81476	-1.38934	0.43726
H	5.20364	-2.50013	-1.36811
H	6.11206	-3.06805	0.02945
C	3.37961	-1.01718	0.26177
H	5.45261	-0.57165	0.08728
H	5.00823	-1.48724	1.51389
C	1.15224	-1.19908	-0.24926
O	0.09519	-1.70037	-0.59354
C	1.33813	0.25282	0.18877
C	0.41275	0.69635	1.29779
O	0.02297	1.82598	1.44375
O	0.12992	-0.30274	2.13372
C	-0.74041	0.02078	3.22764
H	-0.89069	-0.90969	3.76896
H	-0.27586	0.76776	3.87182
H	-1.69126	0.39851	2.84899
C	2.82724	0.34357	0.63045
C	3.58575	1.49494	0.00317
C	3.78437	1.53725	-1.37981
C	4.10009	2.52083	0.79308
C	4.79937	3.57811	0.21287
C	4.99237	3.61414	-1.16363
C	4.48245	2.58933	-1.96028
H	3.38965	0.73990	-2.00398
H	3.95005	2.49363	1.86764
H	5.19146	4.37183	0.83860
H	5.53622	4.43513	-1.61649
H	4.63102	2.61108	-3.03393
H	2.89001	0.44989	1.71970
H	1.15259	0.89965	-0.67203
H	1.88607	-3.91979	-0.22115
H	2.68193	-3.38056	-1.68814
I	-2.36777	-0.56207	-0.44462
I	-4.80426	0.56446	-0.25889

6.6.24 Iodine-Complex Nazarov Product **15–I_2** (*trans* configuration, CO_2Me coordination)

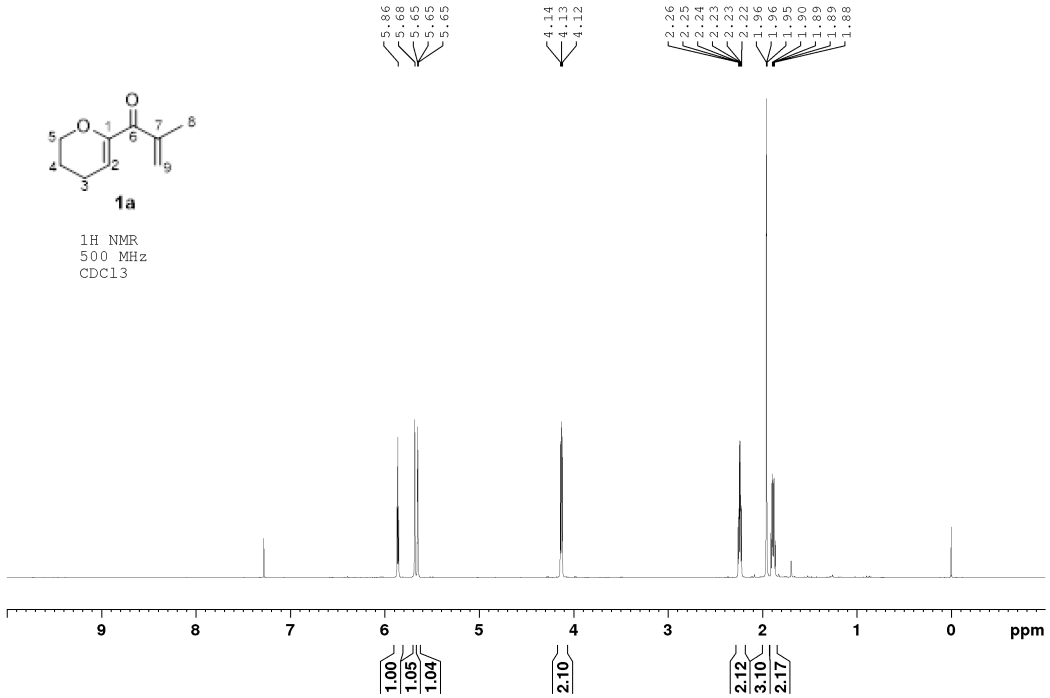
SCF energy:	–1474.959716
Zero-point correction:	+0.318521
Enthalpy correction:	+0.341808
Free energy correction:	+0.259659
Truhlar's Delta G correction:	+0.268685
Grimme's Delta G correction:	+0.266831

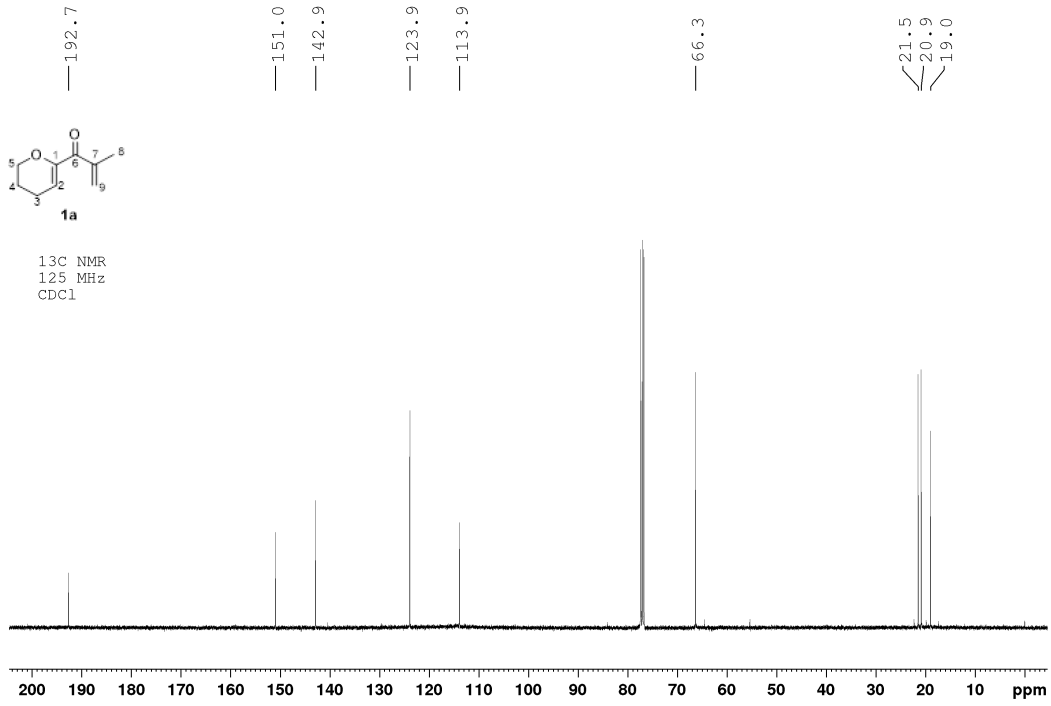
Cartesian Coordinates

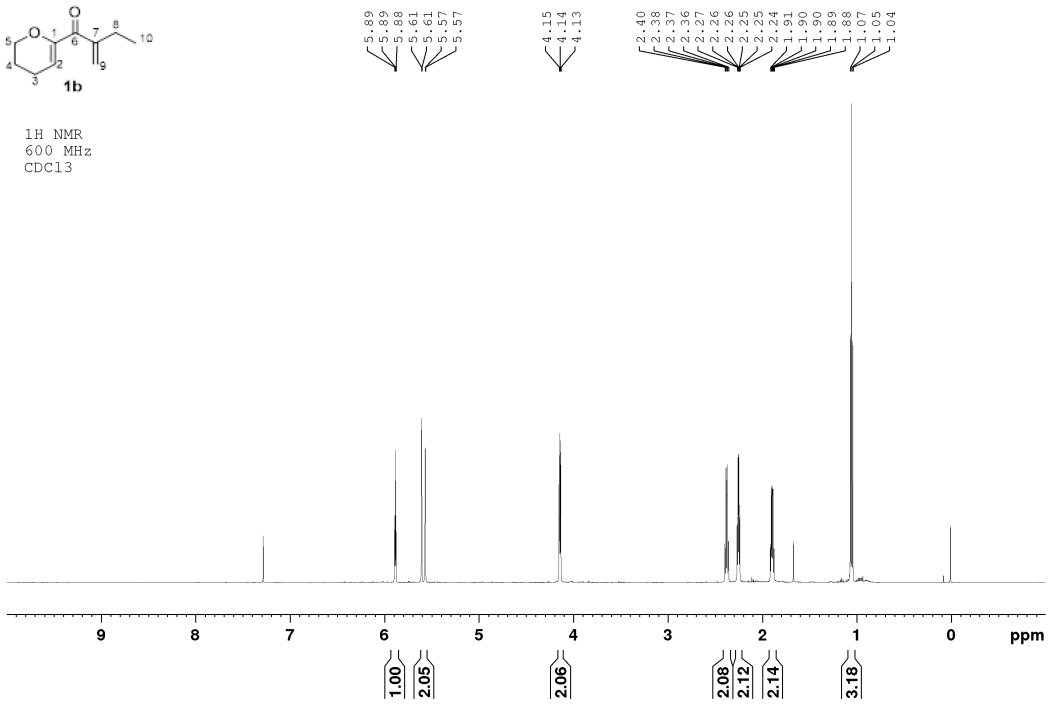
C	-0.96232	-0.51640	1.88066
C	-0.10954	-1.16312	2.92828
C	0.73064	-2.27863	2.29549
C	-0.12292	-3.15825	1.37778
H	1.19800	-2.88204	3.07660
H	1.53791	-1.82694	1.70671
C	-0.68785	-2.34815	0.20524
H	-0.95309	-3.58011	1.95512
H	0.46412	-3.99618	0.99594
C	-1.20939	-1.02753	0.66332
H	-1.47631	-2.89854	-0.31829
H	0.09527	-2.15268	-0.54182
C	-1.55374	0.81877	1.98957
O	-1.48461	1.58620	2.92207
C	-2.27288	1.12975	0.65482
C	-1.67874	2.40236	0.11071
O	-0.58999	2.47438	-0.42031
O	-2.45386	3.45369	0.31541
C	-1.92153	4.72641	-0.09163
H	-0.99574	4.93228	0.44542
H	-2.68393	5.45582	0.16777
H	-1.73859	4.72932	-1.16597
C	-2.01546	-0.10831	-0.23139
C	-3.27877	-0.76442	-0.75460
C	-4.22858	-1.27491	0.13481
C	-3.50372	-0.88323	-2.12488
C	-4.66099	-1.49645	-2.60254
C	-5.60280	-1.99893	-1.71122
C	-5.38354	-1.88650	-0.33889
H	-4.05988	-1.19413	1.20505
H	-2.76967	-0.49290	-2.82251
H	-4.82378	-1.58056	-3.67109
H	-6.50269	-2.47692	-2.08092
H	-6.11242	-2.27828	0.36155
H	-1.39203	0.16622	-1.08933
H	-3.33205	1.28566	0.86273
H	0.52855	-0.40498	3.39204
H	-0.74437	-1.56664	3.72533
I	1.74462	0.86428	-0.48340
I	3.93012	-0.68291	-0.55537

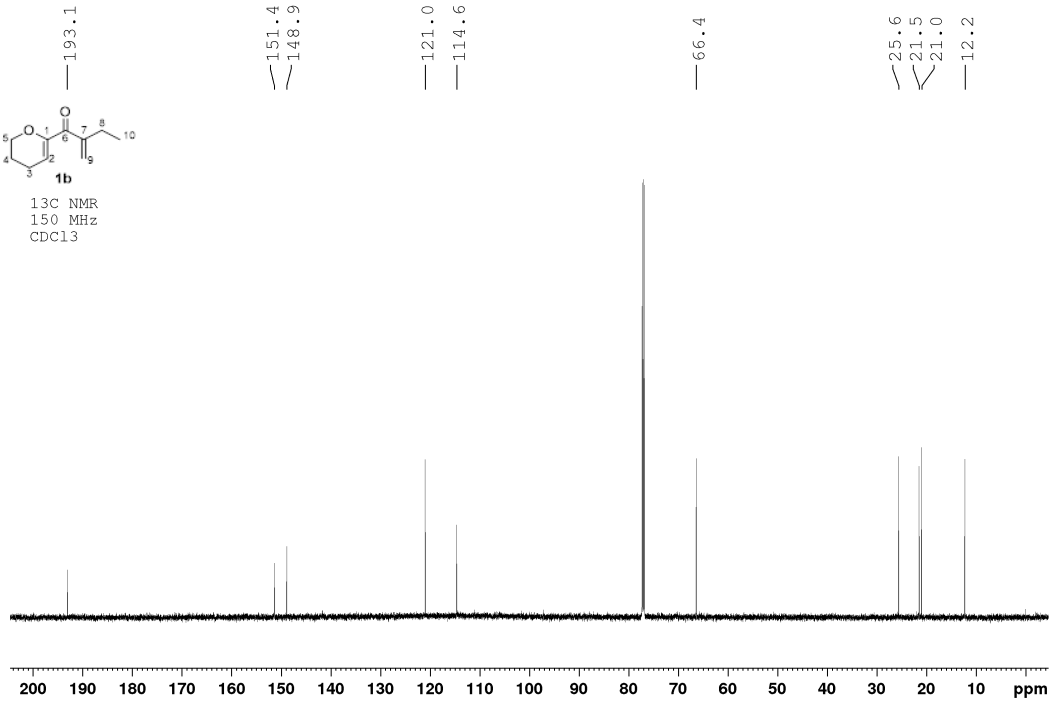
7 Copies of NMR Spectra

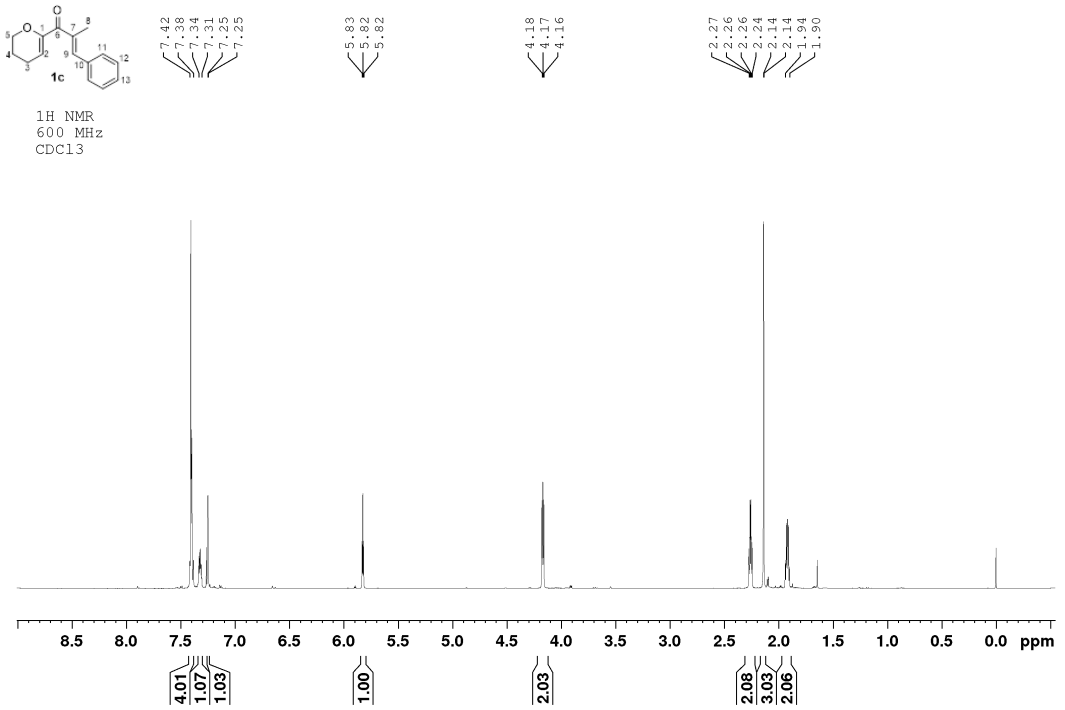
7.1 Divinyl Ketones

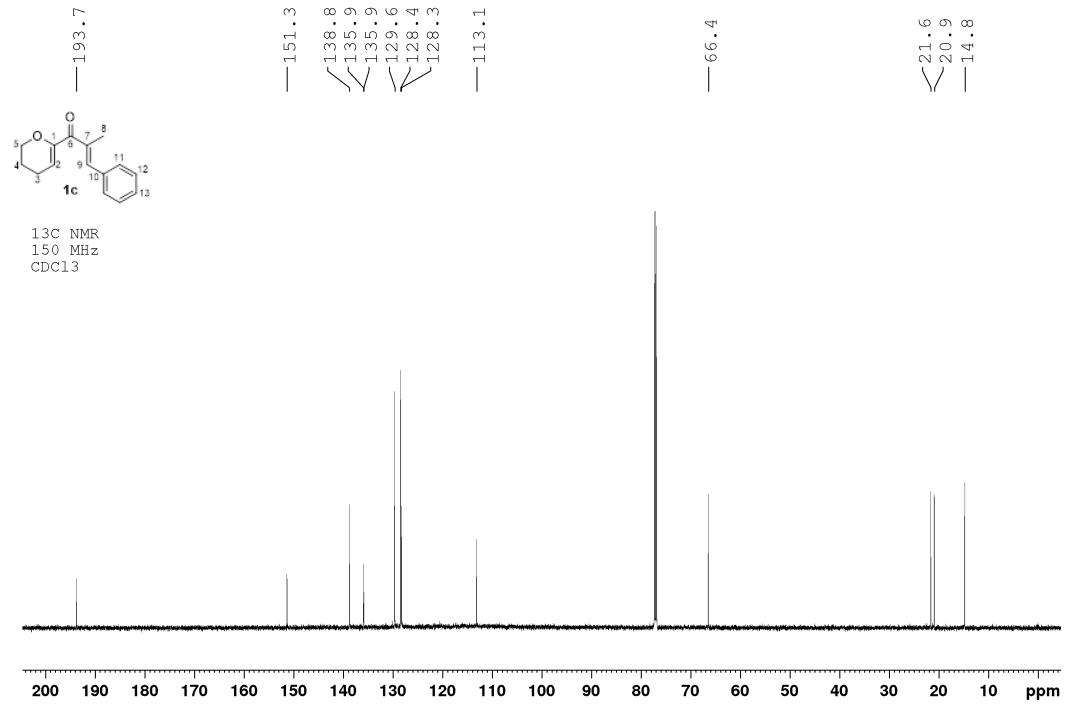


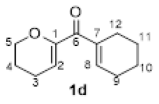



1b
1H NMR
600 MHz
CDCl3
5.89
5.89
5.88
5.61
5.61
5.57
5.57
4.15
4.14
4.13
2.40
2.38
2.37
2.36
2.27
2.26
2.26
2.25
2.25
2.24
1.91
1.90
1.90
1.89
1.88
1.07
1.05
1.04
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.05
2.06
2.08
2.12
2.14
3.18

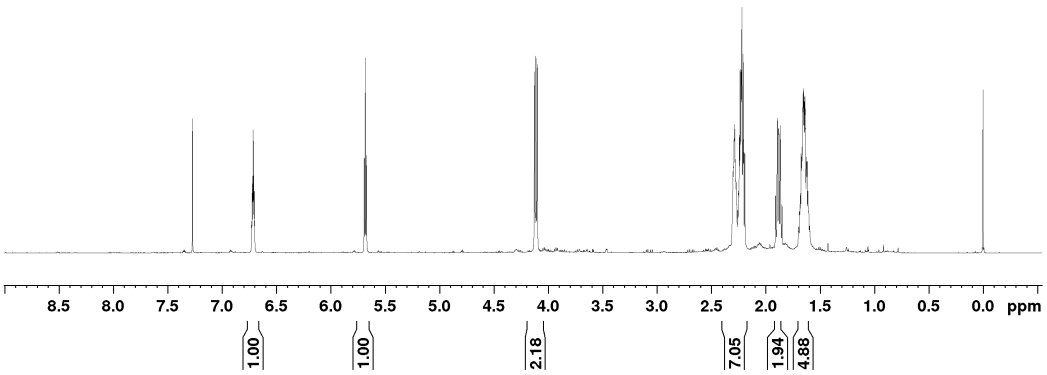

193.1
151.4
148.9
121.0
114.6
66.4
25.6
21.5
21.0
12.2
1b
13C NMR
150 MHz
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

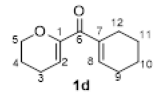

1c
7.42
7.38
7.34
7.31
7.25
7.25
5.83
5.82
5.82
4.18
4.17
4.16
2.27
2.26
2.26
2.24
2.14
2.14
1.94
1.90
1H NMR
600 MHz
CDCl3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
4.01
1.07
1.03
1.00
2.03
2.08
3.03
2.06

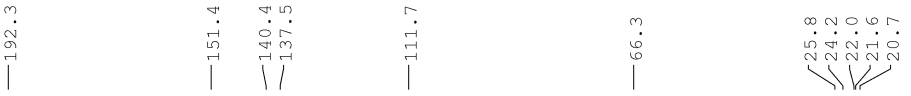

193.7
151.3
138.8
135.9
135.9
129.6
128.4
128.3
113.1
66.4
21.6
20.9
14.8
1c
13C NMR
150 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



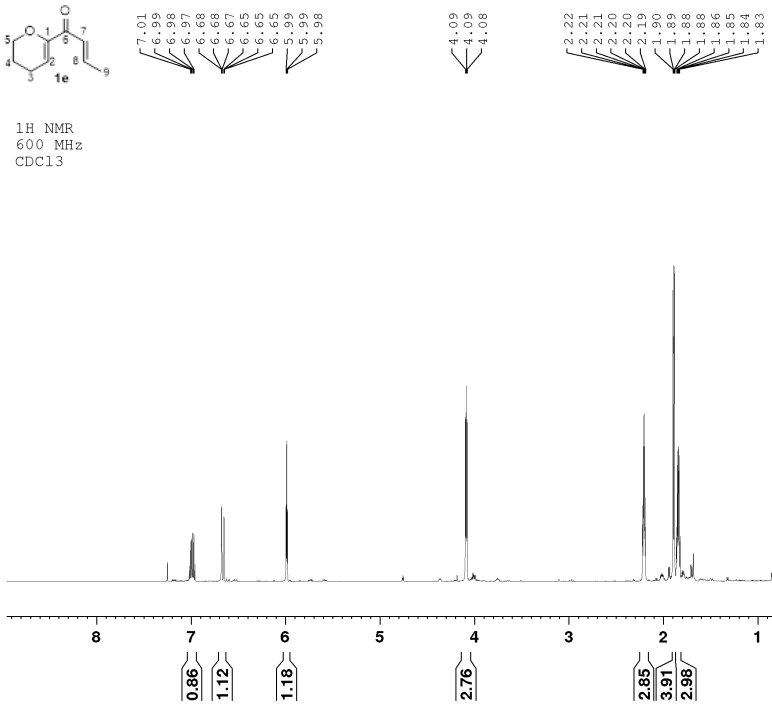
1H NMR
400 MHz
CDCl3

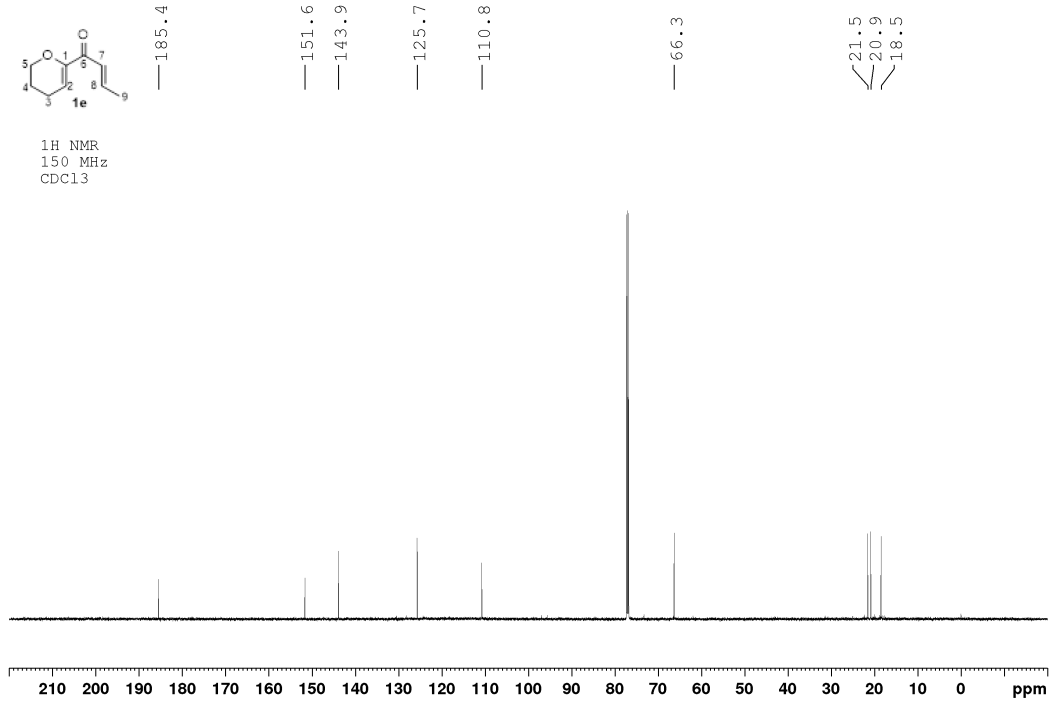


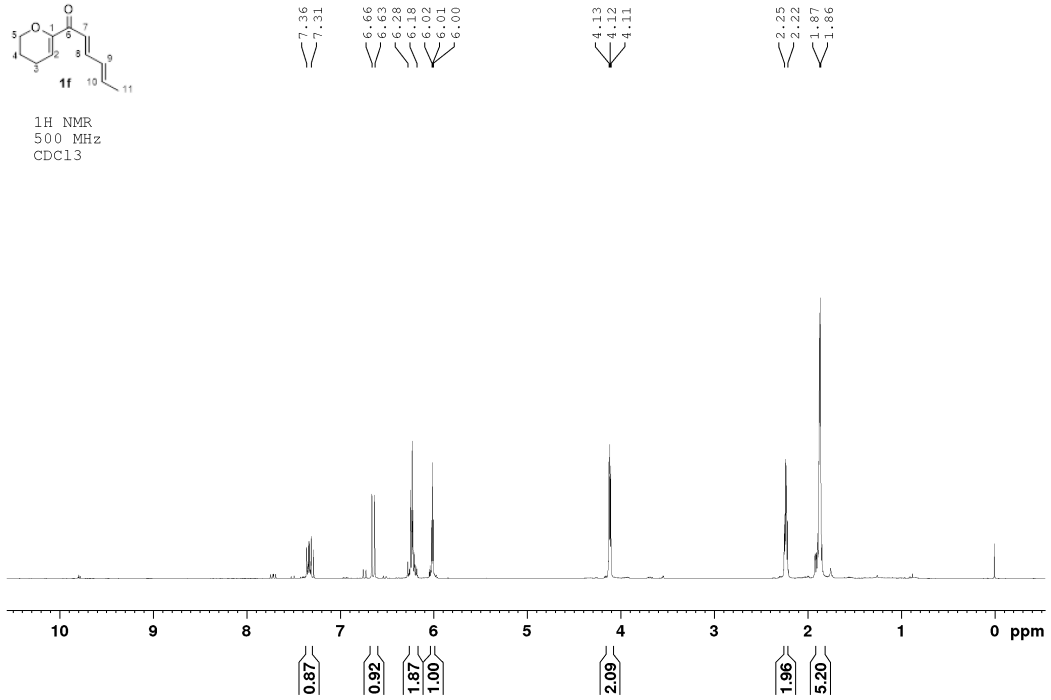


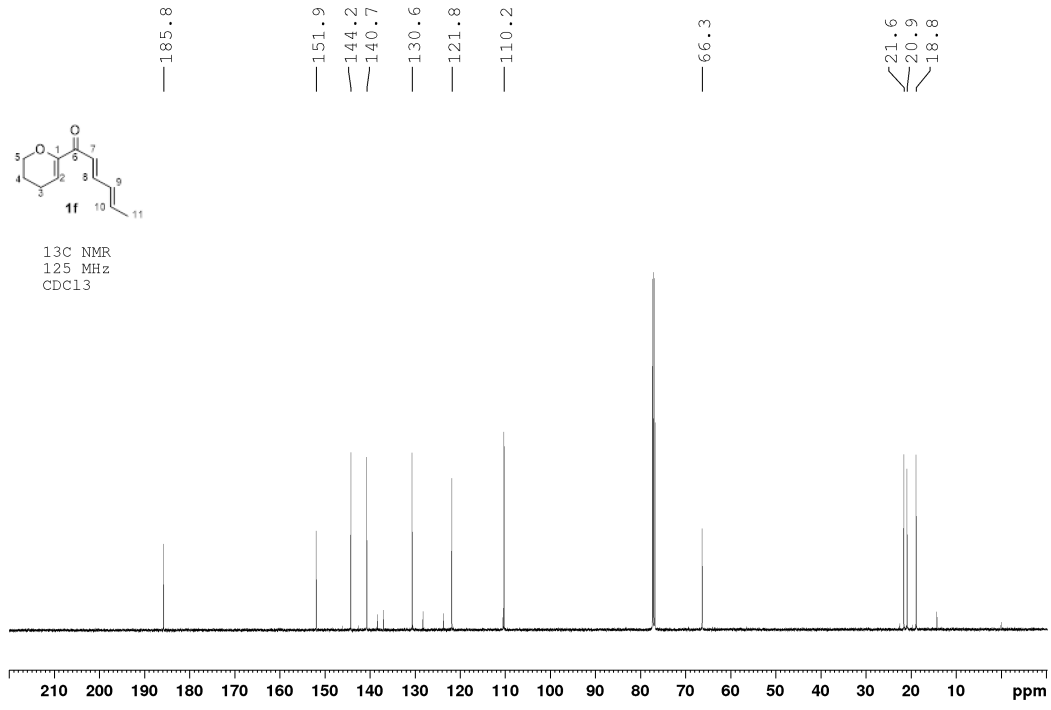


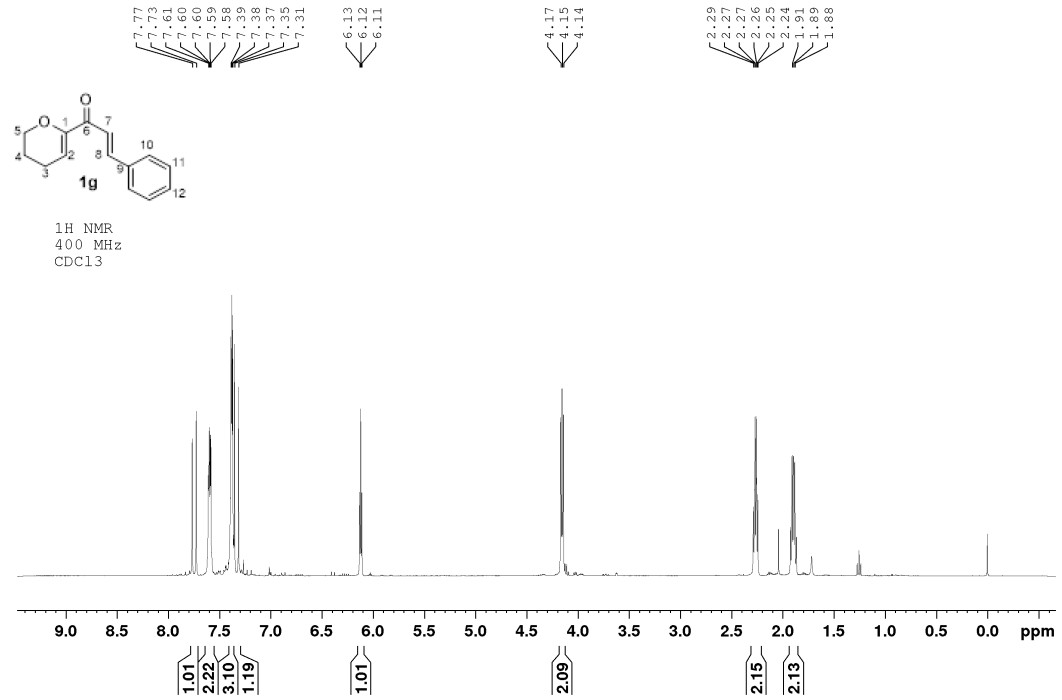
13C NMR
100 MHz
CDCl3

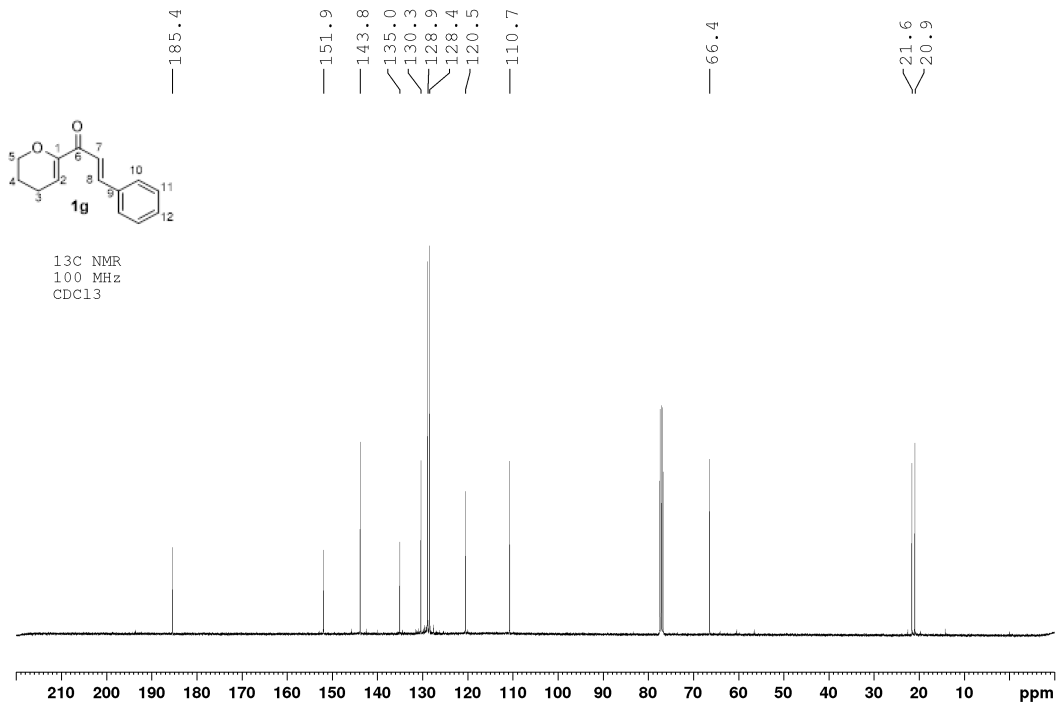

1e
7.01
6.99
6.98
6.97
6.68
6.68
6.67
6.65
6.65
6.65
5.99
5.99
5.98
4.09
4.09
4.08
2.22
2.21
2.21
2.20
2.20
2.19
1.90
1.89
1.88
1.88
1.86
1.85
1.84
1.83
1H NMR
600 MHz
CDCl3
8
7
6
5
4
3
2
1
0
-1
ppm
0.86
1.12
1.18
2.76
2.85
3.91
2.98

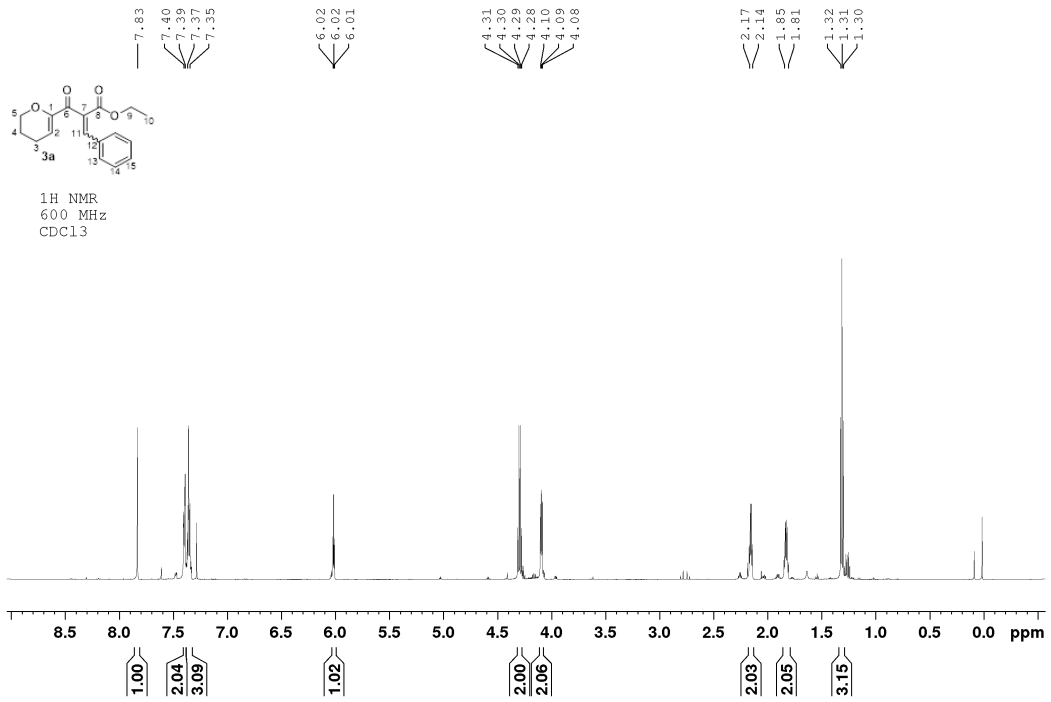

1e
185.4
151.6
143.9
125.7
110.8
66.3
21.5
20.9
18.5
1H NMR
150 MHz
CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

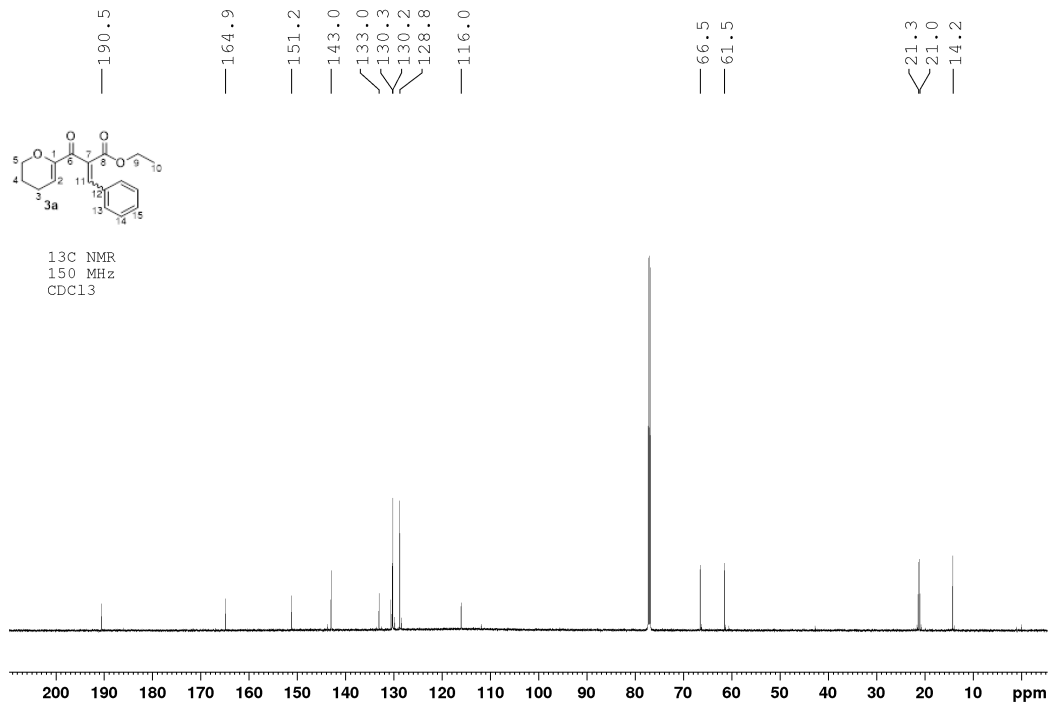

1f
1H NMR
500 MHz
CDCl3
7.36
7.31
6.66
6.63
6.28
6.18
6.02
6.01
6.00
4.13
4.12
4.11
2.25
2.22
1.87
1.86
0.87
0.92
1.87
1.00
2.09
1.96
5.20
ppm

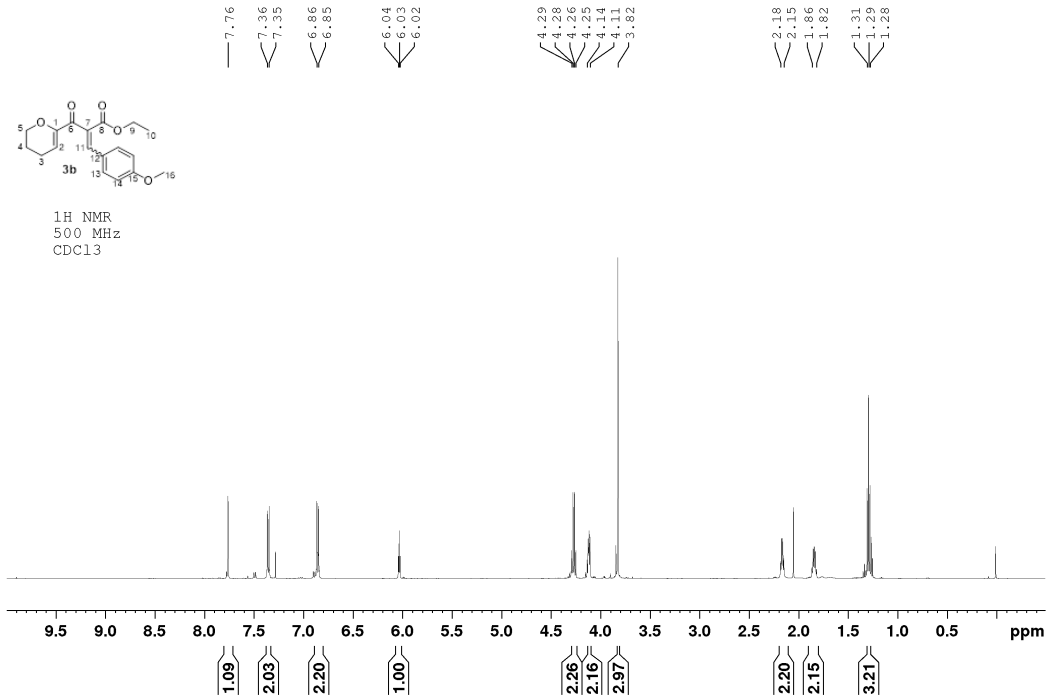

1f
13C NMR
125 MHz
CDCl3
185.8
151.9
144.2
140.7
130.6
121.8
110.2
66.3
21.6
20.9
18.8
ppm

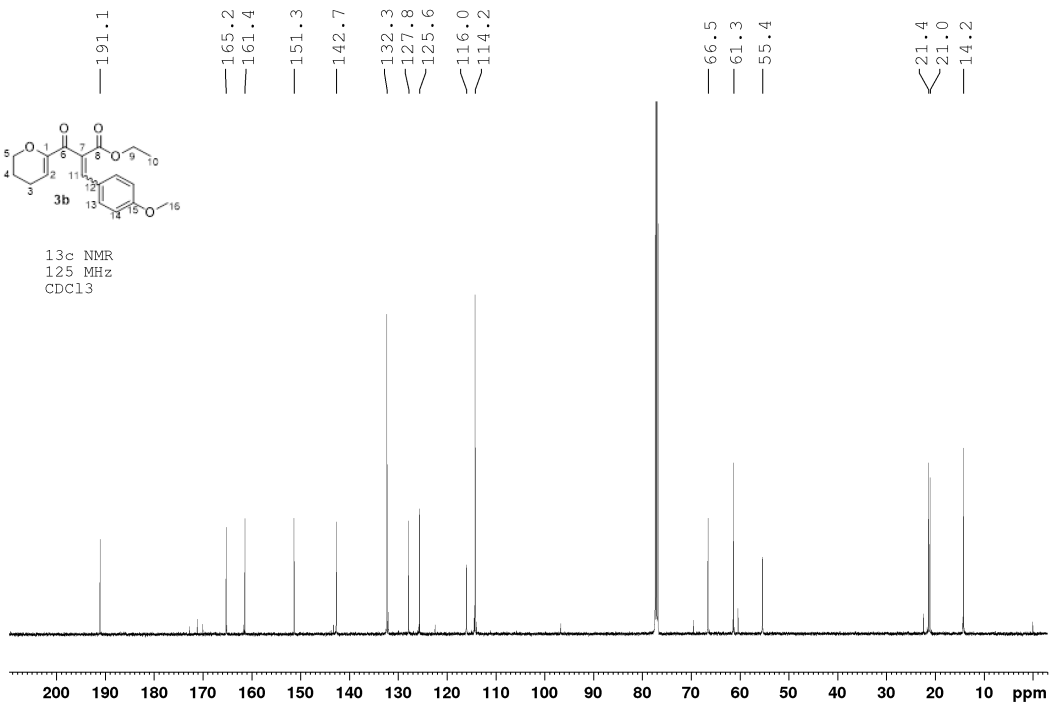

7.77
7.73
7.61
7.60
7.59
7.58
7.39
7.38
7.37
7.35
7.31
6.13
6.12
6.11
4.17
4.15
4.14
2.29
2.27
2.27
2.26
2.25
2.24
1.91
1.89
1.88
1g
1H NMR
400 MHz
CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.01
2.22
3.10
1.19
1.01
2.09
2.15
2.13

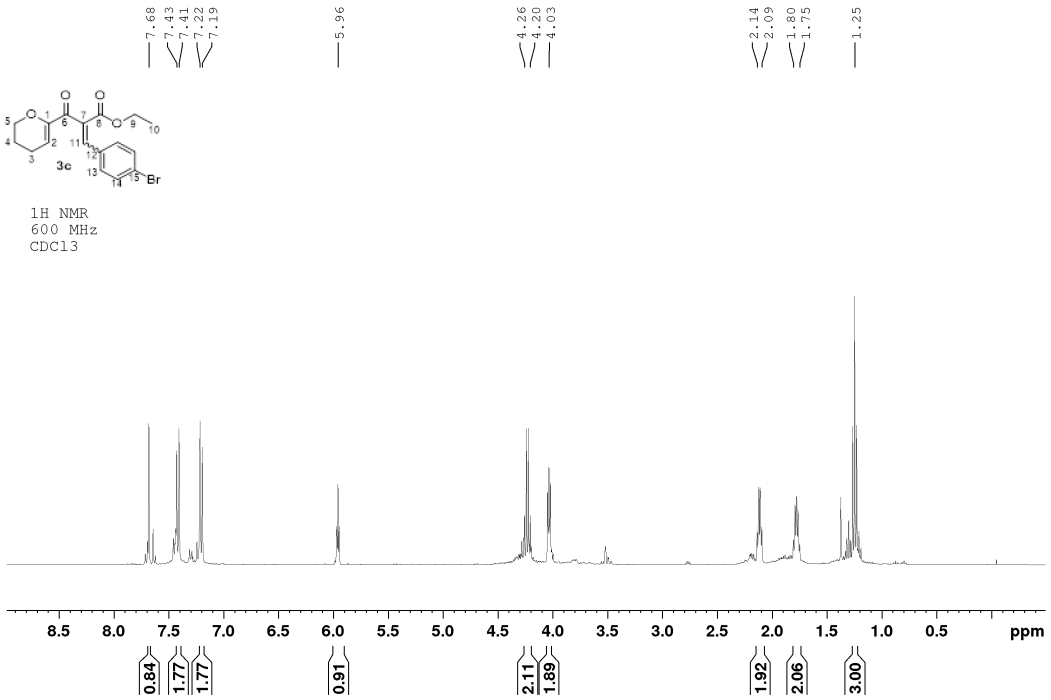

185.4
151.9
143.8
135.0
130.3
128.9
128.4
120.5
110.7
66.4
21.6
20.9
1g
13C NMR
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.83
7.40
7.39
7.37
7.35
6.02
6.02
6.01
4.31
4.30
4.29
4.28
4.10
4.09
4.08
2.17
2.14
1.85
1.81
1.32
1.31
1.30
3a
1H NMR
600 MHz
CDCl3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
2.04
3.09
1.02
2.00
2.06
2.03
2.05
3.15


190.5
164.9
151.2
143.0
133.0
130.3
130.2
128.8
116.0
66.5
61.5
21.3
21.0
14.2
3a
13C NMR
150 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.76
7.36
7.35
6.86
6.85
6.04
6.03
6.02
4.29
4.28
4.26
4.25
4.14
4.11
3.82
2.18
2.15
1.86
1.82
1.31
1.29
1.28
3b
1H NMR
500 MHz
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.09
2.03
2.20
1.00
2.26
2.16
2.97
2.20
2.15
3.21


191.1
165.2
161.4
151.3
142.7
132.3
127.8
125.6
116.0
114.2
66.5
61.3
55.4
21.4
21.0
14.2
3b
13c NMR
125 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.43
7.41
7.22
7.19
5.96
4.26
4.20
4.03
2.14
2.09
1.80
1.75
1.25
3c
Br
1H NMR
600 MHz
CDCl3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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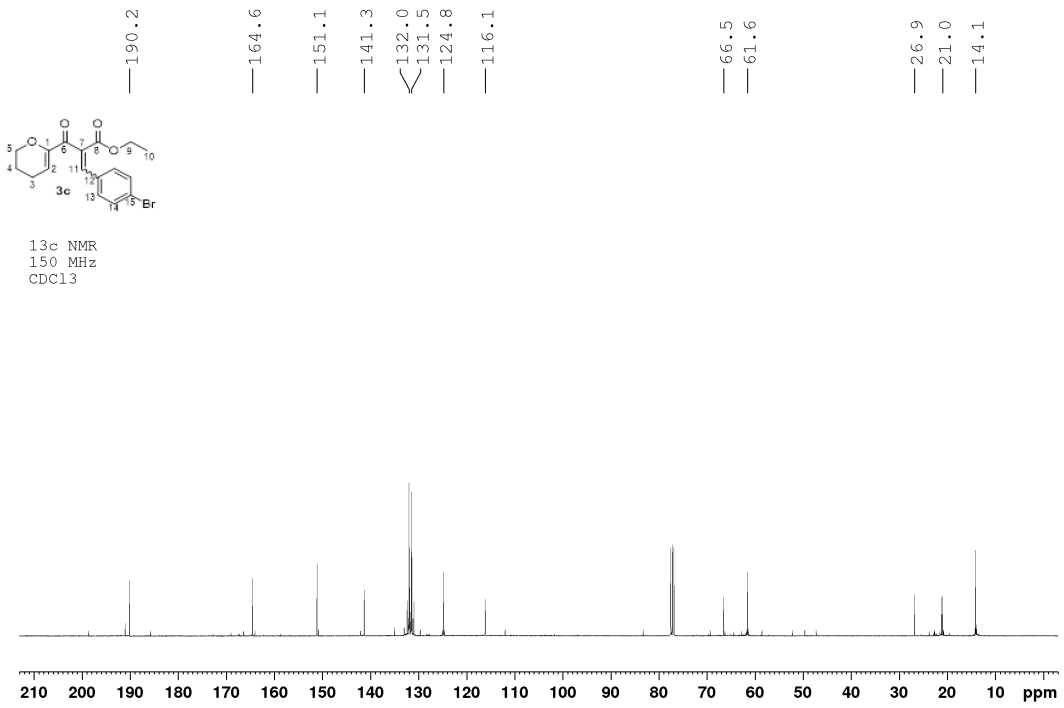
1.77
0.91
2.11
1.89
1.92
2.06
3.00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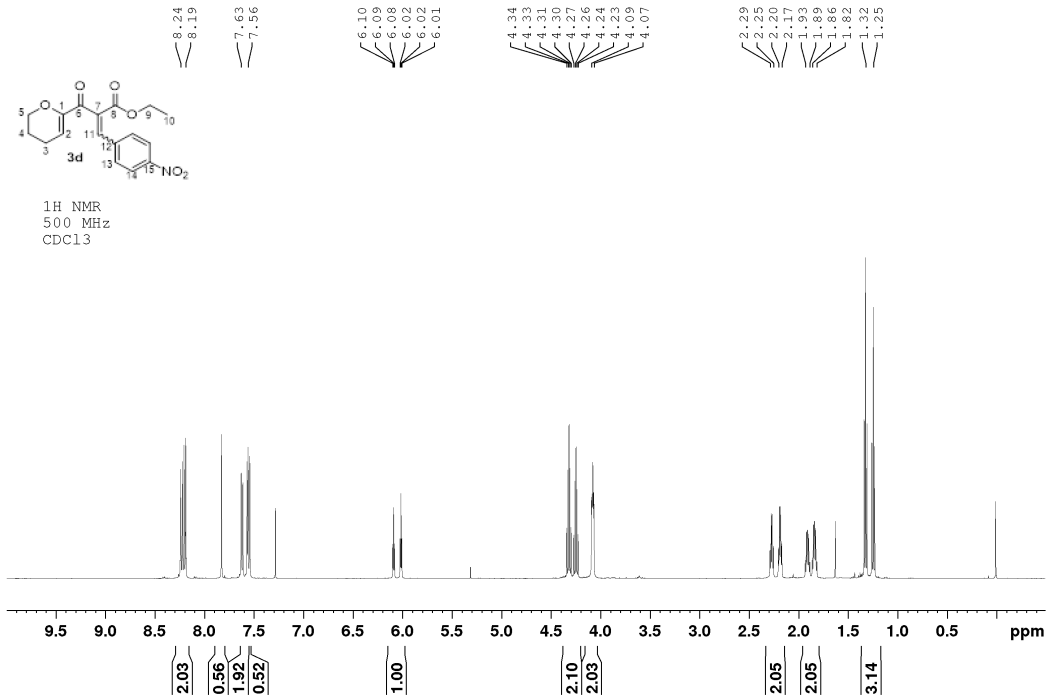
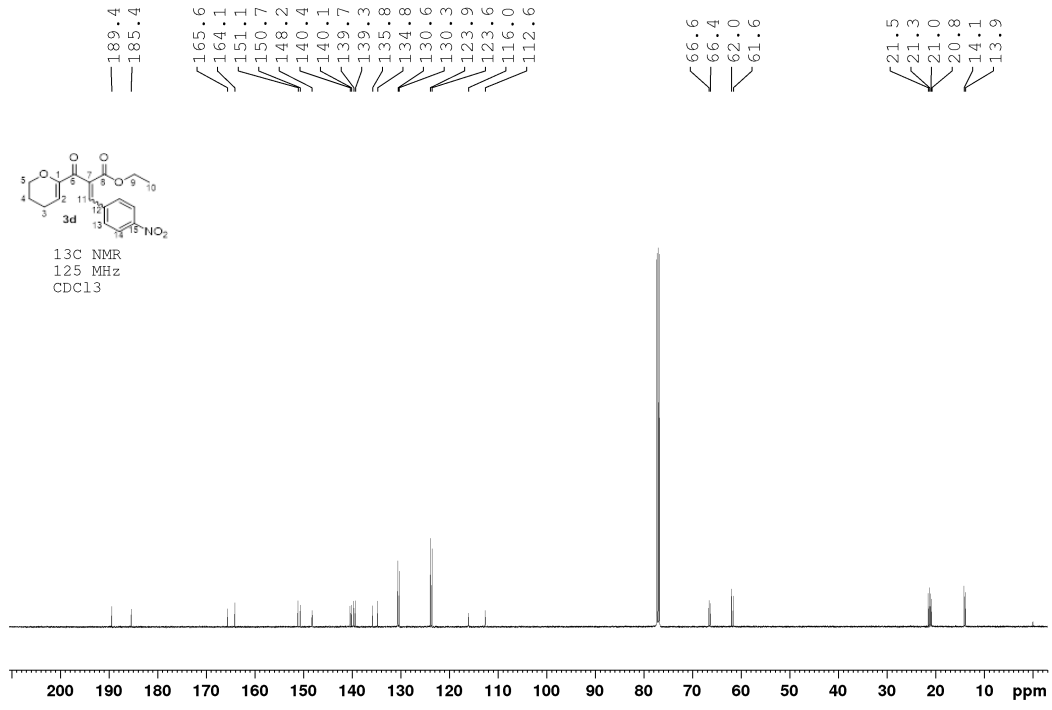
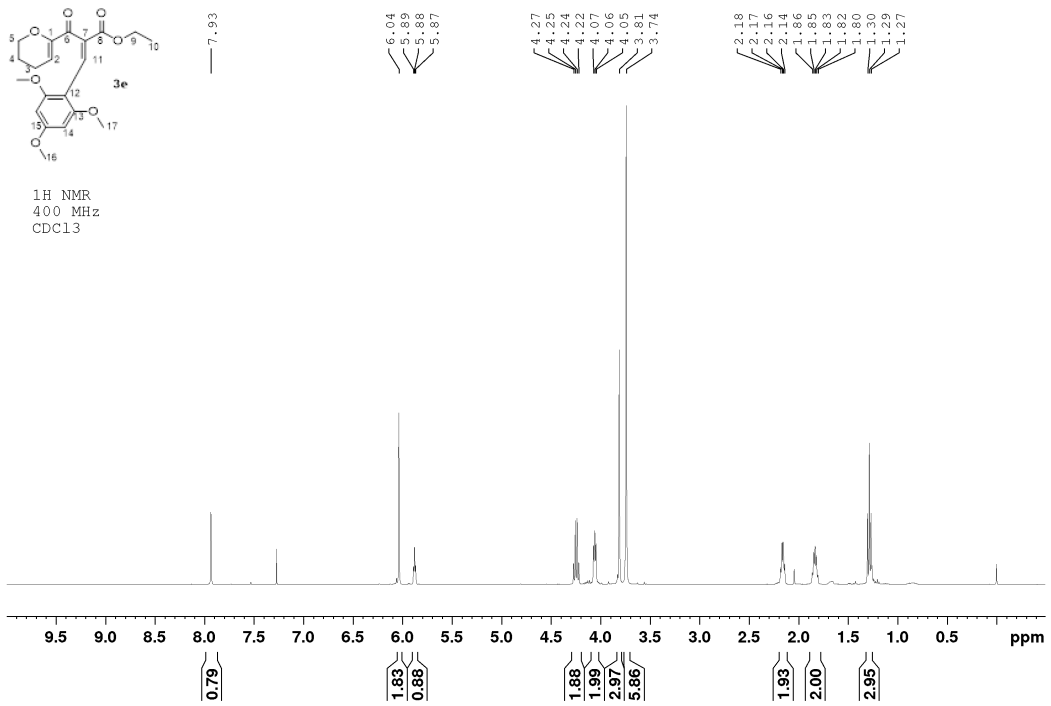
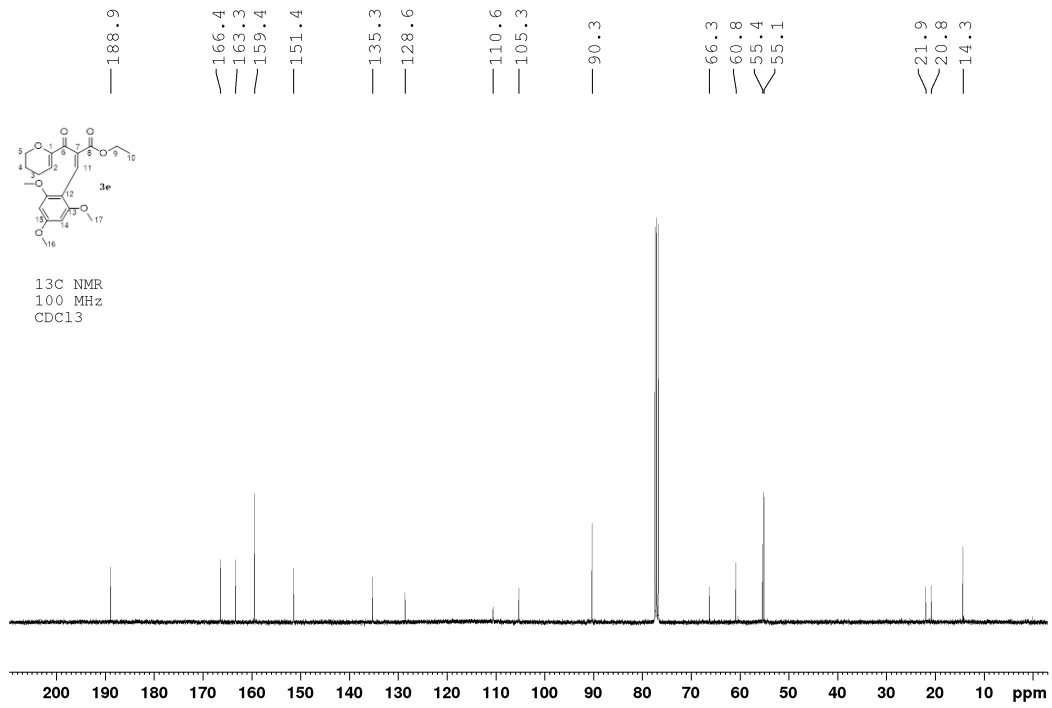
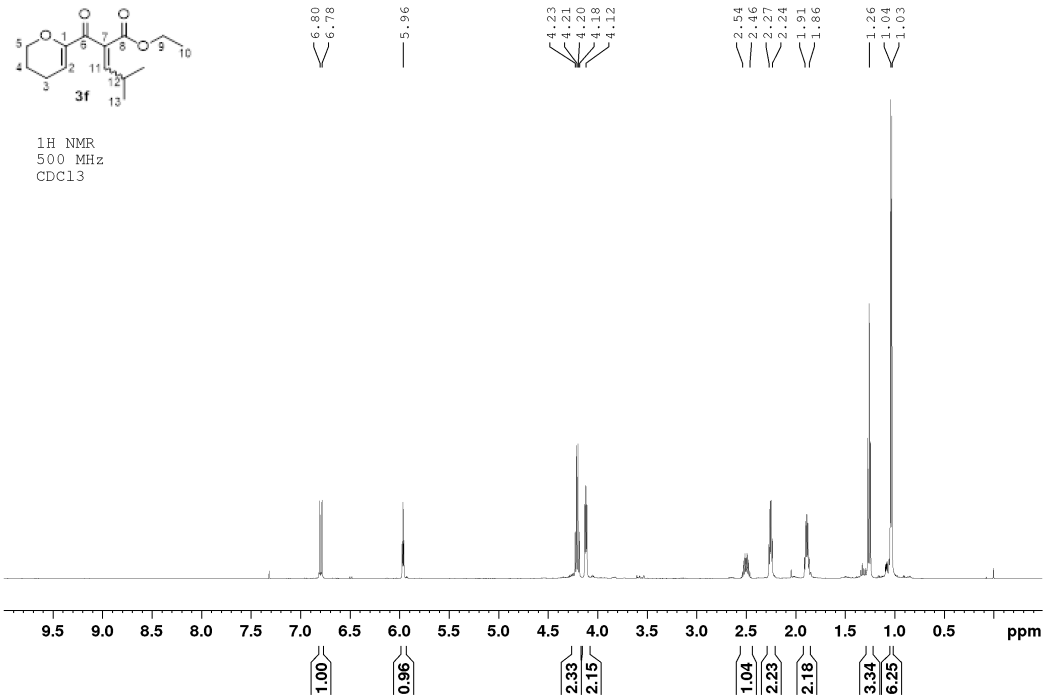
164.6
151.1
141.3
132.0
131.5
124.8
116.1
66.5
61.6
26.9
21.0
14.1
3c
Br
13c NMR
150 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

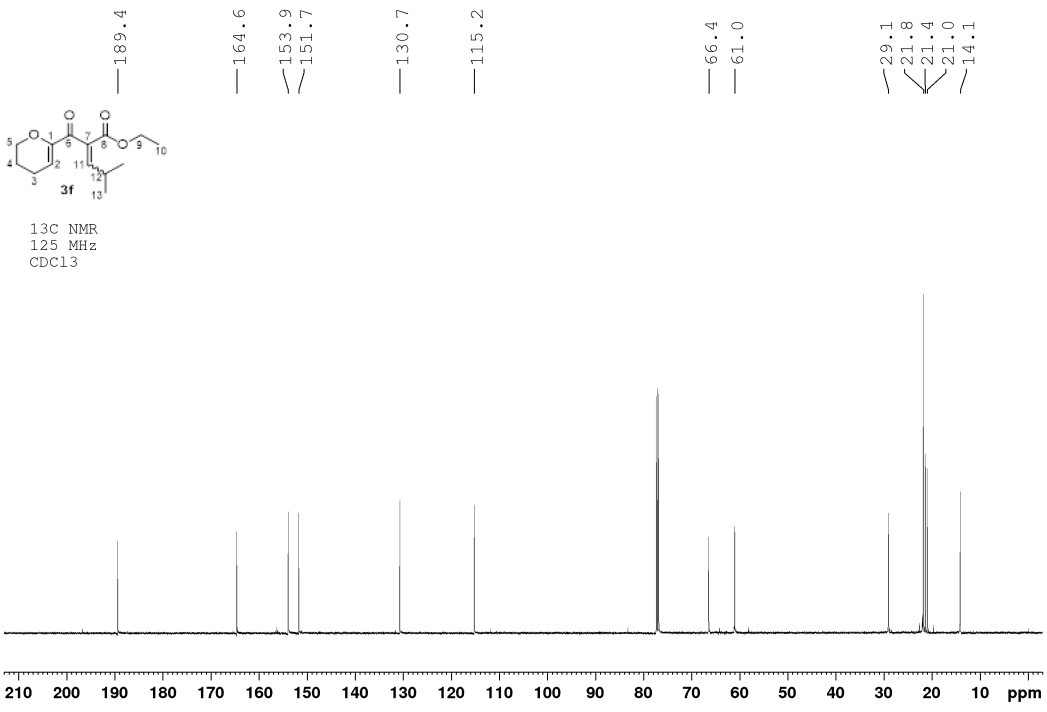

8.24
8.19
7.63
7.56
6.10
6.09
6.08
6.02
6.02
6.01
4.34
4.33
4.31
4.30
4.27
4.26
4.24
4.23
4.09
4.07
2.29
2.25
2.20
2.17
1.93
1.89
1.86
1.82
1.32
1.25
3d
1H NMR
500 MHz
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.03
0.56
1.92
0.52
1.00
2.10
2.03
2.05
2.05
3.14

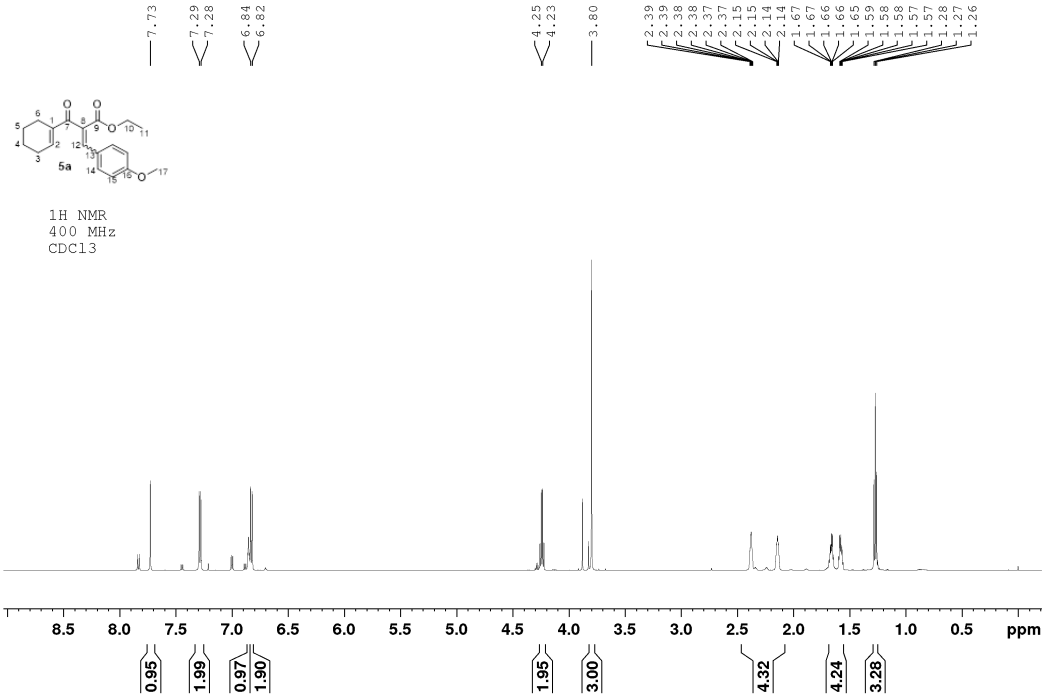

189.4
185.4
165.6
164.1
151.1
150.7
148.2
140.4
140.1
139.7
139.3
135.8
134.8
130.6
130.3
123.9
123.6
116.0
112.6
66.6
66.4
62.0
61.6
21.5
21.3
21.0
20.8
14.1
13.9
3d
13C NMR
125 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

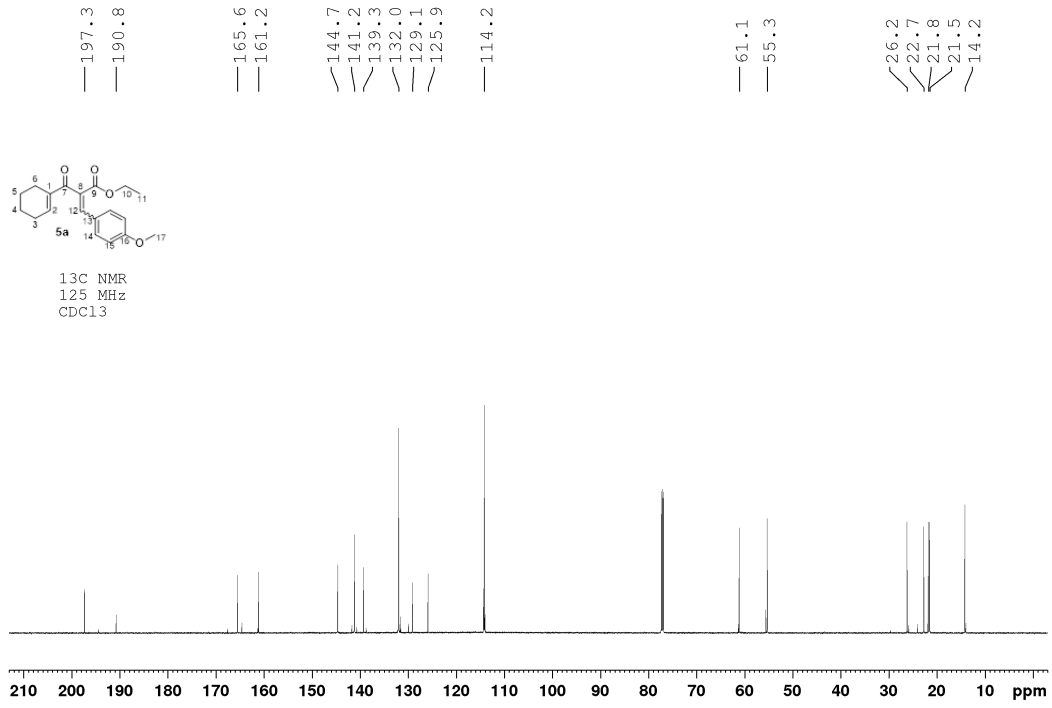

7.93
6.04
5.89
5.88
5.87
4.27
4.25
4.24
4.22
4.07
4.06
4.05
3.81
3.74
2.18
2.17
2.16
2.14
1.86
1.85
1.83
1.82
1.80
1.30
1.29
1.27
3e
1H NMR
400 MHz
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.79
1.83
0.88
1.88
1.99
2.97
5.86
1.93
2.00
2.95

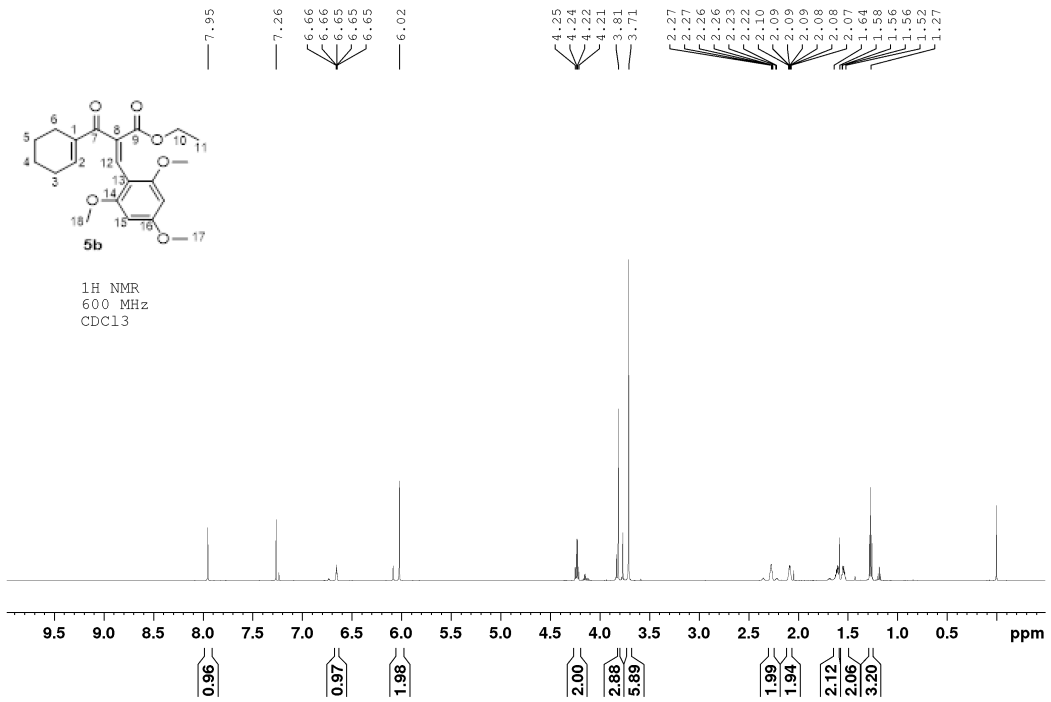

188.9
166.4
163.3
159.4
151.4
135.3
128.6
110.6
105.3
90.3
66.3
60.8
55.4
55.1
21.9
20.8
14.3
3e
13C NMR
100 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

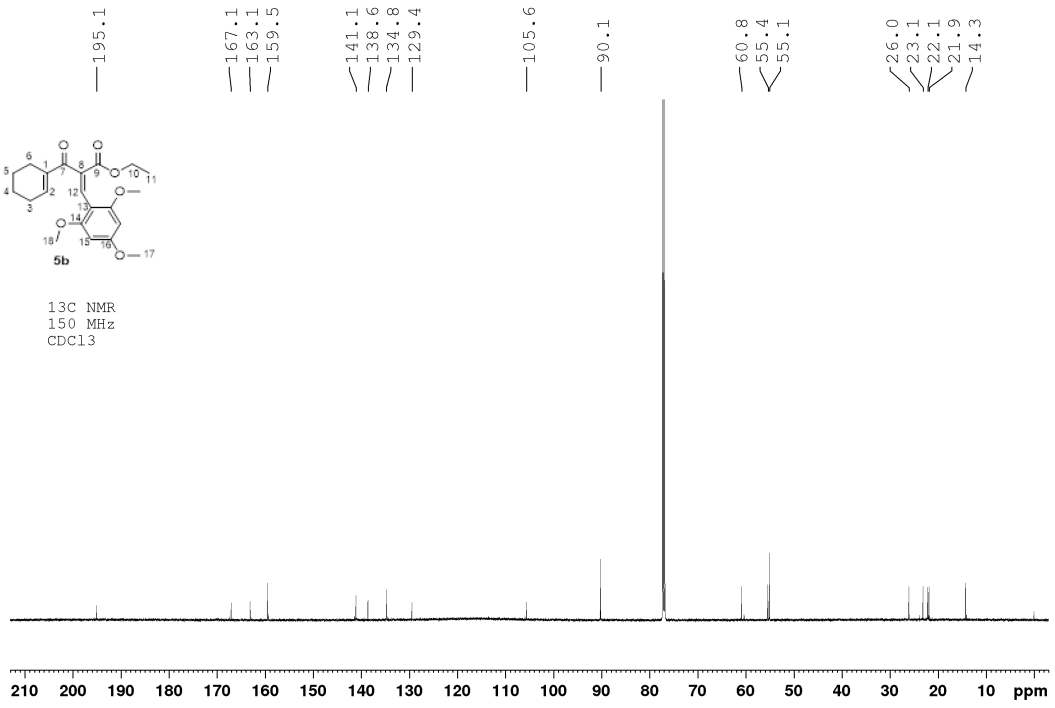

3f
1H NMR
500 MHz
CDCl3
6.80
6.78
5.96
4.23
4.21
4.20
4.18
4.12
2.54
2.46
2.27
2.24
1.91
1.86
1.26
1.04
1.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
0.96
2.33
2.15
1.04
2.23
2.18
3.34
6.25

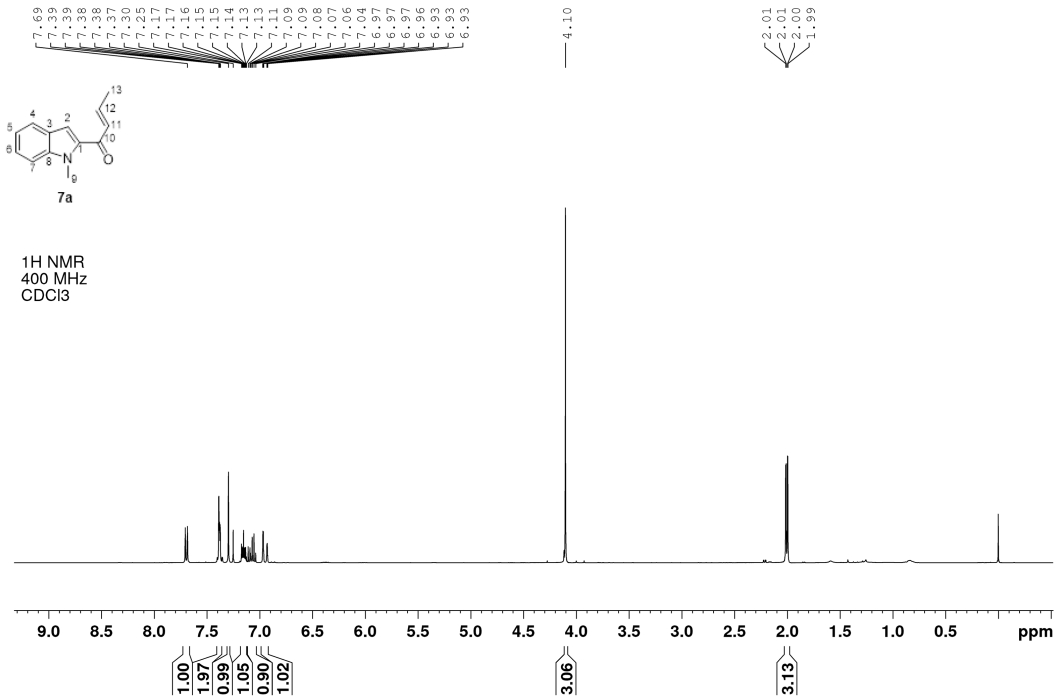

189.4
164.6
153.9
151.7
130.7
115.2
66.4
61.0
29.1
21.8
21.4
21.0
14.1
3f
13C NMR
125 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

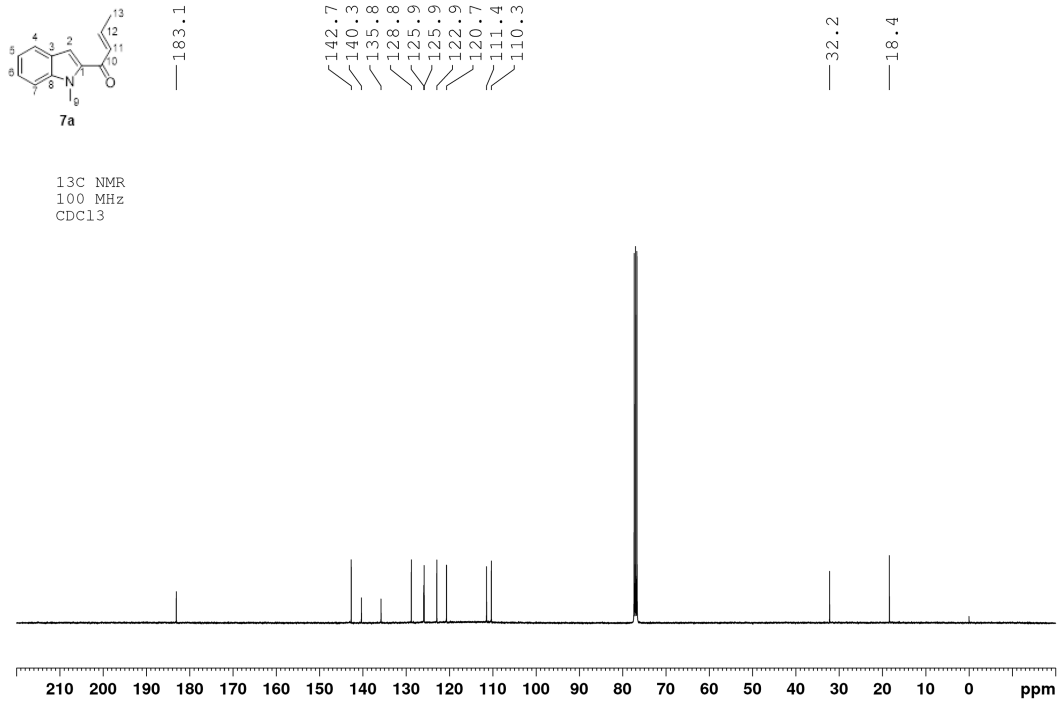

7.73
7.29
7.28
6.84
6.82
4.25
4.23
3.80
2.39
2.39
2.38
2.38
2.37
2.37
2.15
2.15
2.14
2.14
1.67
1.67
1.66
1.66
1.65
1.59
1.58
1.58
1.57
1.57
1.28
1.27
1.26
5a
1H NMR
400 MHz
CDCl3
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.95
1.99
0.97
1.90
1.95
3.00
4.32
4.24
3.28

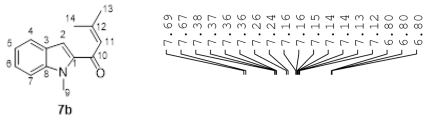

197.3
190.8
165.6
161.2
144.7
141.2
139.3
132.0
129.1
125.9
114.2
61.1
55.3
26.2
22.7
21.8
21.5
14.2
5a
13C NMR
125 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.95
7.26
6.66
6.66
6.65
6.65
6.65
6.02
4.25
4.24
4.22
4.21
3.81
3.71
2.27
2.27
2.26
2.26
2.23
2.22
2.10
2.09
2.09
2.09
2.08
2.08
2.07
1.64
1.58
1.56
1.56
1.52
1.27
5b
1H NMR
600 MHz
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.96
0.97
1.98
2.00
2.88
5.89
1.99
1.94
2.12
2.06
3.20


195.1
167.1
163.1
159.5
141.1
138.6
134.8
129.4
105.6
90.1
60.8
55.4
55.1
26.0
23.1
22.1
21.9
14.3
5b
13C NMR
150 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

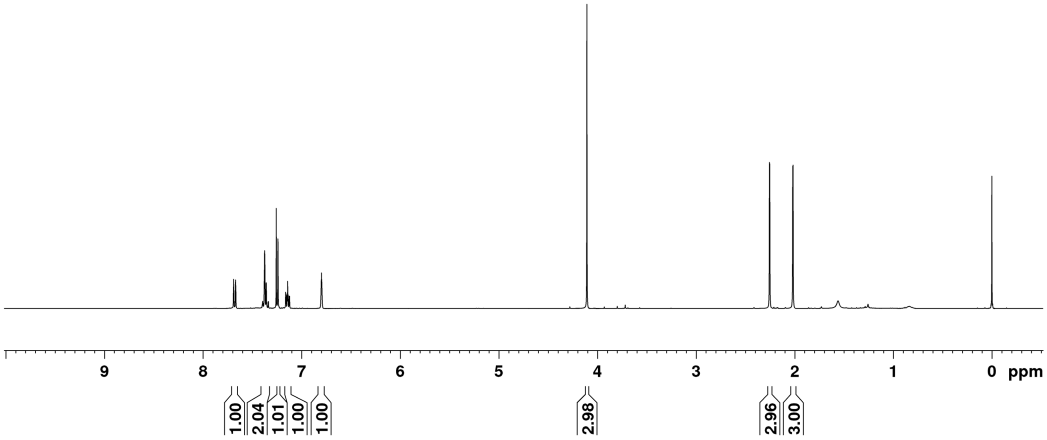

7.69
7.39
7.39
7.38
7.38
7.37
7.30
7.25
7.17
7.17
7.16
7.15
7.15
7.14
7.13
7.13
7.11
7.09
7.09
7.08
7.07
7.06
7.04
6.97
6.97
6.96
6.93
6.93
4.10
2.01
2.01
2.00
1.99
7a
1H NMR
400 MHz
CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.97
0.99
1.05
0.90
1.02
3.06
3.13

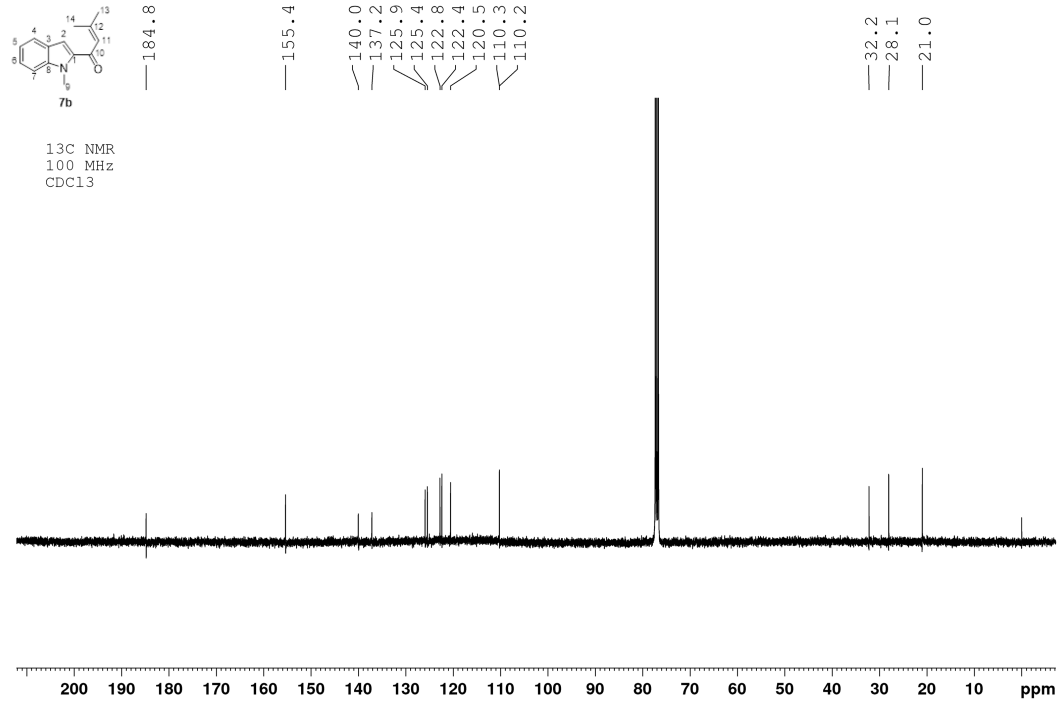

183.1
142.7
140.3
135.8
128.8
125.9
125.9
122.9
120.7
111.4
110.3
32.2
18.4
7a
13C NMR
100 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



7b

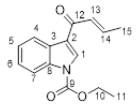
1H NMR
400 MHz
CDCl3





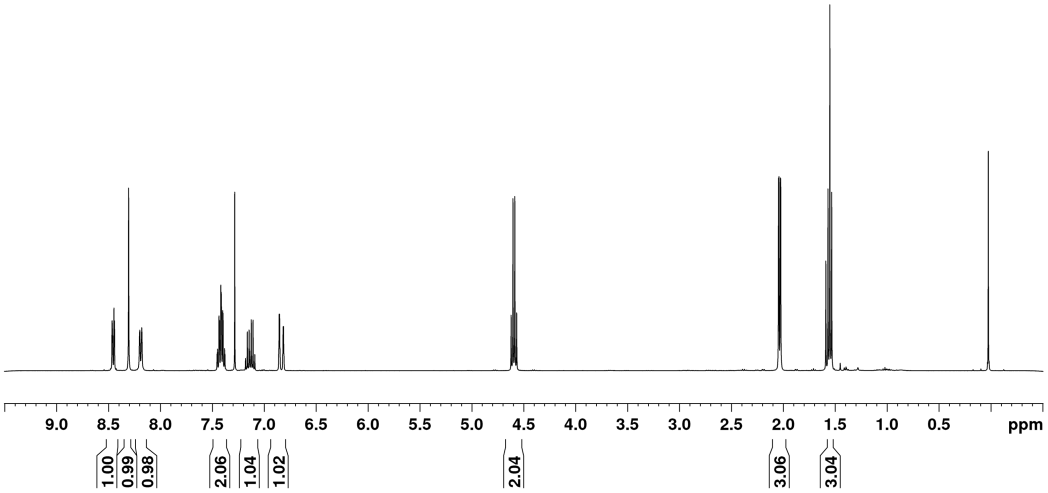
7b

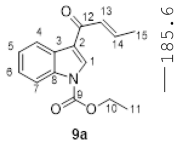
13C NMR
100 MHz
CDCl3



9a

1H NMR
400 MHz
CDCl3

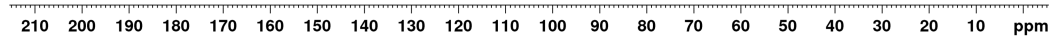


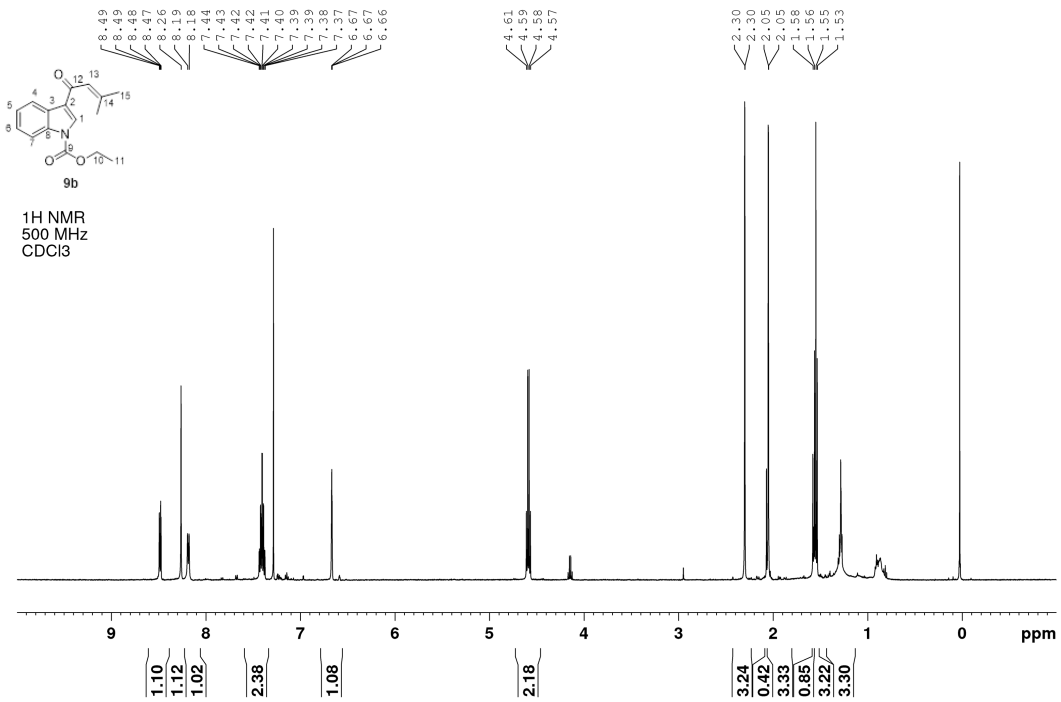


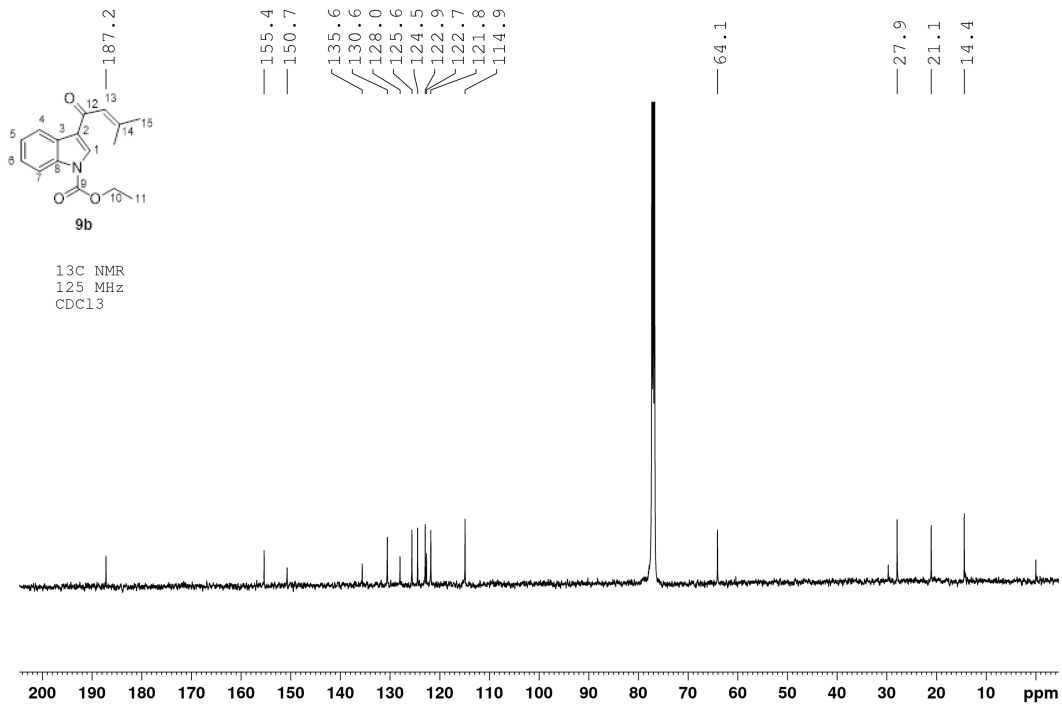
9a

13C NMR
125 MHz
CDCl3

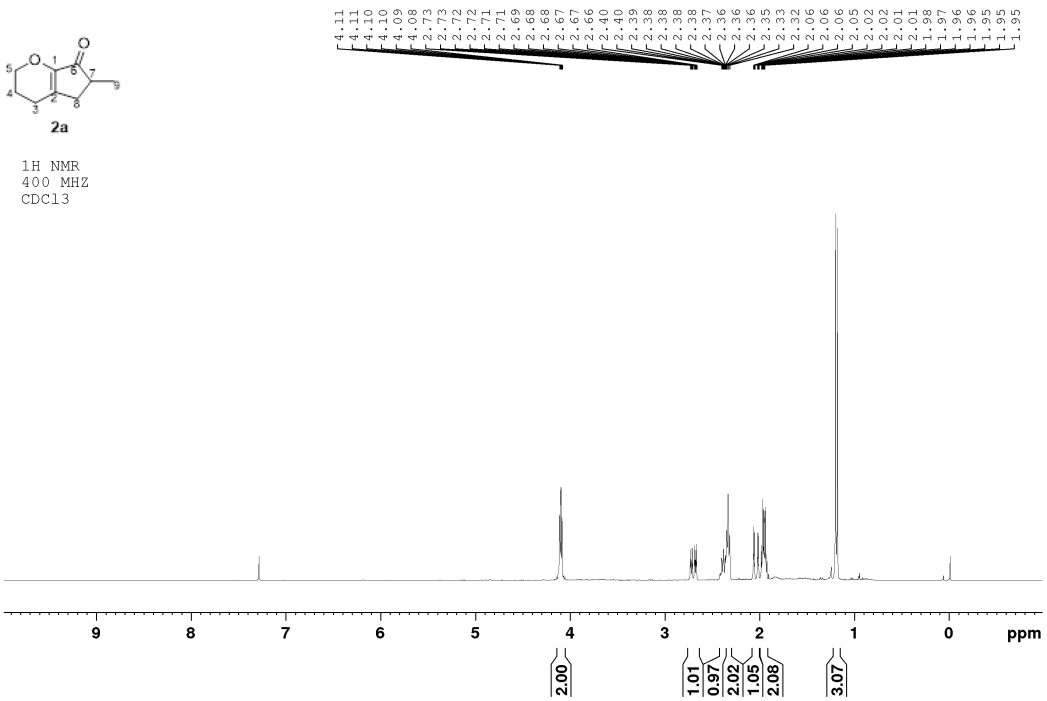
185.6
150.6
142.7
135.7
131.3
128.3
127.9
125.8
124.6
123.0
121.3
114.9
64.2
18.4
14.4

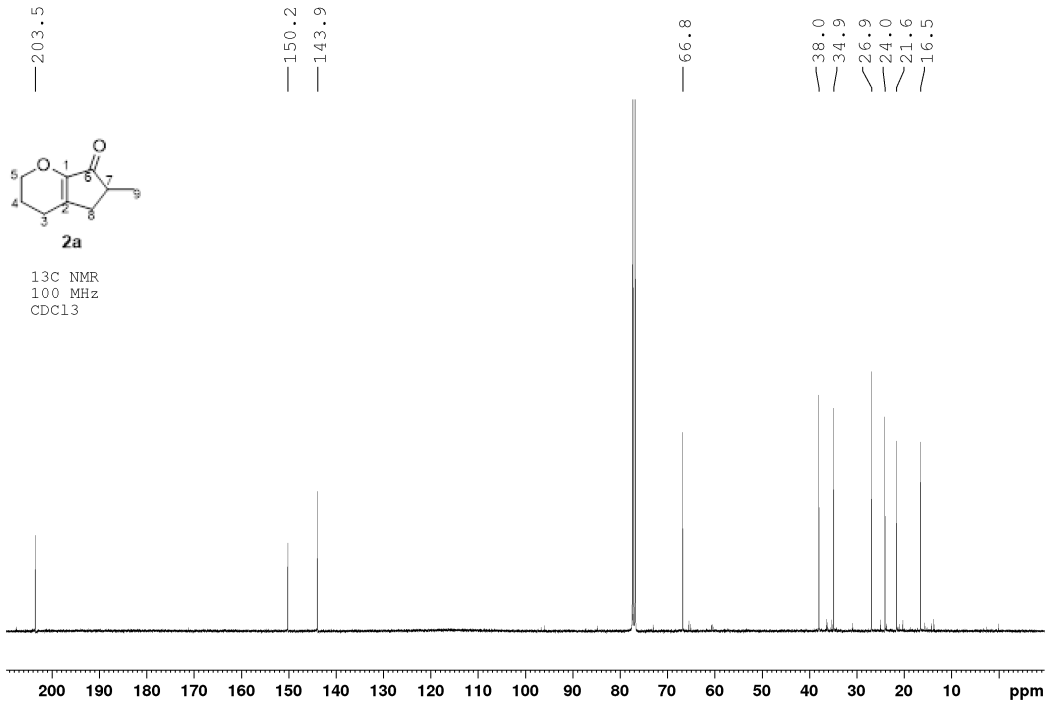


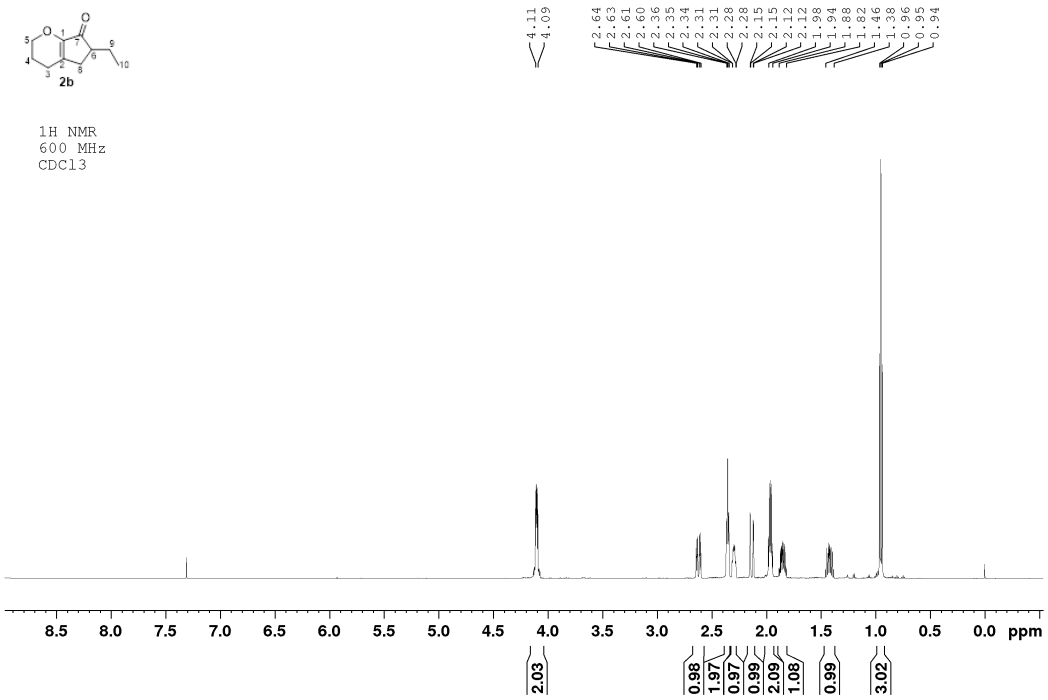

8.49
8.49
8.48
8.47
8.26
8.19
8.18
7.44
7.43
7.42
7.42
7.41
7.40
7.39
7.39
7.38
7.37
6.67
6.67
6.66
4.61
4.59
4.58
4.57
2.30
2.30
2.05
2.05
1.58
1.56
1.55
1.53
9b
1H NMR
500 MHz
CDCl3
9
8
7
6
5
4
3
2
1
0
ppm
1.10
1.12
1.02
2.38
1.08
2.18
3.24
0.42
3.33
0.85
3.22
3.30

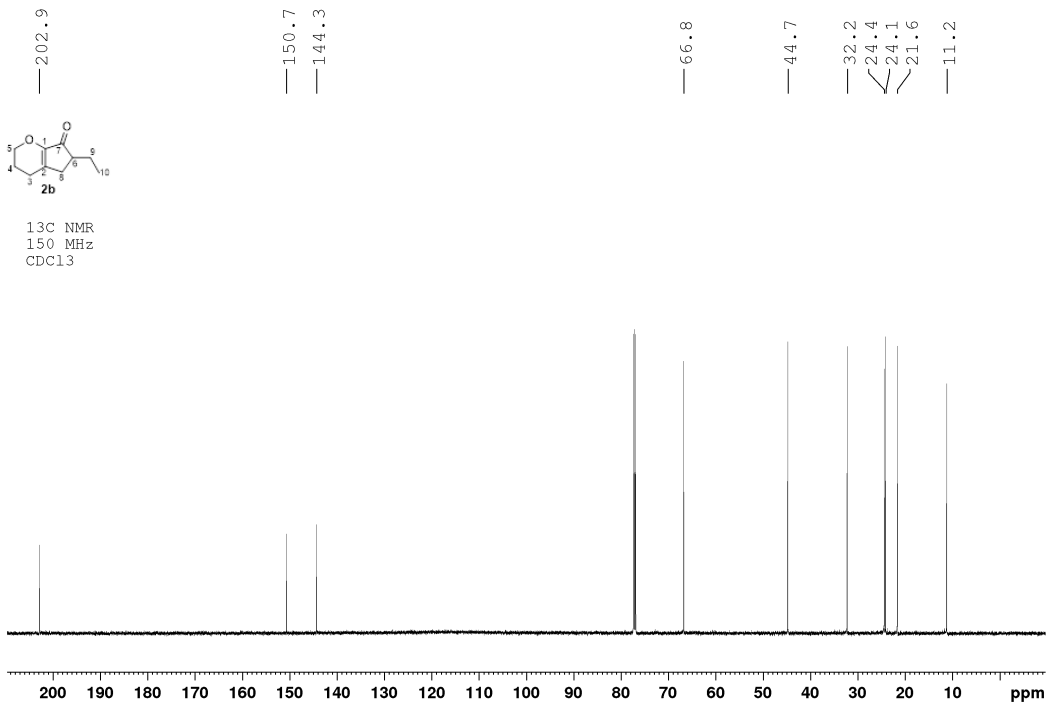

187.2
155.4
150.7
135.6
130.6
128.0
125.6
124.5
122.9
122.7
121.8
114.9
64.1
27.9
21.1
14.4
9b
13C NMR
125 MHz
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

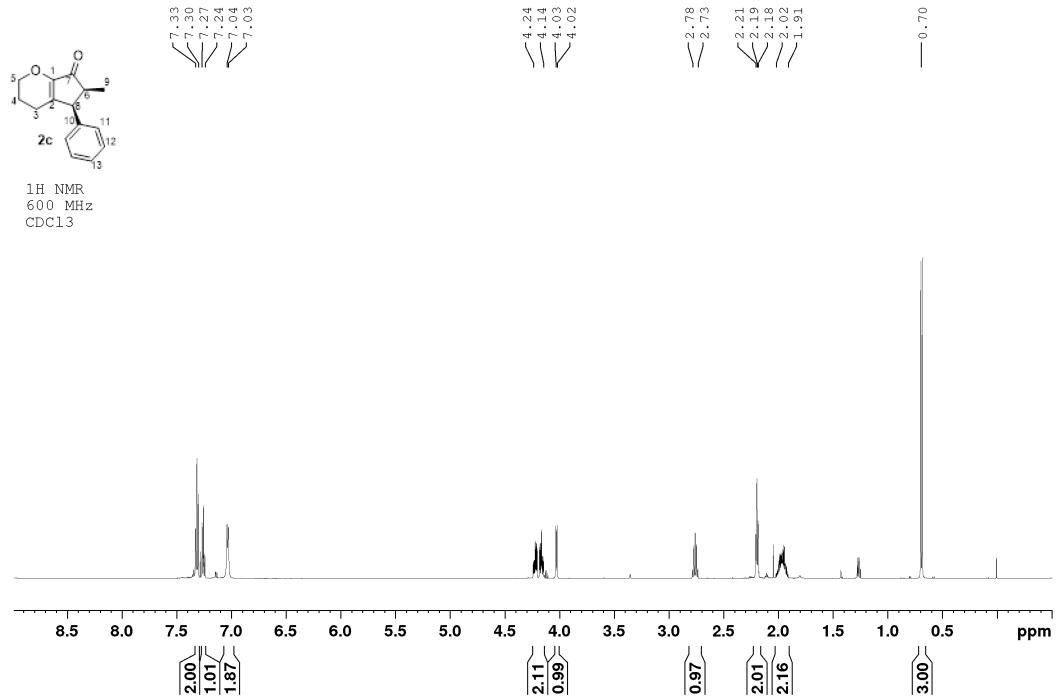
7.2 Nazarov Products

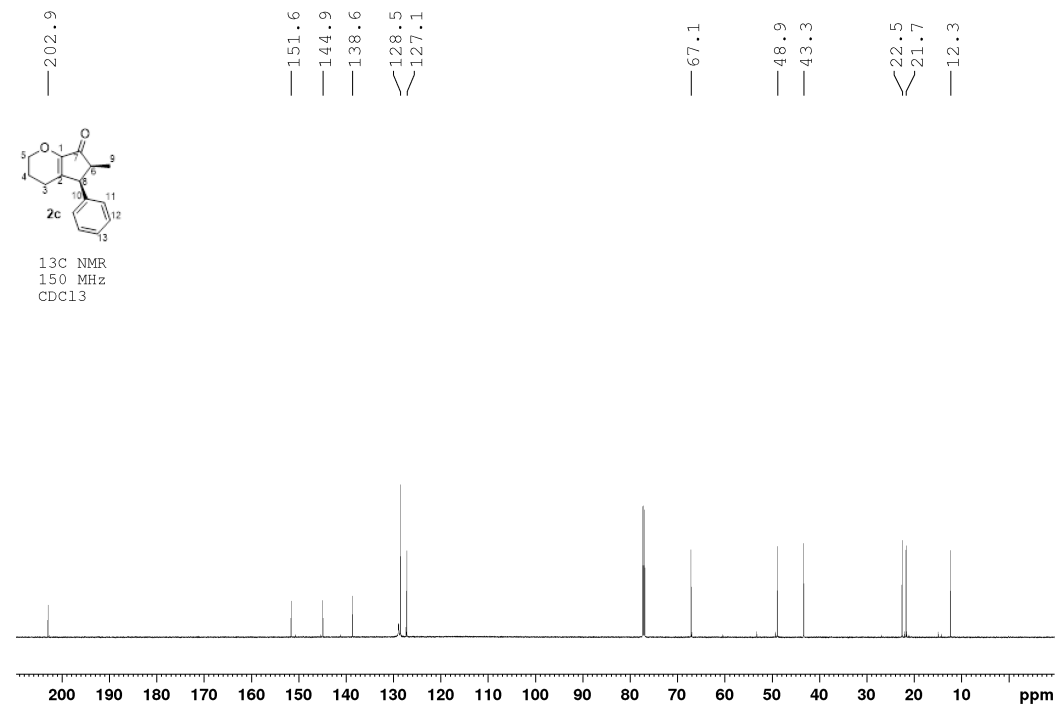


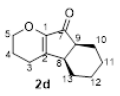



2b
1H NMR
600 MHz
CDCl3
4.11
4.09
2.64
2.63
2.61
2.60
2.36
2.35
2.34
2.31
2.31
2.28
2.28
2.15
2.15
2.12
2.12
1.98
1.94
1.88
1.82
1.46
1.38
0.96
0.95
0.94
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.03
0.98
1.97
0.97
0.99
2.09
1.08
0.99
3.02


202.9
150.7
144.3
66.8
44.7
32.2
24.4
24.1
21.6
11.2
2b
13C NMR
150 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

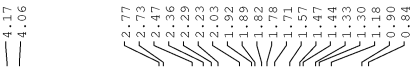

7.33
7.30
7.27
7.24
7.04
7.03
4.24
4.14
4.03
4.02
2.78
2.73
2.21
2.19
2.18
2.02
1.91
0.70
2c
1H NMR
600 MHz
CDC13
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
1.01
1.87
2.11
0.99
0.97
2.01
2.16
3.00

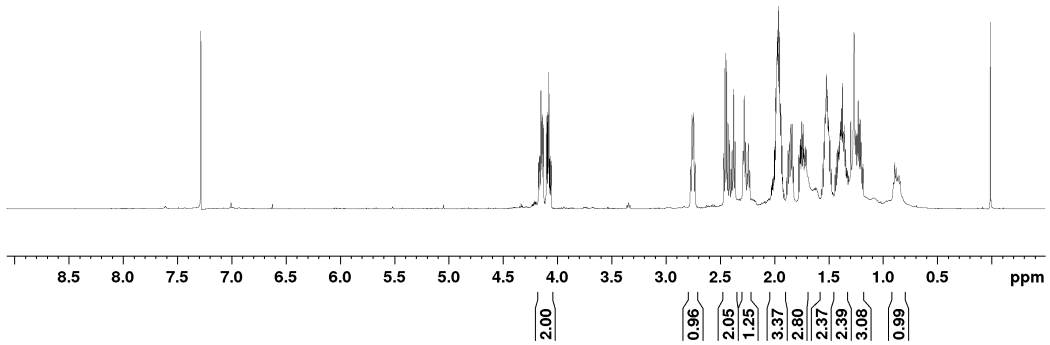

202.9
151.6
144.9
138.6
128.5
127.1
67.1
48.9
43.3
22.5
21.7
12.3
2c
13C NMR
150 MHz
CDC13
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



2d

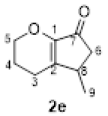
1H NM
500 M
CDCl3





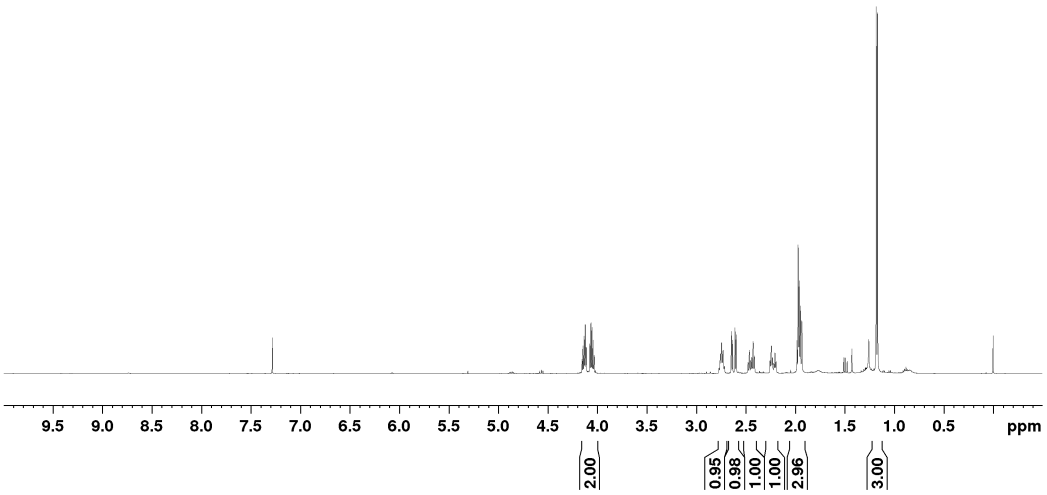
2d

13C NMR
125 MHz
CDCl3



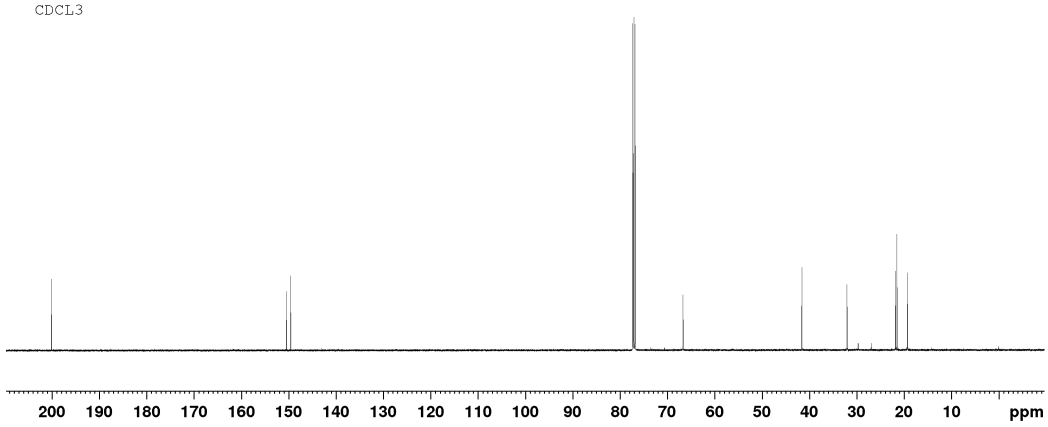
2e

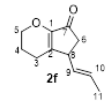
1H NMR
500 MHz
CDCl3



2e

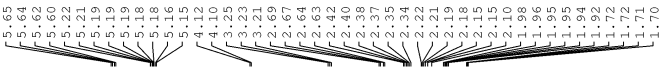
13C NMR
125 MHz
CDCL3

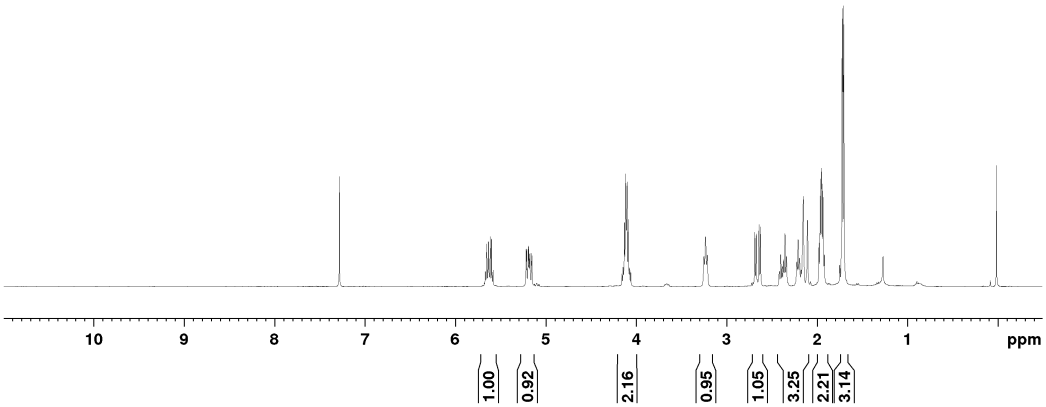


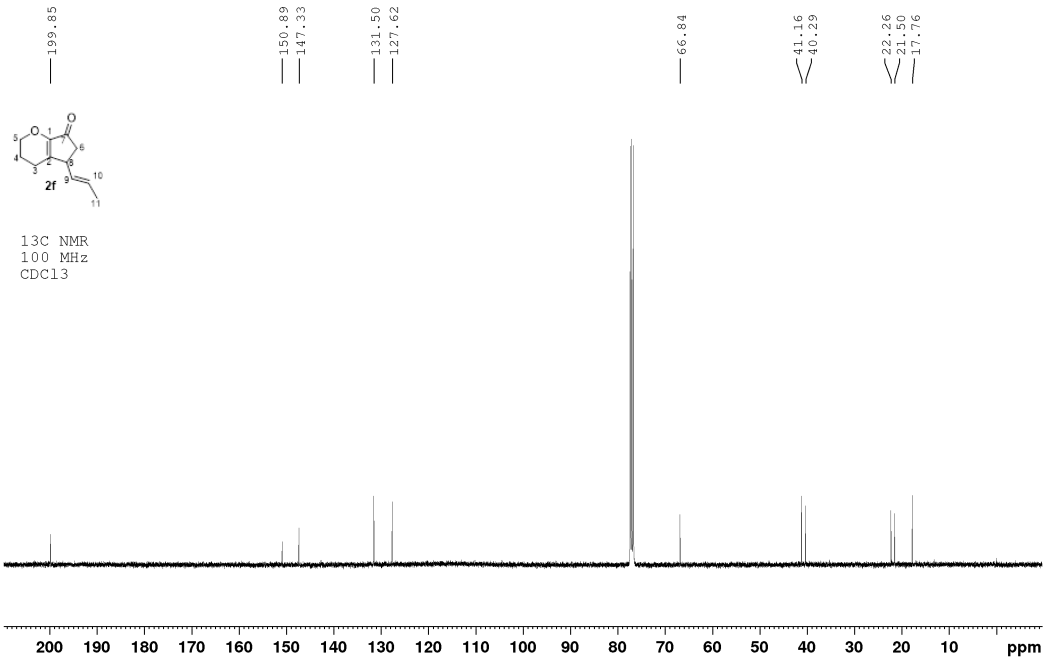


2f

1H NMR
400 MHz
CDCl3

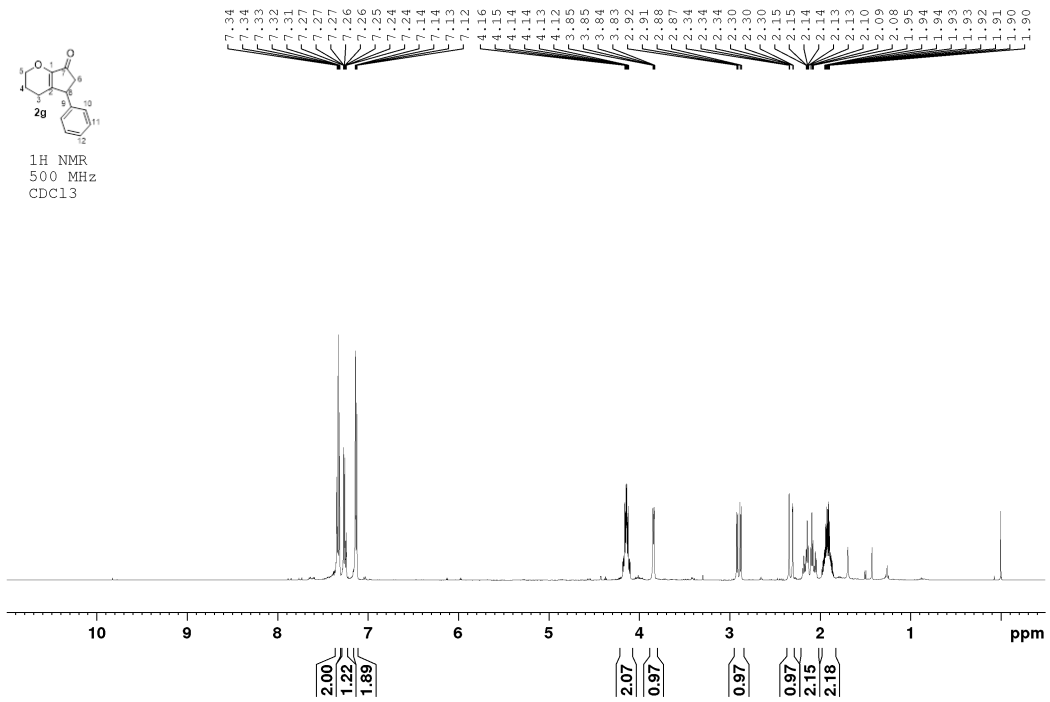






2f

13C NMR
100 MHz
CDCl3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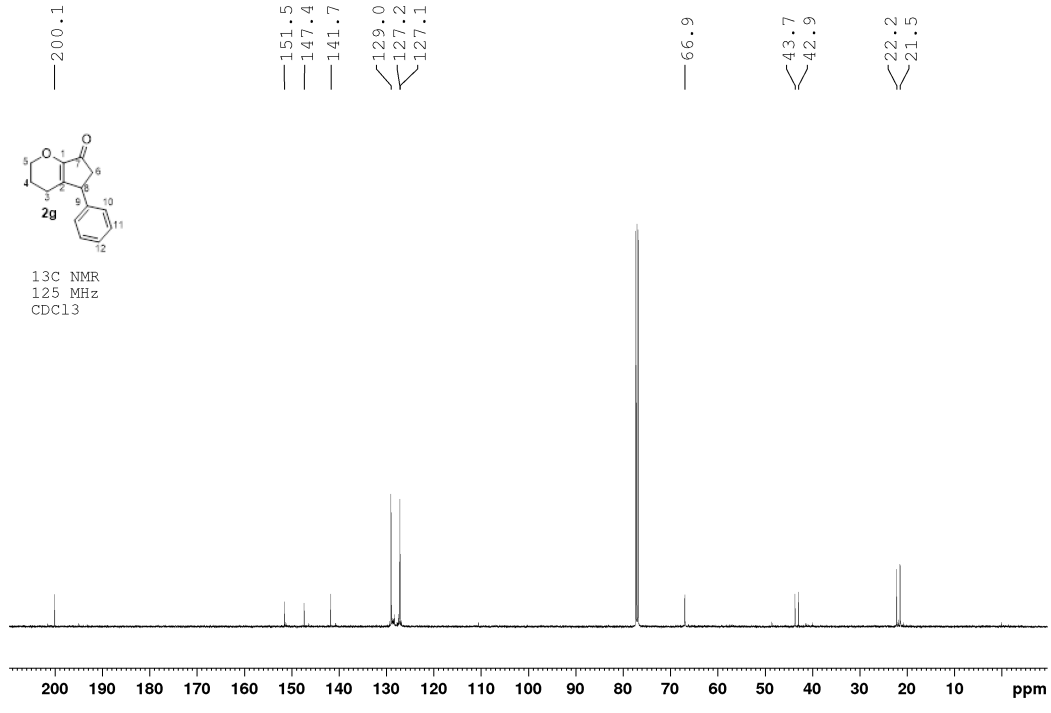
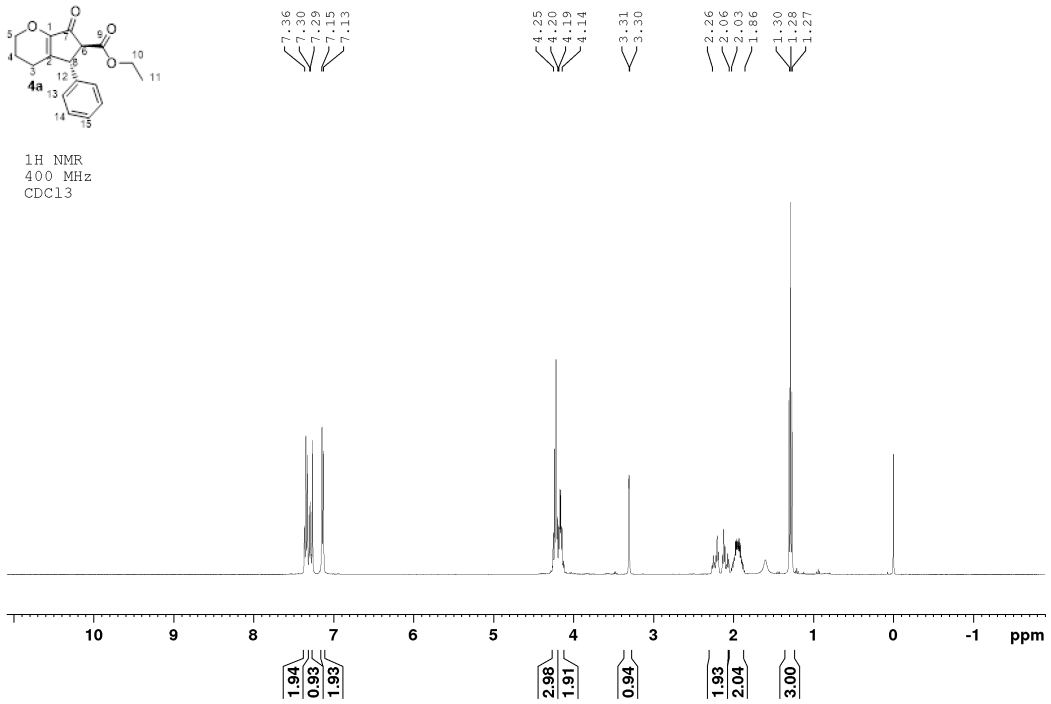
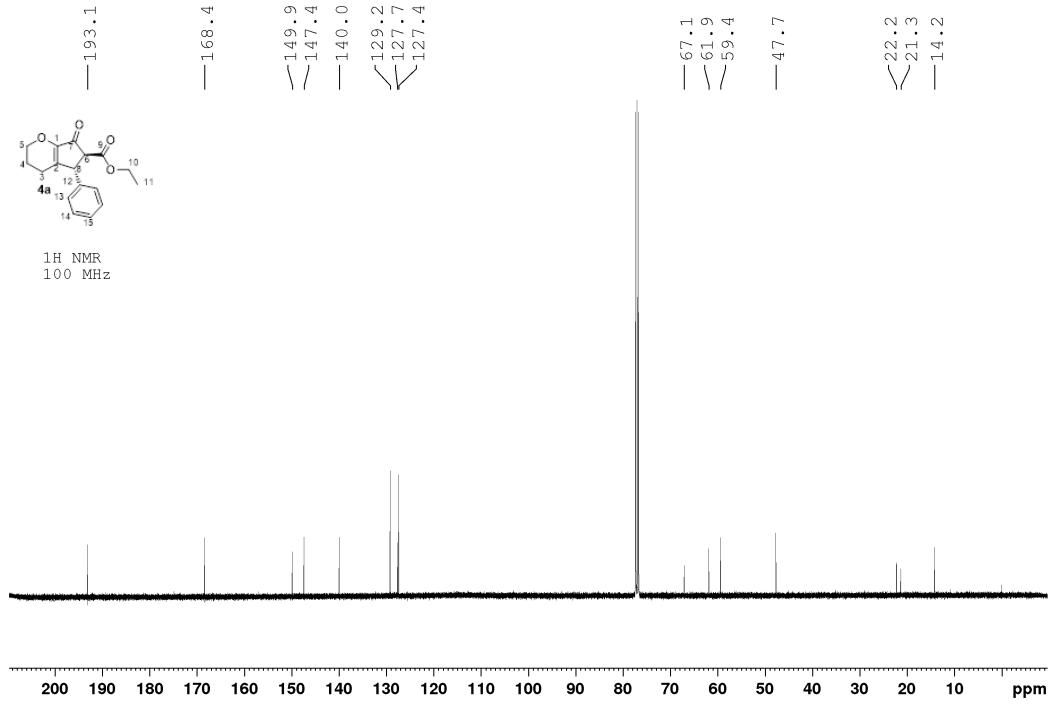
7.33
7.32
7.31
7.27
7.27
7.27
7.26
7.26
7.25
7.24
7.24
7.14
7.14
7.13
7.12
4.16
4.15
4.14
4.14
4.13
4.12
3.85
3.85
3.84
3.83
2.92
2.91
2.88
2.87
2.34
2.34
2.34
2.30
2.30
2.15
2.15
2.14
2.13
2.13
2.10
2.09
2.08
1.95
1.94
1.93
1.93
1.92
1.91
1.90
1.90
2g
1H NMR
500 MHz
CDCl3
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.22
1.89
2.07
0.97
0.97
0.97
2.15
2.18


200.1
151.5
147.4
141.7
129.0
127.2
127.1
66.9
43.7
42.9
22.2
21.5
2g
13C NMR
125 MHz
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.36
7.30
7.29
7.15
7.13
4.25
4.20
4.19
4.14
3.31
3.30
2.26
2.06
2.03
1.86
1.30
1.28
1.27
1H NMR
400 MHz
CDCl3
10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.94
0.93
1.93
2.98
1.91
0.94
1.93
2.04
3.00


193.1
168.4
149.9
147.4
140.0
129.2
127.7
127.4
67.1
61.9
59.4
47.7
22.2
21.3
14.2
1H NMR
100 MHz
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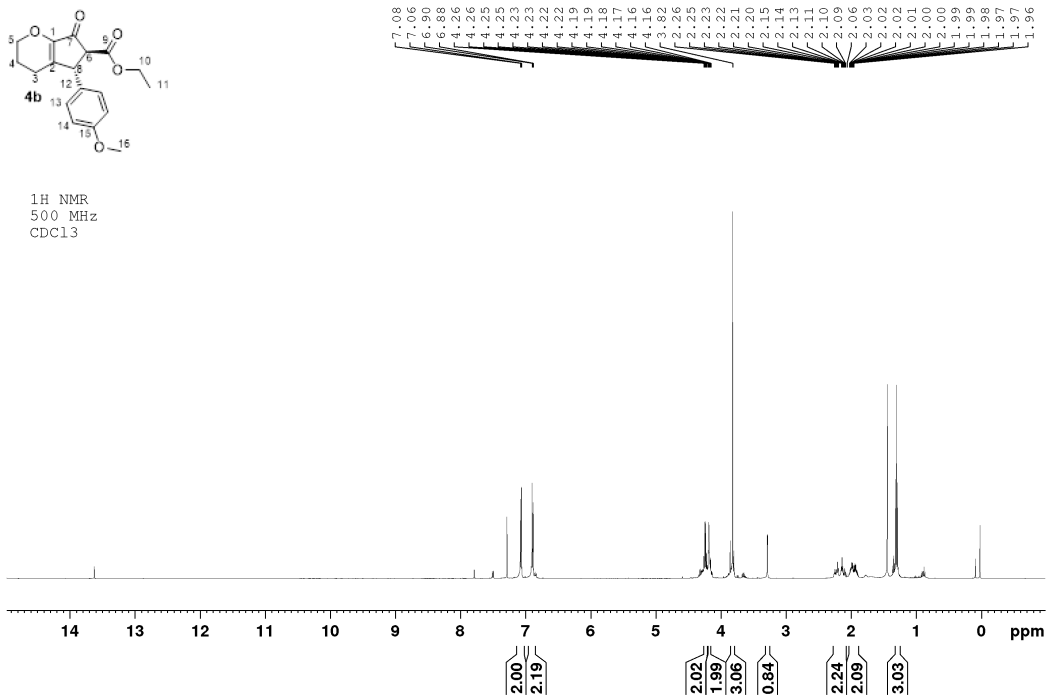
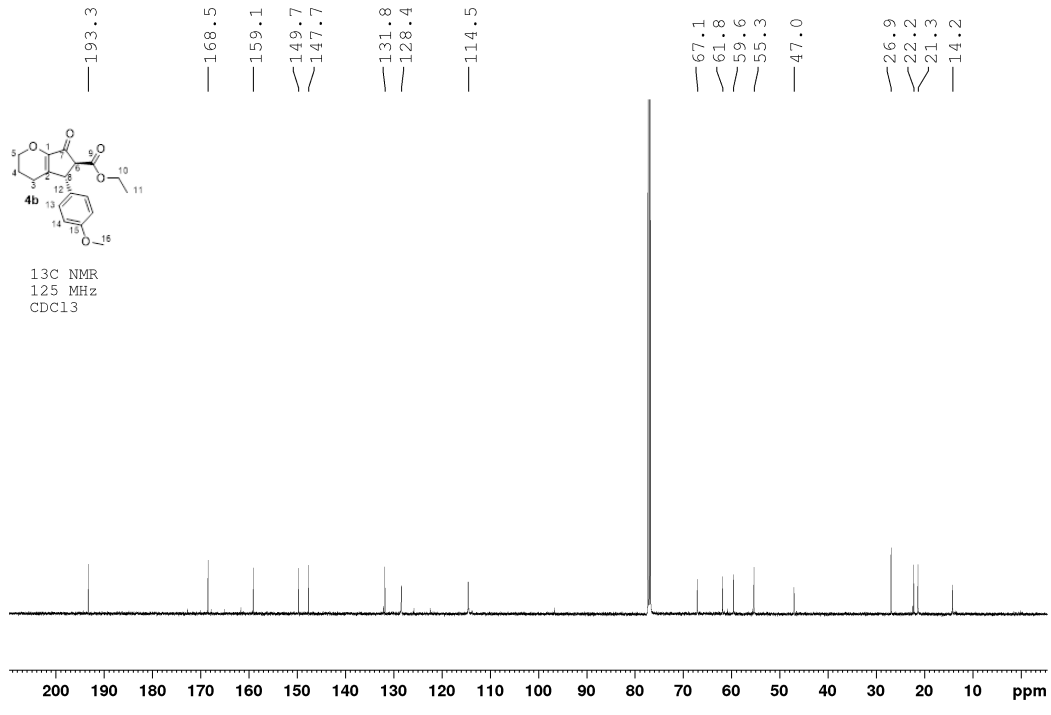

4b
1H NMR
500 MHz
CDCl3
7.08
7.06
6.90
6.88
4.26
4.26
4.25
4.25
4.23
4.23
4.22
4.22
4.19
4.19
4.18
4.17
4.16
4.16
3.82
2.26
2.25
2.23
2.22
2.21
2.20
2.15
2.14
2.13
2.11
2.10
2.09
2.06
2.03
2.02
2.02
2.01
2.00
2.00
1.99
1.99
1.98
1.97
1.97
1.96
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.19
2.02
1.99
3.06
0.84
2.24
2.09
3.03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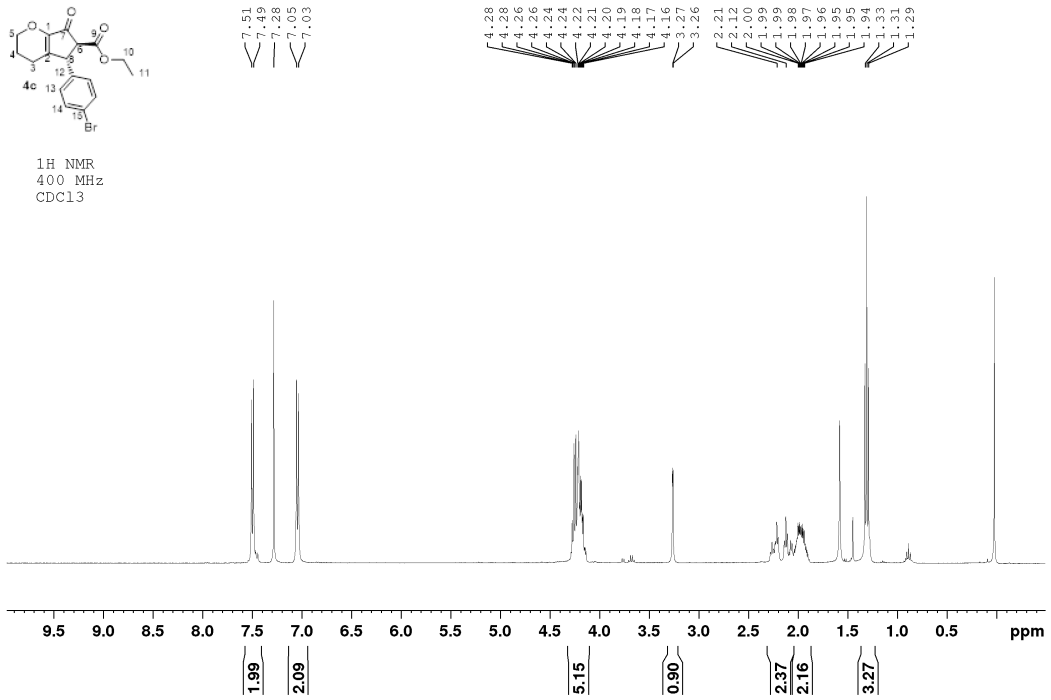
168.5
159.1
149.7
147.7
131.8
128.4
114.5
67.1
61.8
59.6
55.3
47.0
26.9
22.2
21.3
14.2
4b
13C NMR
125 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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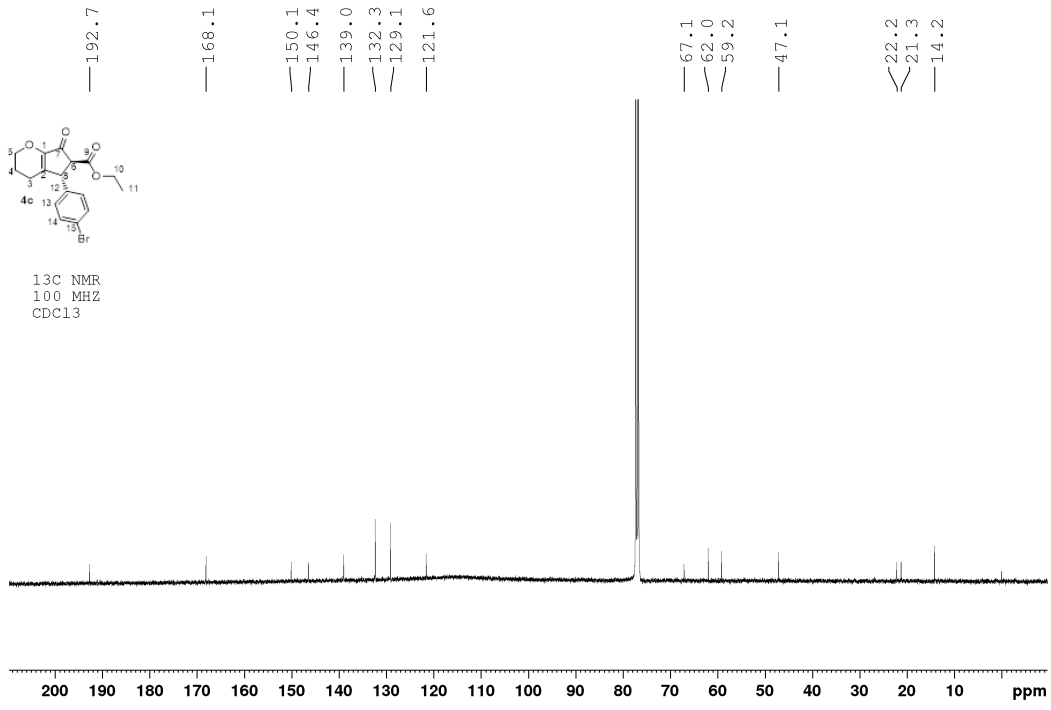
7.49
7.28
7.05
7.03
4.28
4.28
4.26
4.26
4.24
4.24
4.22
4.21
4.20
4.19
4.18
4.17
4.16
3.27
3.26
2.21
2.12
2.00
1.99
1.99
1.98
1.97
1.96
1.95
1.95
1.94
1.33
1.31
1.29
4c
1H NMR
400 MHz
CDCl3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.99
2.09
5.15
0.90
2.37
2.16
3.27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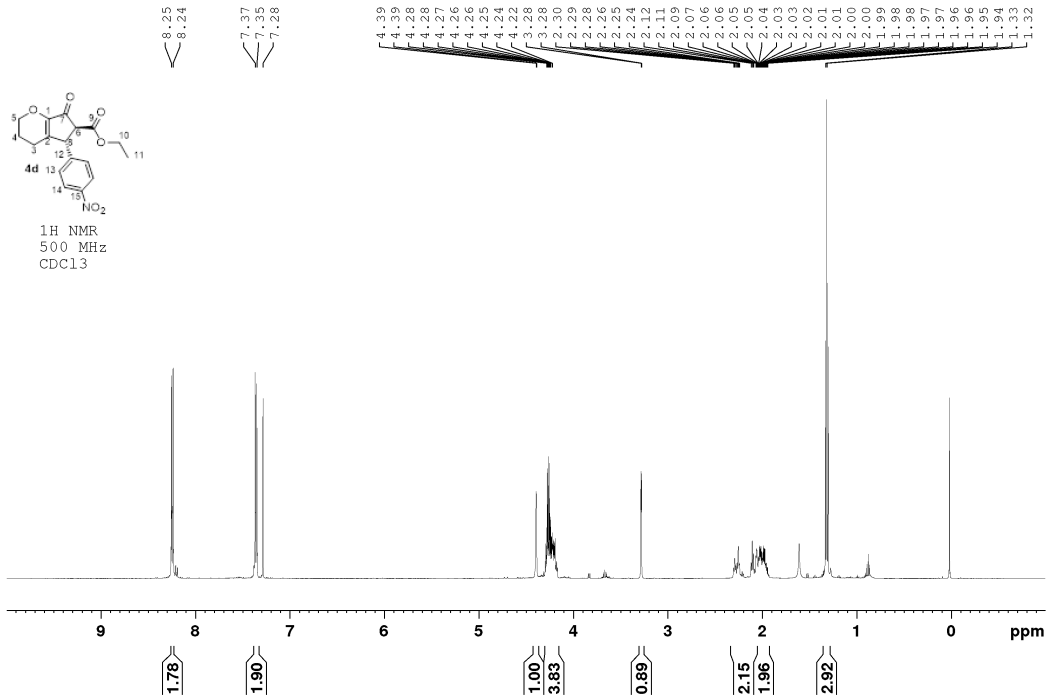
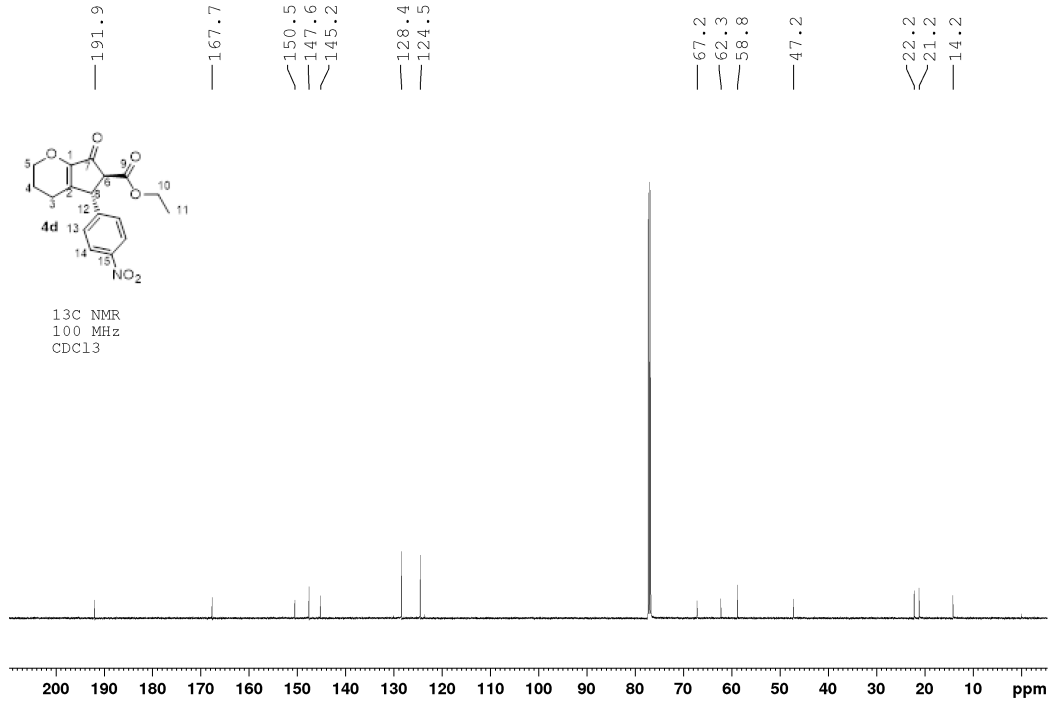
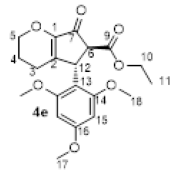
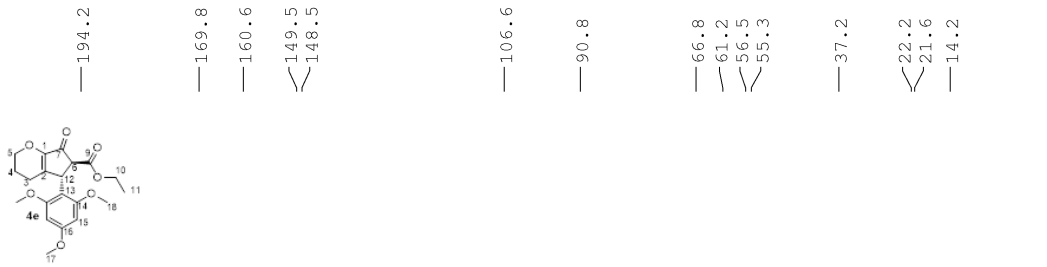
168.1
150.1
146.4
139.0
132.3
129.1
121.6
67.1
62.0
59.2
47.1
22.2
21.3
14.2
4c
13C NMR
100 MHZ
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.25
8.24
7.37
7.35
7.28
4.39
4.39
4.28
4.28
4.27
4.26
4.26
4.25
4.24
4.22
3.28
3.28
2.30
2.29
2.28
2.26
2.25
2.24
2.12
2.11
2.09
2.07
2.06
2.06
2.05
2.05
2.04
2.03
2.02
2.01
2.01
2.00
2.00
1.99
1.98
1.98
1.97
1.97
1.96
1.96
1.95
1.94
1.33
1.32
4d
1H NMR
500 MHz
CDCl3
9
8
7
6
5
4
3
2
1
0
ppm
1.78
1.90
1.00
3.83
0.89
2.15
1.96
2.92

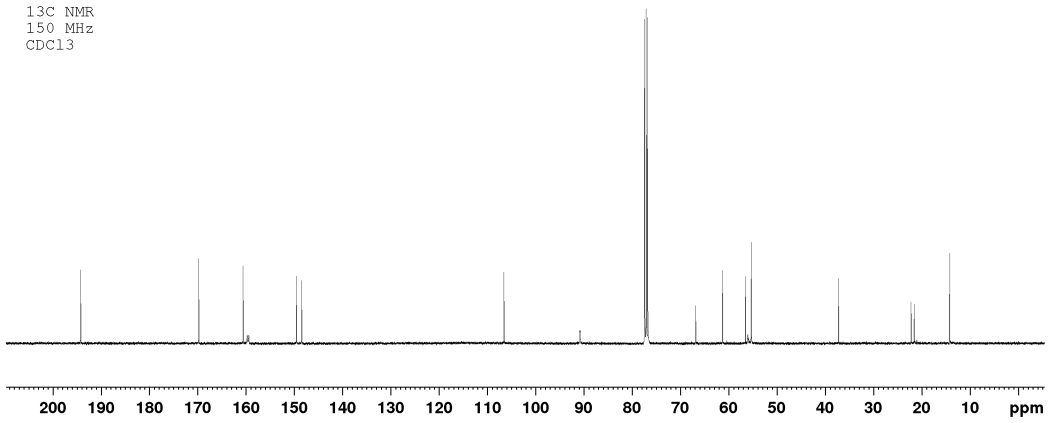

191.9
167.7
150.5
147.6
145.2
128.4
124.5
67.2
62.3
58.8
47.2
22.2
21.2
14.2
4d
13C NMR
100 MHz
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

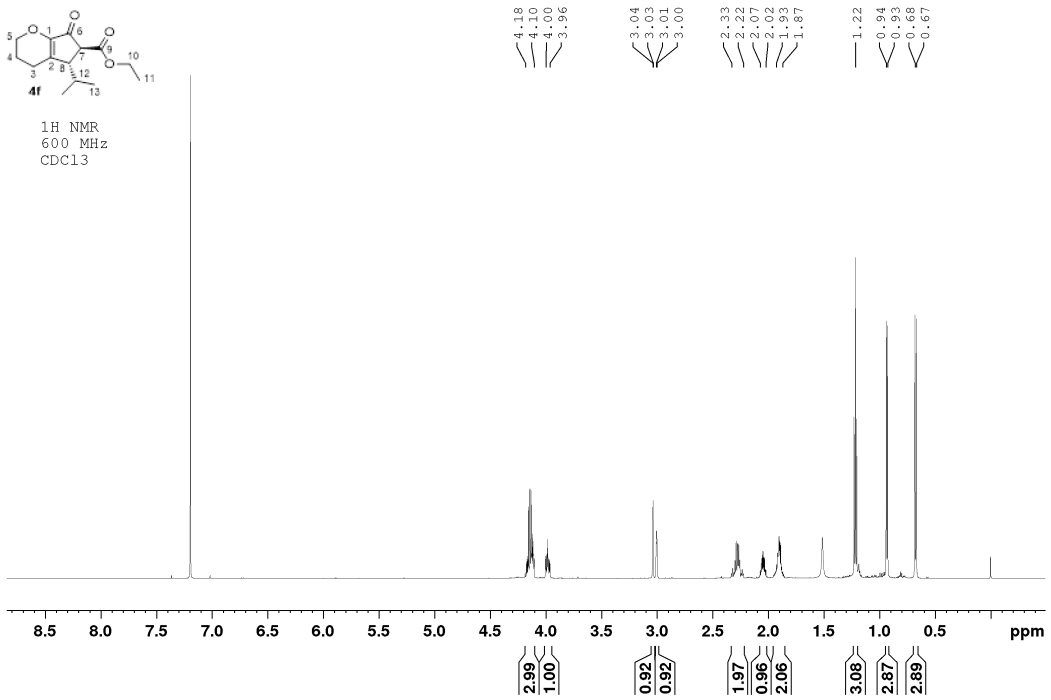


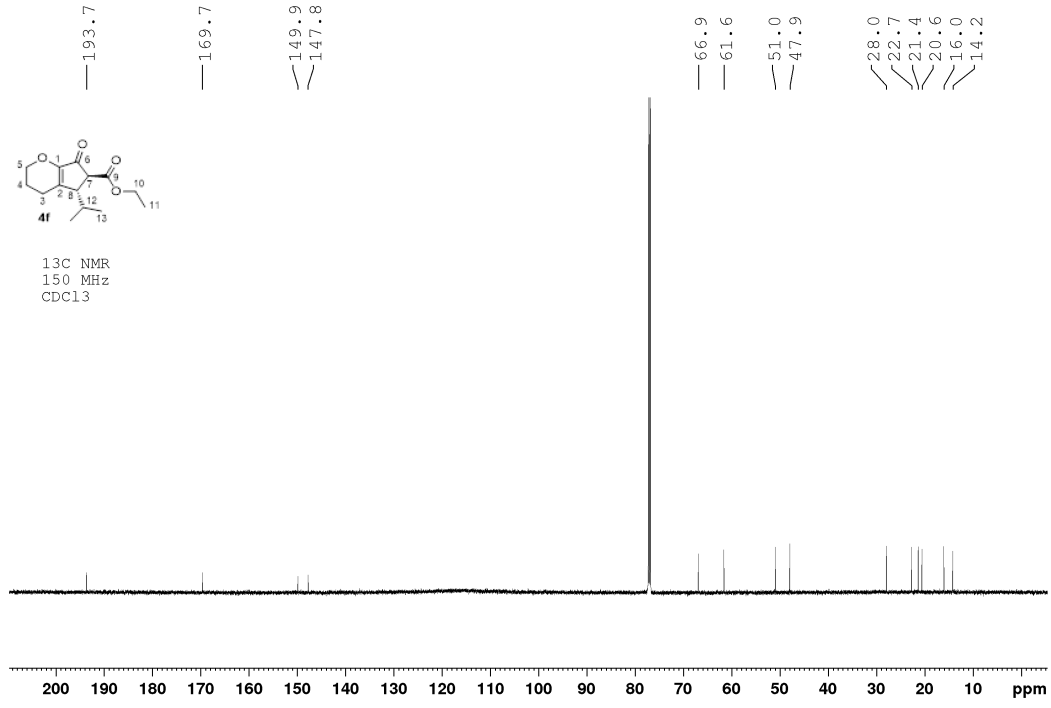
1H NMR
600 MHz
CDCl3

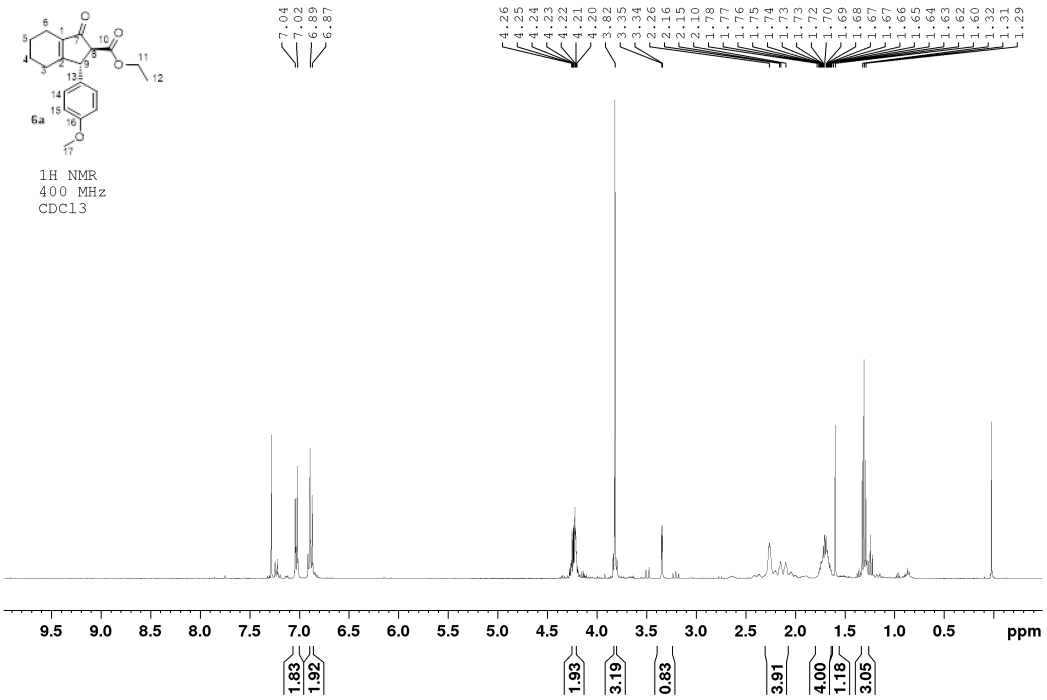


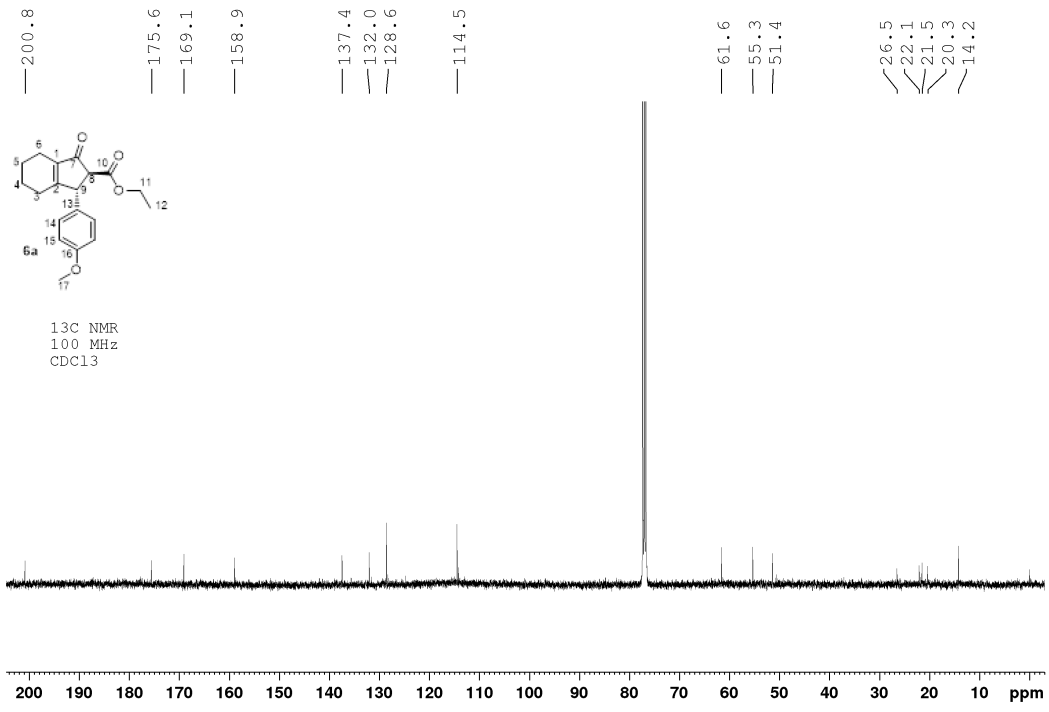
13C NMR
150 MHz
CDCl3

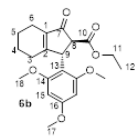



4f
1H NMR
600 MHz
CDCl3
4.18
4.10
4.00
3.96
3.04
3.03
3.01
3.00
2.33
2.22
2.07
2.02
1.93
1.87
1.22
0.94
0.93
0.68
0.67
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.99
1.00
0.92
0.92
1.97
0.96
2.06
3.08
2.87
2.89

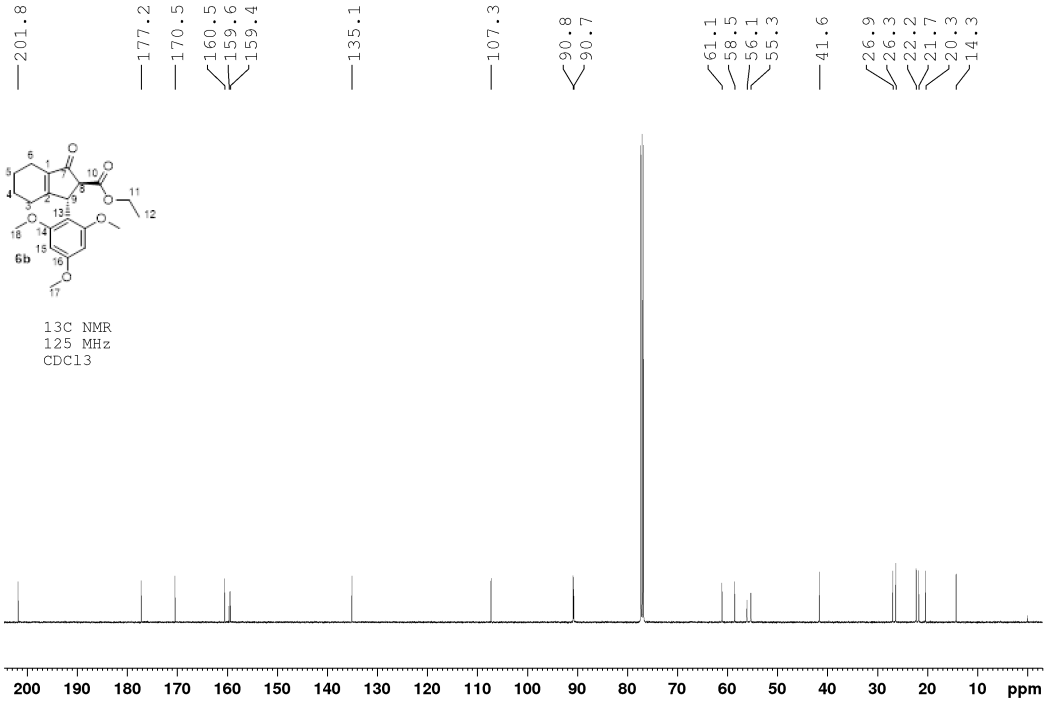

193.7
169.7
149.9
147.8
66.9
61.6
51.0
47.9
28.0
22.7
21.4
20.6
16.0
14.2
4f
13C NMR
150 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


1H NMR
400 MHz
CDCl3
7.04
7.02
6.89
6.87
4.26
4.25
4.24
4.23
4.22
4.21
4.20
3.82
3.35
3.34
2.26
2.16
2.15
2.10
1.78
1.77
1.76
1.75
1.74
1.73
1.72
1.70
1.69
1.68
1.67
1.66
1.65
1.64
1.63
1.62
1.60
1.32
1.31
1.29
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.83
1.92
1.93
3.19
0.83
3.91
4.00
1.18
3.05

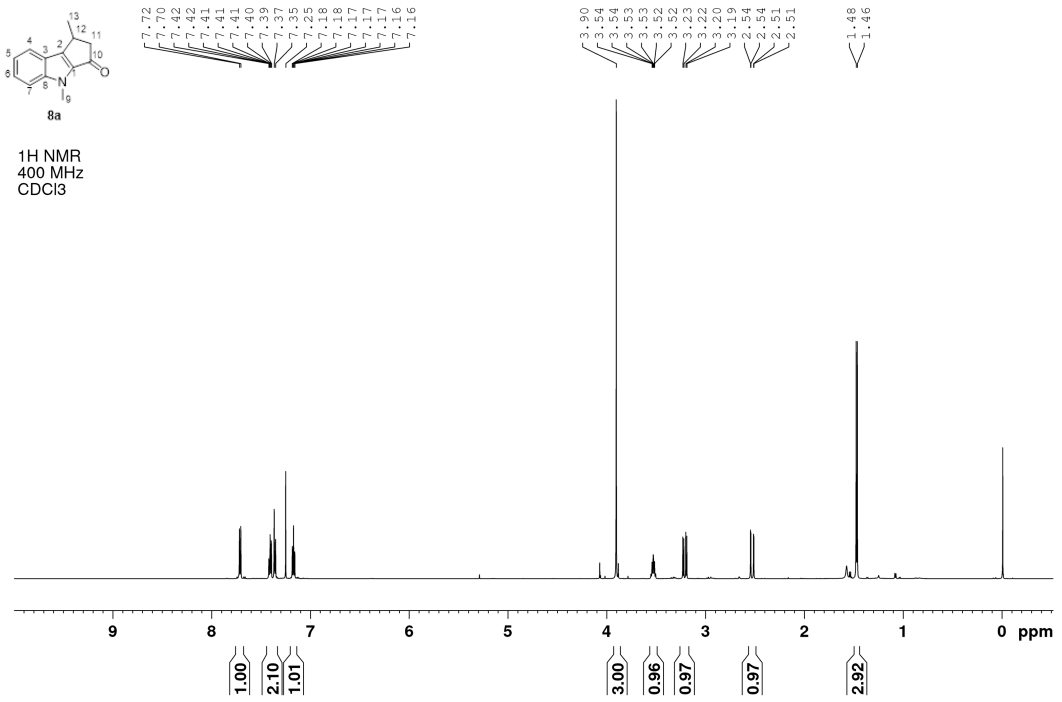

200.8
175.6
169.1
158.9
137.4
132.0
128.6
114.5
61.6
55.3
51.4
26.5
22.1
21.5
20.3
14.2
13C NMR
100 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

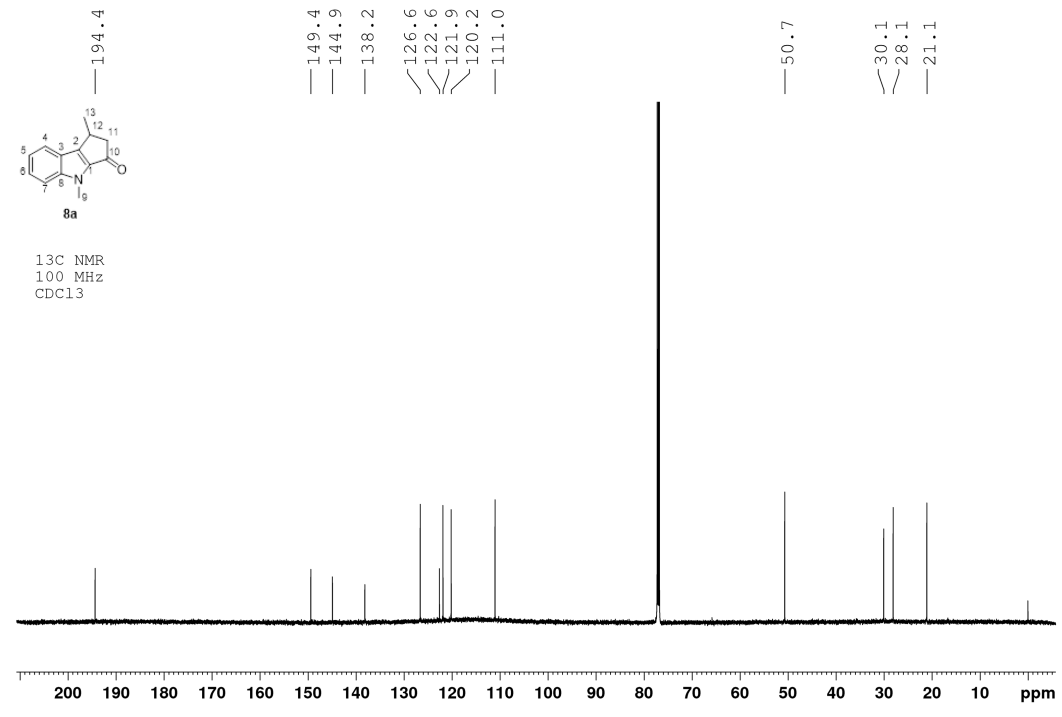


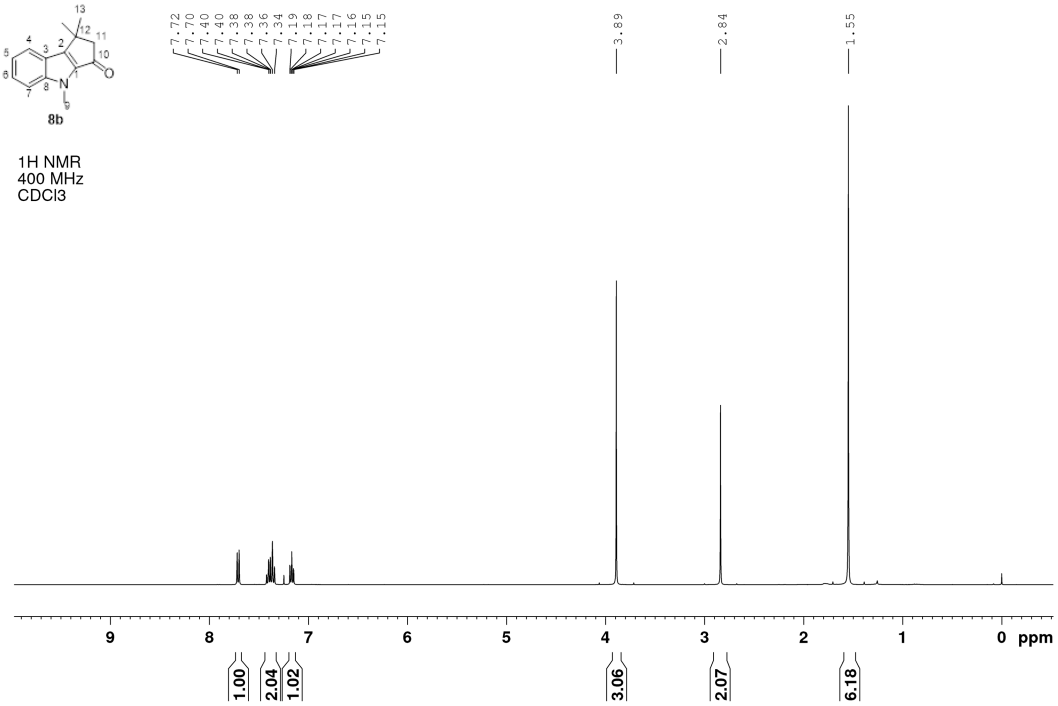
1H NMR
500 MHz
CDCl3

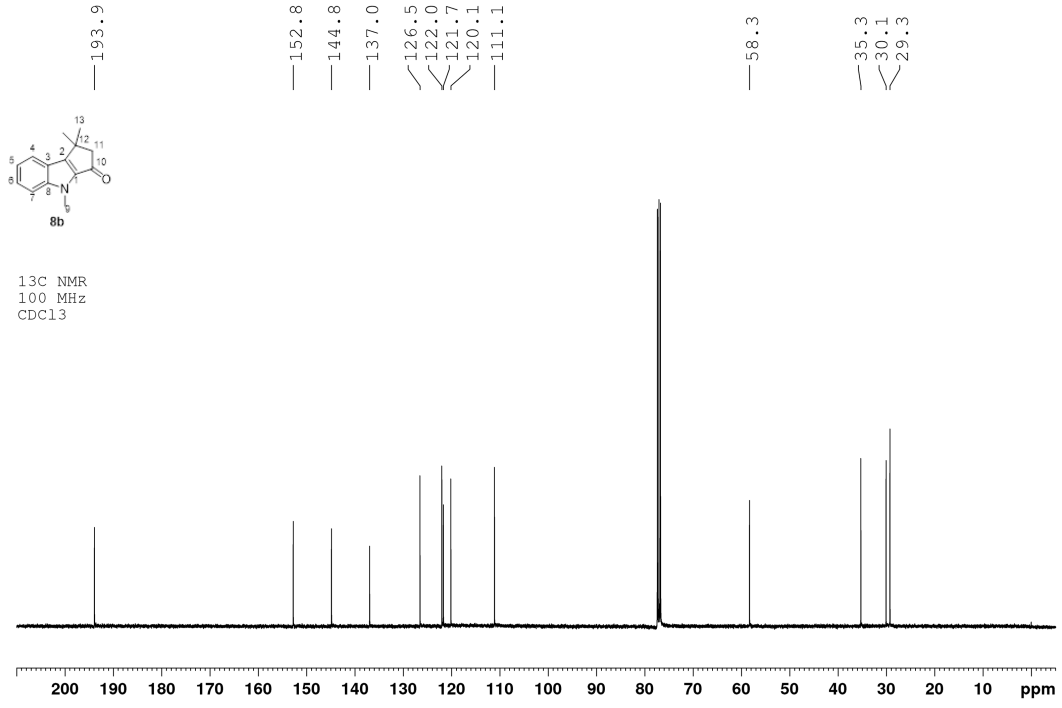


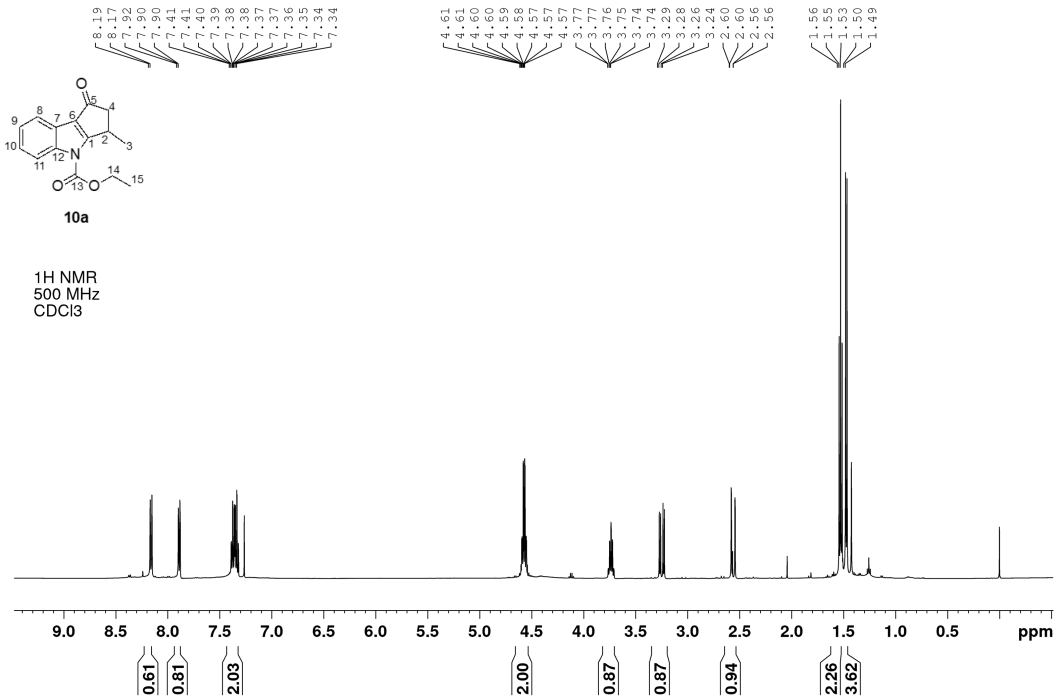
13C NMR
125 MHz
CDCl3

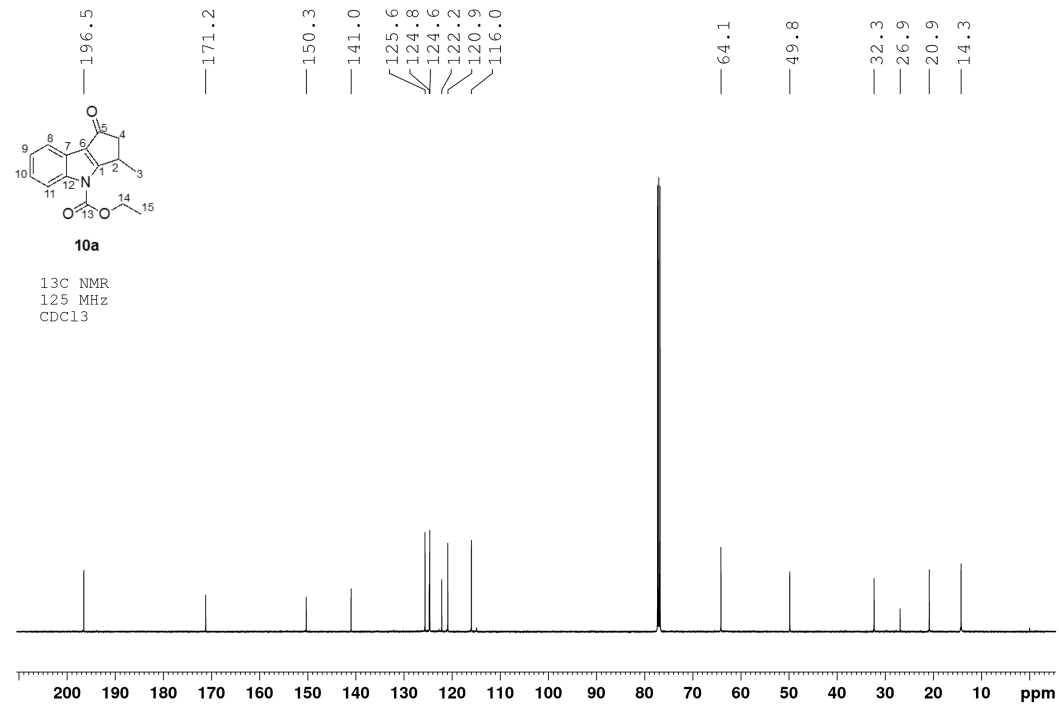

8a
1H NMR
400 MHz
CDCl3
7.72
7.70
7.42
7.42
7.41
7.41
7.41
7.40
7.39
7.37
7.35
7.25
7.18
7.18
7.17
7.17
7.17
7.16
7.16
3.90
3.54
3.54
3.53
3.53
3.52
3.52
3.23
3.22
3.20
3.19
2.54
2.54
2.51
2.51
1.48
1.46
9
8
7
6
5
4
3
2
1
0 ppm
1.00
2.10
1.01
3.00
0.96
0.97
0.97
2.92

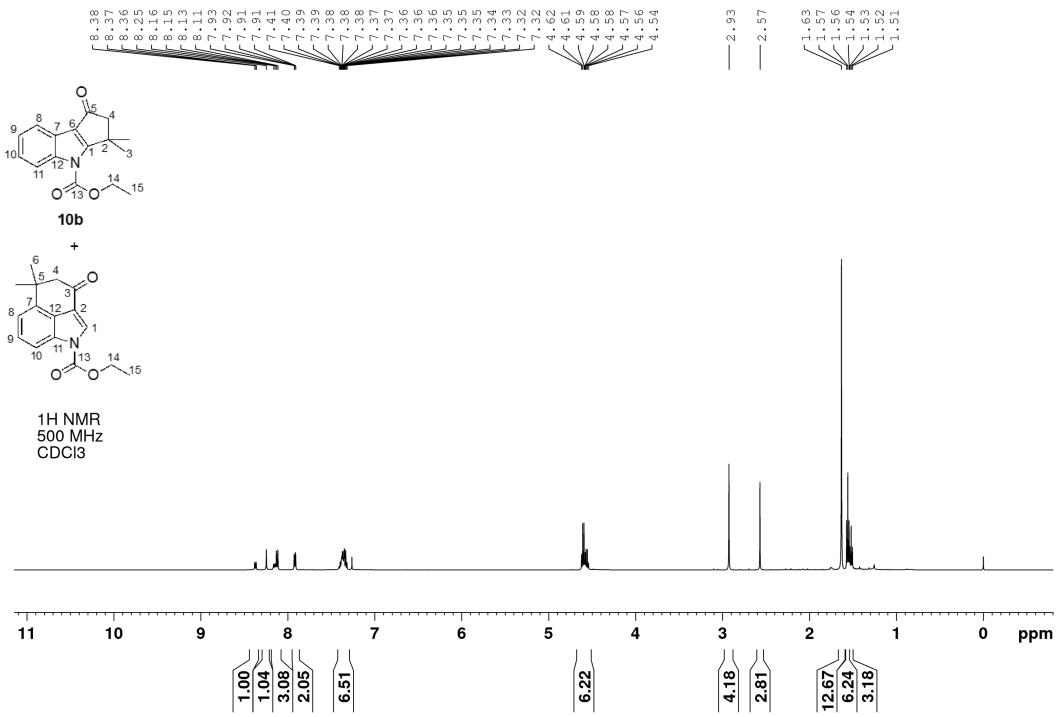

194.4
149.4
144.9
138.2
126.6
122.6
121.9
120.2
111.0
50.7
30.1
28.1
21.1
8a
13C NMR
100 MHz
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

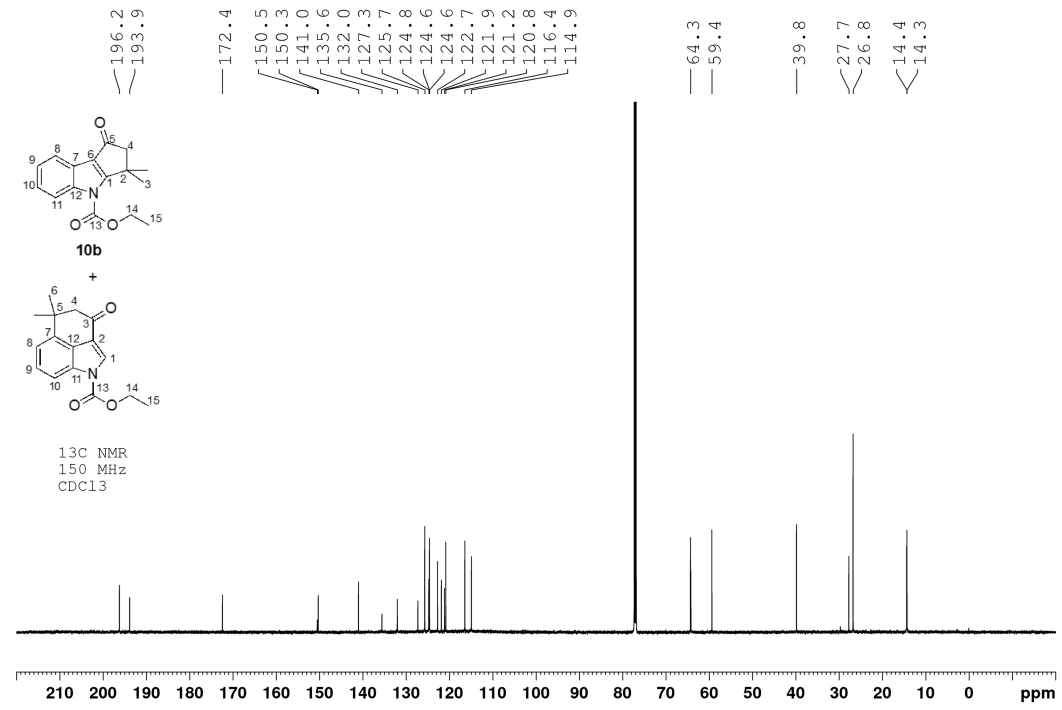

8b
1H NMR
400 MHz
CDCl3
7.72
7.70
7.40
7.38
7.38
7.36
7.34
7.19
7.18
7.17
7.17
7.16
7.15
7.15
3.89
2.84
1.55
9
8
7
6
5
4
3
2
1
0 ppm
1.00
2.04
1.02
3.06
2.07
6.18


8b
13C NMR
100 MHz
CDCl3
193.9
152.8
144.8
137.0
126.5
122.0
121.7
120.1
111.1
58.3
35.3
30.1
29.3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.19
8.17
7.92
7.90
7.41
7.40
7.39
7.38
7.37
7.36
7.35
7.34
4.61
4.60
4.59
4.58
4.57
3.77
3.76
3.75
3.74
3.29
3.28
3.26
3.24
2.60
2.56
1.56
1.55
1.53
1.50
1.49
10a
1H NMR
500 MHz
CDCl3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.61
0.81
2.03
2.00
0.87
0.87
0.94
2.26
3.62


196.5
171.2
150.3
141.0
125.6
124.8
124.6
122.2
120.9
116.0
64.1
49.8
32.3
26.9
20.9
14.3
10a
13C NMR
125 MHz
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10b
+
1H NMR
500 MHz
CDCl3
ppm


10b
+
13C NMR
150 MHz
CDCl3
ppm

8 References

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