Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.
This journal is © the Partner Organisations 2021

Bifunctional squaramides with benzyl-like fragments: analysis of CH···π interactions by Multivariate Linear Regression model and Quantum Chemical Topology

Howard, Díaz-Salazar, Eddy I. Jiménez, Wilmer E. Vallejo Narváez, Tomás Rocha-Rinza, Marcos Hernández-Rodríguez*

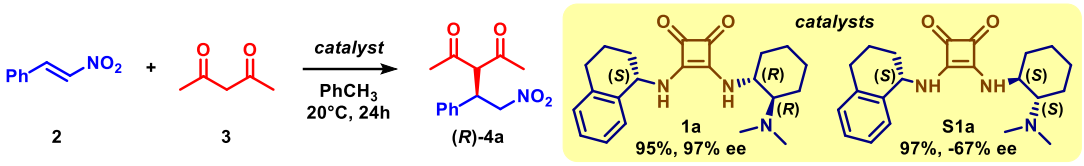
Instituto de Química, Universidad Nacional Autónoma de México
Circuito Exterior, Ciudad Universitaria, Del. Coyoacán, 04510 Cd. Mx., México

Supporting Information Table of Contents

1. **Evaluation of squaramides and thioureas on the Michael addition** **S2**
2. **Calculation of parameters and Multivariate Linear Regression model** **S3**
3. **Effect of the temperature** **S14**
4. **Kinetic studies** **S14**
5. **Transition states modeling and quantum chemical topology analyses** **S15**
6. **Experimental procedures for the synthesis of bifunctional organocatalysts and its evaluation in Michael additions** **S22**
7. **References** **S32**
8. **NMR spectra** **S35**
9. **CSP-HPLC traces** **S77**
10. **XYZ coordinates and electronic energies of the calculated structures** **S96**

1. Evaluation of squaramides and thioureas on the Michael addition

A study between the diastereomeric squaramides **1a** and **S1a** showed that **1a** had the correct combination of stereochemistry between the cyclohexane and the tetrahydronaphtyl fragments (Scheme S1).



Scheme S1. Catalytic activity evaluation of diastereoisomeric squaramides.

The modeled geometries of these catalysts showed a structural difference: the phenyl ring in **1a** is on the same side as the diamino group whereas in the diastereoisomeric **S1a** catalyst it is on the opposite side (Figure S1). This difference establishes the better catalytic performance of the squaramide **1a** due to the occurrence of the non-covalent interactions discussed in the main body of the paper. This behavior has also been observed for thioureas.[1]

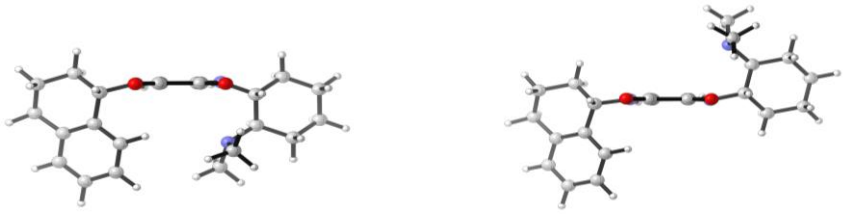
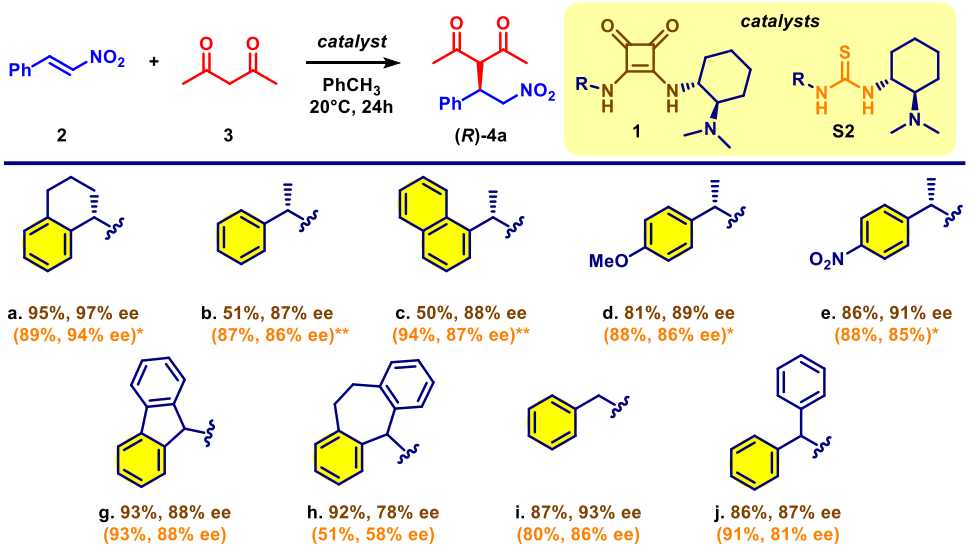


Figure S1. Top view of diastereoisomeric catalysts, left **1a** and right **S1a**.



Scheme S2. Catalysts screening (**1** and **S2**) on the Michael addition of 2,4-pentanedione to *trans*-β-nitrostyrene. Yields and ee for squaramides **1** and **S2** are shown in brown and in orange within parentheses, respectively. The reactions were performed on a 0.25 mmol scale of *trans*-β-nitrostyrene, 2 eq. of 2,4-pentanedione, 0.75 mL of solvent and a catalytic load of 1 mol% for squaramides and 5 mol% for thioureas catalysts. *ref 1a, **ref 1b.

2. Calculation of parameters and Multivariate Linear Regression model

2.1. General considerations

Geometry optimizations, frequency calculations and the computation of all the necessary parameters were carried out using the Gaussian 09 software, Revision D.01[2] at the B97-D/def2-TZVP[3] level of theory. All of the optimized geometries were confirmed by frequency computations as local minima (zero imaginary frequencies), except for the optimized geometries with a frozen dihedral angle (α = 39.30°). Structural representations were generated with CYLview.[4] Multidimensional regression analyses were performed using Excel®.

2.2. Calculation of E_C parameters

The modeled TS of thioureas **S2a** and **S2b** are almost superimposable and had a similar dihedral angles $N_{(1)}$-C-$C_{(ipso)}$-$C_{(ortho)}$ (α). We found that the optimized geometry of the thiourea **S2a** is closer to the conformation in the TS, due to the conformational rigidity of the tetrahydronaphtyl group. (Figure S2).[1b]

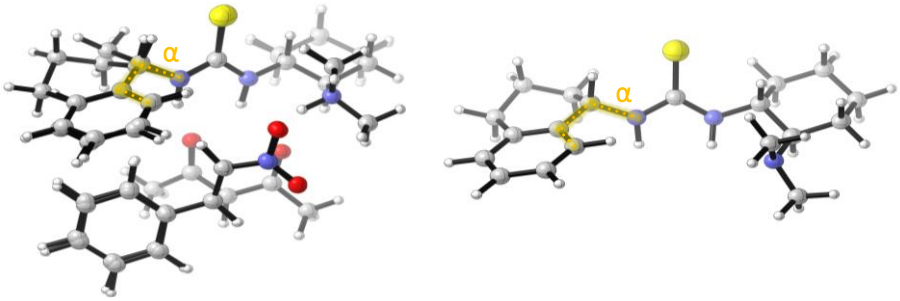


Figure S2. (Left) Superimposable transition states for thioureas **S2a** and **S2b**. (Right) Optimized thiourea **S2a** in the basal state. XYZ coordinates reported in ref 1b.

Hence, we considered that squaramides **1** with different benzyl (and benzyl-like) substituents would present a TS with a similar "active conformation" that allows the formation of CH···π interactions. This arrangement can be evaluated by the dihedral angle α. The value found in the modeled geometry of **1a** (α = 39.30°) could be very similar to the optimum value. Therefore, from the most stable local minima, we fix the dihedral angle α to the active conformation and measure the difference in energy and label it as E_C. We followed the next protocol to compute the E_C parameter:

A) We optimized the lowest energy conformer (**A**) of each catalyst and we confirmed the occurrence of a local minimum by frequency calculations.
B) The geometry of each catalyst (except **1a**) was optimized with frozen dihedral angle α = 39.30° to look for a new conformer (**B**).
C) The energy difference between both conformers defines E_C parameter ($E_C = E(B) - E(A)$).

NOTE: When two conformers of the complexes are possible due to the presence of *ortho* or *meta* substituents on the phenyl ring, two E_C values were calculated. Both values were weighted according to the protocol established in section 2.3 (only conformers within an E_C value less than of 2.0 kcal/mol were considered).

The geometries of the conformers used to determine the E_C parameter are shown in Figure S3.

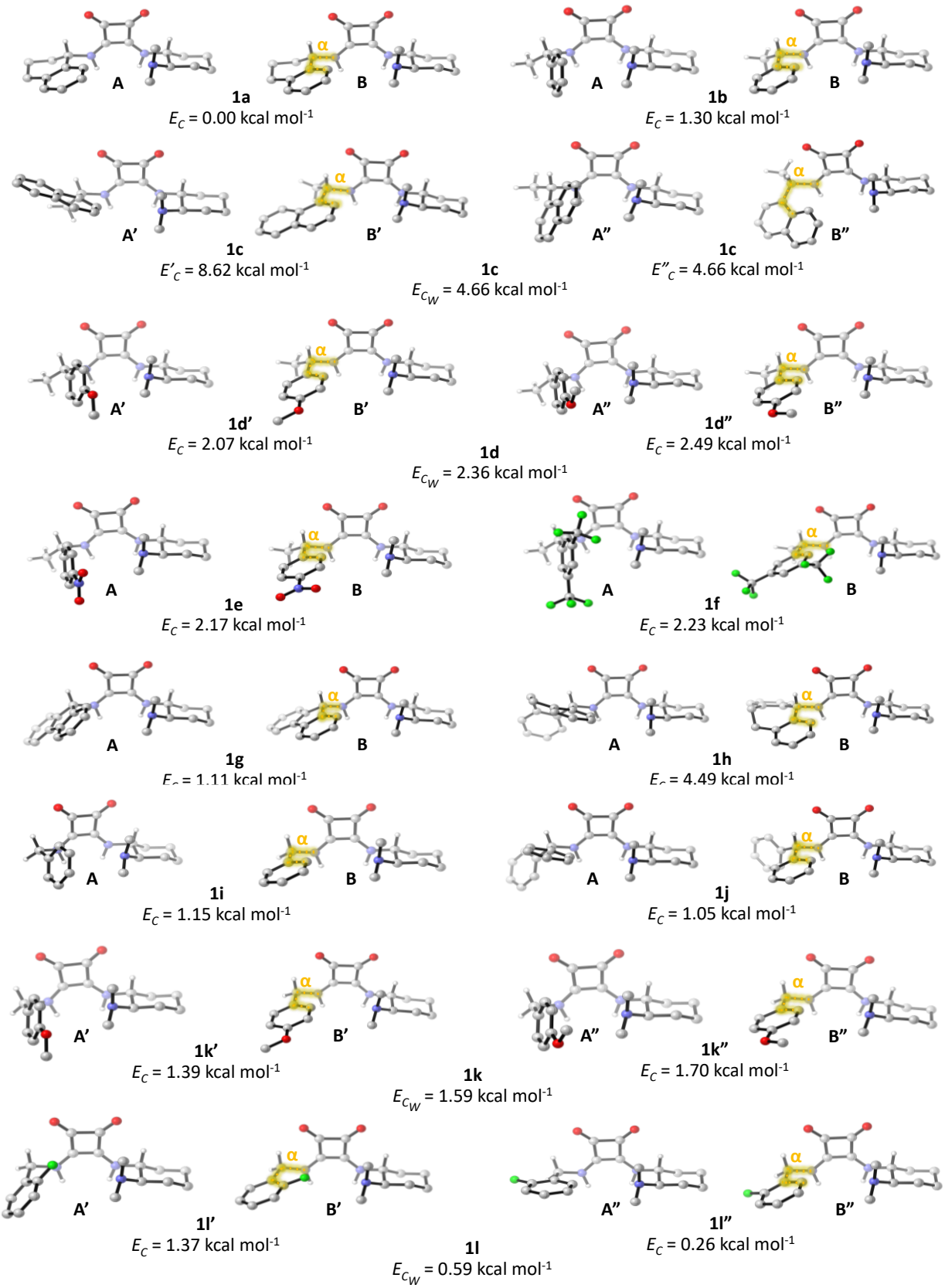


Figure S3. Conformers of the catalysts with their respective values of E_C.

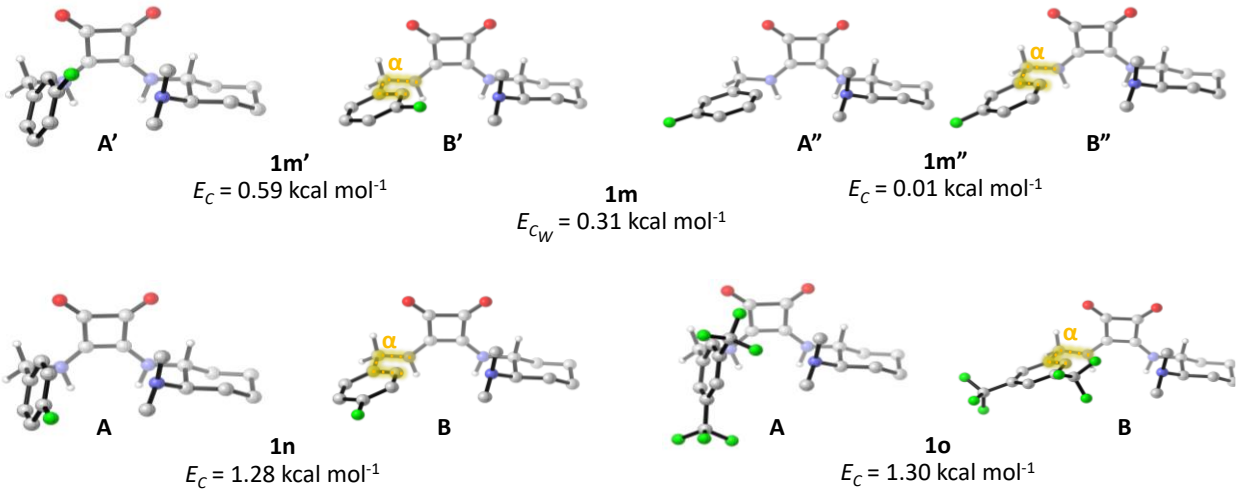


Figure S3 (continuation). Conformers of the catalysts with their respective values of E_C. We considered α = 39.30° for all the B-conformers.

2.3. Calculation of π-parameters

The B-rotamer of the catalysts is the active conformation to form CH···π interactions. Thus, we considered this rotamer to determine π-parameters following the Sigman's protocol:[5]

A) The separate components P (probe) and Cat (squaramide catalyst) of the complex were optimized at the B97D/def2TZVP level of theory. The energies of these components were labeled as $\boldsymbol{E_P}$ and $\boldsymbol{E_{Cat}}$.

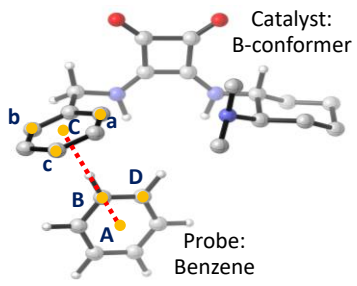
B) The components P and Cat were placed together in such a way that form CH···π interactions (see Figure S4). The geometry is fixed and the distance between the centroids of the rings (x) is scanned (steps of 0.05 Å) to obtain the energy (y) of the complex.

C) The obtained curve is fitted with a fourth degree polynomial function ($ax^4 + bx^3 + cx^2 + dx + e = y$).

D) The roots of the polynomial were calculated using the function roots in Matlab® and the array corresponding to the derivative of the polynomial. The stationary point corresponding to the energy minimum is defined as the interaction distance $\boldsymbol{D\pi}$.

E) The substitution of $\boldsymbol{D\pi}$ in the original polynomial function renders the minimum energy of the complex $\boldsymbol{E_{Comp}}$ ($a\boldsymbol{D\pi}^4 + b\boldsymbol{D\pi}^3 + c\boldsymbol{D\pi}^2 + d\boldsymbol{D\pi} + e = \boldsymbol{E_{Comp}}$).

F) Finally, the interaction energy $\boldsymbol{E\pi}$ is calculated using the formula $\boldsymbol{E\pi} = \boldsymbol{E_{Comp}} - \boldsymbol{E_P} - \boldsymbol{E_{Cat}}$.



- B-conformer of the catalysts and benzene were used as a probe.
- **A** center of the probe arene.
- **C** center of the catalyst arene.
- Angle **ABC** = 180°.
- The plane **abc** is perpendicular to the line **BC**.
- The dihedral angle **aCBD** = 0°.
- The variable x is defined as the distance **AC**.

Figure S4. Geometrical requirements for the calculation of π-parameters.

When two conformers of the complexes can coexist due to the presence of *ortho* or *meta* substituents on the aryl ring, two ***Dπ*** and two ***Eπ*** values were computed. $D\pi_d$ and $D\pi_D$ are defined as the distances relative to the complexes with the lowest and highest ***Dπ***, respectively. In the same fashion, $E\pi_d$ and $E\pi_D$ are the interaction energies corresponding to the complexes with distances $D\pi_d$ and $D\pi_D$, respectively. $D\pi_W$ and $E\pi_W$ are the energy-weighted interaction distance and energy calculated with equation 1. Only conformers within an energy range of 2.0 kcal mol^{-1} were considered. The importance of each conformer is quantified by the coefficients c_X, which are calculated according to the Boltzmann distribution over the two considered conformers (equation 2).

$$P_W = c_d P_d + c_D P_D \quad \textbf{Equation 1}$$

where **P** is the parameter to study (***Eπ***, ***Dπ***, E_C, **ω**, etc.)

$$c_X = \frac{\exp[-E\pi_X/\mathrm{RT}]}{\exp[-E\pi_d/\mathrm{RT}]+\exp[-E\pi_D/\mathrm{RT}]} \quad \textbf{Equation 2}$$

where **X** = d, D

The structures of the π-complexes with their interaction energies and distances values are shown in Figure S5.

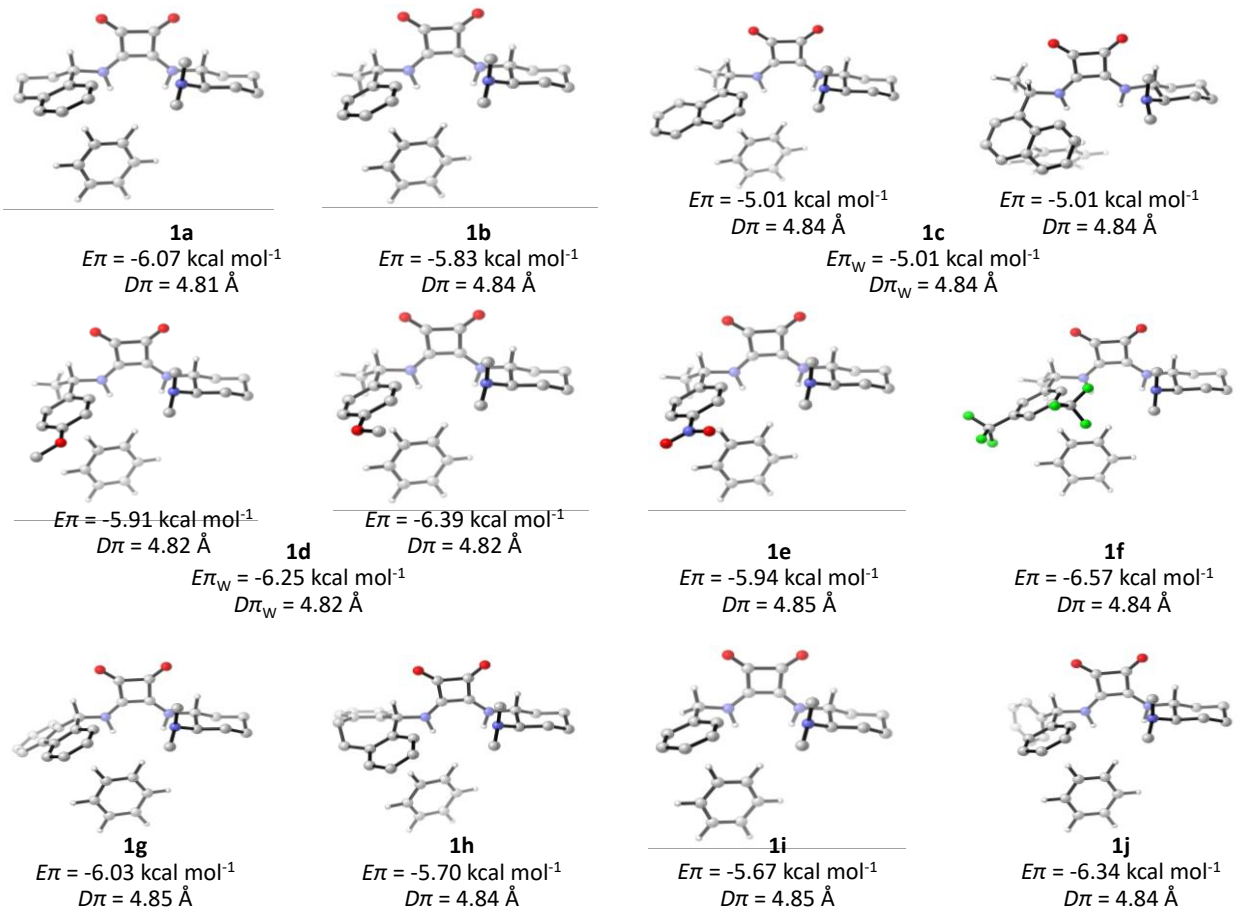


Figure S5. Complexes used to determine π-parameters.

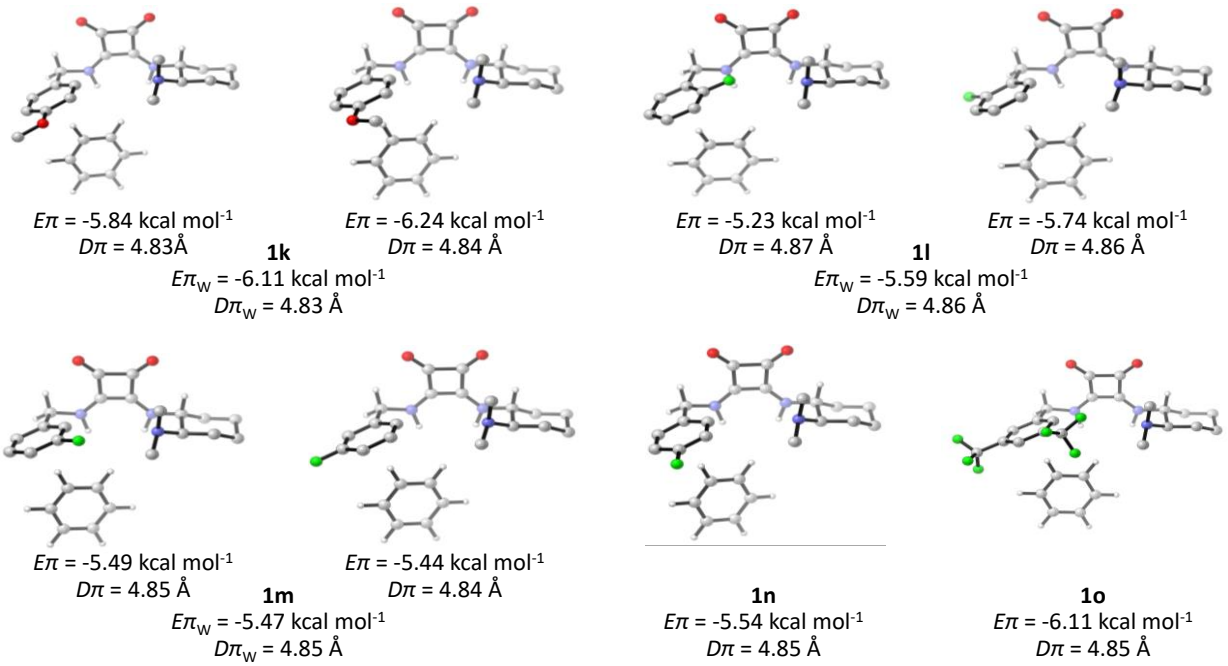


Figure S5 (continuation). Complexes used to determine π-parameters.

2.4. Other parameters collected.

Other steric parameters were determined using the B-conformer of the catalysts. In particular, we calculated sterimol[6] parameters for the aryl and benzyl groups, B-conformer of the squaramide **1i** is described as a graphical example in Figure S6.

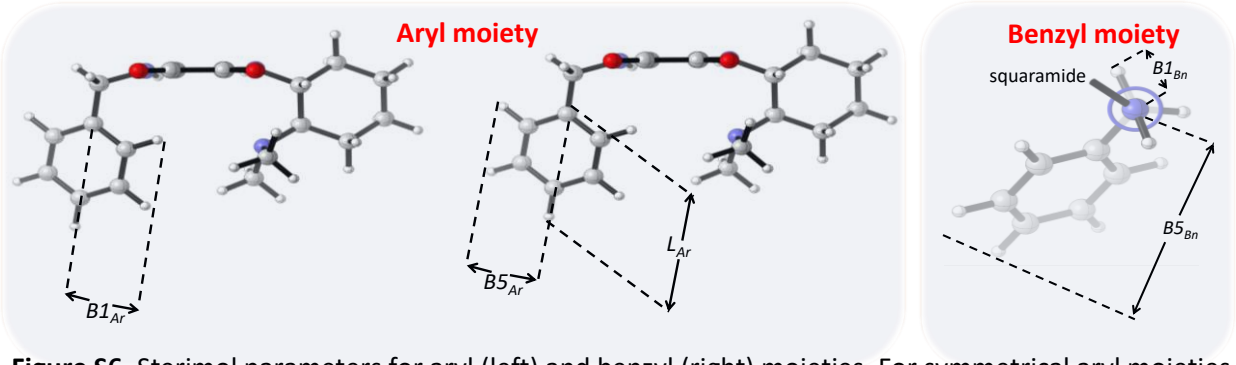
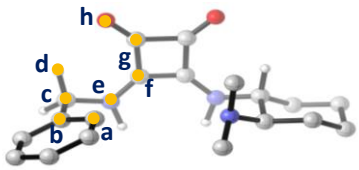


Figure S6. Sterimol parameters for aryl (left) and benzyl (right) moieties. For symmetrical aryl moieties $B1_{Ar}$ and $B5_{Ar}$ have the same value. Benzyl moiety is shown in Newman perspective.

$\boldsymbol{L_{Ar}}$, $\boldsymbol{B1_{Ar}}$ and $\boldsymbol{B5_{Ar}}$ are the length, minimum width and maximum width of the aryl group, respectively. In the same way, $\boldsymbol{B1_{Bn}}$ and $\boldsymbol{B5_{Bn}}$ are the minimum width and maximum width of the whole benzyl group.

The dihedral angles were measured from the optimized structures as shown in the Figure S7.



- Diedral angle **abce** = α = 39.3° (locked)
- Diedral angle **abcd** = β
- Diedral angle **bcef** = γ
- Diedral angle **cefg** = δ
- Diedral angle **efgh** = ω

Figure S7. Geometrical parameters

Finally, to establish a linear free-energy relationship we measured indirectly $\Delta\Delta G^{\neq}$ from the experimental enantiomeric ratio (er). We used the formula $\Delta G^{\neq}$ = [–RT ln(major enantiomer)] – [–*RT* ln(minor enantiomer)] where *R* is the ideal gas constant, and *T* is temperature (293.15 K). Table S1 shows er and $\Delta\Delta G^{\neq}$ values as well as the values of all parameters computed.

Table S1. Parameters collected for the development of the MLR models.

cat	er[a]		ΔΔG≠	E_π	D_π	E_C	β	γ	δ	ω	$B1_{Ar}$	$B5_{Ar}$	L_{Ar}	$B1_{Bn}$	$B5_{Bn}$
1a	98.365	1.635	2.385	-6.074	4.812	0.000	-76.409	-95.036	-17.751	0.337	2.153	3.466	3.902	1.477	5.480
1b	93.660	6.340	1.568	-5.827	4.838	1.962	-75.318	-96.172	-17.275	0.573	2.156	2.156	3.912	1.476	5.530
1c	94.006	5.994	1.603	-5.011	4.841	4.658	-75.210	-143.488	-8.635	0.642	2.131	4.655	3.936	1.479	6.502
1d	94.714	5.286	1.680	-6.247	4.818	2.360	-75.376	-94.960	-17.941	0.440	2.151	2.151	6.004	1.479	7.587
1e	95.237	4.763	1.744	-5.944	4.846	2.169	-75.257	-92.829	-17.653	0.463	2.159	2.159	4.859	1.479	6.839
1f	95.165	4.835	1.735	-6.574	4.843	2.233	-75.252	-94.057	-10.955	1.147	3.595	3.595	4.232	1.477	6.563
1g	93.928	6.072	1.595	-6.029	4.854	1.113	-78.263	-84.031	-23.443	0.948	2.156	4.240	3.866	1.479	5.155
1h	88.827	11.173	1.207	-5.697	4.838	4.494	-73.949	-107.696	-10.886	0.707	2.139	4.204	3.890	1.478	5.735
1i	96.654	3.346	1.958	-5.669	4.853	1.146	-80.185	-91.678	-19.534	0.329	2.155	2.155	3.900	1.470	5.350
1j	93.673	6.327	1.569	-6.345	4.837	1.046	-75.509	-97.012	-15.608	-0.053	2.145	2.145	3.896	1.474	5.560
1k	95.223	4.777	1.742	-6.109	4.833	1.593	-80.125	-91.038	-19.797	0.180	2.153	2.153	5.994	1.470	7.372
1l	95.701	4.299	1.806	-5.591	4.860	0.587	-80.357	-94.121	-16.201	0.225	2.143	2.379	3.917	1.467	5.385
1m	97.218	2.782	2.069	-5.469	4.845	0.315	-80.204	-90.572	-19.227	0.355	2.153	2.346	3.906	1.468	5.389
1n	96.135	3.865	1.871	-5.543	4.854	1.278	-80.176	-91.068	-19.519	0.482	2.149	2.149	4.141	1.470	5.681
1o	97.342	2.658	2.096	-6.110	4.853	1.303	-80.209	-90.448	-13.906	1.376	3.592	3.592	4.173	1.469	6.516
1p	-	-	-	-5.491	4.825	4.232	-73.242	-	-	-	2.431	-	-	-	-
1q	-	-	-	-6.556	4.802	2.563	-80.761	-	-	-	3.583	-	-	-	-
1r	-	-	-	-5.293	4.818	2.446	-80.460	-	-	-	2.419	-	-	-	-
1s	-	-	-	-5.058	4.858	0.137	-80.190	-	-	-	2.431	-	-	-	-
1t	-	-	-	-5.046	4.883	0.309	-80.229	-	-	-	2.436	-	-	-	-
1u	-	-	-	-7.295	4.782	0.011	-76.422	-	-	-	2.438	-	-	-	-

[a]er was determined by CSP-HPLC

2.5. Multivariate linear regression model

We found a single correlation with a qualitative agreement between E_C parameter and $\Delta\Delta G^{\neq}$ was found (R^2 = 0.518, Figure S8, left). On the other hand, the cross-term $E\pi E_C$ showed a correlation with R^2 = 0.561 (Figure S8, right).

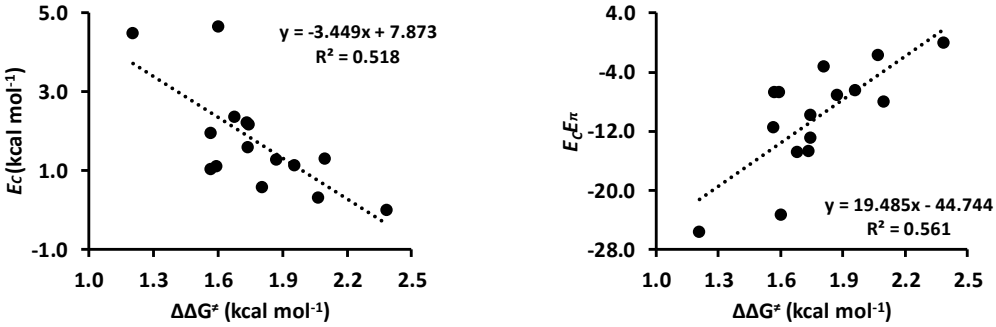


Figure S8. Single correlations between $\Delta\Delta G^{\neq}$ with E_C (left) and $E\pi E_C$ (right).

Multiple linear regression models were developed using the Data Analysis ToolPack in Excel®, some models are represented in (Figure S9).

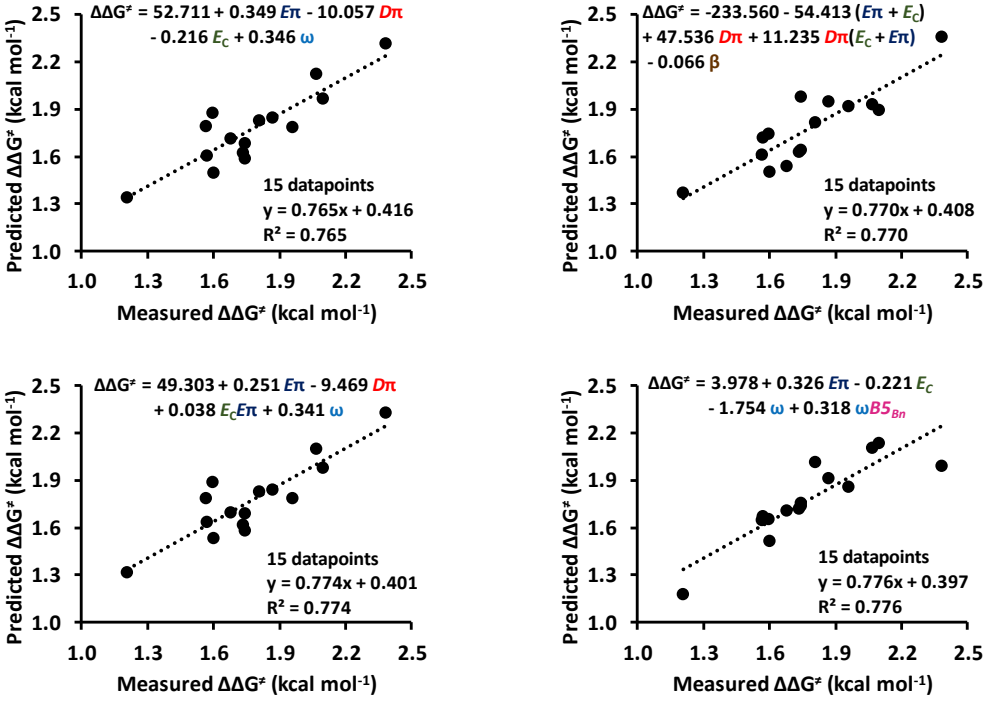


Figure S9. Representative MLR models involving $\Delta\Delta G^{\neq}$.

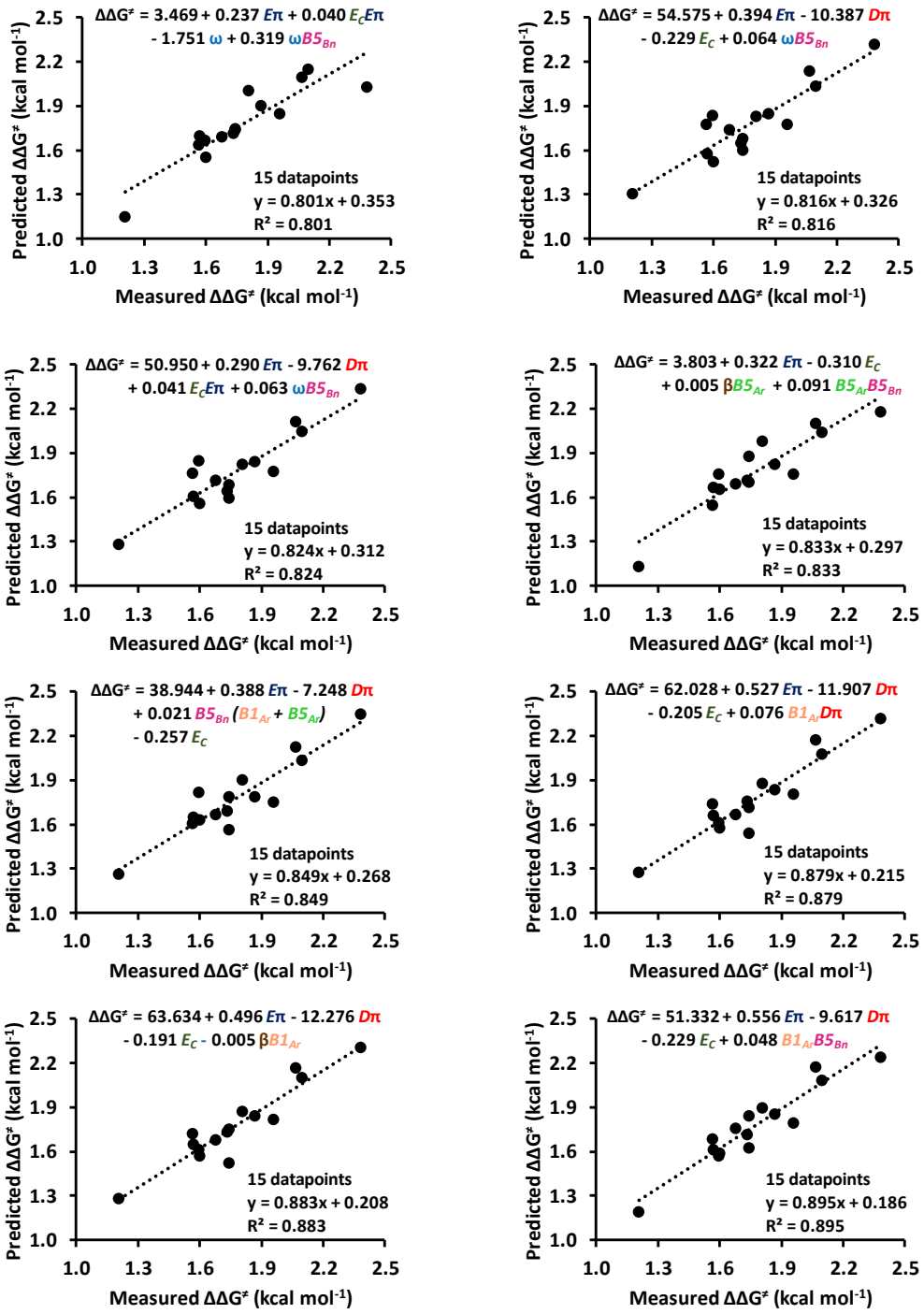


Figure S9 (continuation). Representative MLR models involving $\Delta\Delta G^{\neq}$.

After several attempts we found three possible MLR models that could explain the behavior of the catalysts (Figure S10). A good linear correlation between the Predicted $\Delta\Delta G^{\neq}$ and the Measured $\Delta\Delta G^{\neq}$ indicates that the models adequately describe the system under study. The validation of the models (leave-one-out L1O and leave-two-out L2O cross-validation) was a decisive factor in choosing between one model or another. L1O- and L2O-values close to R^2 prove the statistical robustness of the model. Thus,

we employed the model in Figure S10b (Figure 3 in the manuscript) to continue with our study. This model predicts well the behavior of most of the catalysts. The equation is composed of four terms: ***Eπ*** and ***Dπ*** describes the strength of the NCI, the term $E_C E\pi$ is related with conformational effects, and the cross-term $\beta B1_{Ar}$ accounts for geometrical/steric requirements.

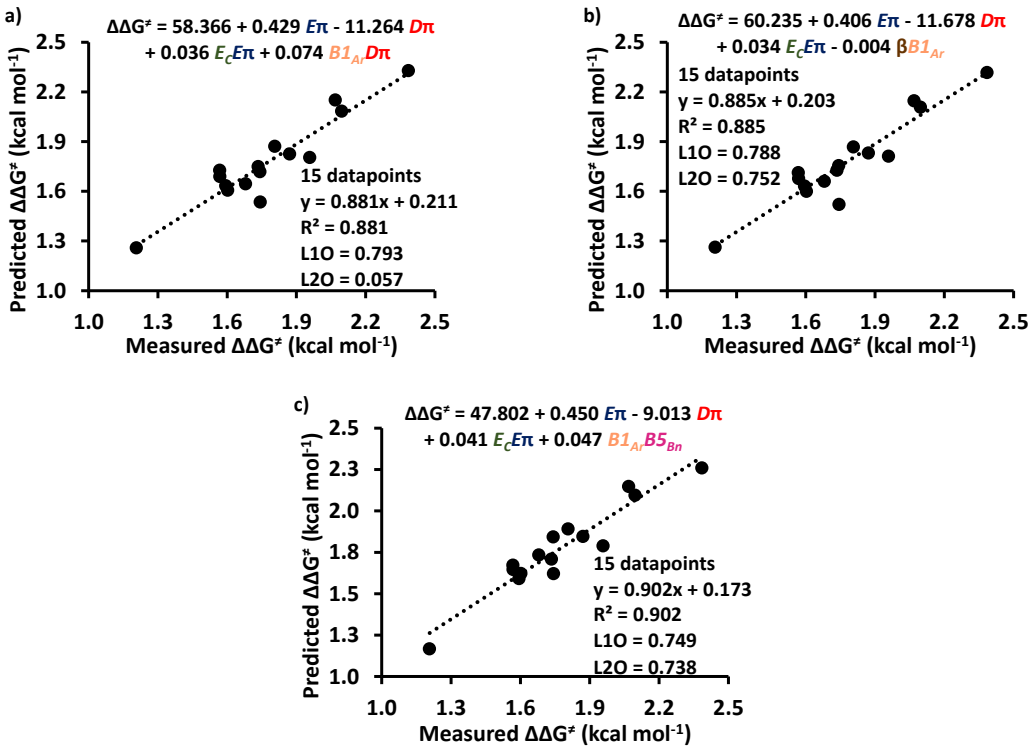


Figure S10. Candidate MLR models.

Table S2. Data corresponding to the MLR model in Figure S10b.

cat	Parameters				Measured ΔΔG≠	Predicted ΔΔG≠
	E_π	D_π	$E_C E_\pi$	$\beta B1_{Ar}$	(kcal mol^{-1})	(kcal mol^{-1})
1a	-6.074	4.812	0.000	-164.484	2.385	2.343
1b	-5.827	4.838	-11.430	-162.411	1.568	1.690
1c	-5.011	4.841	-23.343	-160.263	1.603	1.598
1d	-6.247	4.818	-14.743	-162.156	1.680	1.640
1e	-5.944	4.846	-12.895	-162.481	1.744	1.521
1f	-6.574	4.843	-14.681	-270.509	1.735	1.713
1g	-6.029	4.854	-6.711	-168.700	1.595	1.584
1h	-5.697	4.838	-25.599	-158.146	1.207	1.221
1i	-5.669	4.853	-6.496	-172.824	1.958	1.790
1j	-6.345	4.837	-6.637	-161.961	1.569	1.636
1k	-6.109	4.833	-9.734	-172.513	1.742	1.733
1l	-5.591	4.860	-3.285	-172.169	1.806	1.843
1m	-5.469	4.845	-1.720	-172.680	2.069	2.156
1n	-5.543	4.854	-7.085	-172.314	1.871	1.813
1o	-6.110	4.853	-7.964	-288.102	2.096	2.126

Table S2 (continuation). Data corresponding to the MLR model in Figure S10b.

cat	Parameters				Measured $\Delta\Delta G^{\neq}$	Predicted $\Delta\Delta G^{\neq}$
	E_π	D_π	$E_C E_\pi$	$\beta B1_{Ar}$	(kcal mol^{-1})	(kcal mol^{-1})
1p	-5.491	4.825	-23.236	-178.072	-	1.671
1q	-6.556	4.802	-16.802	-289.399	-	2.221
1r	-5.293	4.818	-12.947	-194.615	-	2.261
1s	-5.058	4.858	-0.692	-194.966	-	2.299
1t	-5.046	4.883	-1.558	-195.422	-	1.992
1u	-7.295	4.782	-0.078	-186.279	-	2.259

The leave-one-out and leave-two-out cross-validation method was employed to prove that our model is statistically robust as shown in Figure S11.

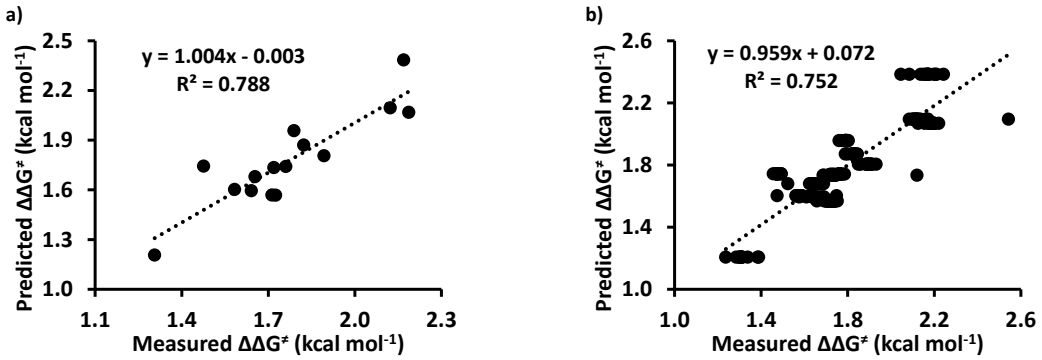


Figure S11. a) Leave-one-out and b) leave-two-out cross-validation methods for model in Figure S10b.

2.6. Other non-covalent interactions

When we analyzed the π-parameters for **1o**, we found a distance $d_{H,F}$ = 2.73 Å between the squaramide and the probe (Figure S12). This value is consistent with CH···FC interactions.[7] That kind of interaction could be present in the TS of the Michael addition catalyzed by **1o**.

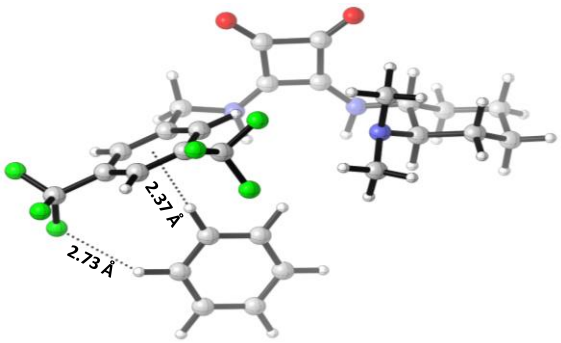


Figure S12. Non-covalent interactions between **1o** and benzene (probe).

3. Effect of the temperature

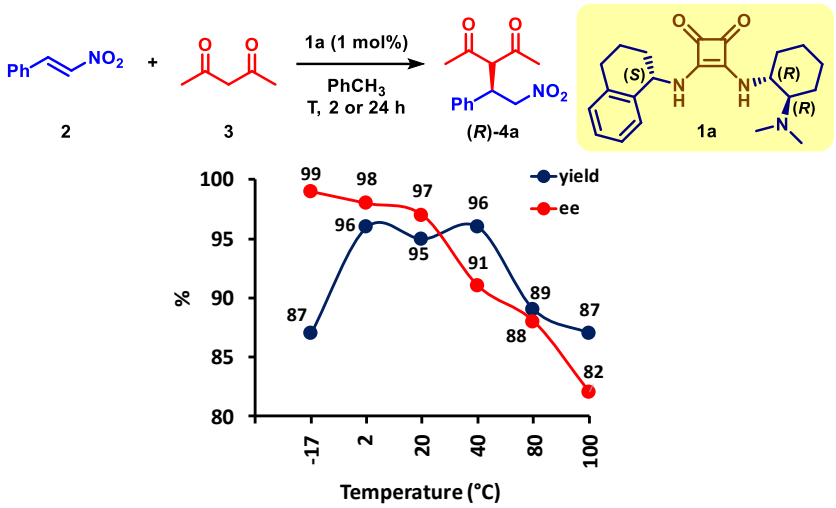
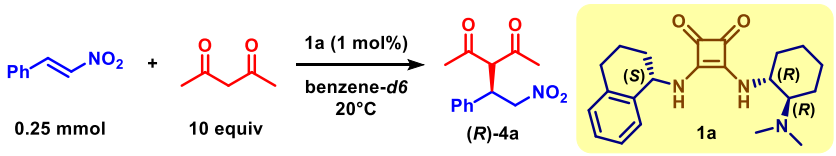


Figure S13. Effect of the temperature in the reaction catalyzed with **1a**.
Temperature = -17, 2 and 20 °C; t = 24 h.
Temperature = 40, 80 and 100 °C; t = 2 h.

4. Kinetic studies



Scheme S3. Reaction carried out in deuterated benzene for kinetic studies performed by ^{1}H NMR.

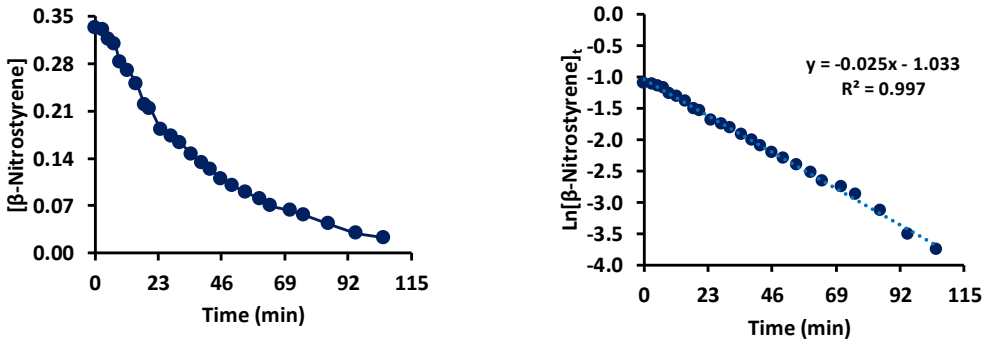


Figure S14. Kinetics of the Michael addition under pseudo-first order conditions. Concentration of β-nitrostyrene as a function of time with catalyst **1a** (left). Plot on a logarithmic scale of the concentration of β-nitrostyrene as the reaction proceeds (right).

Table S3. Comparison of the rate constants of Michael Addition with different catalysts.

Catalyst	Cat (mol%)	k_{obs} (min^{-1})	k_{rel}
Takemoto	5	0.0279[a]	3.100
S2a	5	0.009[b]	1.000
1a	1	0.0253	2.811

[a]Ref 1a, [b]Ref 1b.

5. Transition states modeling and quantum chemical topology analyses

5.1. General considerations

The geometry of all intermediates and transition states were completely optimized with the PCM-(toluene)-B97-D/TZVP[1,8] approximation as implemented in the Gaussian 16, Revision C.01[9]. Structural representations were generated with the package CYLview.[4] Each stationary structure was characterized as a local minimum or a saddle point of first order through the computation of the corresponding harmonic frequencies. Intrinsic reaction coordinate calculations were carried out in all cases to verify that the localized transition state structures connect the two minima on the potential energy surface associated with reactants and products. Single-point energy calculations on the optimized geometries were then evaluated using the same functional (B97-D) and the triple-zeta valence quality def2-TZVP basis set, within the PCM model (toluene). Thermal corrections were calculated from the unscaled vibrational frequencies at the B97-D/TZVP level on the optimized geometries.

The topological analyses of the electron density determined with the method (PCM-(toluene)-B97D/TZVP) were done in accordance with the Quantum Theory of Atoms in Molecules (QTAIM) implemented in the AIMAll[10] program. The QTAIM characterization was done in terms of the properties of electron density $\rho(\mathbf{r})$, the delocalization indexes (DIs), and the hydrogen bond energy according to the Espinosa estimation E_H.[11] All local topological descriptors are computed at intermolecular bond critical points. The IQA energy partition was performed with M06-2x/TZVP//PCM(toluene)-B97-D/TZVP electron densities to get further insights about the chemical bonding of the examined transition states. The IQA calculations were carried out with the AIMAll[10] program.

5.2. Rate-limiting step computation of the Michael addition

The rate of the organocatalyzed addition of 2,4-pentanodione to β-nitrostyrene is determined by the formation of the C-C bond. This step is also responsible for the enantioselectivity of the reaction. Therefore, and to understand in more detail the origins of the stereoselectivity, we computed this reaction path with the PCM-(toluene)-B97-D/def2-TZVP//PCM-(toluene)-B97-D/TZVP level of theory. Energy profiles and theoretical activation barriers are shown in Figure S15 and Table S4, respectively.

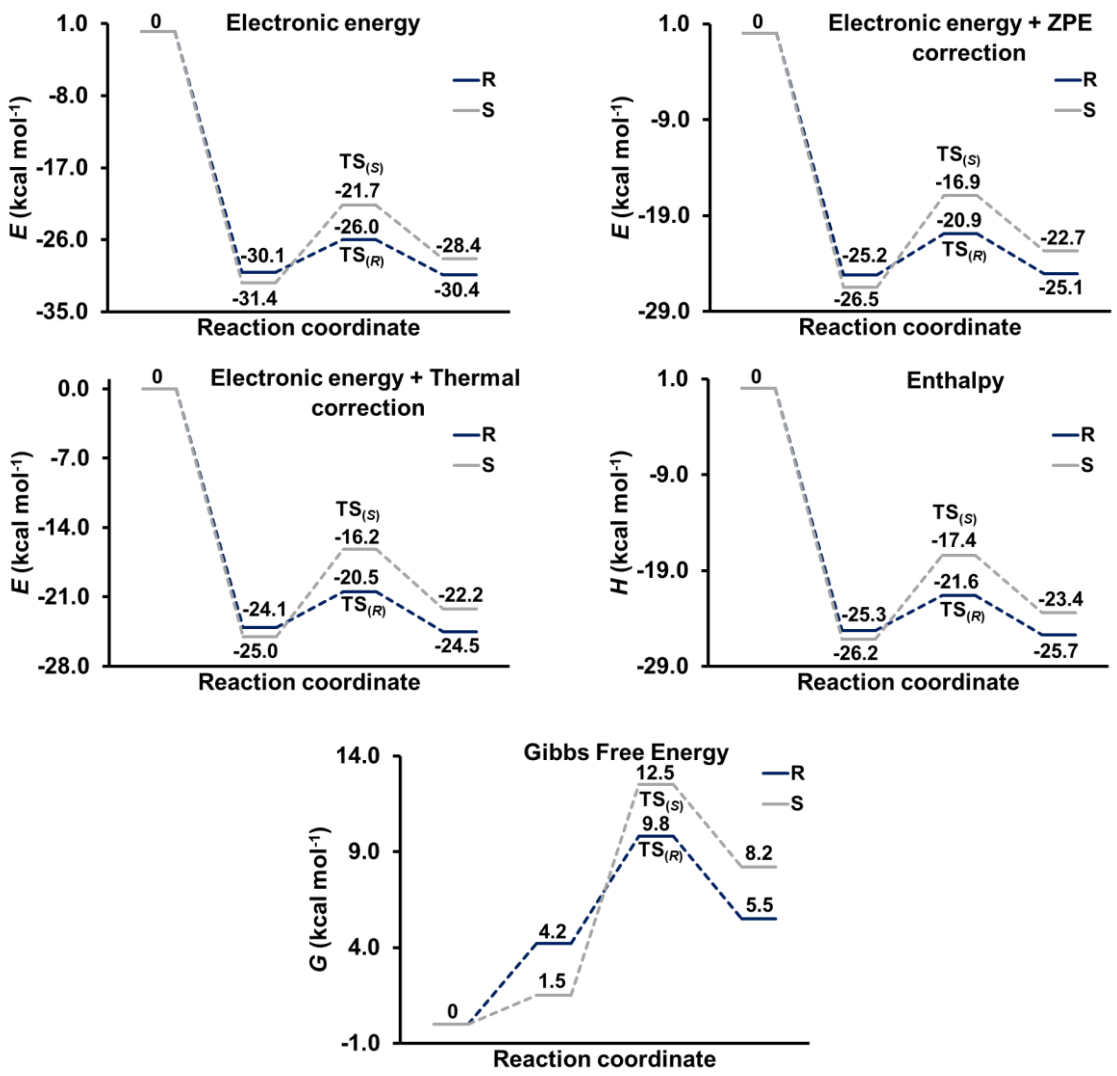
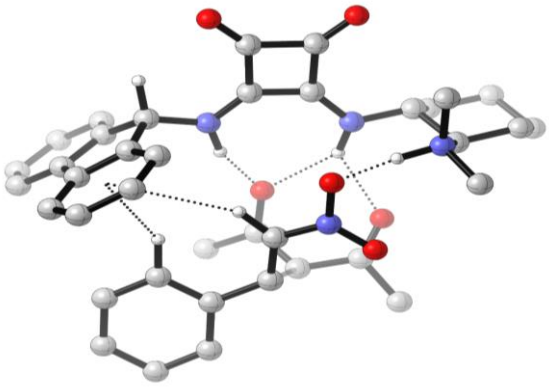


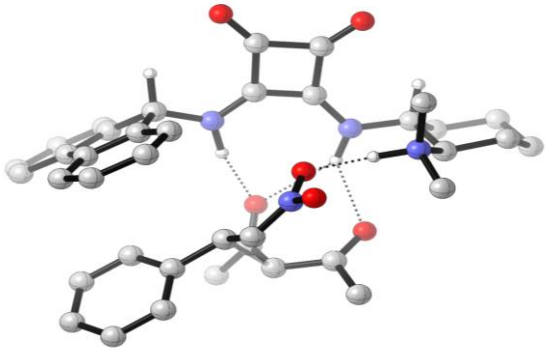
Figure S15. Profiles of relative energies to reactants for the Michael reaction under consideration with catalyst **1a**. The full description of the approximationand basis set is: PCM-(toluene)-B97-D/def2-TZVP//PCM-(toluene)-B97-D/TZVP. The values are reported in kcal mol^{-1}.

Table S4. Theoretical activation barriers in kcal mol^{-1}, electronic energy ($E_e^{\neq}$), with zero-point energy correction ($E^{\neq}$), plus thermal correction at 298.15 K ($E^{\neq}_{298K}$), enthalpy ($H^{\neq}$) and Gibbs free energy ($G^{\neq}$), of the enantiodetermining step of the addition of 2,4-pentanodione to β-nitrostyrene with catalyst **1a**.

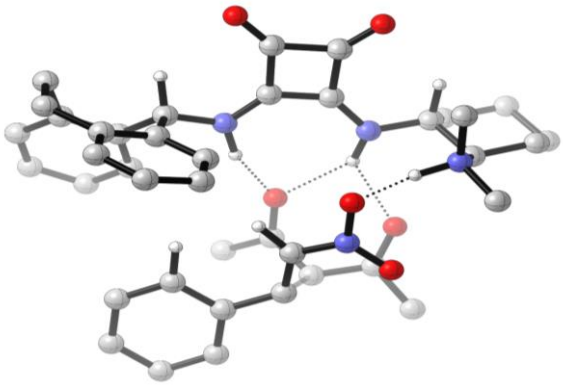
Energy	E_a *(R)*	E_a *(S)*	ΔE_a
$E_e^{\neq}$	-26.0	-21.7	4.3
$E^{\neq}$	-20.9	-16.9	4.0
$E^{\neq}_{298K}$	-20.5	-16.2	4.3
$H^{\neq}$	-21.6	-17.4	4.2
$G^{\neq}$	9.8	12.5	2.7



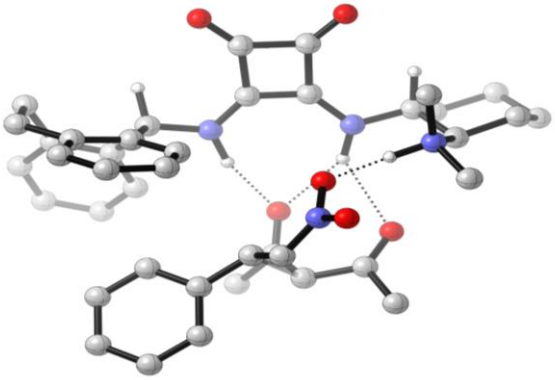
$TS_{(R)}$-1g
(-24.93)



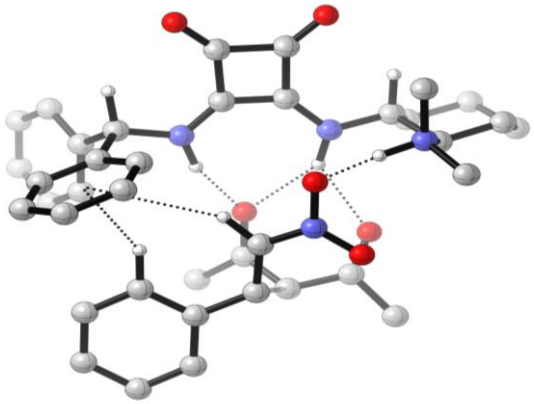
$TS_{(S)}$-1g
(-22.08)



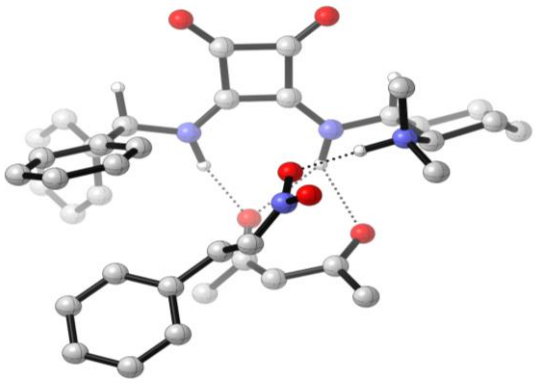
$TS_{(R)}$-1h
(-22.86)



$TS_{(S)}$-1h
(-21.84)

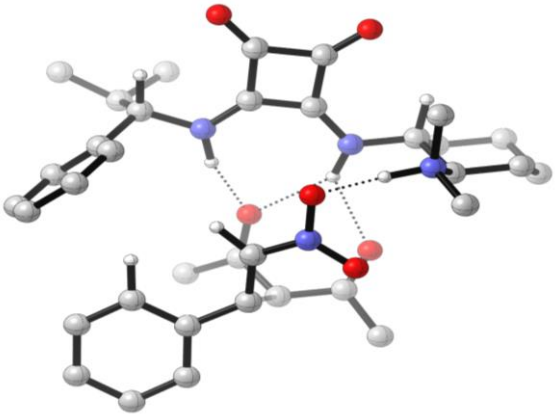


$TS_{(R)}$-1j
(-24.53)

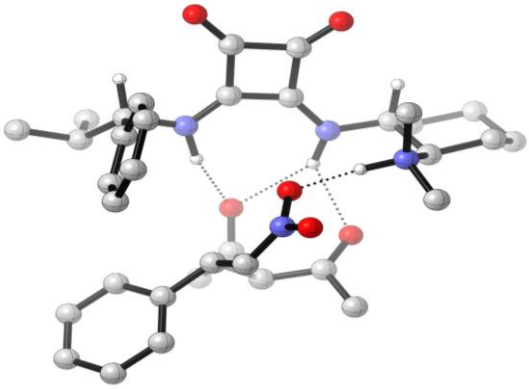


$TS_{(S)}$-1j
(-21.48)

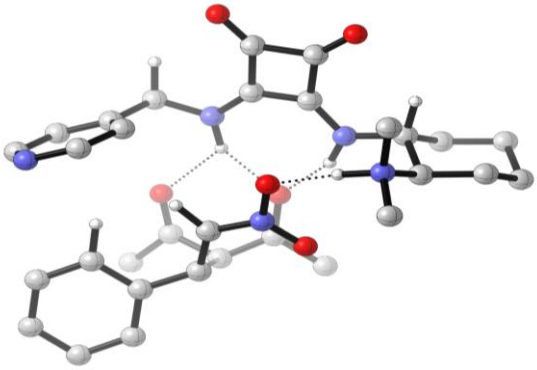
Figure S16. Diastereomeric transition state geometries found for the Michael addition of 2,4-pentanedione to *trans*-β-nitrostyrene catalyzed with squaramides **1g**, **1h**, **1j**, **1p** and **1s**. Relative electronic energies, in kcal mol^{-1}, are shown in parentheses.



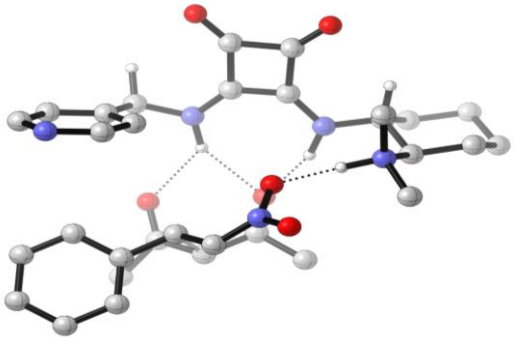
$TS_{(R)}$-1p
(-21.17)



$TS_{(S)}$-1p
(-17.68)



$TS_{(R)}$-1s
(-26.46)



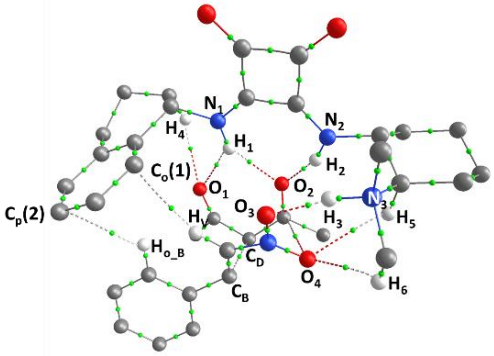
$TS_{(S)}$-1s
(-21.78)

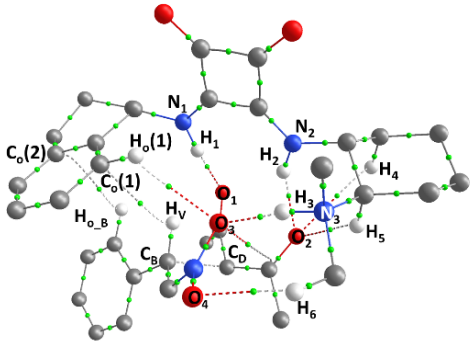
Figure S16 (continuation). Diastereomeric transition state geometries found for the Michael addition of 2,4-pentanedione to *trans*-β-nitrostyrene catalyzed with squaramides **1g**, **1h**, **1j**, **1p** and **1s**. Relative electronic energies, in kcal mol^{-1}, are shown in parentheses.

5.3. Analysis of the transition states by Quantum Theory of Atoms in Molecules (QTAIM)

We performed the QTAIM analysis to quantify and recognize the interactions involved in the transition states to generate the *R*- and *S*-products through the reaction with the catalyst **1a**. According to QTAIM data (Table S5), the $TS_{(R)}$ exhibits stronger interactions than its counterpart $TS_{(S)}$, e.g. $H_2\cdots O_2$ and $H_3\cdots O_3$. Additionally, the formation of the *R*-product yields a bifurcated hydrogen bond among H_1, H_2 and O_1 atoms, which is not present in $TS_{(R)}$. Those interactions in the former TS are stronger than they are in latter as indicated by the electron density $\rho(\mathbf{r})$, delocalization indexes (DIs) and hydrogen bond energies (E_{HB}) values, which are descriptors related to the strength of the association. The magnitude of E_{HB}, indicates that H···O contacts are stronger in the formation of $TS_{(R)}$ than in the generation of $TS_{(S)}$. This trend of HB strength is also observed for electron density and DIs values.

Table S5. Selected QTAIM data of the $TS_{(R)}$ and $TS_{(S)}$.





Interaction	$TS_{(R)}$-1a $\rho(r)$	DI	E_H	$TS_{(S)}$-1a $\rho(r)$	DI	E_H
$H_1\cdots O_1$	1.06	2.9	-1.85	2.58	7.9	-6.43
$H_1\cdots O_2$	1.63	4.8	-3.29	-	-	-
$H_2\cdots O_2$	3.66	10.3	-10.57	2.35	6.7	-5.68
$H_3\cdots O_3$	5.59	14.6	-17.35	4.88	12.9	-14.84
$H_4\cdots O_1$	0.99	3.9	-1.91	-	-	-
$C_o(1)\cdots H_V$	0.95	3.0	-1.41	0.69	1.6	-1.10
$C_p(2)\cdots H_{o_B}$	0.74	1.7	-1.22	-	-	-
$C_o(2)\cdots H_{o_B}$	-	-	-	0.96	2.0	-1.57
$H_o(1)\cdots O_3$	-	-	-	0.67	2.5	-1.13
$H_4\cdots O_2$	-	-	-	0.38	1.5	-0.66
$H_5\cdots O_2$	-	-	-	1.27	5.1	-2.32
$H_5\cdots O_4$	0.86	3.0	-1.47	-	-	-
$H_6\cdots O_4$	1.02	3.6	-1.85	1.21	4.8	-2.16
$C_B\cdots C_D$	6.76	44.0	-12.02	6.65	44.1	-11.73

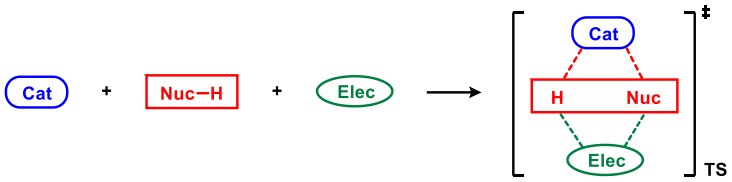
Values for the electron density ρ(r) and the delocalization index DI in hundredths of atomic units and EH in kcal mol^{-1}.

5.4. Interacting quantum atoms energy partition

The Interacting Quantum Atoms (IQA) method is an electronic energy partition, E, in one (E_{net}^{A}) and two atoms ($E_{int}^{A\cdots B}$) terms[12] as indicated in Equation 3.

$$E = \sum_{A} E_{net}^{A} + \sum_{A}\sum_{B>A} E_{int}^{A\cdots B}, \qquad \textbf{Equation 3}$$

where the sums run over atomic regions. E_{net}^{A} and $E_{int}^{A\cdots B}$ are designated as (i) the IQA net energy of atom A and (ii) the IQA interaction energy between two atoms, A and B.[13] IQA energies can be calculated using the QTAIM spatial partition with DFT electron densities, using the same program (AIMAll).[10] This approach yields the total DFT electronic energy according to equation 3. Considering that the IQA approach is invariant with respect to the assembly of QTAIM atoms in molecules, the energy of a trimolecular complex



$$Cat + Nuc + Elec \rightleftarrows Cat \cdots Nuc \cdots Elec \qquad \textbf{Equation 4}$$

Where Cat = catalyst, Nuc = nucleophile and $Elec$ = electrophile.

can be written as

$$\Delta E = E^{Cat\cdots Nuc\cdots Elec} - \left(E_{iso}^{Cat} + E_{iso}^{Nuc} + E_{iso}^{Elec}\right). \qquad \textbf{Equation 5}$$

This equation can be rewritten as follows

$$\Delta E = \sum_{species} E_{def}^{species} + E_{int}^{Cat\cdots Nuc} + E_{int}^{Cat\cdots Elec} + E_{int}^{Nuc\cdots Elec}, \qquad \textbf{Equation 6}$$

where

$$E_{def}^{species} = E_{net}^{species} - E_{iso}^{species} \qquad \textbf{Equation 7}$$

$E_{def}^{species}$ is related to the changes of the electron density and the nuclear geometry associated with the interaction of monomer (Cat, Nuc or $Elec$) with other molecules and $E_{iso}^{species}$ denotes the energy of the isolated species.

We can write ΔE as pairwise contributions

$$\begin{aligned}\Delta E = \Bigg\{ & E_{int}^{Cat\cdots Nuc}\left[1 + \left(\frac{E_{def}^{Cat}}{E_{int}^{Cat\cdots Nuc} + E_{int}^{Cat\cdots Elec}}\right) + \left(\frac{E_{def}^{Nuc}}{E_{int}^{Nuc\cdots Cat} + E_{int}^{Nuc\cdots Elec}}\right)\right] \\ & + E_{int}^{Cat\cdots Elec}\left[1 + \left(\frac{E_{def}^{Cat}}{E_{int}^{Cat\cdots Nuc} + E_{int}^{Cat\cdots Elec}}\right) + \left(\frac{E_{def}^{Elec}}{E_{int}^{Elec\cdots Cat} + E_{int}^{Elec\cdots Nuc}}\right)\right] \\ & + E_{int}^{Nuc\cdots Elec}\left[1 + \left(\frac{E_{def}^{Nuc}}{E_{int}^{Nuc\cdots Cat} + E_{int}^{Nuc\cdots Elec}}\right)\right. \\ & \left. + \left(\frac{E_{def}^{Elec}}{E_{int}^{Elec\cdots Cat} + E_{int}^{Elec\cdots Nuc}}\right)\right]\Bigg\},\end{aligned} \qquad \textbf{Equation 8}$$

Furthermore, $E_{int}^{M\cdots N}$ term can be divided into

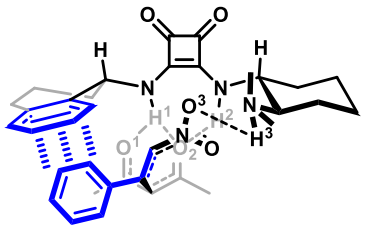
$$E_{int}^{M\cdots N} = E_{Class}^{M\cdots N} - E_{XC}^{M\cdots N} \qquad \textbf{Equation 9}$$

$E_{Class}^{M\cdots N}$ is the electrostatic component and $E_{XC}^{M\cdots N}$ is the exchange-correlation term, which are the ionic and covalent contributions of the interactions between M and N, respectively.

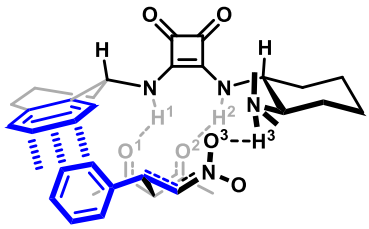
Deformation energies of Cat, Nuc and $Elec$ were considered to obtain the IQA pairwise contributions to ΔE (presented in Table 4 of the manuscript), while Table S5 shows the IQA total interaction energies of the relevant Non-Covalent Interactions involved in the diastereomeric transition states.

In Table S6, the analysis exposed that the formation energy in $TS_{(R)}$ (-29.5 kcal mol^{-1}) is superior to that in $TS_{(S)}$ (-20.8 kcal mol^{-1}). This difference arises because of the coupling between catalyst **1a** and the electrophile as well as the interaction electrophile···nucleophile which are stronger in the $TS_{(R)}$. Interestingly, the interaction energy shows that the covalence between electrophile···nucleophile is higher in *R* than in *S*, which may indicate that the formation of the C-C bond is better in the first case. In general terms, the HBs present in the $TS_{(R)}$ are greater in number and strength, which agrees with the topological data in Table S5 for these interactions (Table S7). On the other hand, a stronger π-interaction is present in $TS_{(R)}$. Something to highlight is that the coulombic component has a greater impact on $TS_{(R)}$ than on $TS_{(S)}$, which may be due to the proximity between the phenyl rings. In conclusion, the data obtained by IQA showed that $TS_{(R)}$ is a reactive specie of low energy (compared to $TS_{(S)}$), in this way the activation barrier decreased, and the reaction is highly selective. These computational results agree with the experimental data obtained.

Table S6. Formation energies of diastereomeric TSs of the IQA partition.[a]



$TS_{(R)}$-1a

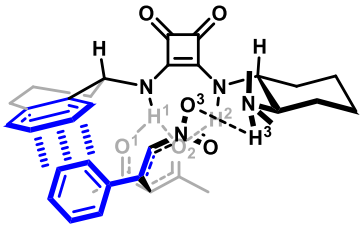


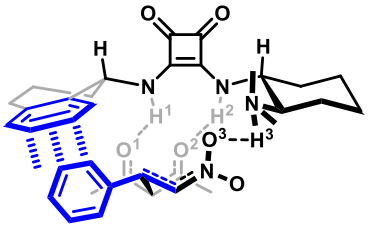
$TS_{(S)}$-1a

Interaction	*IQA energies (kcal mol^{-1})*			*IQA energies (kcal mol^{-1})*		
	Classical	**XC**	**E_{int} total**	**Classical**	**XC**	**E_{int} total**
cat···elec	-4.5	-14.6	-19.1	-3.6	-14.3	-18.0
cat···nuc	3.2	10.6	13.9	3.4	13.4	16.8
elec···nuc	-5.1	-19.2	-24.3	-3.7	-16.0	-19.7
TS formation energy			**-29.5**			**-20.8**

[a] cat = catalyst, elec = electrophile, Nuc = nucleophile, Classical = electrostatic contribution, XC = Exchange-Correlation term related to the level of covalence. IQA interaction among catalyst, nucleophile and electrophile. Deformation energies were considered.

Table S7. IQA total interaction energies between atoms and fragments in respective TSs.





Interaction	$TS_{(R)}$ *IQA energies (kcal mol^{-1})*			$TS_{(S)}$ *IQA energies (kcal mol^{-1})*		
	Classical	XC	E_{int} total	Classical	XC	E_{int} total
$H_1\cdots O_1$	-74.5	-3.2	-77.7	-85.3	-9.9	-95.2
$H_1\cdots O_2$	-82.6	-5.6	-88.2	-	-	-
$H_2\cdots O_2$	-97.5	-13.3	-110.8	-87.8	-8.2	-96.0
$H_3\cdots O_3$	-72.8	-20.5	-93.3	-70.9	-17.9	-88.8
Ar···ArCH=CH	-6.8	-22.2	-29.0	-2.4	-22.4	-24.8

IQA energies are shown in three sections: classical, XC and E_{int}. The classical component indicates the coulombic interaction, while XC designates its degree of covalence. E_{int} corresponds to the total interaction energy.

6. Experimental procedures for the synthesis of bifunctional organocatalysts and its evaluation in Michael additions

6.1. General methods

Starting materials were purchased from Sigma-Aldrich and used as received. Reactions were monitored by thin-layer chromatography (TLC) on silica gel plates F254 and the spots were detected either by UV absorption, Seebach's stain or $KMnO_4$. Flash column chromatography was carried out with silica gel 60 (0.4/0.63 mm, 230-400 mesh). ^1H and ^{13}C NMR spectra were recorded at ambient temperature using Bruker Fourier-300 MHz, Jeol Eclipse-300 MHz, and Bruker Avance III-400 MHz spectrometers. Chemical shifts (δ) are reported in ppm relative to residual solvent signals ($CDCl_3$ = δ 7.26 for ^1H NMR, δ 77.16 for ^{13}C NMR. DMSO-d_6 = δ 2.50 for ^1H NMR, δ 39.52 for ^{13}C NMR) or TMS as internal reference (δ 0.0) and coupling constants are in hertz (Hz). Mass spectra were obtained by direct analysis in real time (DART) in a JEOL AccuTOF JMST100LC spectrometer with TOF mass analyzer. CSP-HPLC analyses were performed using the indicated chiral column and UV detector. The FT-IR spectral data were recorded in a Bruker ATR in the 450-4000 cm^{-1} range. Uncorrected melting points were determined in a Fisher Johns melting point apparatus. Catalysts **1i**[14] and **1o**[15] used in this work were synthetized according to the reported procedures.

6.2. Synthesis of organocatalysts

General procedure for the isothiocyanate synthesis (S3g-j). The corresponding amine (2 mmol, 1 eq) was dissolved in 20 mL of CH_2Cl_2 and 20 mL of a saturated aqueous solution of $NaHCO_3$. Thiophosgene 0.17 mL (2.2 mmol, 1.1 eq) was added via syringe to the organic layer. The biphasic mixture was stirred for 1h at room temperature. After the separation of the two layers, the aqueous fraction was extracted with CH_2Cl_2 (2 x 15 mL). The combined organic layers were dried and concentrated. The product was purified by flash chromatography with a mixture of hexane/EtOAc, 95:5.

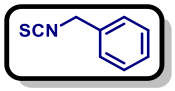
9-Isothiocyanate-9*H*-fluorene (**S3g**).

White solid (200.9 mg, 45% yield). **mp:** 88–90 °C. **IR (KBr):** $\tilde{\nu}_{max}$ cm^{-1} = 3433, 3042, 2183, 2153, 2102, 1449, 1293, 736, 680. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.69 (d, *J* = 7.5 Hz, 2H), 7.64 (d, *J* = 7.4 Hz, 2H), 7.45 (t, *J* = 7.4 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 2H), 5.71 (s, 1H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 140.96, 140.17, 129.76, 128.29, 124.96, 120.51, 115.11, 59.99. **DART (positive):** *m/z* (%) = 165 (100) $[M\text{-}NCS]^+$. **HRMS (DART/TOF):** = m/z $[M\text{-}NCS]^+$ calcd for $C_{13}H_9^\bullet$ 165.0704; found 165.0711.

5-isothiocyanate-10,11-dihydro-5*H*-dibenzo[a,d][7]annulene (**S3h**).

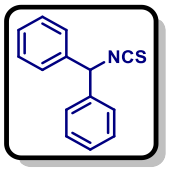
Semi-solid orange (336.7 mg, 67% yield). **IR (KBr):** $\tilde{\nu}_{max}$ cm^{-1} = 3436, 3067, 2938, 2197, 2149, 2097, 1485, 1456, 1340, 828, 754, 628. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.46 – 7.36 (m, 2H), 7.26 – 7.13 (m, 6H), 6.31 (s, 1H), 3.37 – 3.12 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 138.00, 136.36, 130.64, 128.84, 126.77, 115.11, 63.97, 32.07. **DART (positive):** *m/z* (%) = 193 (100) $[M\text{-}NCS]^+$. **HRMS (DART/TOF):** = m/z $[M\text{-}NCS]^+$ calcd for $C_{15}H_{13}^\bullet$ 193.1017; found 193.1020.

Benzyl isothiocyanate (**S3i**).



Yellow oil (274.5 mg, 92% yield). **IR (film):** $\tilde{\nu}_{max}$ cm^{-1} = 3383, 3031, 2921, 2166, 2089, 1667, 1452, 1346, 1135, 698. **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 7.64 – 7.19 (m, 5H), 4.69 (s, 2H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ = 134.29, 132.15, 129.03, 128.44, 126.90, 48.73. **DART (positive):** *m/z* (%) = 150 (11) $[M+H]^+$, 91 (100). **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for C_8H_8NS 150.0377; found 150.0387. The analytical date are in agreement with those reported previously in the literature.[16]

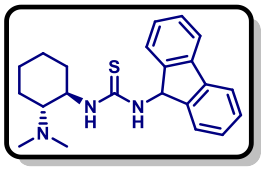
Diphenylmethyl isothiocyanate (**S3j**).



Yellow oil (351.5 mg, 78% yield). **IR (film):** $\tilde{\nu}_{max}$ cm^{-1} = 3062, 3030, 2073, 1658, 1493, 1451, 1278, 1135, 1074, 745, 698. **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 7.43 – 7.14 (m, 10H), 5.97 (s, 1H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ = 139.30, 130.17, 129.03, 128.42, 126.70, 64.70. **DART (positive):** *m/z* (%) = 167 (100) $[M\text{-}NCS]^+$. **HRMS (DART/TOF):** = m/z $[M\text{-}NCS]^+$ calcd for $C_{13}H_{11}^\bullet$ 167.0861; found 167.0858.

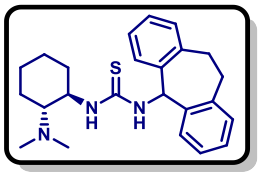
General procedure for the thiourea synthesis (S2g-j). The corresponding isothiocyanate (2 mmol, 1 equiv) was dissolved in 7 mL of CH_2Cl_2. The (*R,R*)-*N,N*-dimethyl-2-aminocyclohexaneamine (2.4 mmol, 1.2 equiv.) was added and stirred overnight at room temperature. The reaction mixture was concentrated and the catalyst purified by flash chromatography with EtOAc as eluent followed by a mixture CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1.

1-((1*R*,2*R*)-2-(Dimethylamino)cyclohexyl)-3-(9*H*-fluoren-9-yl)thiourea (**S2g**).



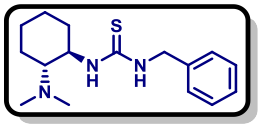
Beige solid (636.0 mg, 87% yield). **mp:** 88–90 °C. $[\alpha]_D^{25}$ +76.5° (*c* 0.52, $CHCl_3$). **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 7.86 – 7.56 (m, 4H), 7.47 – 7.17 (m, 4H), 7.05 – 6.60 (m, 1H), 4.06 – 3.77 (m, 1H), 3.28 – 2.79 (m, 2H), 2.75 – 2.55 (m, 1H), 2.42 – 2.26 (m, 1H), 2.16 (s, 6H), 1.87 – 1.65 (m, 3H), 1.25 – 1.08 (m, 4H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ = 184.53, 140.45, 128.64, 128.59, 127.76, 127.70, 125.57, 119.92, 67.39, 60.05, 55.74, 39.55, 33.12, 31.06, 24.50, 22.69. **DART (positive):** *m/z* (%) = 366 (100) $[M+H]^+$, 183 (67), 143 (63). **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{22}H_{28}N_3S$ 366.2004; found 366.1995.

1-(10,11-Dihydro-5H-dibenzo[a,d][7]annulen-5-yl)-3-((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)thiourea (**S2h**).



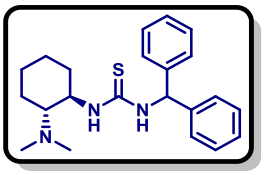
Slightly yellow solid (385.7 mg, 49% yield). **mp:** 125–127 °C. $[\alpha]_D^{25}$ +46.0° (*c* 1.3, $CHCl_3$). **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 7.67 – 7.56 (m, 1H), 7.53 – 7.32 (m, 2H), 7.25 – 7.00 (m, 7), 6.76 (s, 1H), 4.17 (s, 1H), 3.45 – 3.13 (m, 4H), 2.90 (s, 1H), 2.54 – 2.22 (m, 7H), 2.00 – 1.79 (m, 2H), 1.78 – 1.59 (m, 1H), 1.34 – 1.13 (m, 4H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ = 181.58, 139.03, 138.73, 138.49, 130.73, 130.25, 128.16, 127.95, 126.44, 126.38, 67.03, 61.55, 55.54, 39.77, 32.81, 32.30, 24.68, 24.35, 22.76. **DART (positive):** *m/z* (%) = 394 (52) $[M+H]^+$, 183 (100), 143 (49). **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{24}H_{32}N_3S$ 394.2317; found 394.2309.

1-Benzyl-3-((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)thiourea (**S2i**).



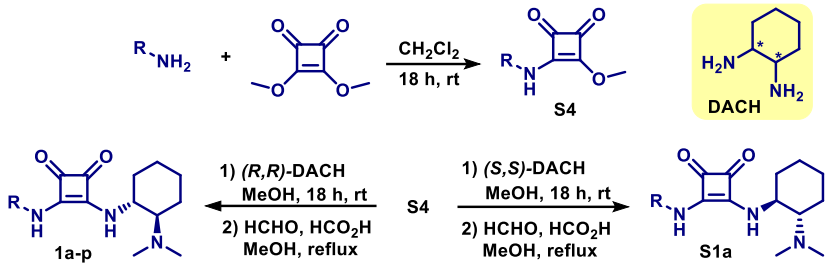
Hygroscopic yellow solid (536.2 mg, 92% yield). $[\alpha]_D^{25}$ +40.1° (*c* 0.72, $CHCl_3$) (lit.[17] *S*,*S* enantiomer, $[\alpha]_D^{25}$ -41.4° (*c* 1.0, $CHCl_3$)). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.99 (s, 1H), 7.36 – 7.20 (m, 5H), 6.91 (s, 1H), 4.73 – 4.53 (m, 2H), 4.02 – 3.81 (m, 1H), 2.65 – 2.53 (m, 1H), 2.38 (s, 1H), 2.20 (s, 6H), 1.90 – 1.74 (m, 2H), 1.74 – 1.63 (m, 1H), 1.32 – 1.11 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 182.68, 137.91, 128.68, 127.85, 127.52, 67.11, 55.66, 48.69, 39.83, 33.09, 24.78, 24.52, 22.17. **DART (positive):** *m/z* (%) = 292 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{16}H_{26}N_3S$ 292.1847; found 292.1856.

1-Benzhydryl-3-((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)thiourea (**S2j**).

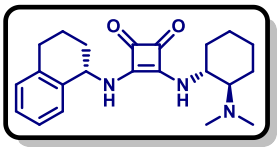


White solid (713.0 mg, 97% yield). **mp:** 78–80 °C. $[\alpha]_D^{25}$ +30.0° (*c* 1.0, $CHCl_3$). **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 7.51 – 7.13 (m, 10H), 6.78 (br, 1H), 6.33 (br, 1H), 3.92 – 3.62 (m, 1H), 2.48 (s, 2H), 2.05 (s, 6H), 1.90 – 1.73 (m, 2H), 1.73 – 1.56 (m, 1H), 1.37 – 1.00 (m, 4H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ = 182.21, 141.05, 128.78, 128.70, 127.65, 127.58, 67.09, 62.16, 56.01, 39.65, 32.85, 24.82, 24.40, 22.22. **DART (positive):** *m/z* (%) = 368 (100) $[M+H]^+$, 143 (69). **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{22}H_{29}N_3S$ 368.2160; found 368.2142.

General procedure for the squaramide synthesis (1a-p). Dimethylsquarate (**8**; 142.1 mg, 1.00 mmol), and the corresponding amine (**7a-f**; 1.00 mmol) were dissolved in 5 mL of CH_2Cl_2 and stirred at room temperature. After 18 h, the reaction mixture was filtered, and the filtrate was washed with 1 M $HCl_{(aq)}$. The organic layer was dried with Na_2SO_4, filtered, and concentrated to afford **9a-f**. The solid obtained above was dissolved in MeOH (5 mL). Subsequently, **(*R*,*R*)-DACH** or **(*S*,*S*)-DACH** (148.5 mg, 1.30 mmol) was added at ambient temperature and the reaction mixture was stirred for 18 h at the same temperature. Then, 37% aqueous formaldehyde (0.90 mL, 12.00 mmol) and formic acid (0.91 mL, 24.00 mmol) was added at room temperature. The reaction mixture was then stirred under refluxed for 24 h, basified with 6 M aqueous NaOH to pH 12 and extracted three times with CH_2Cl_2. The combined organic layers were dried over anhydrous Na_2SO_4, filtrated and concentrated in vacuo. The residue was purified by recrystallization from MeOH to give the respective compound.

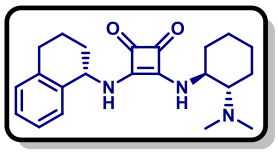


3-(((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)amino)-4-(((*S*)-1,2,3,4-tetrahydronaphthalen-1-yl)amino)cyclobut-3-ene-1,2-dione (**1a**).



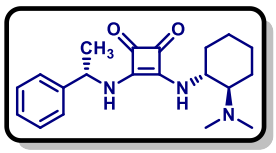
White solid (187.4 mg, 51% yield after three steps). $[\alpha]_D^{25}$ -147.9° (*c* 0.53, DMF). **^{1}H NMR (300 MHz, DMSO-*d*$_6$):** δ =7.93 (d, *J* = 8.4 Hz, 1H), 7.32 – 7.11 (m, 5H), 5.21 (bs, 1H), 3.73 (bs, 1H), 2.88 – 2.68 (m, 2H), 2.37 – 2.23 (m, 1H), 2.15 (s, 6H), 2.12 – 1.56 (m, 8H), 1.31 – 1.10 (m, 4H). **^{13}C NMR (75 MHz, DMSO-*d*$_6$):** δ = 182.08, 181.86, 167.45, 166.47, 136.93, 136.39, 129.29, 129.15, 127.55, 126.31, 66.14, 54.08, 50.85, 39.91, 34.95, 30.87, 28.47, 24.48, 24.36, 21.19, 18.33. **DART (positive):** *m/z* (%) = 368 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{22}H_{30}N_3O_2$ 368.2338; found 368.2336.

3-(((1*S*,2*S*)-2-(dimethylamino)cyclohexyl)amino)-4-(((*S*)-1,2,3,4-tetrahydronaphthalen-1-yl)amino)cyclobut-3-ene-1,2-dione (**S1a**).



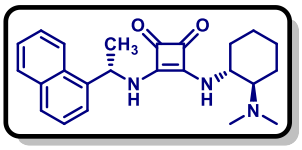
White solid (154.3 mg, 42% yield after three steps). $[\alpha]_D^{25}$ -26.0° (*c* 0.55, DMF). **^{1}H NMR (300 MHz, DMSO-*d*$_6$):** δ = 7.83 (d, *J* = 8.6 Hz, 1H), 7.30 – 7.10 (m, 5H), 5.19 (bs, 1H), 3.75 (bs, 1H), 2.88 – 2.66 (m, 2H), 2.35 – 2.23 (m, 1H), 2.17 (s, 6H), 2.12 – 1.57 (m, 8H), 1.31 – 1.09 (m, 4H). **^{13}C NMR (75 MHz, DMSO-*d*$_6$):** δ = 182.03, 181.79, 167.44, 166.57, 136.84, 136.46, 129.01, 128.91, 127.39, 126.21, 66.20, 54.06, 51.04, 40.00, 34.78, 30.94, 28.47, 24.44, 24.35, 21.43, 18.79. **DART (positive):** *m/z* (%) = 368 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{22}H_{30}N_3O_2$ 368.2338; found 368.2337.

3-(((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)amino)-4-(((*S*)-1-phenylethyl)amino)cyclobut-3-ene-1,2-dione (**1b**).



White solid (136.6 mg, 40% yield after three steps). **^{1}H NMR (300 MHz, DMSO-*d*$_6$):** δ = 7.84 (bs, 1H), 7.43 – 7.25 (m, 6H), 5.22 (bs, 1H), 3.75 (bs, 1H), 2.42 – 2.27 (m, 1H), 2.15 (s, 1H), 2.09 – 1.93 (m, 1H), 1.85 – 1.60 (m, 3H), 1.54 (d, *J* = 6.5 Hz, 3H), 1.32 – 1.06 (m, 4H). **^{13}C NMR (75 MHz, DMSO-*d*$_6$):** δ = 182.19, 181.65, 167.47, 166.65, 143.43, 128.69, 127.44, 126.15, 125.94, 66.19, 54.08, 52.62, 39.91, 34.83, 24.45, 24.38, 22.94, 21.33. **DART (positive):** *m/z* (%) = 342 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{19}H_{26}N_3O_2$ 342.21815; found 342.21668.

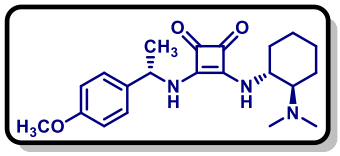
3-(((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)amino)-4-(((*S*)-1-naphthalen-1-yl)amino)cyclobut-3-ene-1,2-dione (**1c**).



White solid (168.3 mg, 43% yield after three steps). **^{1}H NMR (300 MHz, DMSO-*d*$_6$):** δ = 8.15 (d, *J* = 8.3 Hz, 1H), 8.03 – 7.85 (m, 3H), 7.67 – 7.50 (m, 4H), 7.31 (bs, 1H), 6.21 – 5.95 (m, 1H), 3.73 (bs, 1H), 2.36 – 2.20 (m, 1H), 2.12 (s, 7H), 1.85 – 1.56 (m, 6H), 1.31 – 1.05 (m, 4H). **^{13}C NMR (75 MHz, DMSO-*d*$_6$):** δ = 182.21, 181.86, 167.61, 166.64, 138.62, 133.58, 130.16, 128.86, 128.16, 126.68, 125.93, 125.53, 122.94, 122.72, 66.19, 54.10, 48.57, 39.90, 34.84, 24.44, 24.34, 22.91, 21.35. **DART (positive):** *m/z* (%) =

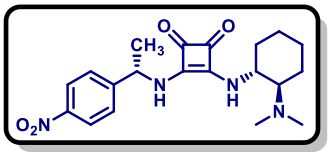
371 (15), 392 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{24}H_{30}N_3O_2$ 392.23380; found 392.23330.

3-(((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)amino)-4-(((*S*)-1-(4methoxyphenyl)ethyl)amino)cyclobut-3-ene-1,2-dione (**1d**).



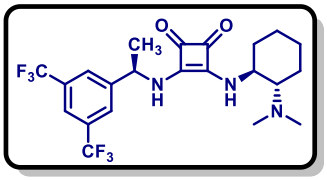
White solid (222.89 mg, 60% yield after three steps). **^{1}H NMR (300 MHz, DMSO-*d*$_6$):** δ = 7.99 (bs, 1H), 7.49 (bs, 1H), 7.32 (d, *J* = 8.7 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 5.18 (bs, 1H), 3.74 (s, 3H), 3.33 (s, 1H), 2.38 – 2.24 (m, 1H), 2.14 (s, 6H), 2.08 – 1.96 (m, 1H), 1.82 – 1.59 (m, 3H), 1.51 (d, *J* = 6.8 Hz, 3H), 1.32 – 1.08 (m, 4H). **^{13}C NMR (75 MHz, DMSO-*d*$_6$):** δ = 182.08, 181.65, 167.44, 166.63, 158.54, 135.56, 127.41, 114.00, 66.14, 55.11, 54.04, 52.03, 39.91, 34.81, 24.45, 24.41, 22.88, 21.39. **DART (positive):** *m/z* (%) = 372 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{24}H_{30}N_3O_2$ 372.22872; found 372.22883.

3-(((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)amino)-4-(((*S*)-1-(4-nitrophenyl)ethyl)amino)cyclobut-3-ene-1,2-dione (**1e**).



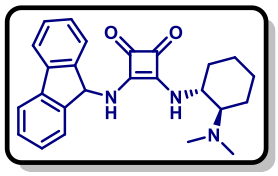
Yellow solid (112.1 mg, 29% yield after three steps). **^{1}H NMR (300 MHz, DMSO-*d*$_6$):** δ = 8.25 (d, *J* = 8.8 Hz, 2H), 7.98 (bs, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.36 (bs, 1H), 5.35 (bs, 1H), 3.76 (bs, 1H), 2.40 – 2.25 (m, 1H), 2.15 (s, 6H), 2.08 – 1.99 (bs, 1H), 1.82 – 1.59 (m, 3H), 1.57 (d, *J* = 7.0 Hz, 3H), 1.33 – 1.08 (m, 4H). **^{13}C NMR (75 MHz, DMSO-*d*$_6$):** δ = 182.31, 181.62, 167.73, 166.61, 151.37, 146.71, 127.46, 123.93, 66.15, 54.17, 52.20, 52.03, 39.95, 34.74, 24.45, 24.37, 22.57, 21.38. **DART (positive):** *m/z* (%) = 206 (45), 238 (20), 355 (100), 387 (50) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{24}H_{30}N_3O_2$ 387.20323; found 387.20324.

3-(((*R*)-1-(3,5-bis(trifluoromethyl)phenyl)ethyl)amino)-4-(((1*S*,2*S*)-2-(dimethylamino)cyclohexyl)amino)cyclobut-3-ene-1,2-dione (**1f**).



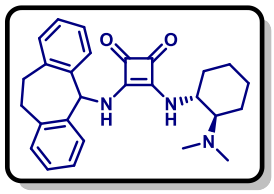
White solid (186.2 mg, 39% yield after three steps). **^{1}H NMR (300 MHz, DMSO-*d*$_6$):** δ = 8.14 – 7.98 (m, 4H), 7.42 (bs, 1H), 5.41 (bs, 1H), 3.78 (bs, 1H), 2.40 – 2.27 (m, 1H), 2.15 (s, 6H), 2.07 – 1.91 (m, 1H), 1.85 – 1.62 (m, 3H), 1.60 (d, *J* = 6.8 Hz, 3H), 1.33 – 1.08 (m, 4H). **^{13}C NMR (75 MHz, DMSO-*d*$_6$):** δ = 182.76, 181.67, 167.93, 166.62, 147.51, 130.54 (q, *J* = 32.8 Hz), 127.12, 123.30 (q, *J* = 272.8 Hz), 121.24, 66.19, 54.26, 52.06, 39.91, 34.64, 24.48, 24.38, 22.58, 21.67. **DART (positive):** *m/z* (%) = 478 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{22}H_{26}F_6N_3O_2$ 478.19292; found 478.19356.

3-((9H-fluoren-9-yl)amino)-4-(((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)amino)cyclobut-3-ene-1,2-dione (**1g**).



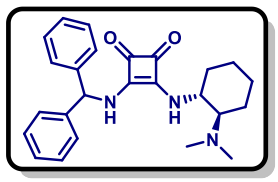
Yellow solid (16.1 mg, 4% yield after three steps). **^{1}H NMR (300 MHz, DMSO-*d*$_6$):** δ = 8.00 (bs, 1H), 7.90 (d, *J* = 7.5 Hz, 2H), 7.62 (t, *J* = 8.8 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.38 (td, *J* = 7.4, 3.5 Hz, 2H), 7.24 (bs, 1H), 6.13 (bs, 1H), 3.72 (bs, 1H), 2.38 – 2.24 (m, 1H), 2.15 (s, 6H), 2.12 – 1.97 (m, 1H), 1.81 – 1.57 (m, 3H), 1.33 – 1.07 (m, 4H). **^{13}C NMR (75 MHz, DMSO-*d*$_6$):** δ = 182.42, 182.09, 168.32, 167.27, 143.82, 139.83, 129.12, 128.09, 125.44, 120.39, 66.12, 58.25, 54.12, 39.98, 34.70, 24.46, 24.28, 21.31. **DART (positive):** *m/z* (%) = 188 (53), 402 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{22}H_{30}N_3O_2$ 402.21815; found 402.21748.

3-((10,11-dihydro-5H-dibenzo[a,d][7]annulen-5-yl)amino)-4-(((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)amino)cyclobut-3-ene-1,2-dione (**1h**).



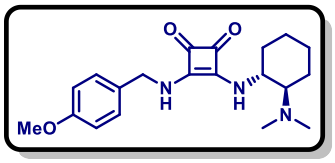
White solid (107.4 mg, 25% yield after three steps). $[\alpha]_D^{25}$ -62.5° (*c* 0.57, DMF). **^{1}H NMR (700 MHz, DMSO-*d*$_6$):** δ = 8.40 (d, *J* = 9.4 Hz, 1H), 7.44 – 7.36 (m, 3H), 7.27 – 7.19 (m, 6H), 6.54 (d, *J* = 9.3 Hz, 1H), 3.80 – 3.71 (m, 1H), 3.37 – 3.30 (m, 2H), 3.12 – 3.03 (m, 2H), 2.31 (td, *J* = 10.3, 9.9, 3.1 Hz, 1H), 2.15 (s, 6H), 2.07 – 2.02 (m, 1H), 1.82 – 1.59 (m, 3H), 1.27 – 1.11 (m, 4H). **^{13}C NMR (176 MHz, DMSO-*d*$_6$):** δ = 182.31, 181.62, 167.53, 165.80, 138.82, 138.77, 138.69, 138.26, 130.61, 130.23, 128.86, 128.55, 128.12, 128.08, 126.55, 126.49, 66.24, 60.97, 54.16, 40.02, 34.87, 32.19, 31.80, 24.41, 24.39, 21.20. **DART (positive):** *m/z* (%) = 193 (100), 430 (16) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{27}H_{32}N_3O_2$ 430.24945; found 430.24798.

3-(benzhydrylamino)-4-(((1*R*,2*R*)-2-(dimethylamino)cyclohexyl)amino)cyclobut-3-ene-1,2-dione (**1j**).



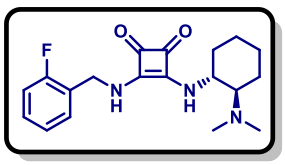
White solid (149.3 mg, 37% yield after three steps). $[\alpha]_D^{25}$ -22.7° (*c* 0.11, DMF). **^{1}H NMR (700 MHz, DMSO-*d*$_6$):** δ = 8.37 (bs, 1H), 7.45 – 7.36 (m, 5H), 7.32 – 7.27 (m, 6H), 6.42 (bs, 1H), 3.76 (bs, 1H), 2.39 – 2.29 (m, 1H), 2.17 (s, 6H), 2.11 – 2.04 (m, 1H), 1.85 – 1.58 (m, 3H), 1.32 – 1.12 (m, 4H). **^{13}C NMR (176 MHz, DMSO-*d*$_6$):** δ = 182.62, 181.70, 167.70, 166.56, 142.00, 128.78, 128.73, 127.54, 127.43, 127.11, 126.93, 126.88, 66.24, 60.26, 54.19, 40.01, 34.80, 24.45, 24.38, 21.40. **DART (positive):** *m/z* (%) = 89 (100), 167 (31), 404 (82) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{25}H_{30}N_3O_2$ 404.23380; found 404.23306.

3-(((1R,2R)-2-(dimethylamino)cyclohexyl)amino)-4-((4-methoxybenzyl)amino)cyclobut-3-ene-1,2-dione (**1k**).



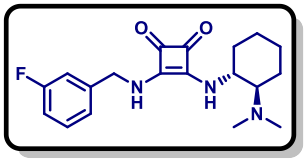
White solid (53.6 mg, 15% yield after three steps). **^{1}H NMR (400 MHz, DMSO-*d*$_6$):** δ = 7.43 (bs, 1H), 7.27 (d, *J* = 8.5 Hz, 2H), 7.20 (bs, 1H), 6.93 (d, *J* = 8.6 Hz, 2H), 4.63 (bs, 2H), 3.79 (bs, 1H), 3.74 (s, 3H), 3.36 – 2.00 (m, 8H), 1.82 – 1.59 (m, 3H), 1.31 – 1.15 (m, 4H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$):** δ = 181.98, 181.59, 167.46, 167.24, 158.69, 130.92, 129.20, 114.07, 66.16, 55.12, 54.02, 46.27, 35.00, 34.77, 24.47, 24.36, 21.38. **DART (positive):** *m/z* (%) = 358 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{20}H_{27}N_3O_3$ 358.21307; found 358.21261.

3-(((1R,2R)-2-(dimethylamino)cyclohexyl)amino)-4-((2-fluorobenzyl)amino)cyclobut-3-ene-1,2-dione (**1l**).



White solid (13.8 mg, 4% yield after three steps). Mixture of rotamers. **^{1}H NMR (400 MHz, DMSO-*d*$_6$):** δ = 7.88 (bs, 1H), 7.49 – 7.36 (m, 3H), 7.32 – 7.13 (m, 2), 4.78 (bs, 2H), 3.76 (bs, 1H), 2.36 – 2.27 (m, 1H), 2.18 – 2.04 (m, 7H), 1.83 – 1.61 (m, 3H), 1.30- 1.12 (m, 4H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$):** δ = 182.22, 182.06, 167.96, 167.72, 130.54, 130.33, 125.23, 116.02, 115.82, 66.64, 54.56, 54.49, 35.47, 35.23, 24.95, 24.91, 21.87. **DART (positive):** *m/z* (%) = 346 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{19}H_{25}FN_3O_2$ 346.19308; found 346.19283.

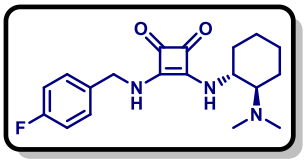
3-(((1R,2R)-2-(dimethylamino)cyclohexyl)amino)-4-((3-fluorobenzyl)amino)cyclobut-3-ene-1,2-dione (**1m**).



White solid (82.9 mg, 24% yield after three steps). **^{1}H NMR (400 MHz, DMSO-*d*$_6$):** δ = 7.88 (bs, 1H), 7.48 – 7.33 (m, 2H), 7.23 – 7.06 (m, 3H), 4.73 (bs, 2H), 3.76 (bs, 1H), 2.36 – 2.28 (m, 1H), 2.16 (s, 6H), 2.09 – 1.97 (m, 1H), 1.82 – 1.59 (m, 3H), 1.31 – 1.11 (m, 4H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$):** δ = 182.24, 181.94, 167.65, 167.24, 162.27 (d, *J* = 244.1 Hz), 141.40, 130.70, 123.72, 114.38 (d, *J* = 21.4 Hz),

114.23 (d, *J* = 20.8 Hz), 66.15, 54.14, 46.18, 39.94, 34.72, 24.48, 24.37, 21.42. **DART (positive):** *m/z* (%) = 346 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{19}H_{25}FN_3O_2$ 346.19308; found 346.19283.

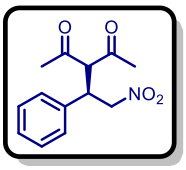
3-(((1R,2R)-2-(dimethylamino)cyclohexyl)amino)-4-((4-fluorobenzyl)amino)cyclobut-3-ene-1,2-dione (**1n**) White solid (48.3 mg, 14% yield after three steps). Mixture of rotamers. **^{1}H NMR (400 MHz, DMSO-*d*$_6$):** δ = 7.88 (bs, 1H), 7.48 – 7.28 (m, 3H), 7.26 – 7.09 (m, 2H), 4.69 (bs, 2H), 3.77 (bs 1H), 2.37 – 1.91 (m, 8H), 1.83 – 1.58 (m, 3H), 1.34 – 1.11 (m, 4H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$):** δ = 182.25, 181.58, 167.29, 167.24, 161.46 (d, *J* = 242.9 Hz), 135.23, 135.08, 129.87 (d, *J* = 8.2 Hz), 129.43, 115.36 (d, *J* = 21.3), 66.16, 57.49, 54.01, 46.00, 34.99, 32.70, 24.46, 21.39. **DART (positive):** *m/z* (%) = 346 (100) $[M+H]^+$. **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{19}H_{25}FN_3O_2$ 346.19308; found 346.19289.



6.3. Michael additions

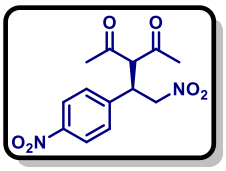
General procedure for conjugate addition reactions. To a solution of nitrostyrene (0.25 mmol) and the respective organocatalyst (1.0 mol%) in toluene (0.76 mL) was added 1,3-dicarbonyl compound (0.50 mmol). After 24 hours the reaction mixture was concentrated and purified by flash chromatography with a mixture of hexane/EtOAc (7:3) to afford the conjugate addition product.

(*R*)-3-(2-Nitro-1-phenylethyl)-pentane-2,4-dione (**4a**).



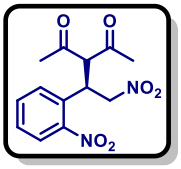
White solid (59.2 mg, 95% yield). **mp:** 110–111°C. $[\alpha]_D^{25}$ -190.3° (*c* 1.19, $CHCl_3$), 97% ee (lit.[18] mp: 112 – 114°C, $[\alpha]_D^{25}$ -175.4° (*c* 1.08, $CHCl_3$), 89% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.36 – 7.12 (m, 5H), 4.68 – 4.59 (m, 2H), 4.37 (d, *J* = 10.7, Hz, 1H), 4.29 – 4.20 (m, 1H), 2.28 (s, 3H), 1.94 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 201.84, 201.12, 136.13, 129.41, 128.62, 128.05, 78.27, 70.77, 42.91, 30.54, 29.71. **HPLC** (Chiralpak IA, hexane/isopropanol 90:10, 1.0 mL/min, 208 nm): t_{major} = 13.183 min, t_{minor} = 10.357 min.

(*R*)-3-(2-Nitro-1-(4-nitrophenyl)ethyl)pentane-2,4-dione (**4b**).



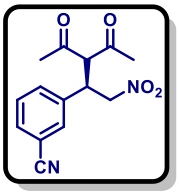
Beige solid (63.3 mg, 86% yield). **mp:** 115–118°C. $[\alpha]_D^{25}$ -101.2° (*c* 1.2, $CHCl_3$), 96% ee (lit.[1a] *S* enantiomer $[\alpha]_D^{25}$ +99.9° (*c* 1.03, $CHCl_3$), 84% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.20 (d, J = 8.8 Hz, 2H), 7.43 (d, J = 8.8 Hz, 2H), 4.76 – 4.65 (m, 2H), 4.45 – 4.35 (m, 2H), 2.33 (s, 3H), 2.04 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 200.93, 200.10, 147.92, 143.83, 129.28, 124.49, 77.43, 70.11, 42.44, 30.67, 30.14. **HPLC** (Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 15.356 min, t_{minor} = 11.679 min.

(*R*)-3-(2-Nitro-1-(2-nitrophenyl)ethyl)pentane-2,4-dione (**4c**).



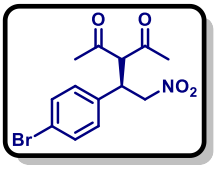
Beige solid (64.7 mg, 88% yield). **mp:** 110–111°C. $[\alpha]_D^{25}$ -107.8° (*c* 1.2, $CHCl_3$), 91% ee (lit.[19] mp: 112 – 114°C, $[\alpha]_D^{25}$ -123.1 ° (*c* 1.0, $CHCl_3$), 97% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.93 (dd, J = 8.1, 1.3 Hz, 1H), 7.59 (td, J = 7.7, 1.3 Hz, 1H), 7.48 (td, J = 8.1, 1.3 Hz, 1H), 7.37 (dd, J = 7.9, 1.1 Hz, 1H), 4.97 (dd, J = 13.3, 7.2 Hz, 1H), 4.84 (dd, J = 13.3, 3.7 Hz, 1H), 4.75 (td, J = 7.9, 7.2, 3.7 Hz, 1H), 4.68 (d, J = 8.7 Hz, 1H), 2.31 (s, 3H), 2.14 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 201.72, 200.68, 149.92, 133.60, 131.36, 129.47, 129.32, 125.65, 76.68, 69.17, 37.25, 31.39, 29.49. **HPLC** (Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 18.655 min, t_{minor} = 15.051 min.

(*R*)-3-(2-nitro-1-(3-cyanophenyl)ethyl)pentane-2,4-dione (**4d**).



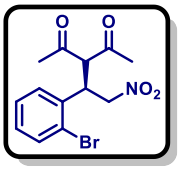
White solid (58.9 mg, 86% yield). $[\alpha]_D^{25}$ -122.3° (*c* 1.3, $CHCl_3$), 91% ee. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.65 – 7.55 (m, 2H), 7.52 – 7.45 (m, 2H), 4.73 – 4.64 (m, 2H), 4.40 (d, J = 10.5 Hz, 1H), 4.36 – 4.28 (m, 1H), 2.32 (s, 3H), 2.03 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 201.04, 200.25, 138.19, 132.76, 132.23, 131.66, 130.24, 118.16, 113.50, 77.51, 70.06, 42.30, 30.65, 30.14. **DART (positive):** *m/z* (%) = 275 (100) $[M+H]^+$, 172 (22), 101 (37). **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{14}H_{14}N_2O_4$ 275.10318; found 275.10325. **HPLC** (Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 19.320 min, t_{minor} = 14.392 min.

(*R*)-3-(1-(4-bromophenyl)-2-nitroethyl)pentane-2,4-dione (**4e**).



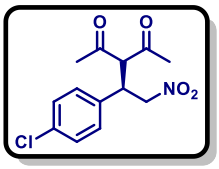
White solid (73.8 mg, 90% yield). $[\alpha]_D^{25}$ -136.5° (*c* 1.28, $CHCl_3$), 98% ee (lit.[19] $[\alpha]_D^{25}$ -143.1° (*c* 1.0, $CHCl_3$), 98% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.46 (d, J = 8.5 Hz, 2H), 7.08 (d, J = 8.4 Hz, 2H), 4.66 – 4.58 (m, 2H), 4.33 (d, J = 10.7 Hz, 1H), 4.22 (dt, J = 10.7, 6.3 Hz, 1H), 2.29 (s, 3H), 1.98 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 201.46, 200.67, 135.24, 132.59, 129.75, 122.73, 77.94, 70.51, 42.31, 30.56, 29.85. **HPLC** (Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 9.720 min, t_{minor} = 6.937 min.

(*R*)-3-(1-(2-bromophenyl)-2-nitroethyl)pentane-2,4-dione (**4f**).



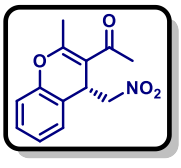
White solid (60.7 mg, 74% yield). **mp:** 82–83°C. $[\alpha]_D^{25}$ -190.9° (*c* 1.95, $CHCl_3$), 97% ee (lit.[19] mp: 87–88°C, $[\alpha]_D^{25}$ -218.5° (*c* 1.0, $CHCl_3$), 98% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.63 (dd, J = 8.0, 1.3 Hz, 1H), 7.29 (td, J = 7.6, 1.3 Hz, 1H), 7.20 – 7.12 (m, 2H), 4.84 (dd, J = 12.2, 6.4 Hz, 1H), 4.78 – 4.71 (m, 1H), 4.67 (dd, J = 12.2, 4.0 Hz, 1H), 4.60 (d, J = 9.6 Hz, 1H), 2.28 (s, 3H), 2.05 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 202.06, 200.99, 135.17, 134.12, 130.07, 128.91, 128.37, 124.66, 76.37, 69.19, 41.18, 31.12, 28.56. **HPLC** (Chiralpak IA, hexane/ethanol 95:5, 0.8 mL/min, 220 nm): t_{major} = 17.510 min, t_{minor} = 13.779 min, 97% ee; $[\alpha]_D^{25}$ -190.9° (*c* 1.95, $CHCl_3$).

(*R*)-3-(1-(4-Chlorophenyl)-2-nitroethyl)pentane-2,4-dione (**4g**).



White solid (65.2 mg, 92% yield). **mp:** 117–118°C. $[\alpha]_D^{25}$ -143.2° (*c* 1.42, $CHCl_3$), 90% ee (lit.[20] mp: 119–121°C, $[\alpha]_D^{25}$ -132.5° (*c* 1.04, $CHCl_3$), 88% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.31 (d, *J* = 8.5 Hz, 2H), 7.14 (d, *J* = 8.5 Hz, 2H), 4.62 (d, J = 6.4 Hz, 2H), 4.33 (d, J = 10.7 Hz, 1H), 4.23 (dt, J = 10.7, 6.3 Hz, 1H), 2.28 (s, 3H), 1.97 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 201.47, 200.71, 134.71, 134.58, 129.62, 129.45, 78.00, 70.54, 42.24, 30.54, 29.84. **HPLC** (Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 9.402 min, t_{minor} = 6.923 min.

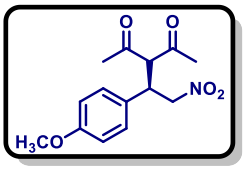
(*R*)-1-(2-methyl-4-(nitromethyl)-4H-chromen-3-yl)ethan-1-one (**4h**).[21]



To a solution of *trans*-2-Hydroxy-β-nitrostyrene (0.25 mmol) and organocatalyst (1.0 mol%) in toluene (0.76 mL) was added 2,4-Pentanedione (0.50 mmol). After 24 hours PTSA monohydrate (20 mol%) were added, and the mixture was heated for 2 h at 100 °C. The solution was cooled to rt, the solvent eliminated under vacuum, and the residue was purified by flash chromatography to afford the product **4h**. Yellow oil (56.8 mg, 92% yield). $[\alpha]_D^{25}$ +19.7° (*c* 0.96, $CHCl_3$), 94% ee (lit.[21] *S* enantiomer $[\alpha]_D^{25}$ -23.7° (*c* 0.5, $CHCl_3$), 98% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.30 – 7.25 (m, 1H), 7.21 – 7.16 (m, 1H), 7.15 – 7.10 (m, 1H), 7.06 (dd, J = 8.2, 1.0 Hz, 1H), 4.68 – 4.62 (m, 1H), 4.52 – 4.45 (m, 1H), 4.40 – 4.33 (m, 1H), 2.47 (s, 3H), 2.46 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 196.87, 163.87, 150.64, 129.07, 128.19, 125.33, 120.73, 116.44, 111.51, 80.31, 35.28,

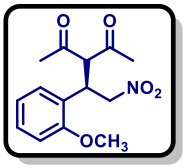
31.02, 21.08. **HPLC** (Chiralcel OD, hexane/isopropanol 90:10, 1.0 mL/min, 254 nm): t_{major} = 12.717 min, t_{minor} = 10.371 min. Absolute configuration was determined by comparing the optical rotation and the retention time of HPLC of **4h** with that of literature data.[21]

(*R*)-3-(1-(4-Methoxyphenyl)-2-nitroethyl)pentane-2,4-dione (**4i**).



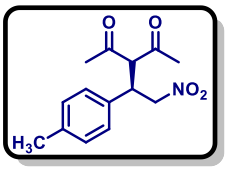
White solid (69.1 mg, 99% yield). **mp:** 117–118°C. $[\alpha]_D^{25}$ -156.1° (*c* 1.22, $CHCl_3$), 92% ee (lit.[19] $[\alpha]_D^{25}$ -191.6° (*c* 1.0, $CHCl_3$), 98% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.11 (d, *J* = 8.7 Hz, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 4.59 (d, J = 6.5 Hz, 2H), 4.33 (d, J = 10.8 Hz, 1H), 4.19 (dt, J = 10.9, 6.4 Hz, 1H), 3.76 (s, 3H), 2.27 (s, 3H), 1.94 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 201.92, 201.27, 159.56, 129.15, 127.76, 114.73, 78.50, 70.91, 55.28, 42.21, 30.46, 29.62. **HPLC** (Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 14.312 min, t_{minor} = 10.417 min.

(*R*)-3-(1-(2Methoxyphenyl)-2-nitroethyl)pentane-2,4-dione (**4j**).



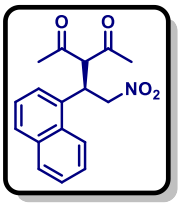
Pale yellow viscous oil (64.9 mg, 93% yield). $[\alpha]_D^{25}$ -199.5° (*c* 1.48, $CHCl_3$) 90% ee, (lit.[20] $[\alpha]_D^{25}$ -200.0° (*c* 0.94, $CHCl_3$) 92% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ =7.26 (td, J = 8.1, 1.7 Hz, 1H), 7.08 (dd, J = 8.0, 1.6 Hz, 1H), 6.92 – 6.85 (m, 2H), 4.79 (dd, J = 12.2, 8.0 Hz, 1H), 4.62 – 4.56 (m, 2H), 4.48 (ddd, J = 10.8, 8.0, 4.3 Hz, 1H), 3.88 (s, 3H), 2.26 (s, 3H), 1.93 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 202.35, 201.67, 157.12, 130.34, 129.82, 123.64, 121.23, 111.35, 76.63, 69.02, 55.52, 39.10, 30.52, 28.91. **HPLC** (Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 11.262 min, t_{minor} = 9.062 min.

(*R*)-3-(2-Nitro-1-(*p*-tolyl)ethyl)pentane-2,4-dione (**4k**).



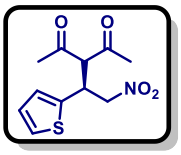
White solid (63.8 mg, 97% yield). **mp:** 98–99°C. $[\alpha]_D^{25}$ -183.4° (*c* 1.07, $CHCl_3$), 97% ee (lit.[20] mp: 101–103°C, $[\alpha]_D^{25}$ -167.7° (*c* 1.5, $CHCl_3$), 89% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.12 (d, J = 8.0 Hz, 2H), 7.06 (d, J = 8.2 Hz, 2H), 4.65 – 4.56 (m, 2H), 4.35 (d, J = 10.8 Hz, 1H), 4.20 (ddd, J = 10.8, 7.3, 5.5 Hz, 1H), 2.30 (s, 3H), 2.28 (s, 3H), 1.94 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 201.96, 201.22, 138.42, 132.96, 130.07, 127.88, 78.45, 70.88, 42.57, 30.51, 29.61, 21.14. **HPLC** (Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 10.933 min, t_{minor} = 8.043 min.

(*R*)-3-(1-(Naphthalen-1-yl)-2-nitroethyl)pentane-2,4-dione (**4l**).



Yellow viscous liquid (65.8 mg, 88% yield). $[\alpha]_D^{25}$ -189.3° (*c* 1.08, $CHCl_3$), 95% ee (lit.[20] $[\alpha]_D^{25}$ -182.0° (*c* 1.10, $CHCl_3$), 95% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.17 (d, J = 8.5 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.81 (d, J = 8.2 Hz, 1H), 7.67 – 7.61 (m, 1H), 7.57 – 7.52 (m, 1H), 7.43 – 7.38 (m, 1H), 7.28 (d, J = 6.8 Hz, 1H), 5.26 – 5.16 (m, 1H), 4.85 – 4.78 (m, 1H), 4.76 – 4.68 (m, 2H), 2.32 (s, 3H), 1.87 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 202.46, 200.91, 134.42, 132.05, 130.92, 129.61, 129.34, 127.50, 126.46, 125.38, 124.92, 122.01, 77.88, 70.59, 36.52, 31.15, 28.77. **HPLC** (Chiralpak IA, hexane/ethanol 85:15, 0.8 mL/min, 220 nm): t_{major} = 14.423 min, t_{minor} = 11.760 min.

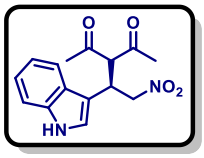
(*S*)-3-(2-Nitro-1-(thiophen-2-yl)ethyl)pentane-2,4-dione (**4m**).



Beige semisolid (58.1 mg, 91% yield). $[\alpha]_D^{25}$ -138.2° (*c* 1.04, $CHCl_3$), 96% ee (lit.[1a] *R* enantiomer $[\alpha]_D^{25}$ +126.5° (*c* 1.10, $CHCl_3$), 89% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.24 (dd, J = 5.1, 1.0 Hz, 1H), 6.96 – 6.91 (m, 1H), 6.91 – 6.87 (m, 1H), 4.67 (d, J = 6.0 Hz, 2H), 4.59 – 4.51 (m, 1H), 4.41 (d, J = 10.1 Hz, 1H), 2.29 (s, 3H), 2.08 (s, 3H). **^{13}C NMR (100**

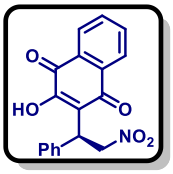
MHz, $CDCl_3$): δ = 201.57, 200.79, 138.58, 127.46, 127.09, 125.82, 78.60, 71.10, 38.33, 30.66, 29.78. **HPLC** (Chiralcel OJ, hexane/ethanol 70:30, 1.0 mL/min, 220 nm): t_{major} = 37.775 min, t_{minor} = 30.539 min.

(*R*)-3-(1-(1H-indol-3-yl)-2-nitroethyl)pentane-2,4-dione (**4n**).[22]



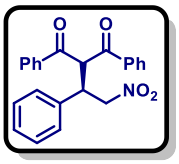
Yellow solid (68.5 mg, 95% yield). **mp**: 267 – 269°C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.26 (bs, 1H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.27 – 7.14 (m, 2H), 6.99 (d, *J* = 2.0 Hz, 1H), 4.81 – 4.64 (m, 2H), 4.63 – 4.52 (m, 2H), 2.30 (s, 3H), 1.94 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 202.84, 202.00, 136.25, 125.71, 123.46, 123.07, 120.54, 118.06, 111.89, 110.44, 77.96, 70.40, 34.62, 30.68, 28.52. **DART (positive):** *m/z* (%) = 289 (17) $[M+H]^+$, 288 (30), 282 (73), 242 (70), 228 (36), 198 (40), 189 (100), 143 (48), 125 (65). **HRMS (DART/TOF):** = m/z $[M+H]^+$ calcd for $C_{15}H_{16}N_2O_4$ 289.11883; found 289.11797. **HPLC** (Chiralpak IC, hexane/ isopropanol 90:10, 1.0 mL/min, 220 nm): t_{major} = 13.113 min, t_{minor} = 11.270 min, 83% ee.

(*S*)-2-Hydroxy-3-(2-nitro-1-phenylethyl)naphthalene-1,4-dione (**5a**).



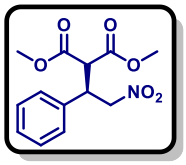
Purified by flash chromatography with a mixture of DCM/EtOAc (9:1). Yellow solid (77.6 mg, 96% yield). **mp:** 148–149°C. $[\alpha]_D^{25}$ +32.4° (*c* 0.72, $CHCl_3$), 97% ee (lit.[23] mp: 147–149°C, $[\alpha]_D^{25}$ +37.0° (*c* 1.0, acetone), 99% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.14 – 8.01 (m, 2H), 7.87 – 7.78 (b, 1H), 7.75 (td, J = 7.6, 1.4 Hz, 1H), 7.67 (td, J = 7.5, 1.3 Hz, 1H), 7.50 – 7.41 (m, 2H), 7.36 – 7.21 (m, 3H), 5.48 (dd, J = 13.3, 9.0 Hz, 1H), 5.31 (dd, J = 9.0, 6.8 Hz, 1H), 5.15 (dd, J = 13.3, 6.8 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 183.83, 181.26, 153.37, 137.67, 135.56, 133.43, 132.74, 129.11, 128.41, 127.97, 127.34, 126.47, 120.94, 76.49, 39.80. **HPLC** (Chiralpak IA, hexane/ethanol 90:10, 0.8 mL/min, 254 nm): t_{major} = 30.107 min, t_{minor} = 43.223 min.

(*R*)-2-(2-Nitro-1-phenylethyl)-1,3-diphenylpropane-1,3-dione (**5b**).



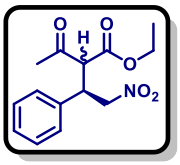
Purified by flash chromatography with a mixture of hexne/EtOAc (85:15). White solid (79.3 mg, 85% yield). $[\alpha]_D^{25}$ -21.7 (*c* 0.92, $CHCl_3$), 98% ee, (lit.[24] $[\alpha]_D^{25}$ -6.5 (*c* 0.25, CH_2Cl_2), 90% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.93 – 7.72 (m, 4H), 7.52 (dt, J = 15.1, 7.4 Hz, 2H), 7.45 – 7.32 (m, 4H), 7.28 – 7.12 (m, 5H), 5.84 (d, J = 8.0 Hz, 1H), 4.99 (d, J = 6.8 Hz, 2H), 4.62 (q, J = 7.2 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 194.36, 193.72, 136.93, 136.33, 135.96, 134.20, 133.92, 129.11, 129.09, 128.96, 128.91, 128.74, 128.39, 128.29, 77.44, 60.03, 44.17. **HPLC** (Chiralpak IA, hexane/ethanol 85:15, 0.8 mL/min, 250 nm): t_{major} = 15.370 min, t_{minor} = 18.270 min.

Dimethyl (*R*)-2-(2-nitro-1-phenylethyl)malonate (**5c**).



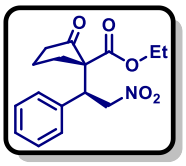
To a solution of *trans*-β-nitrostyrene (0.25 mmol) and the respective organocatalyst (1.0 mol%) in toluene (0.76 mL) was added Dimethyl malonate (0.50 mmol). After 7 days the reaction mixture was concentrated and purified by flash chromatography with a mixture of hexane/EtOAc (85:15) to afford the product **5c**. White solid (46.4 mg, 66% yield). **mp:** 64–65°C. $[\alpha]_D^{25}$ -6.5° (*c* 2.83, $CHCl_3$), 92% ee (lit.[18] mp: 63–64°C, $[\alpha]_D^{25}$ -6.15° (*c* 1.10, $CHCl_3$), 89% ee). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.35 – 7.20 (m, 5H), 4.96 – 4.84 (m, 2H), 4.24 (td, J = 8.9, 5.3 Hz, 1H), 3.87 (d, J = 9.0 Hz, 1H), 3.76 (s, 3H), 3.56 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** 167.96, 167.35, 136.26, 129.14, 128.54, 127.98, 77.48, 54.88, 53.13, 52.95, 43.06. **HPLC** (Chiralpak IC, hexane/ethanol 85:15, 0.6 mL/min, 220 nm): t_{major} = 7.877 min, t_{minor} = 7.020 min.

Ethyl (*3R*)-2-acetyl-4-nitro-3-phenylbutanoate (**5d**).



Purified by flash chromatography with a mixture of hexane/EtOAc (85:15). White semisolid (63.5 mg, 91% yield). Mixture of diastereomers (dr = 75:25). $[\alpha]_D^{25}$ -81.3° (*c* 1.14, $CHCl_3$) (lit.[18] $[\alpha]_D^{25}$ -50.3° (*c* 1.04, $CHCl_3$)). **^{1}H NMR (400 MHz, $CDCl_3$):** δ =7.36 – 7.14 (m, 5H), 4.88 – 4.69 (m, 2H), 4.28 – 3.91 (m, 4H), 2.29 (s, 2.25H), 2.05 (s, 0.75H), 1.27 (t, J = 7.1 Hz, 0.75H), 1.00 (t, J = 7.1 Hz, 2.75H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 201.24, 200.43, 167.62, 166.96, 136.55, 136.50, 129.23, 129.02, 128.44, 128.36, 128.08, 128.00, 77.98, 77.89, 62.30, 62.10, 62.04, 61.78, 42.66, 42.42, 30.37, 30.16, 14.07, 13.76. **HPLC** (Chiralpak IA, hexane/ethanol 85:15, 1.0 mL/min, 220 nm): major diastereomer: t_{major} = 12.053 min, t_{minor} = 7.910 min, 98% ee, minor diastereomer: t_{major} = 9.513 min, t_{minor} = 10.743 min, 93% ee.

Ethyl (*R*)-1-((*S*)-2-nitro-1-phenylethyl)-2-oxocyclopentane-1-carboxylate (**5e**).[14]



Purified by flash chromatography with a mixture of hexane/EtOAc (85:15). Colorless liquid (70.9 mg, 93% yield). Mixture of diastereomers (dr = 97:3). $[\alpha]_D^{25}$ -23.1° (*c* 1.24, $CHCl_3$). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.34 – 7.23 (m, 5H), 5.18 (dd, J = 13.6, 3.9 Hz, 1H), 5.01 (dd, J = 13.6, 10.9 Hz, 1H), 4.24 – 4.17 (m, 2H), 4.08 (dd, J = 10.9, 3.9 Hz, 1H), 2.41 – 2.26 (m, 2H), 2.05 – 1.77 (m, 4H), 1.30 – 1.24 (m, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 212.41, 169.44, 135.52, 129.47, 128.93, 128.41, 76.62, 62.33, 46.35, 38.02, 31.38, 29.84, 19.49, 14.11. **HPLC** (Chiralpak IA, hexane/ethanol 97:3, 0.4 mL/min, 220 nm): major diastereomer: t_{major} = 43.720 min, t_{minor} = 46.080 min, 90% ee, minor diastereomer: t_{major} = 37.240 min, t_{minor} = 40.520 min, 44% ee.

General procedure for catalyst recycling. To a solution of nitrostyrene (0.25 mmol) and the respective organocatalyst (1.0 mol%) in toluene (0.76 mL) was added 1,3-dicarbonyl compound (0.50 mmol). After 24 hours the crude reaction was filtered over a short plug of silica gel. The main product was recovered by washing with ethyl acetate and later the catalyst eluting with a mixture of DCM-MeOH (9:1). The recovered catalyst was dried under vacuum for use it in a subsequent cycle.

General procedure for large-scale conjugate addition reactions. To a solution of nitrostyrene (5 mmol) and the respective catalytic load (0.1–0.01 mol%) in dichloroethane (1.5 mL) was added 1,3-dicarbonyl compound (10.0 mmol). After 24 hours the reaction mixture was concentrated and purified by flash chromatography with a mixture of hexane/EtOAc (7:3) to afford the conjugate addition product.

7. References

[1] (a) E. I. Jiménez, W. E. Vallejo Narváez, C. A. Román-Chavarría, J. Vazquez-Chavez, T. Rocha-Rinza, and M. Hernández-Rodríguez, Bifunctional Thioureas with α-Trifluoromethyl or Methyl Groups: Comparison of Catalytic Performance in Michael Additions, *J. Org. Chem.,* 2016, **81**, 7419; (b) E. I. Jiménez, W. E. Vallejo Narváez, T. Rocha-Rinza, and M. Hernández-Rodríguez, Design and Application of a Bifunctional Organocatalyst Guided by Electron Density Topological Analyses, *Catal. Sci. Technol.,* 2017, **7**, 4470.

[2] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma,

V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[3] (a) S. Grimme, Semiempirical GGA–type density functional constructed with a long–range dispersion correction. *J Comput Chem*, 2006, **27**, 1787; (b) S. E. Wheeler, Local Nature of Substituent Effects in Stacking Interactions, *J. Am. Chem. Soc*., 2011, **133**, 10262.

[4] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).

[5] M, Orlandi, J. A. S. Coelho, M. J. Hilton, F. D. Toste, and M. S. Sigman, Parametrization of Non-covalent Interactions for Transition State Interrogation Applied to Asymmetric Catalysis, *J. Am. Chem. Soc*., 2017, **139**, 6803.

[6] A. V. Brethomé, S. P. Fletcher, and R. S. Paton, Conformational Effects on Physical-Organic Descriptors: The Case of Sterimol Steric Parameters, *ACS Catal*., 2019, **9**, 2313.

[7] (a) D. O'Hagan, Understanding organofluorine chemistry. An introduction to the C–F bond, *Chem. Soc. Rev.,* 2008, **37**, 308. (b) H.-J. Schneider, Hydrogen bonds with fluorine. Studies in solution, in gas phase and by computations, conflicting conclusions from crystallographic analyses, *Chem. Sci.,* 2012, **3**, 1381. (c) P. A. Champagne, J. Desroches, and J.-F. Paquin, Organic Fluorine as a Hydrogen-Bond Acceptor: Recent Examples and Applications, *Synthesis*, 2015, **47**, 306.

[8] B. J. Rooks, M. R. Hass, D. Sepúlveda, T. Lu, and S. E. Wheeler, Prospects for the Computational Design of Bipyridine *N*,*N*'-Dioxide Catalysts for Asymetric Propargylation Reactions, *ACS Catal*, 2015, **5**, 272.

[9] Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[10] AIMALL (Version 16.10.31), Keith, T. A.; TK Gristmill Software, Overland Park KS, USA, 2016 (aim.tkgristmill.com)

[11] E. Espinosa, E. Molins, and C. Lecomte, Hydrogen bond strengths revealed by topological analyses of experimentally observed electron densities, *Chem. Phys. Lett.,* 1998, **285**, 170.

[12] M. A. Blanco, A. Martín Pendás and E. Francisco, *J. Chem. Theory Comput*., 2005, **1**, 1096.

[13] J. M. Guevara-Vela, R. Chávez-Calvillo, M. García-Revilla, J. Hernández-Trujillo, O. Christiansen, E. Francisco, Á. Martín Pendás and T. Rocha-Rinza, *Chem. Eur. J.*, 2013, **19**, 14304.

[14] B. Kotai, G. Kardos, A. Hamza, V. Farkas, I. Papai, and T. Soos, On the Mechanism of Bifunctional Squaramide–Catalyzed Organocatalytic Michael Addition: A Protonated Catalyst as an Oxyanion Hole, *Chem. Eur. J*., 2014, **20**, 5631.

[15] D. Mailhol, M. D. M. Sanchez Duque, W. Raimondi, D. Bonne, T. Constantieux, Y. Coquerel, and J. Rodriguez, Enantioselective Organocatalytic Michael Addition of Cyclobutanones to Nitroalkenes, *Adv. Synth. Catal*., 2012, **354**, 3523.

[16] Ł. Janczewski, A. Gajda, S. Frankowski, T. M. Goszczyński, T. Gajda, T3P®–A Benign Desulfurating Reagent in the Synthesis of Isothiocyanates, *Synthesis*, 2018, **50**, 1141.

[17] C. Yang, E.-G. Zhang, X. Li, J.-P. Cheng, Asymmetric Conjugate Addition of Benzofuran-2-ones to Alkyl 2-Phthalimidoacrylates: Modeling Structure-Stereoselectivity Relationships with Steric and Electronic Parameters, *Angew. Chem. Int. Ed.*, 2016, **55**, 6506.

[18] T. Okino, Y. Hoashi, T. Furukawa, X. Xu, and Y. Takemoto, Enantio- and Diastereoselective Michael Reaction of 1,3-Dicarbonyl Compounds to Nitroolefins Catalyzed by a Bifunctional Thiourea, *J. Am. Chem. Soc*., 2005, **127**, 119.

[19] J. P. Malerich, K. Hagihara, and V. H. Rawal, Chiral Squaramide Derivatives are Excellent Hydrogen Bond Donor Catalysts, *J. Am. Chem. Soc*., 2008, **130**, 14416.

[20] P. Gao, C. Wang, Y. Wu, Z. Zhou, and C. Tang, Sugar–Derived Bifunctional Thiourea Organocatalyzed Asymmetric Michael Addition of Acetylacetone to Nitroolefins, *Eur. J. Org. Chem*., 2008, **2008**, 4563.

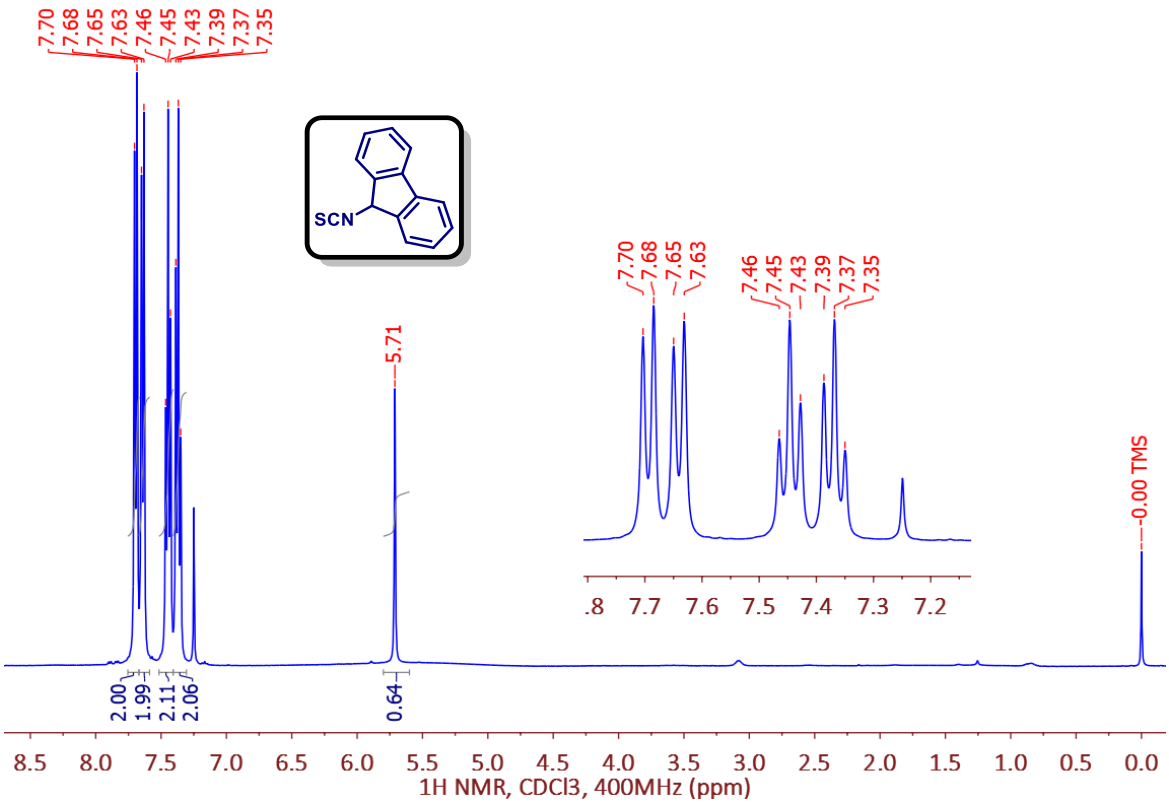
[21] J. M. Andrés, J. Losada, A. Maestro, P. Rodríguez-Ferrer, and R. Pedrosa, Supported and Unsupported Chiral Squaramides as Organocatalysts for Stereoselective Michael Additions: Synthesis of Enantiopure Chromenes and Spirochromanes, *J. Org. Chem*., 2017, **82**, 8444.

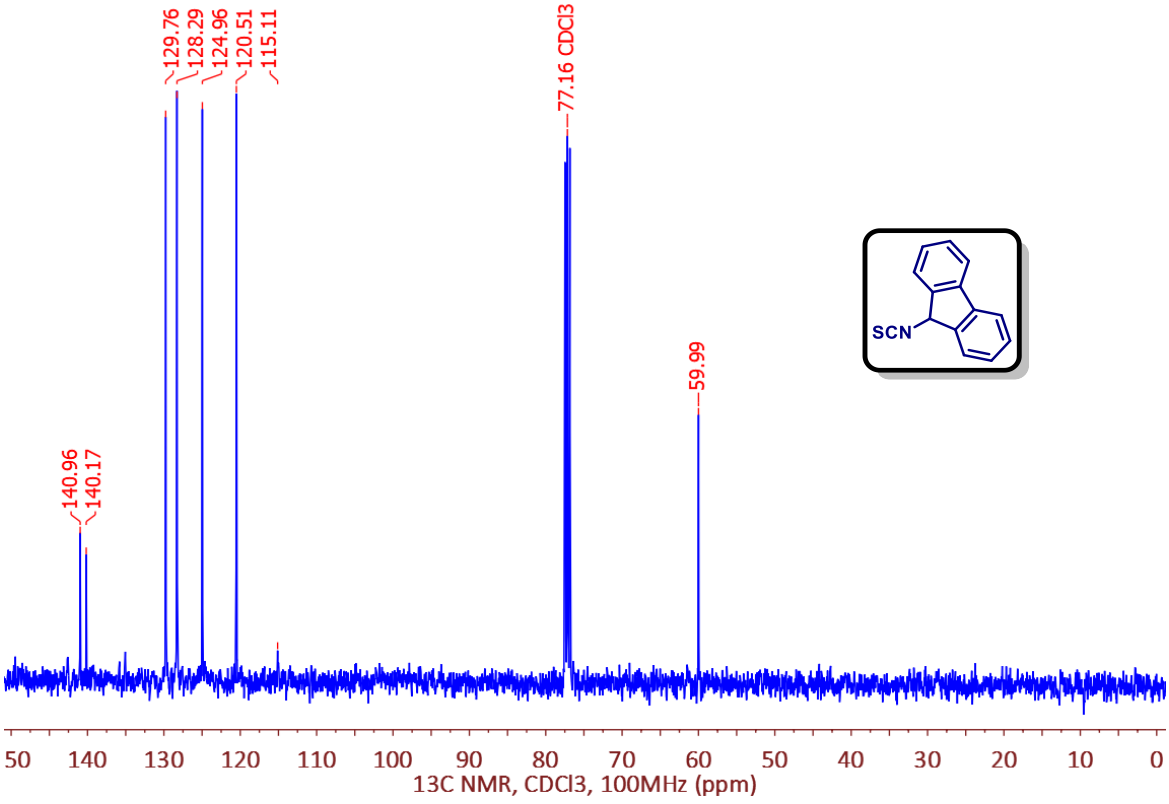
[22] Racemic produc is reported: (a) A. V. Aksenov, N. A. Aksenov, A. A. Skomorokhov, I. V. Aksenova, G. D. Gryaznov, L. G. Voskressensky, and M. A. Rubin, Michael addition to unprotected 3-(2-nitrovinyl)indoles under the conditions of microwave synthesis, *Chem. Heterocycl. Comp.,* 2016, **52**, 923. (b) N. A. Aksenov, A. A. Skomorokhov, A. V. Aksenov, L. G. Voskressensky, and M. A. Rubin, Michael addition to 3-(2-nitrovinyl)indoles–route toward aliphatic nitro compounds with heterocyclic substituents, *Chem Heterocycl Comp.,* 2019, **55**, 541.

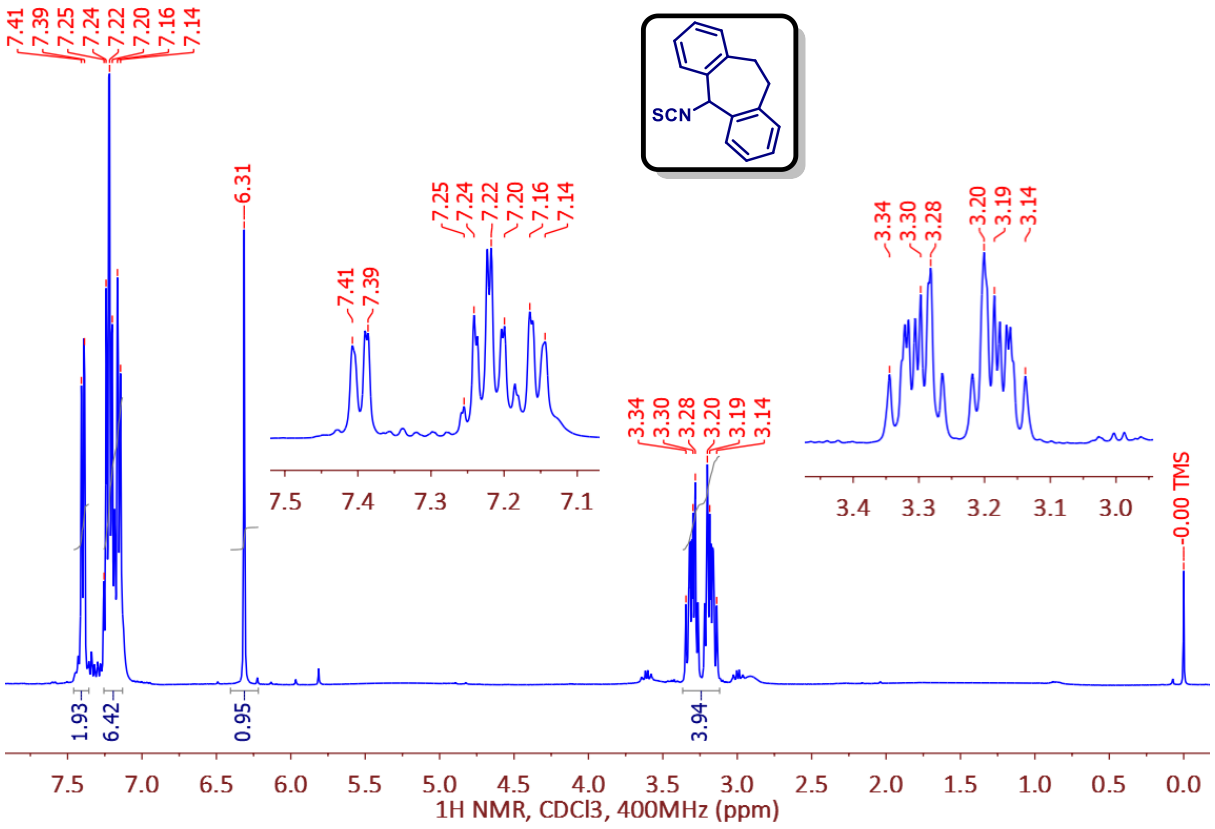
[23] R. Wu, X. Chang, A. Lu, Y. Wang, G. Wu, H. Song, Z. Zhou, and C. Tang, Chiral (thio)phosphorodiamides as excellent hydrogen bond donor catalysts in the asymmetric Michael addition of 2-hydroxy-1,4-naphthoquione to nitroolefins, *Chem. Commun.,* 2011, **47**, 5034.

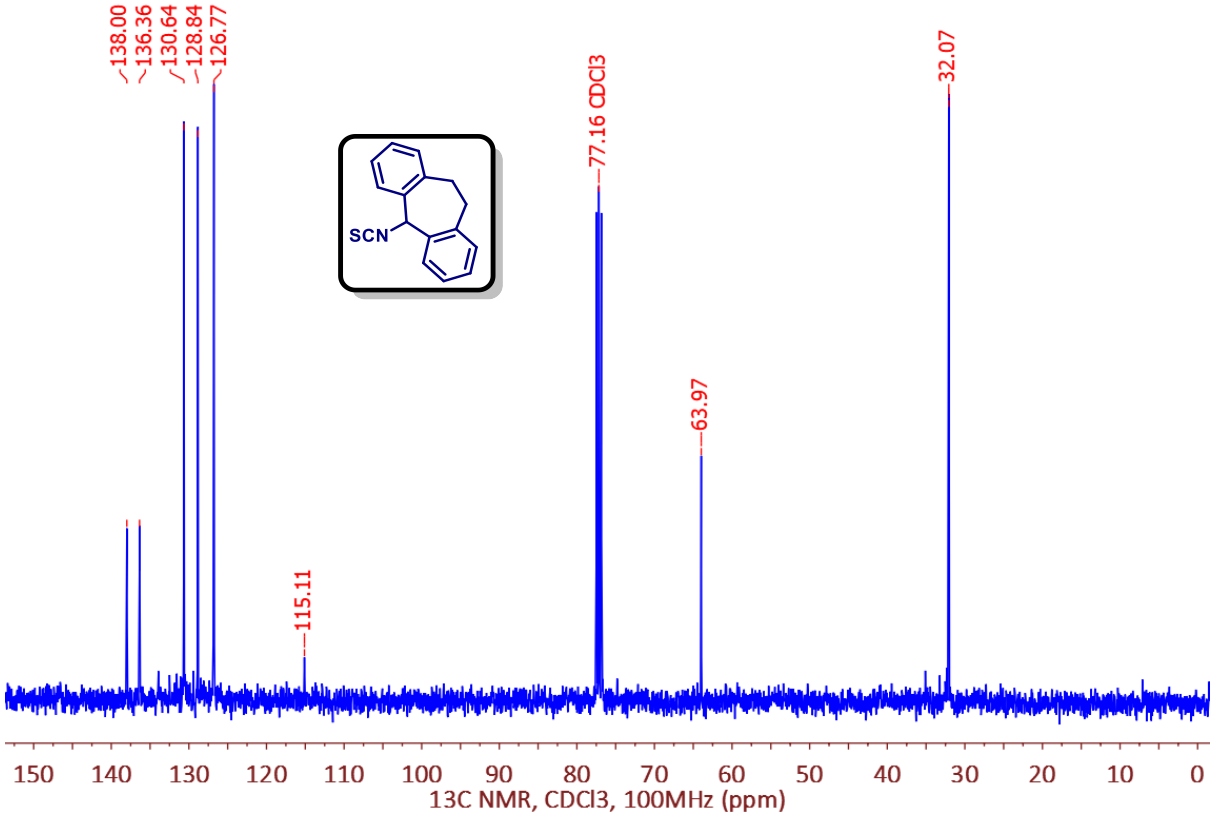
[24] M, Işık, M. Y. Unver, and C. Tanyeli, Modularly Evolved 2-AminoDMAP/Squaramides as Highly Active Bifunctional Organocatalysts in Michael Addition, *J. Org. Chem*., 2015, **80**, 828.

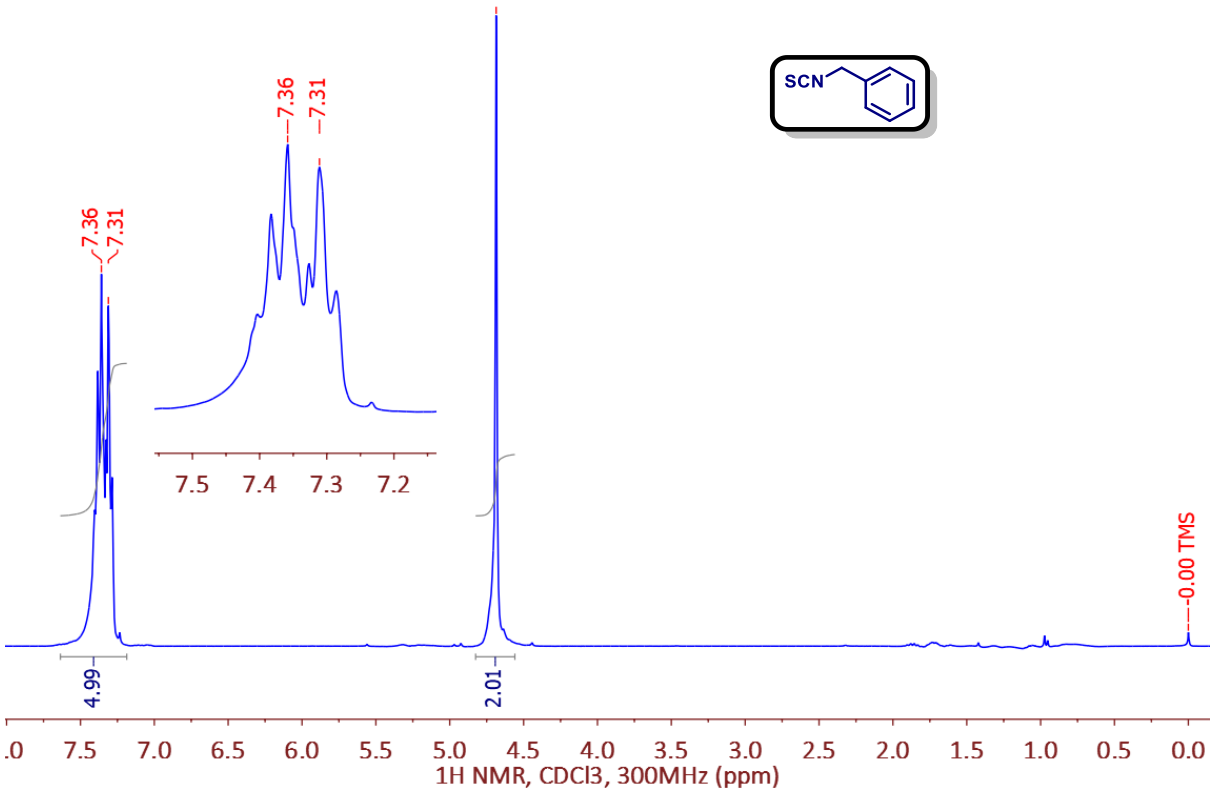
8. NMR spectra

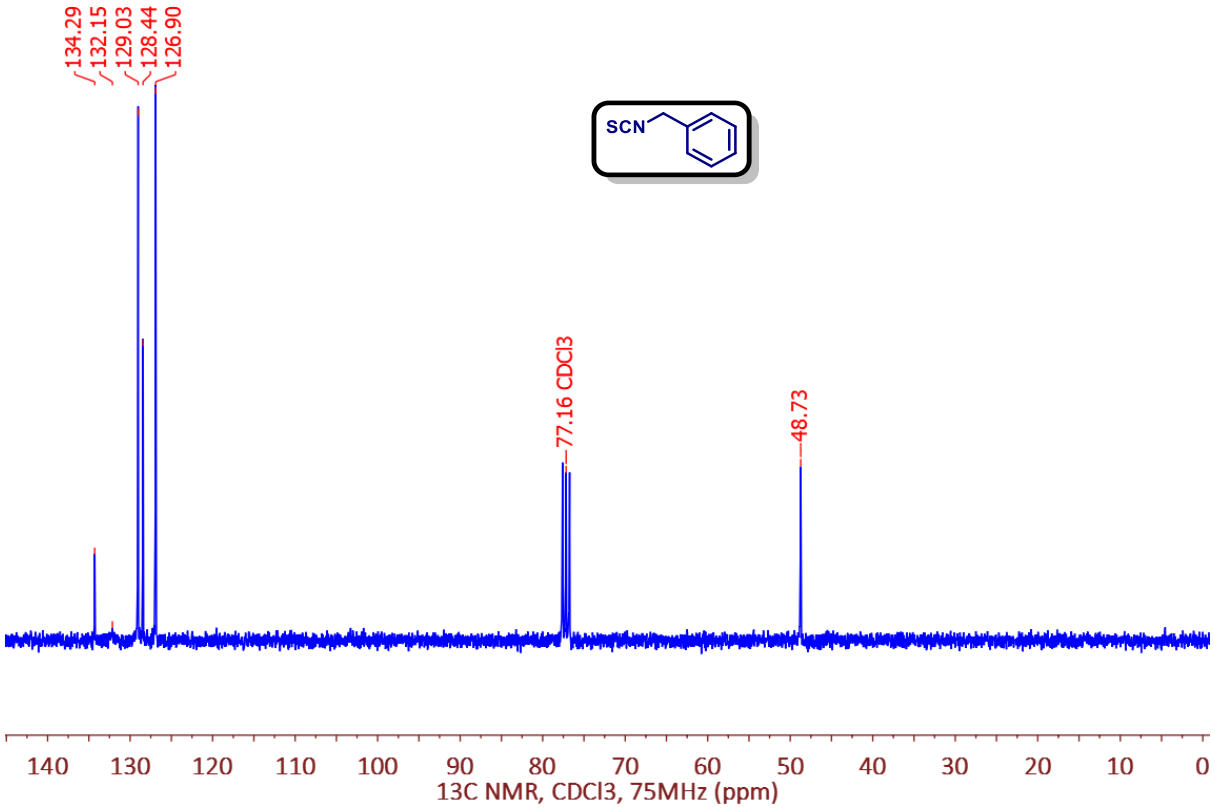


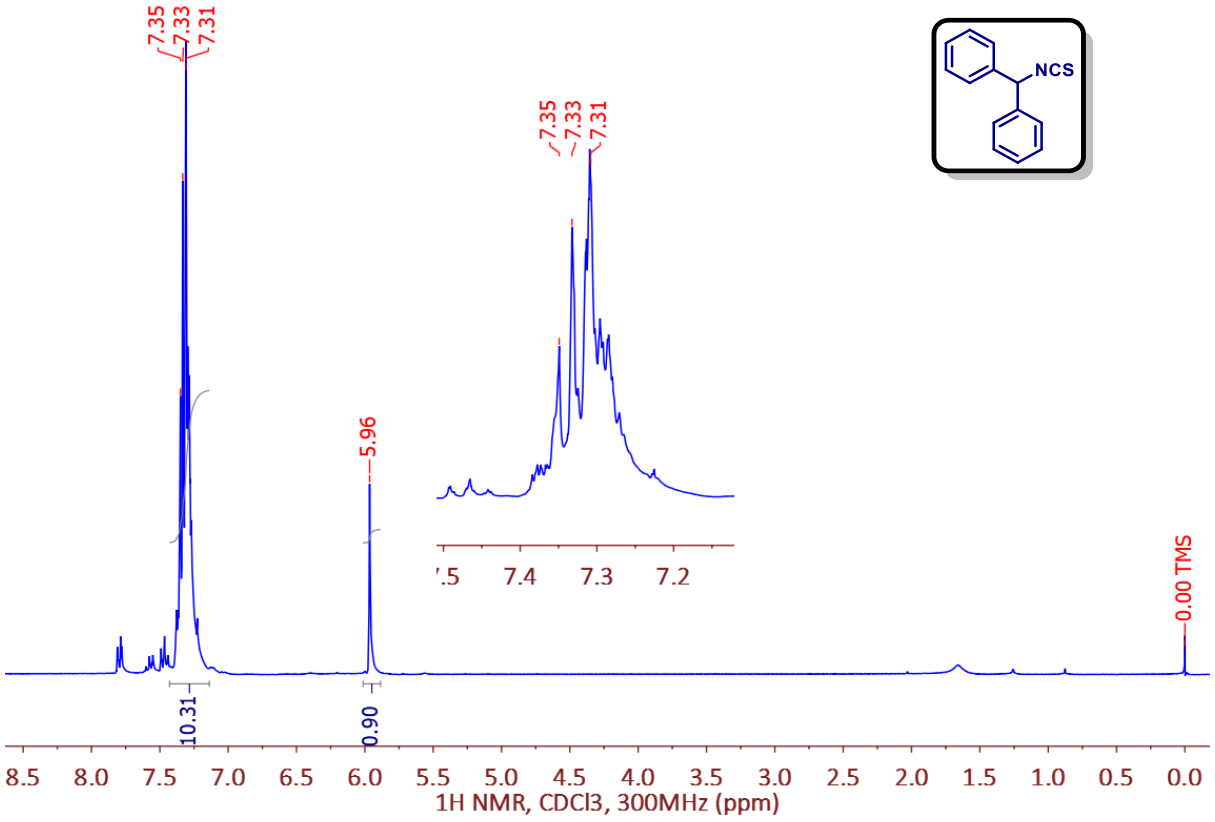


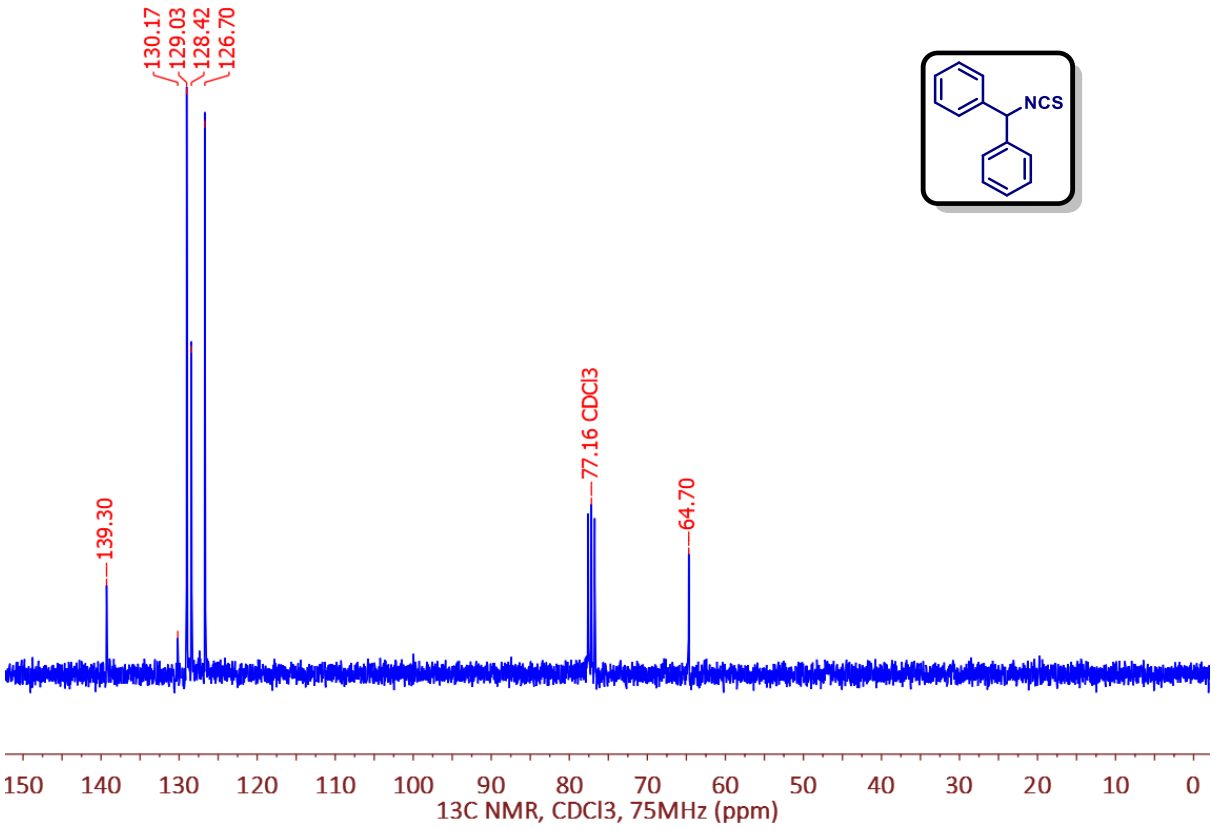

7.41
7.39
7.25
7.24
7.22
7.20
7.16
7.14
6.31
3.34
3.30
3.28
3.20
3.19
3.14
0.00 TMS
SCN
1.93
6.42
0.95
3.94
1H NMR, CDCl3, 400MHz (ppm)

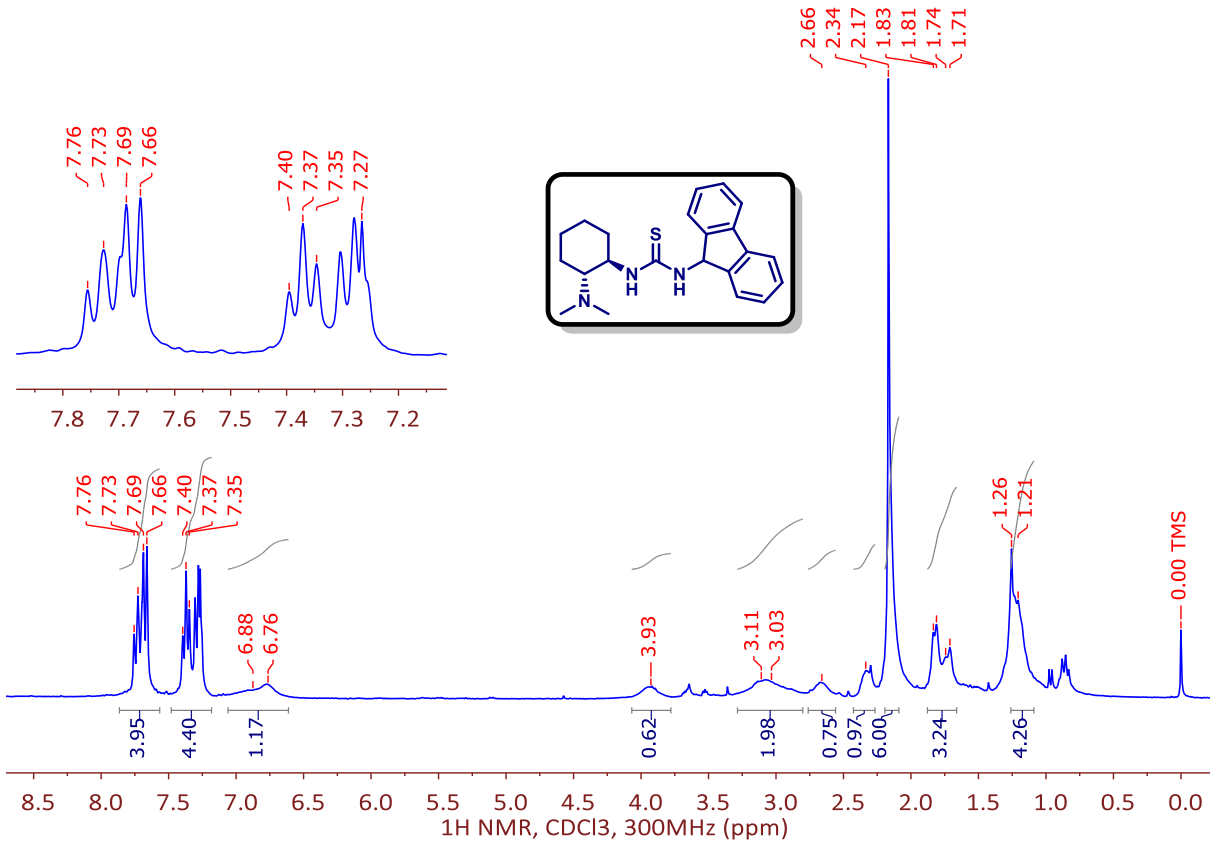

138.00
136.36
130.64
128.84
126.77
77.16 CDCl3
32.07
63.97
115.11
SCN
13C NMR, CDCl3, 100MHz (ppm)

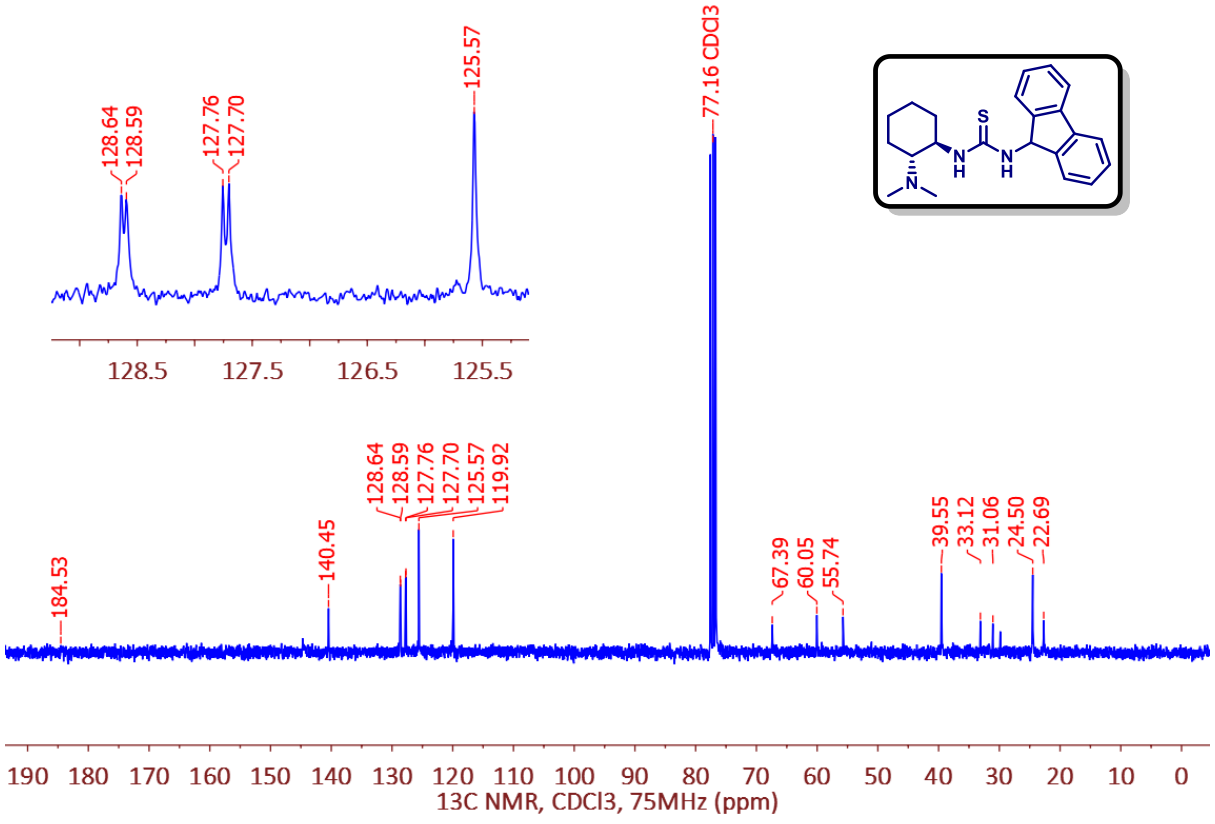

SCN
7.36
7.31
7.5
7.4
7.3
7.2
0.00 TMS
4.99
2.01
1H NMR, CDCl3, 300MHz (ppm)

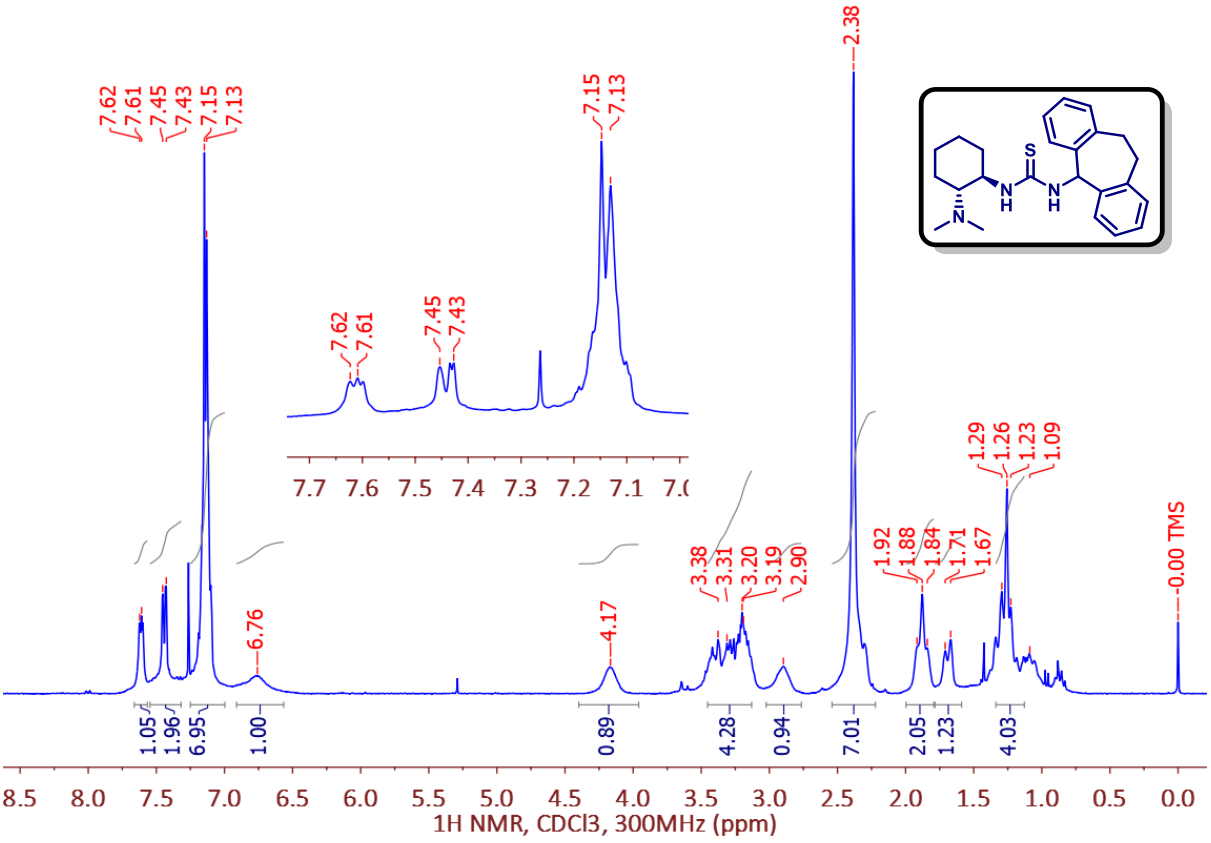

134.29
132.15
129.03
128.44
126.90
SCN
77.16 CDCl3
48.73
13C NMR, CDCl3, 75MHz (ppm)

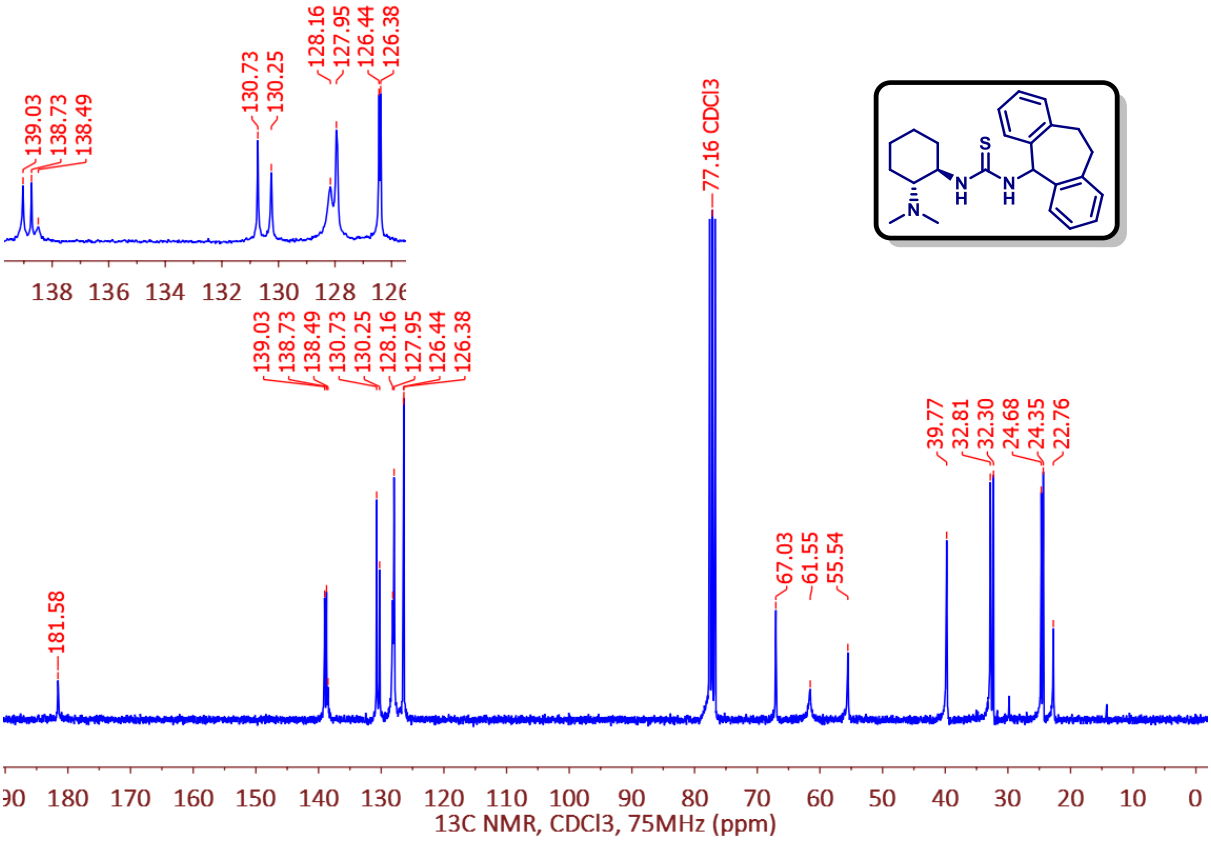

7.35
7.33
7.31
NCS
5.96
0.00 TMS
10.31
0.90
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 300MHz (ppm)

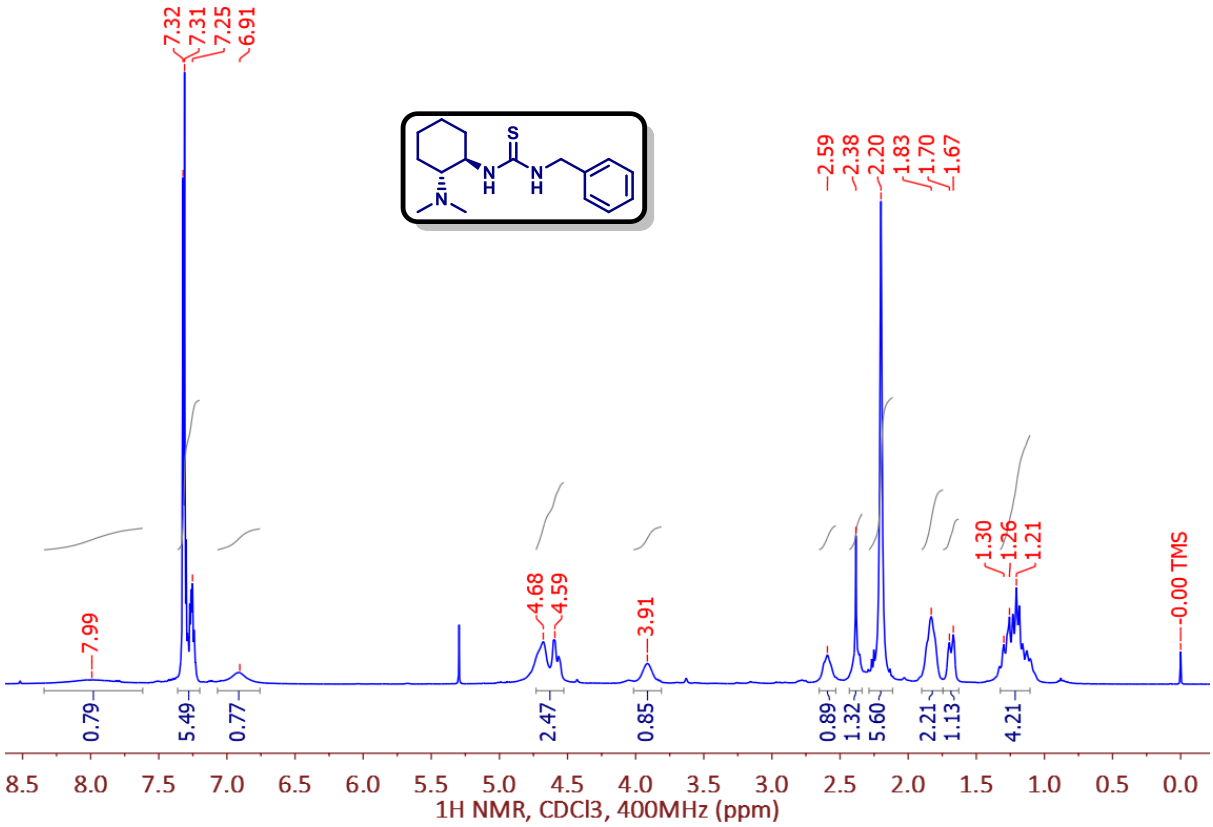

130.17
129.03
128.42
126.70
NCS
139.30
77.16 CDCl3
64.70
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 75MHz (ppm)

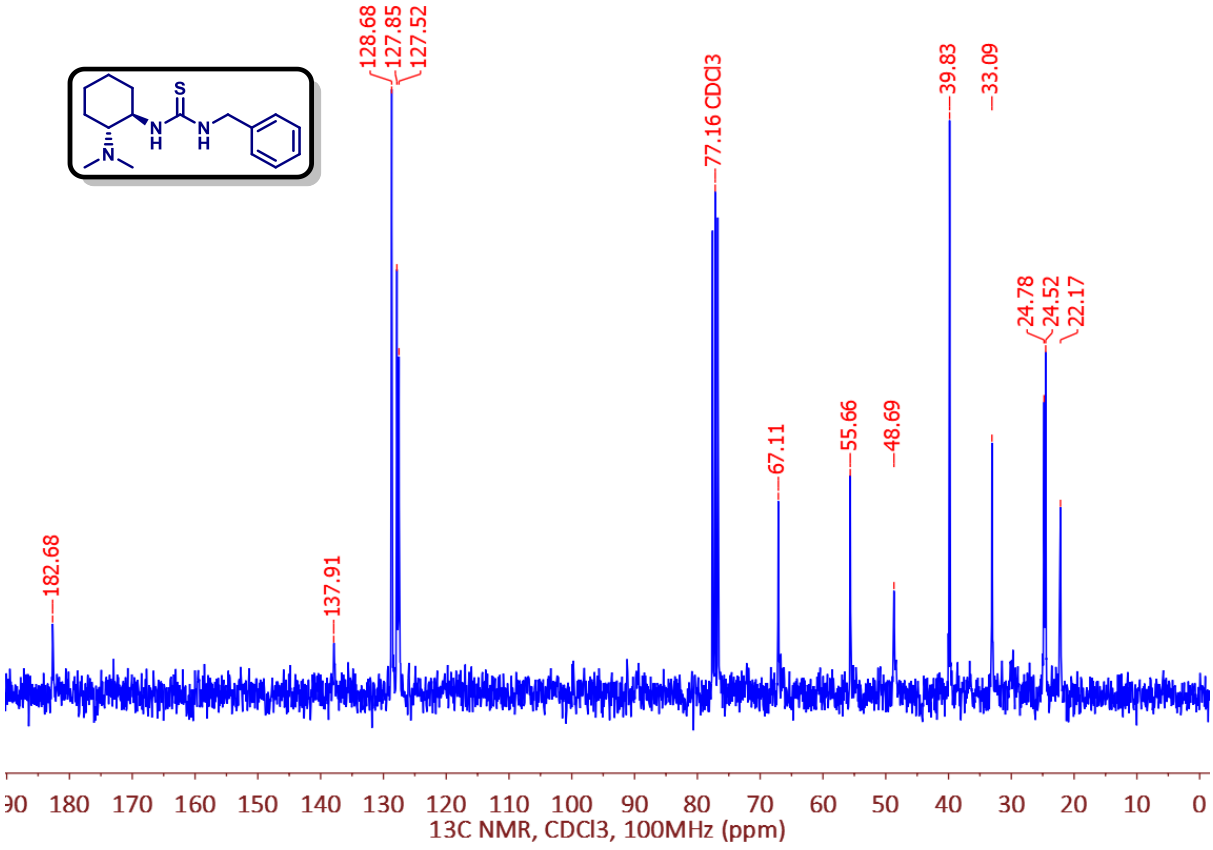

7.76
7.73
7.69
7.66
7.40
7.37
7.35
7.27
7.8 7.7 7.6 7.5 7.4 7.3 7.2
2.66
2.34
2.17
1.83
1.81
1.74
1.71
6.88
6.76
3.93
3.11
3.03
1.26
1.21
0.00 TMS
3.95
4.40
1.17
0.62
1.98
0.75
0.97
6.00
3.24
4.26
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 300MHz (ppm)

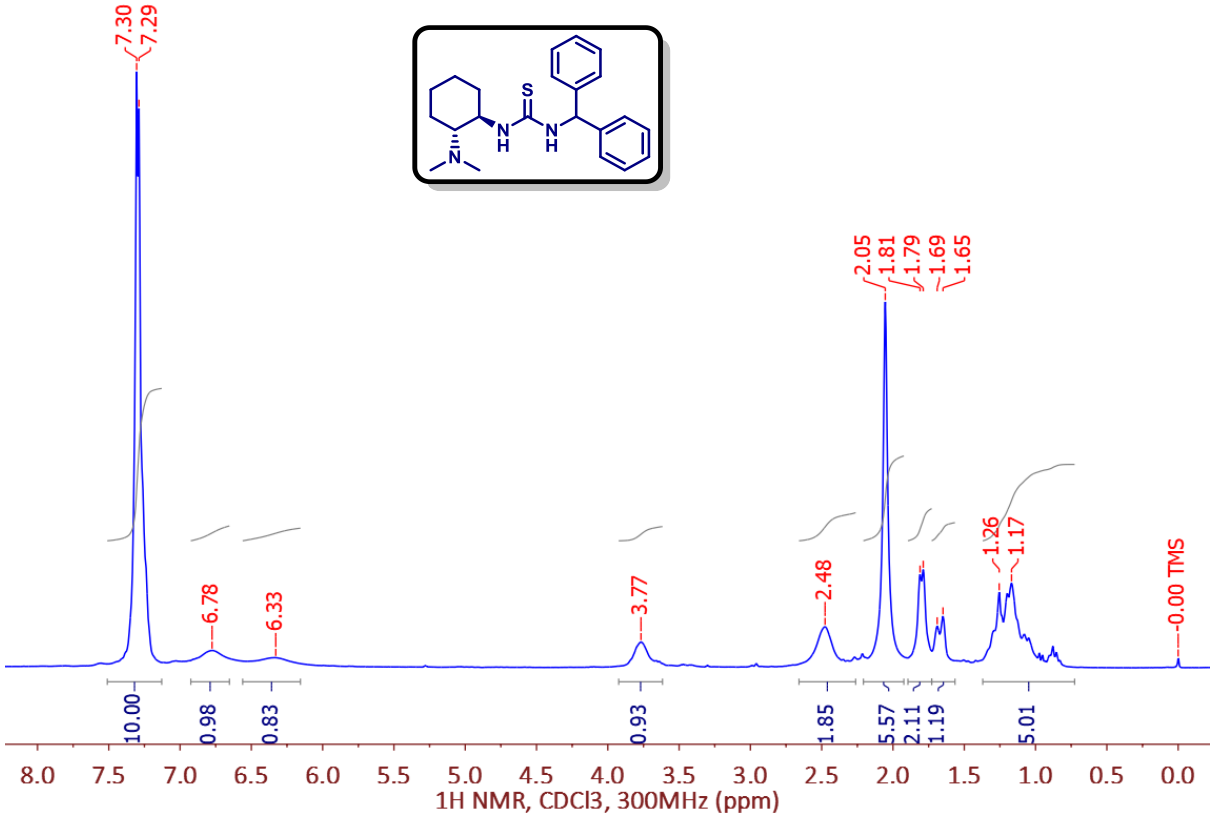

128.64
128.59
127.76
127.70
125.57
128.5 127.5 126.5 125.5
77.16 CDCl3
184.53
140.45
128.64
128.59
127.76
127.70
125.57
119.92
67.39
60.05
55.74
39.55
33.12
31.06
24.50
22.69
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 75MHz (ppm)

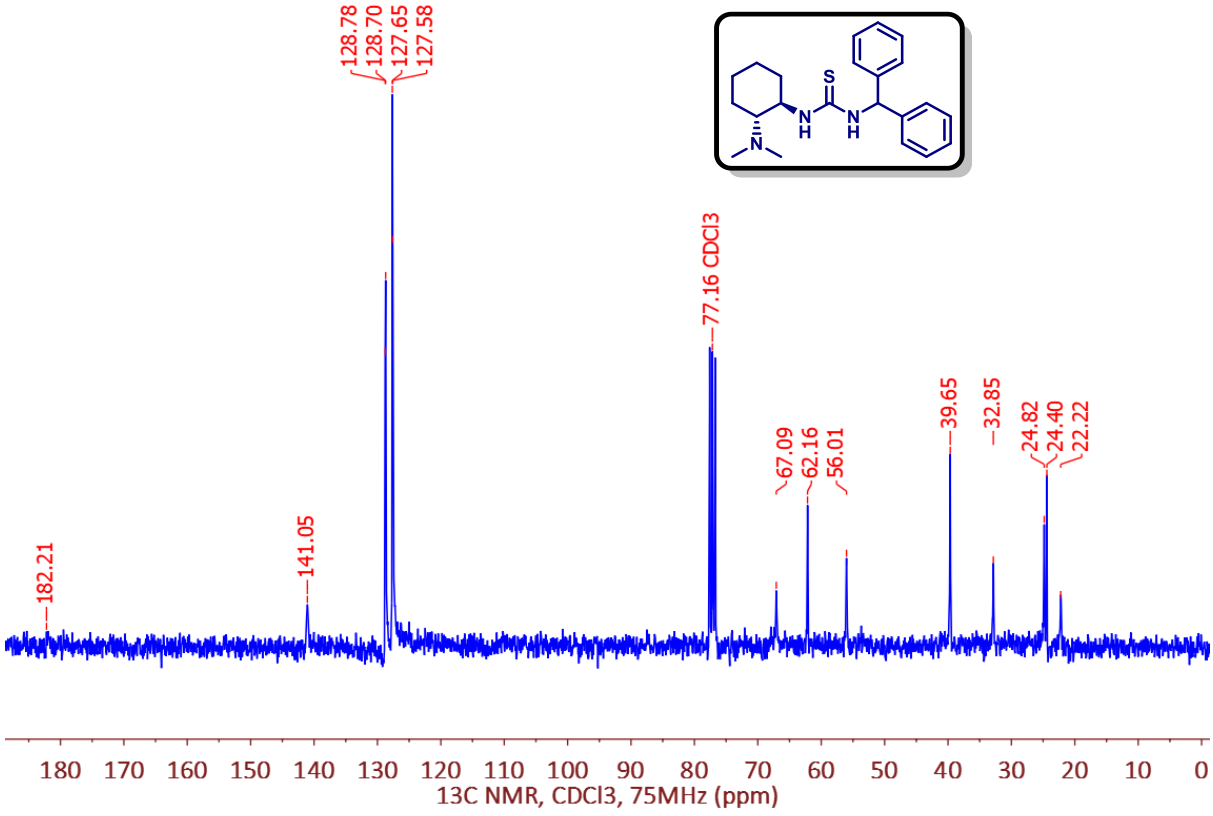

7.62
7.61
7.45
7.43
7.15
7.13
2.38
6.76
4.17
3.38
3.31
3.20
3.19
2.90
1.92
1.88
1.84
1.71
1.67
1.29
1.26
1.23
1.09
0.00 TMS
1.05
1.96
6.95
1.00
0.89
4.28
0.94
7.01
2.05
1.23
4.03
1H NMR, CDCl3, 300MHz (ppm)

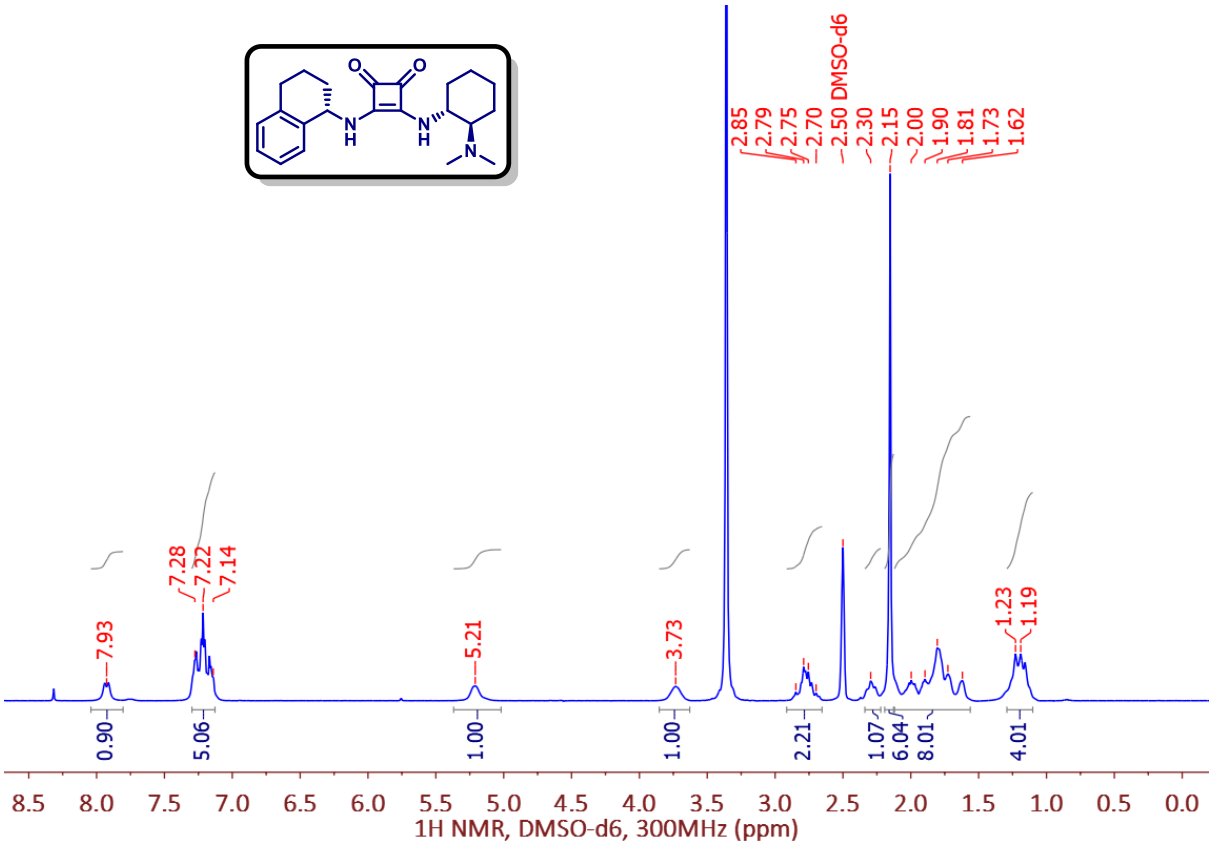

139.03
138.73
138.49
130.73
130.25
128.16
127.95
126.44
126.38
77.16 CDCl3
181.58
67.03
61.55
55.54
39.77
32.81
32.30
24.68
24.35
22.76
13C NMR, CDCl3, 75MHz (ppm)

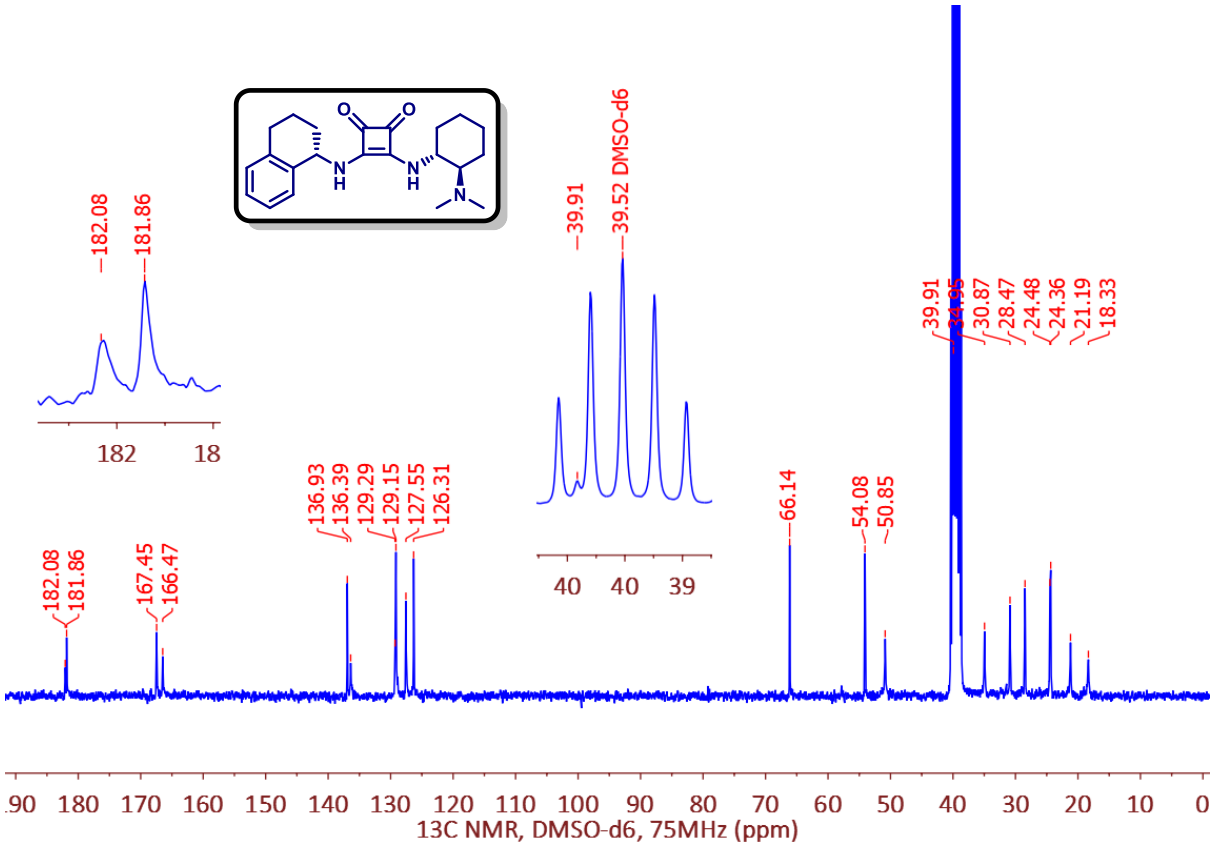

7.32
7.31
7.25
6.91
7.99
4.68
4.59
3.91
2.59
2.38
2.20
1.83
1.70
1.67
1.30
1.26
1.21
0.00 TMS
0.79
5.49
0.77
2.47
0.85
0.89
1.32
5.60
2.21
1.13
4.21
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)

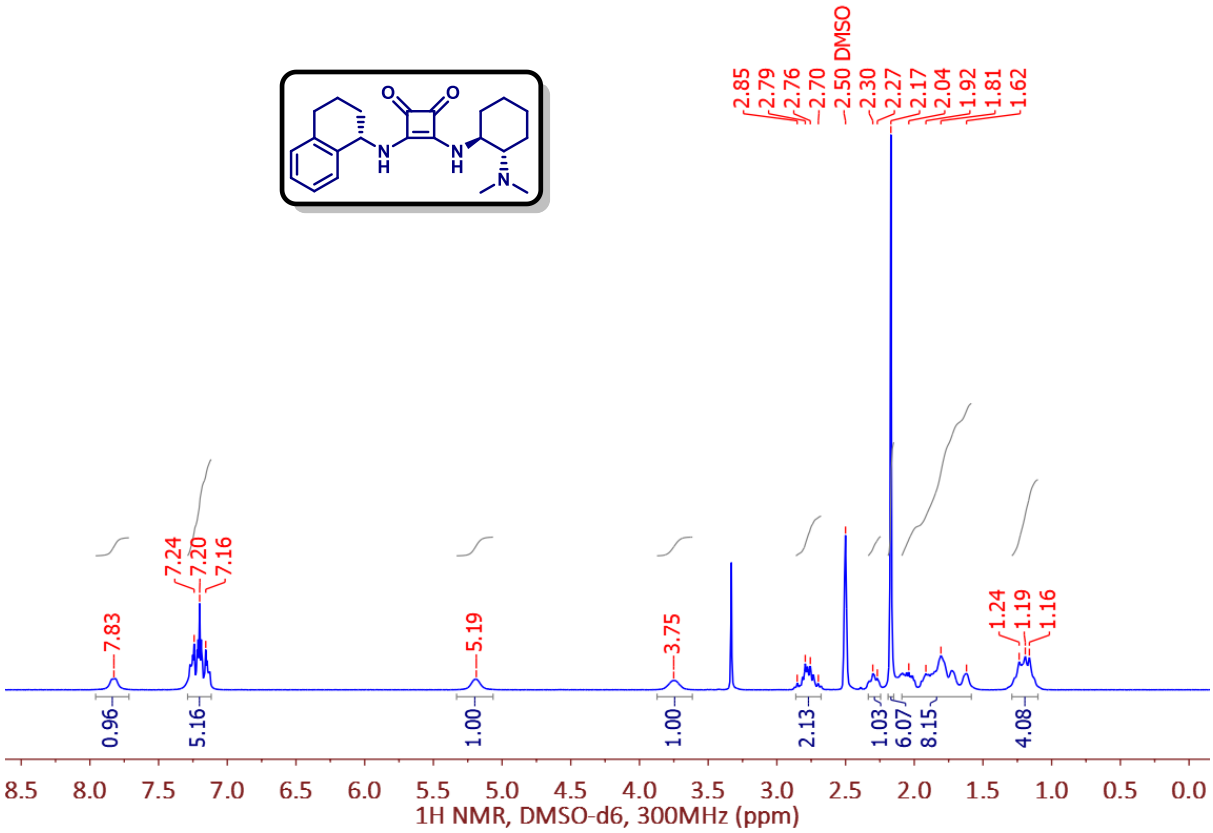

128.68
127.85
127.52
77.16 CDCl3
39.83
33.09
24.78
24.52
22.17
67.11
55.66
48.69
182.68
137.91
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)

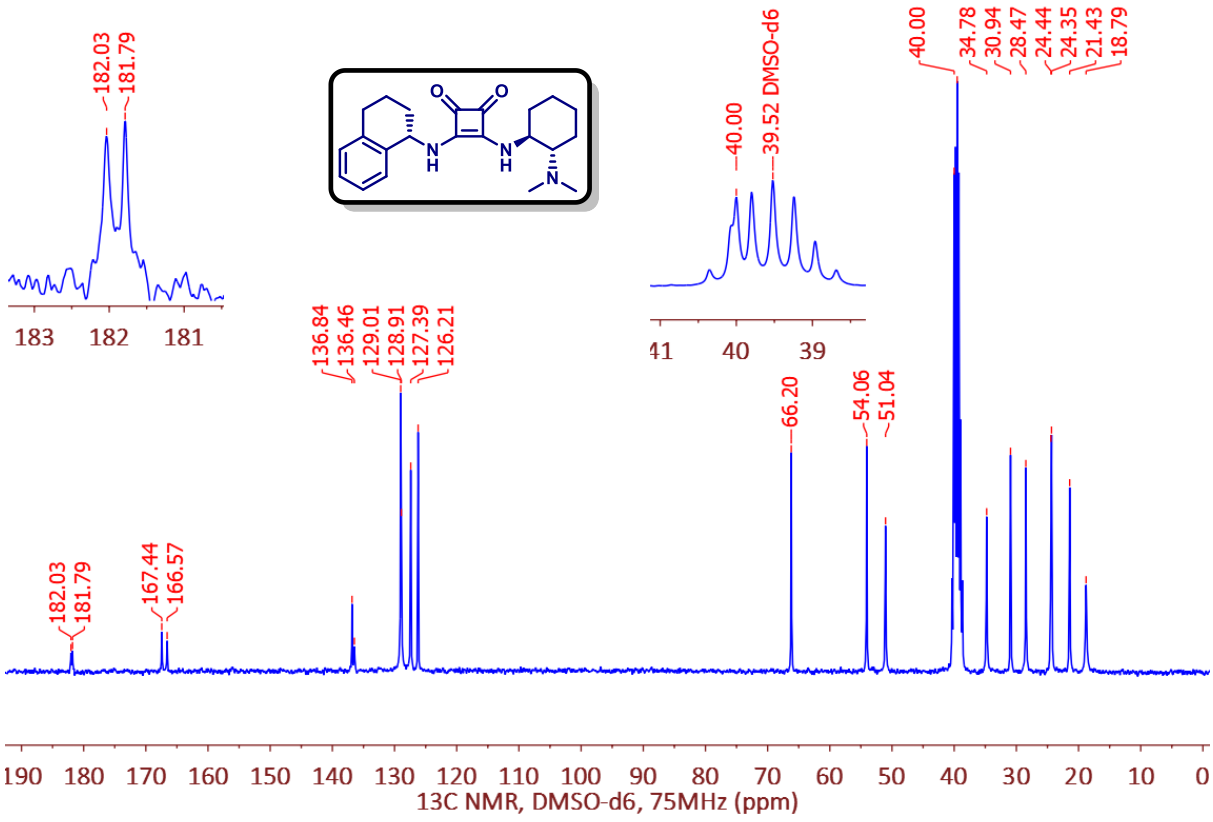

7.30
7.29
6.78
6.33
3.77
2.48
2.05
1.81
1.79
1.69
1.65
1.26
1.17
0.00 TMS
10.00
0.98
0.83
0.93
1.85
5.57
2.11
1.19
5.01
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 300MHz (ppm)

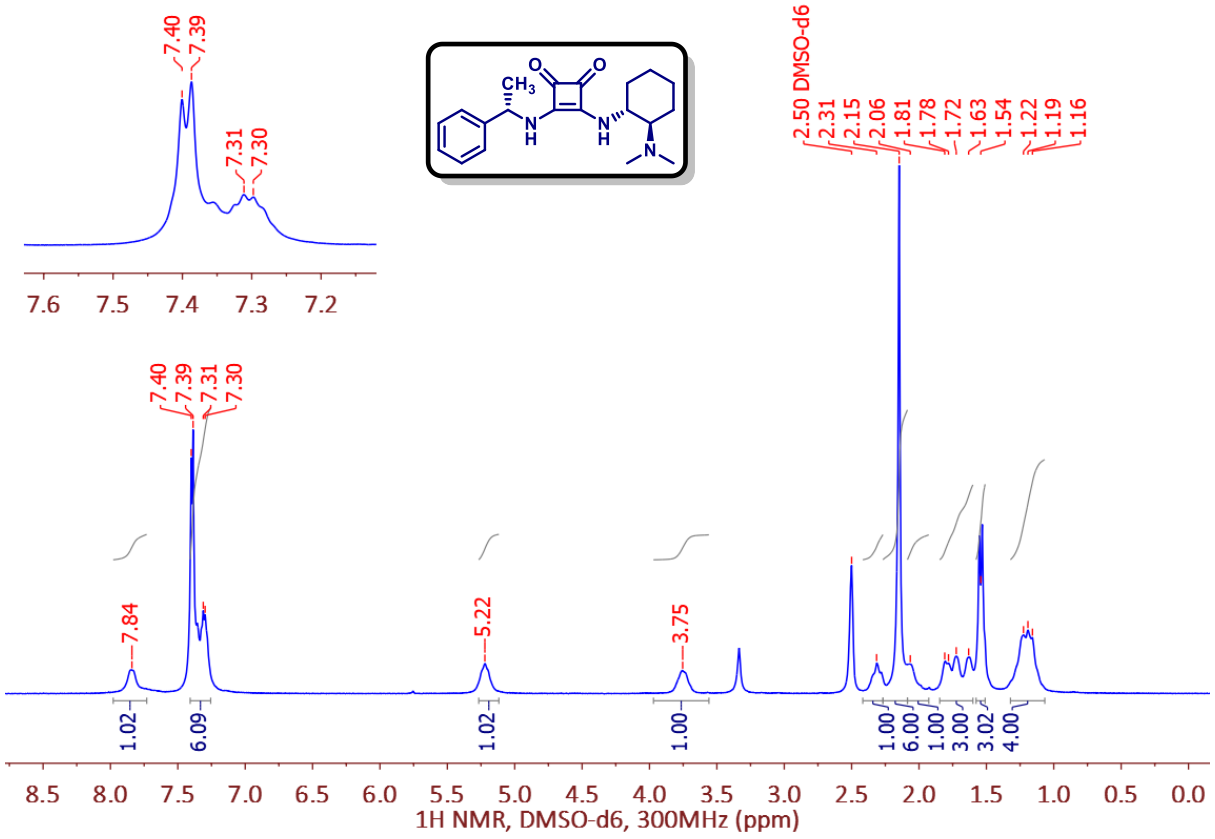

128.78
128.70
127.65
127.58
77.16 CDCl3
182.21
141.05
67.09
62.16
56.01
39.65
32.85
24.82
24.40
22.22
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 75MHz (ppm)

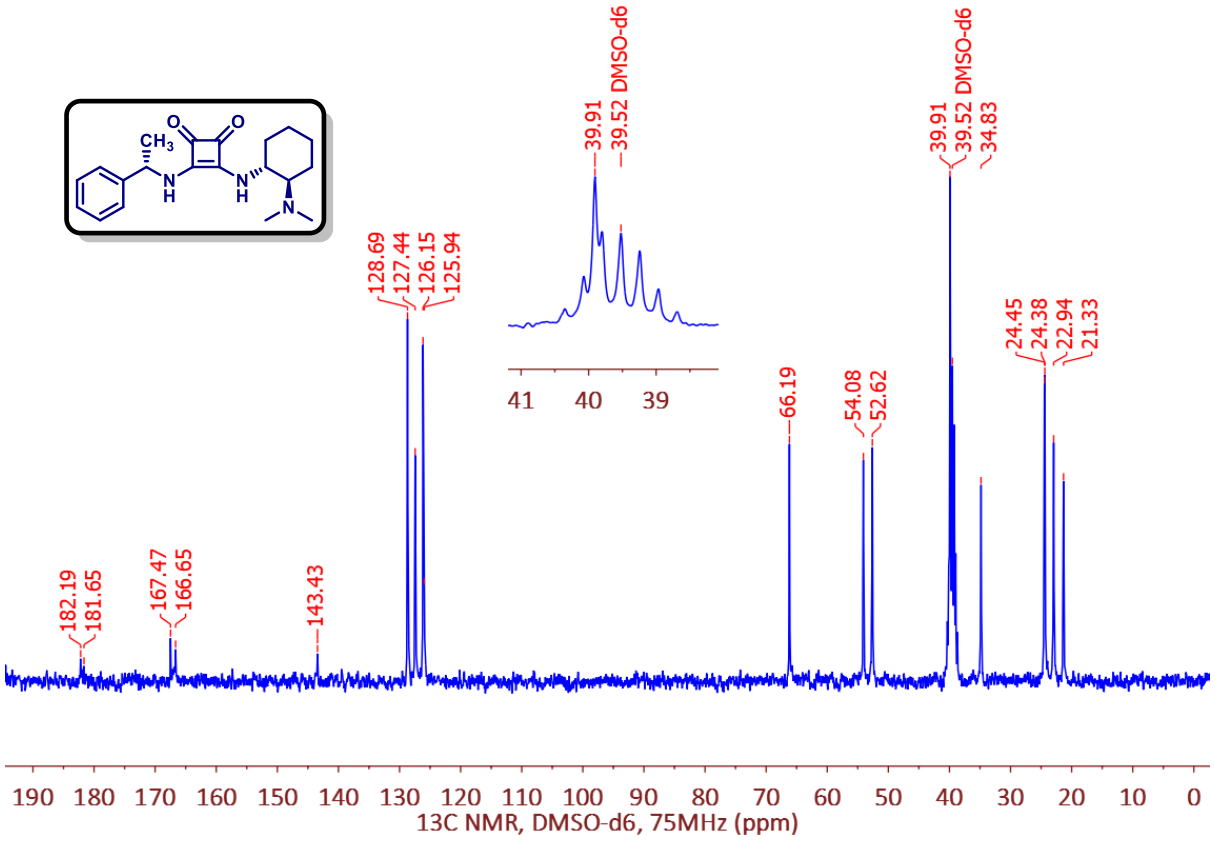

2.85
2.79
2.75
2.70
2.50 DMSO-d6
2.30
2.15
2.00
1.90
1.81
1.73
1.62
7.93
7.28
7.22
7.14
5.21
3.73
1.23
1.19
0.90
5.06
1.00
1.00
2.21
1.07
6.04
8.01
4.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 300MHz (ppm)

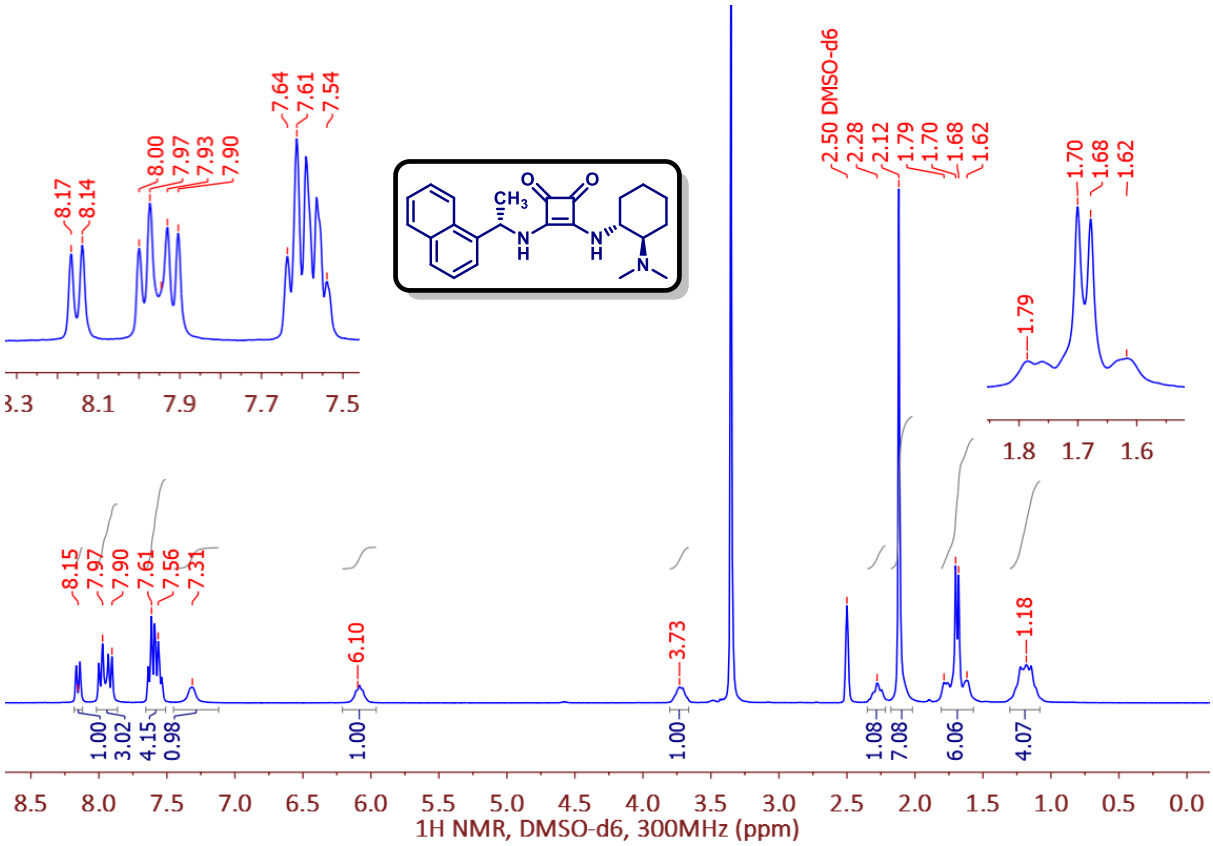

182.08
181.86
182
18
39.91
39.52 DMSO-d6
40 40 39
39.91
34.95
30.87
28.47
24.48
24.36
21.19
18.33
136.93
136.39
129.29
129.15
127.55
126.31
66.14
54.08
50.85
182.08
181.86
167.45
166.47
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 75MHz (ppm)

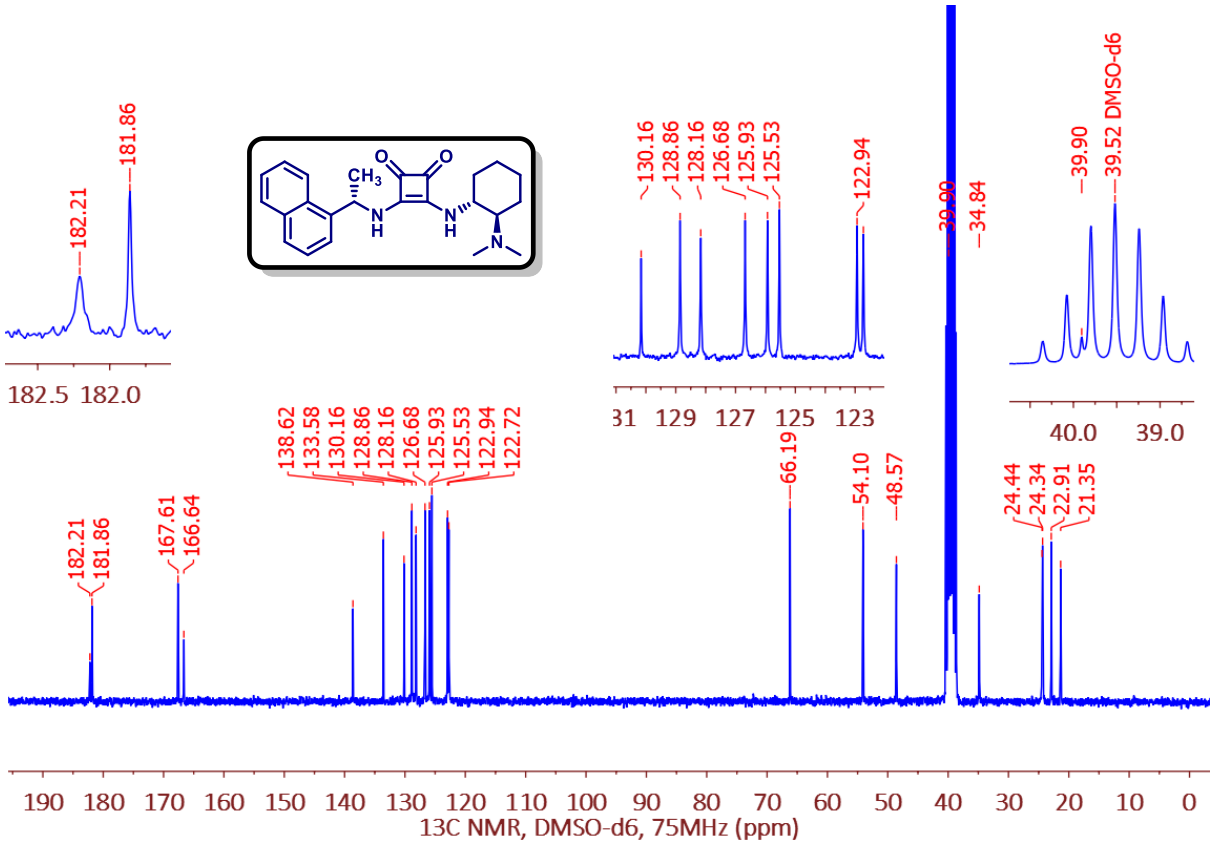

2.85
2.79
2.76
2.70
2.50 DMSO
2.30
2.27
2.17
2.04
1.92
1.81
1.62
7.83
7.24
7.20
7.16
5.19
3.75
1.24
1.19
1.16
0.96
5.16
1.00
1.00
2.13
1.03
6.07
8.15
4.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 300MHz (ppm)

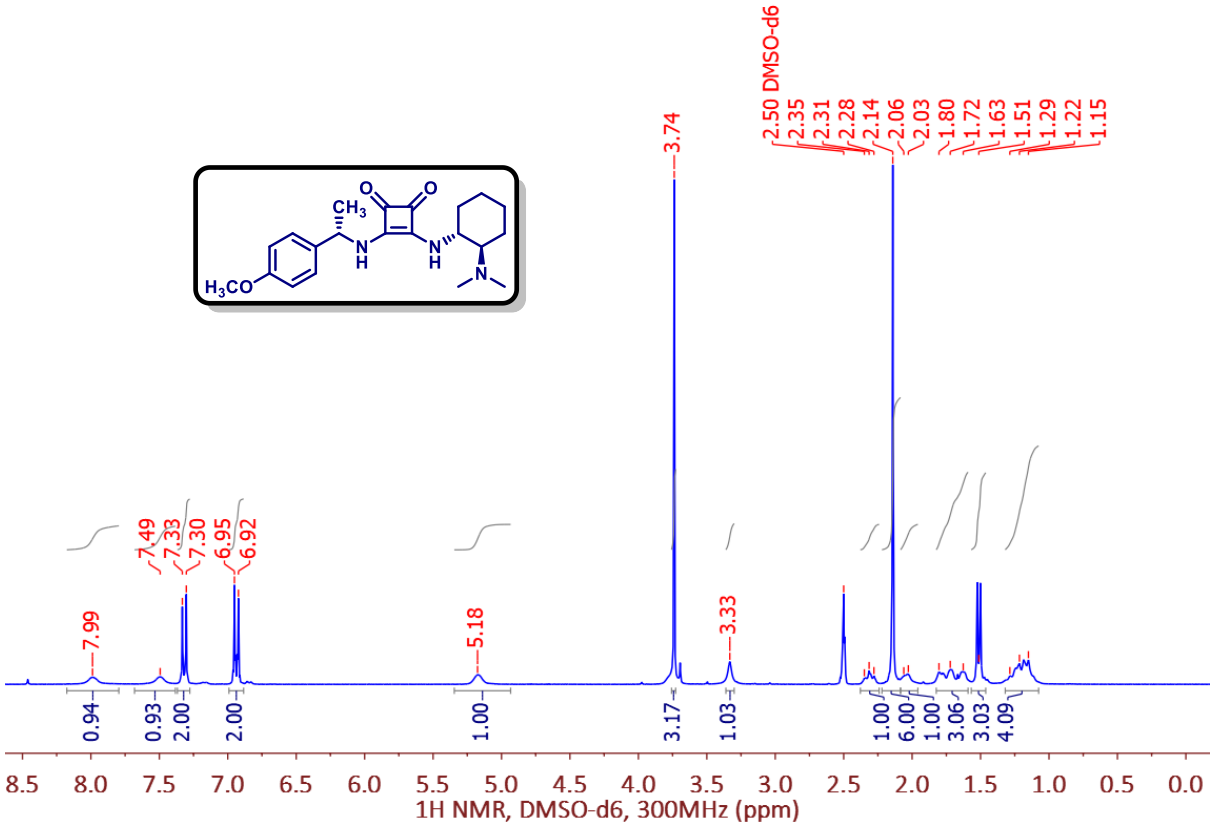

182.03
181.79
183 182 181
40.00
39.52 DMSO-d6
41 40 39
40.00
34.78
30.94
28.47
24.44
24.35
21.43
18.79
136.84
136.46
129.01
128.91
127.39
126.21
66.20
54.06
51.04
182.03
181.79
167.44
166.57
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 75MHz (ppm)

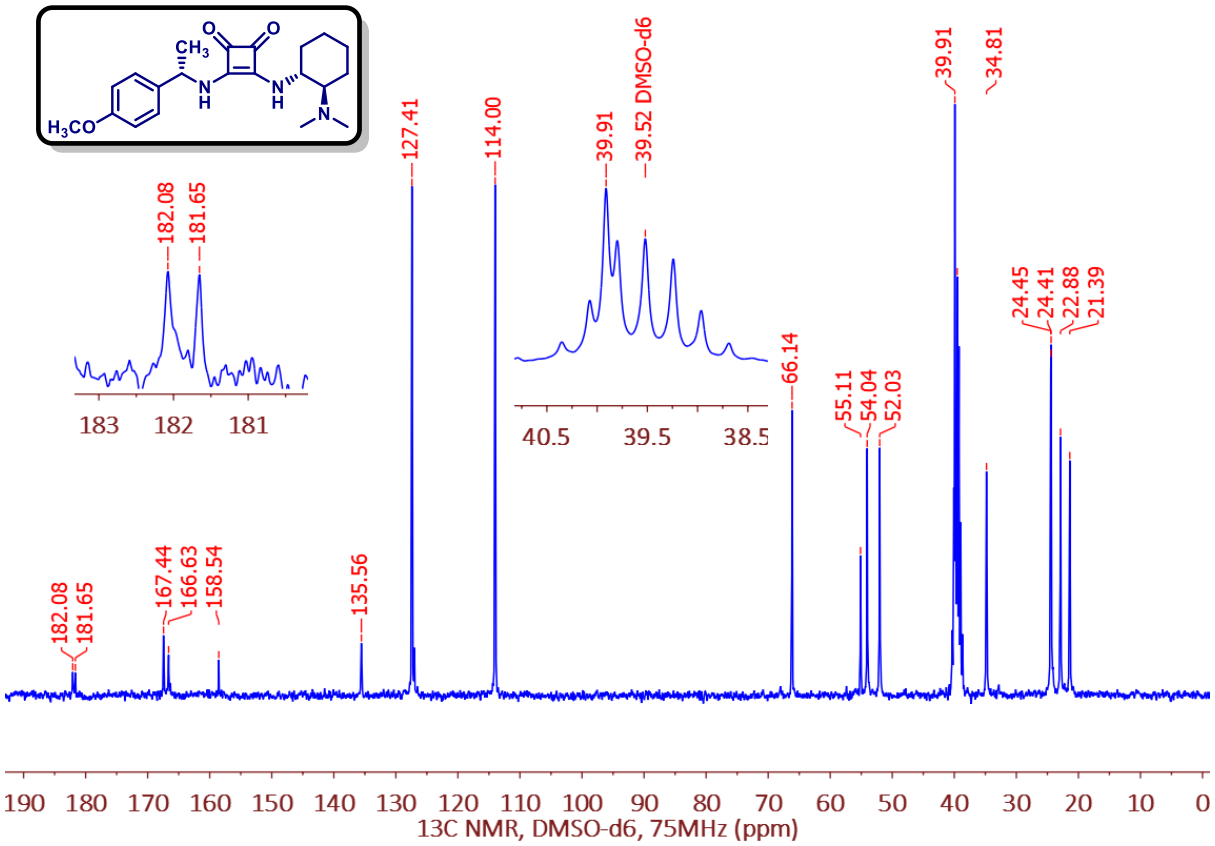

7.40
7.39
7.31
7.30
7.6
7.5
7.4
7.3
7.2
2.50 DMSO-d6
2.31
2.15
2.06
1.81
1.78
1.72
1.63
1.54
1.22
1.19
1.16
7.84
5.22
3.75
1.02
6.09
1.02
1.00
1.00
6.00
1.00
3.00
3.02
4.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 300MHz (ppm)

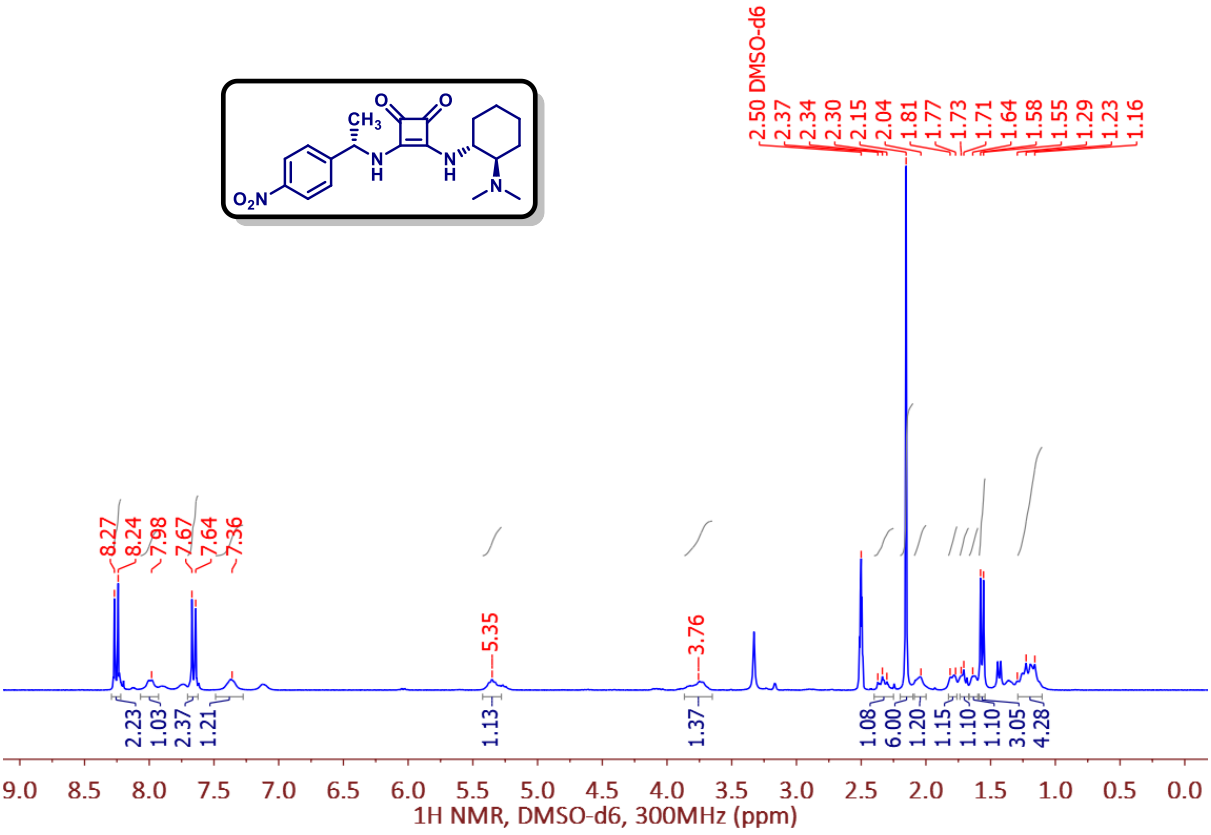

39.91
39.52 DMSO-d6
41
40
39
39.91
39.52 DMSO-d6
34.83
128.69
127.44
126.15
125.94
66.19
54.08
52.62
24.45
24.38
22.94
21.33
182.19
181.65
167.47
166.65
143.43
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 75MHz (ppm)

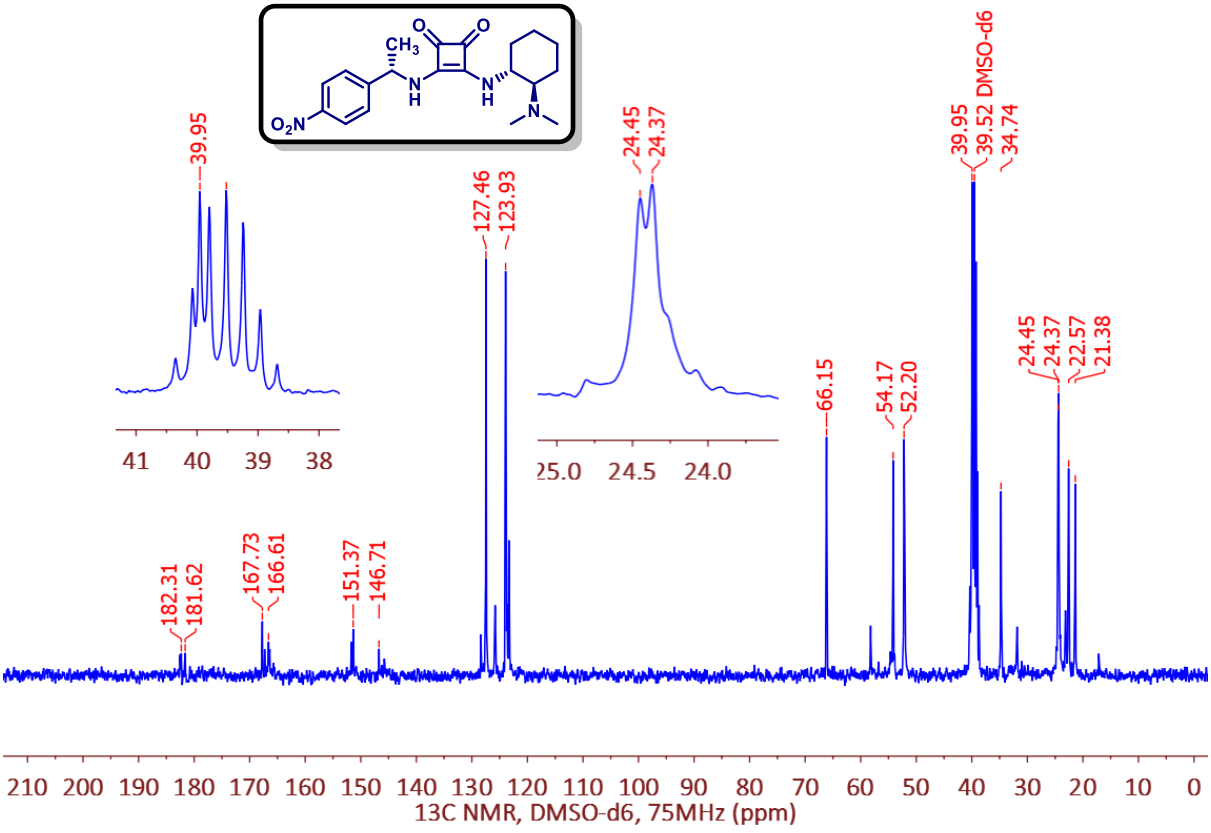

8.17
8.14
8.00
7.97
7.93
7.90
7.64
7.61
7.54
2.50 DMSO-d6
2.28
2.12
1.79
1.70
1.68
1.62
8.15
7.97
7.90
7.61
7.56
7.31
6.10
3.73
1.18
1.00
3.02
4.15
0.98
1.00
1.00
1.08
7.08
6.06
4.07
1H NMR, DMSO-d6, 300MHz (ppm)

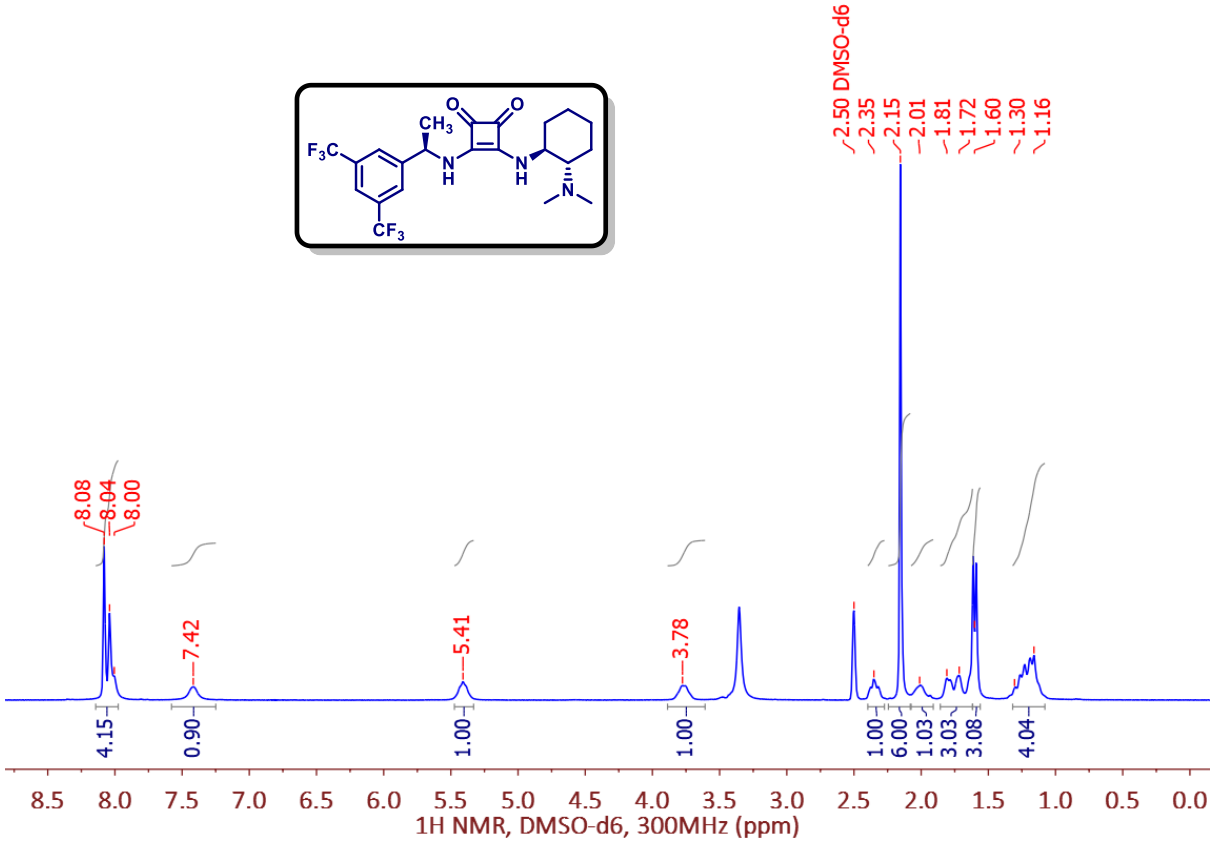

182.21
181.86
130.16
128.86
128.16
126.68
125.93
125.53
122.94
39.90
34.84
39.90
39.52 DMSO-d6
138.62
133.58
130.16
128.86
128.16
126.68
125.93
125.53
122.94
122.72
66.19
54.10
48.57
24.44
24.34
22.91
21.35
182.21
181.86
167.61
166.64
13C NMR, DMSO-d6, 75MHz (ppm)

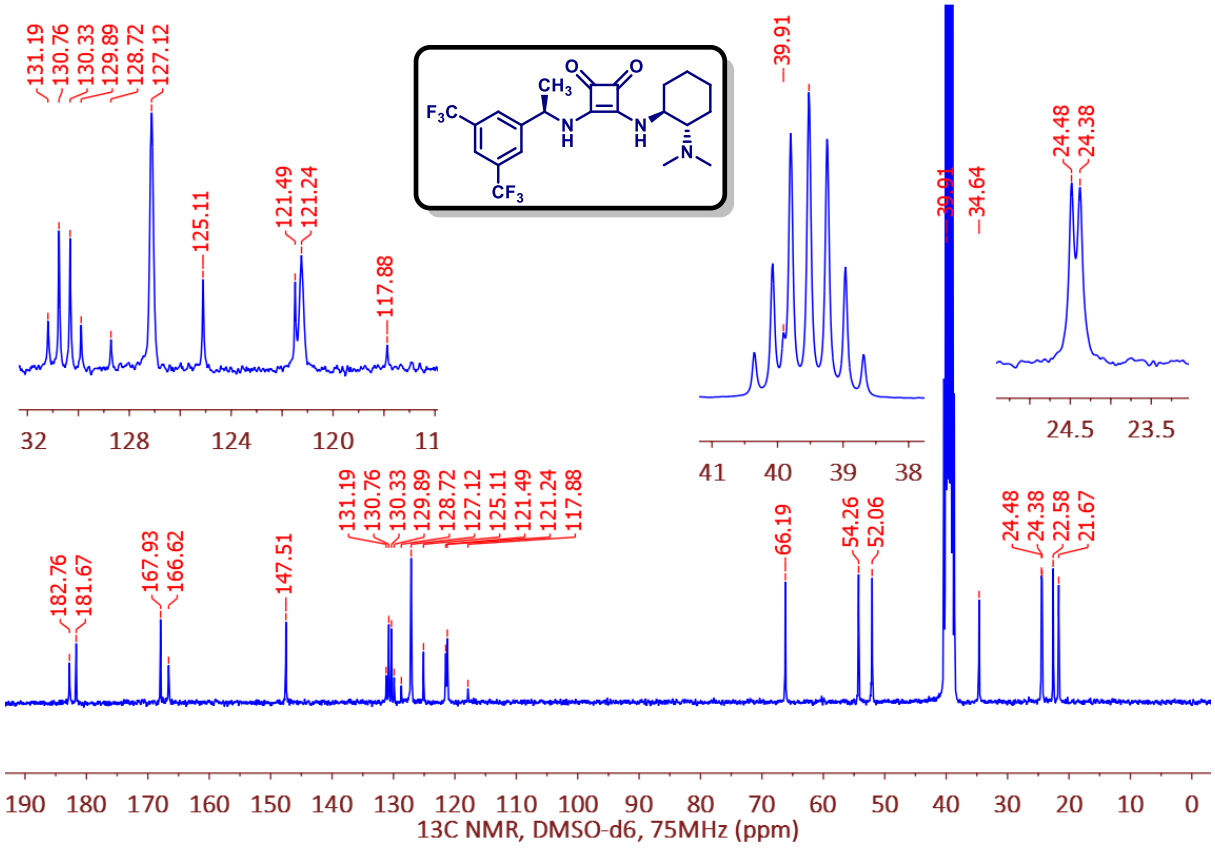

2.50 DMSO-d6
3.74
7.99
7.49
7.33
7.30
6.95
6.92
5.18
3.33
1H NMR, DMSO-d6, 300MHz (ppm)

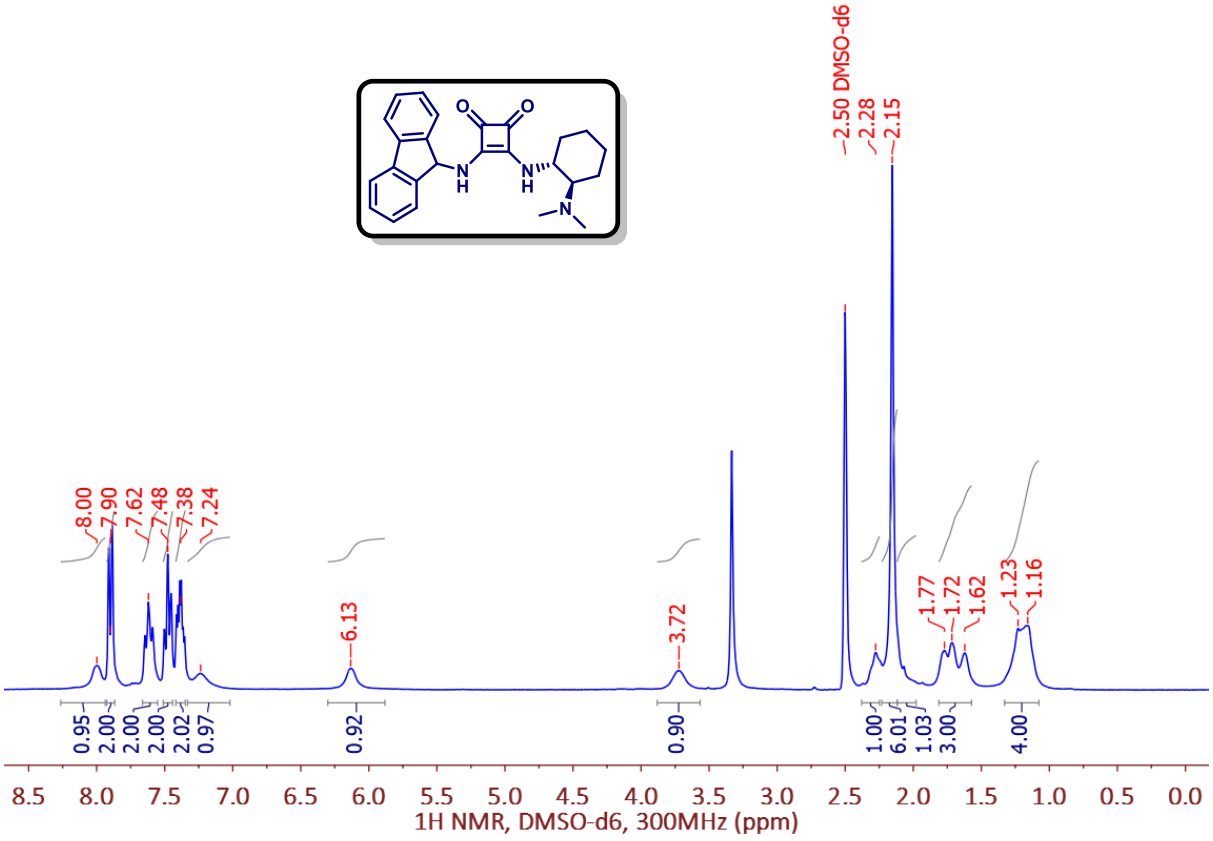

127.41
114.00
39.91
39.52 DMSO-d6
182.08
181.65
66.14
55.11
54.04
52.03
167.44
166.63
158.54
135.56
24.45
24.41
22.88
21.39
13C NMR, DMSO-d6, 75MHz (ppm)

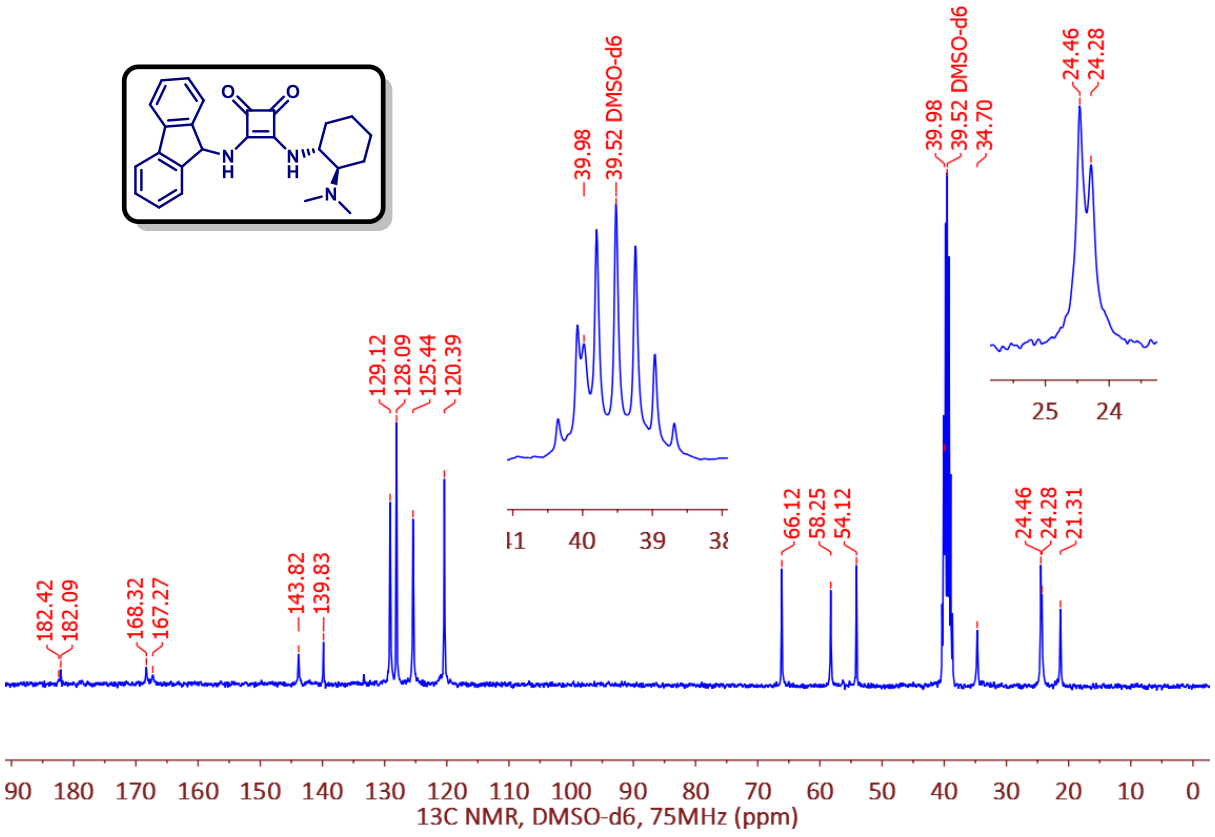

2.50 DMSO-d6
2.37
2.34
2.30
2.15
2.04
1.81
1.77
1.73
1.71
1.64
1.58
1.55
1.29
1.23
1.16
8.27
8.24
7.98
7.67
7.64
7.36
5.35
3.76
2.23
1.03
2.37
1.21
1.13
1.37
1.08
6.00
1.20
1.15
1.10
1.10
3.05
4.28
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 300MHz (ppm)

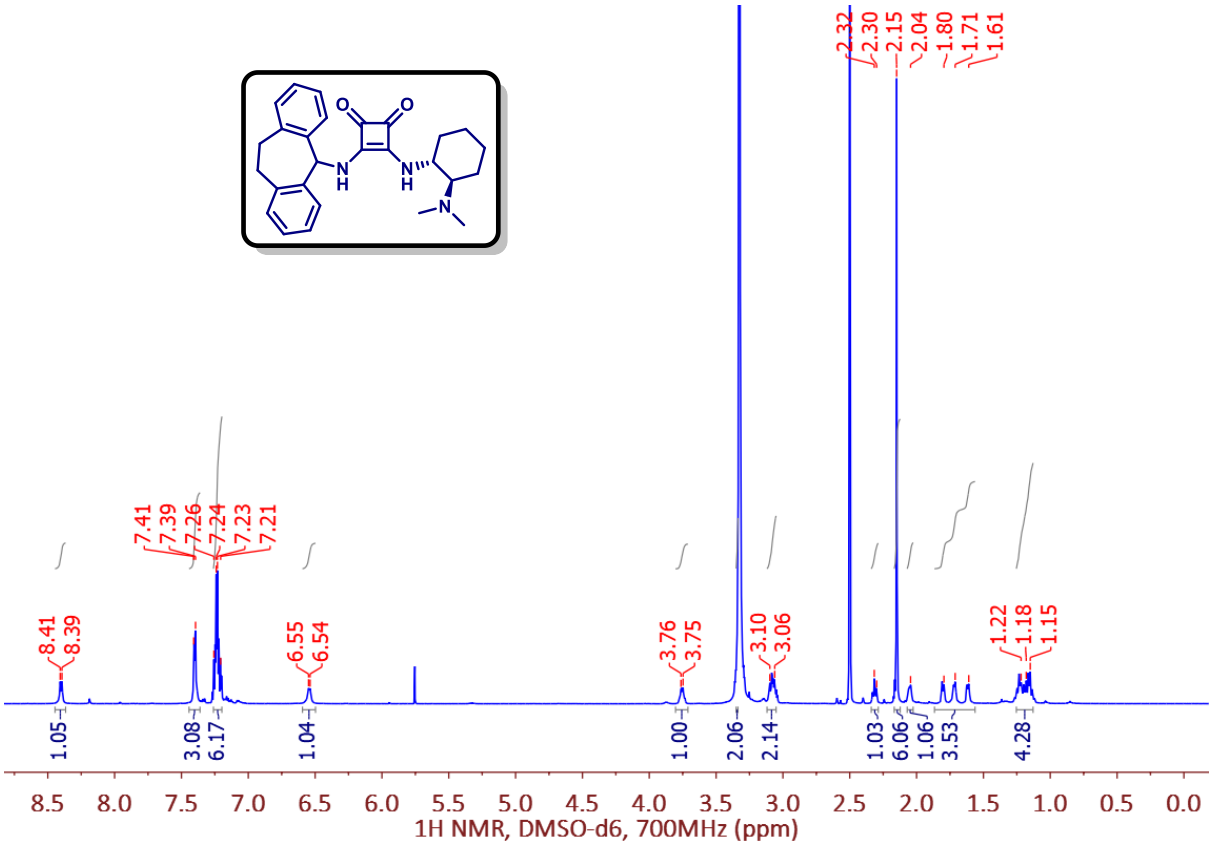

39.95
24.45
24.37
39.95
39.52 DMSO-d6
34.74
127.46
123.93
66.15
54.17
52.20
24.45
24.37
22.57
21.38
182.31
181.62
167.73
166.61
151.37
146.71
41 40 39 38
25.0 24.5 24.0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 75MHz (ppm)

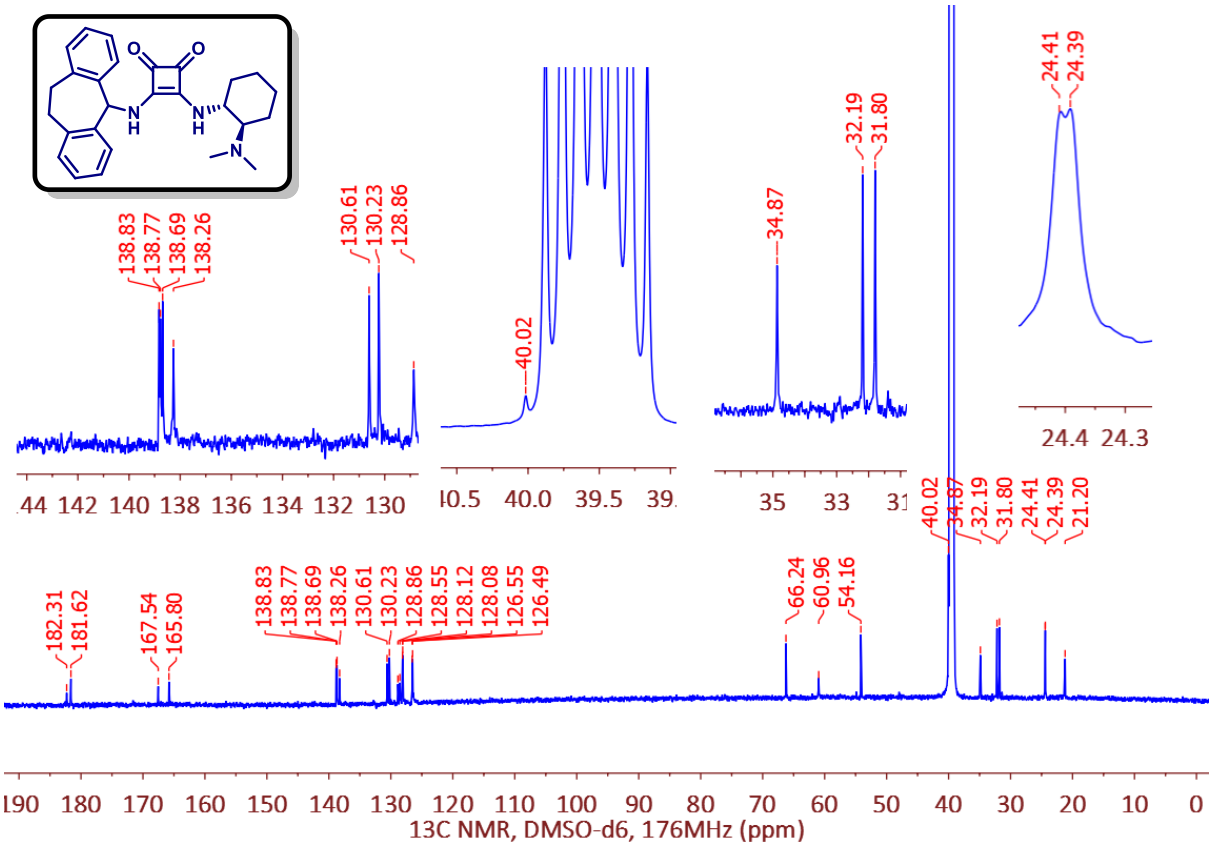

2.50 DMSO-d6
2.35
2.15
2.01
1.81
1.72
1.60
1.30
1.16
8.08
8.04
8.00
7.42
5.41
3.78
4.15
0.90
1.00
1.00
1.00
6.00
1.03
3.03
3.08
4.04
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 300MHz (ppm)

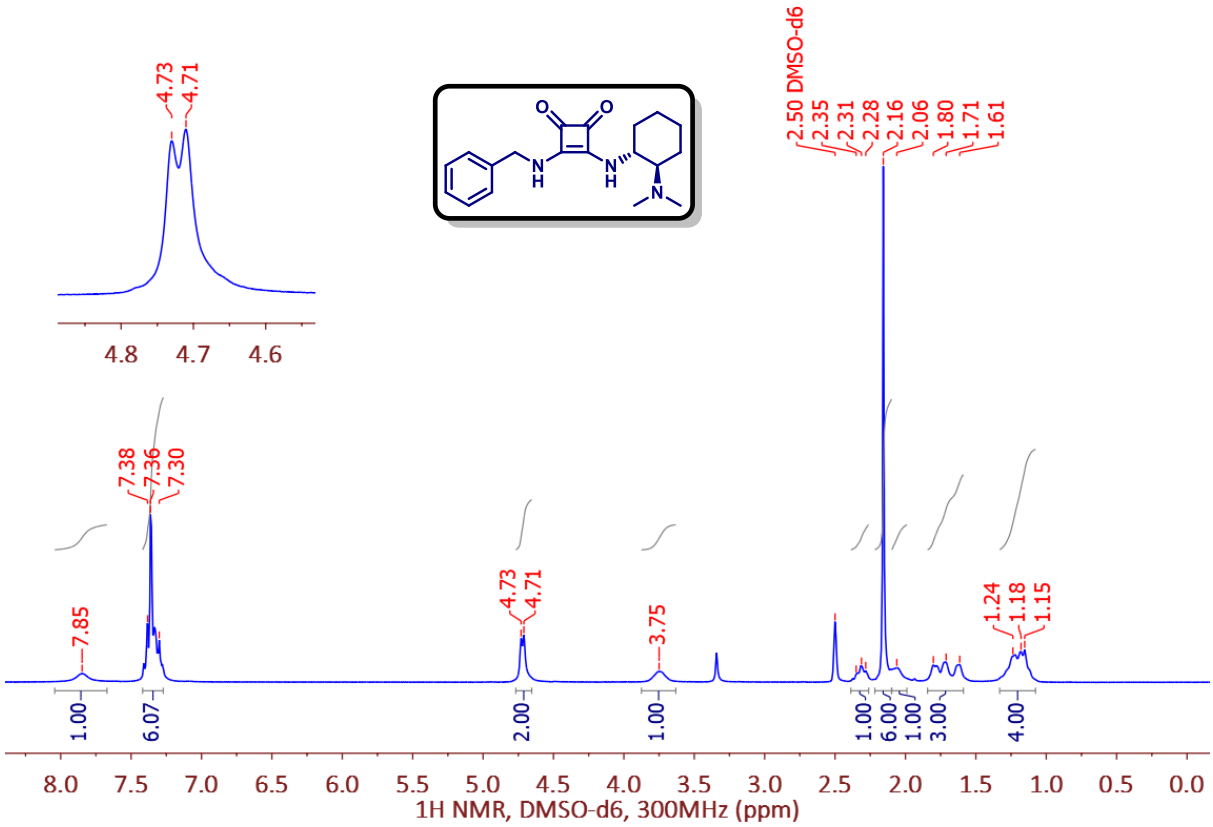

131.19
130.76
130.33
129.89
128.72
127.12
125.11
121.49
121.24
117.88
39.91
34.64
24.48
24.38
182.76
181.67
167.93
166.62
147.51
66.19
54.26
52.06
22.58
21.67
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 75MHz (ppm)

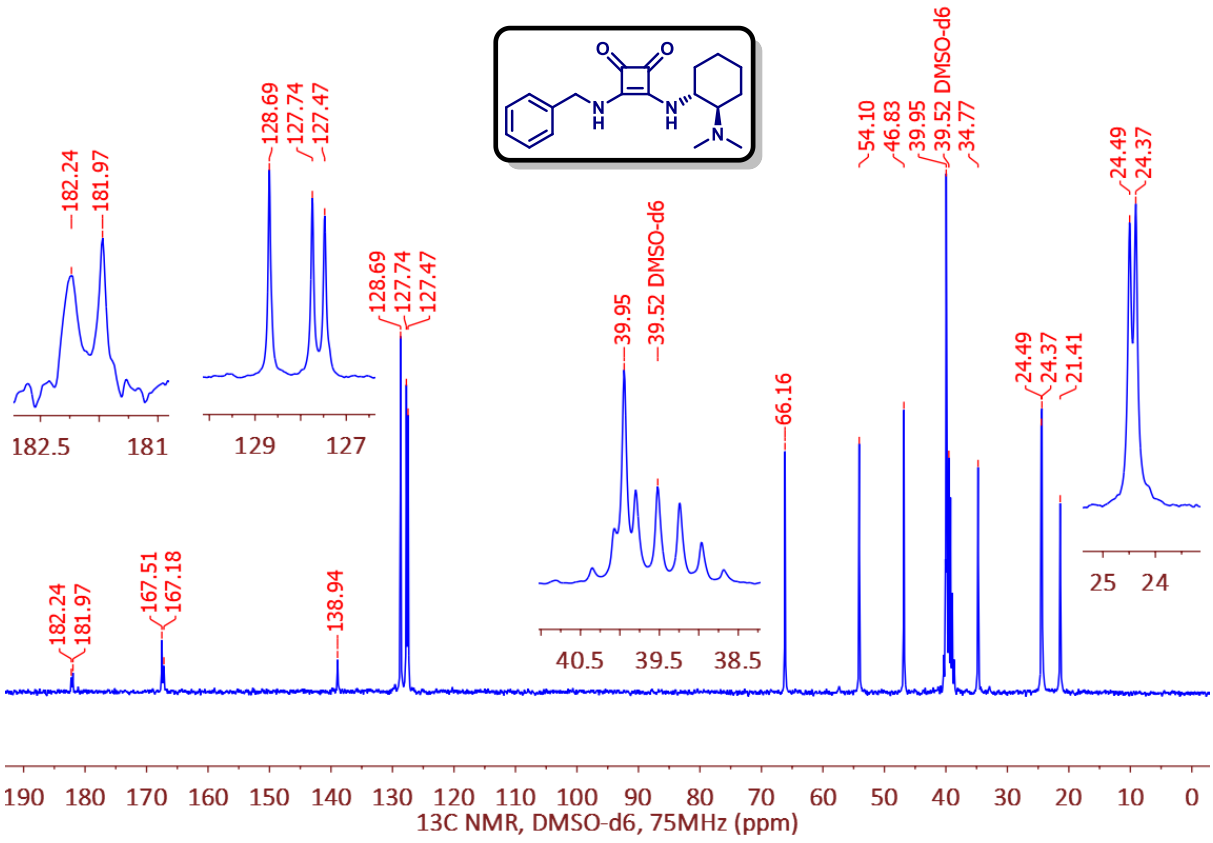

8.00
7.90
7.62
7.48
7.38
7.24
6.13
3.72
2.50 DMSO-d6
2.28
2.15
1.77
1.72
1.62
1.23
1.16
0.95
2.00
2.00
2.00
2.02
0.97
0.92
0.90
1.00
6.01
1.03
3.00
4.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 300MHz (ppm)

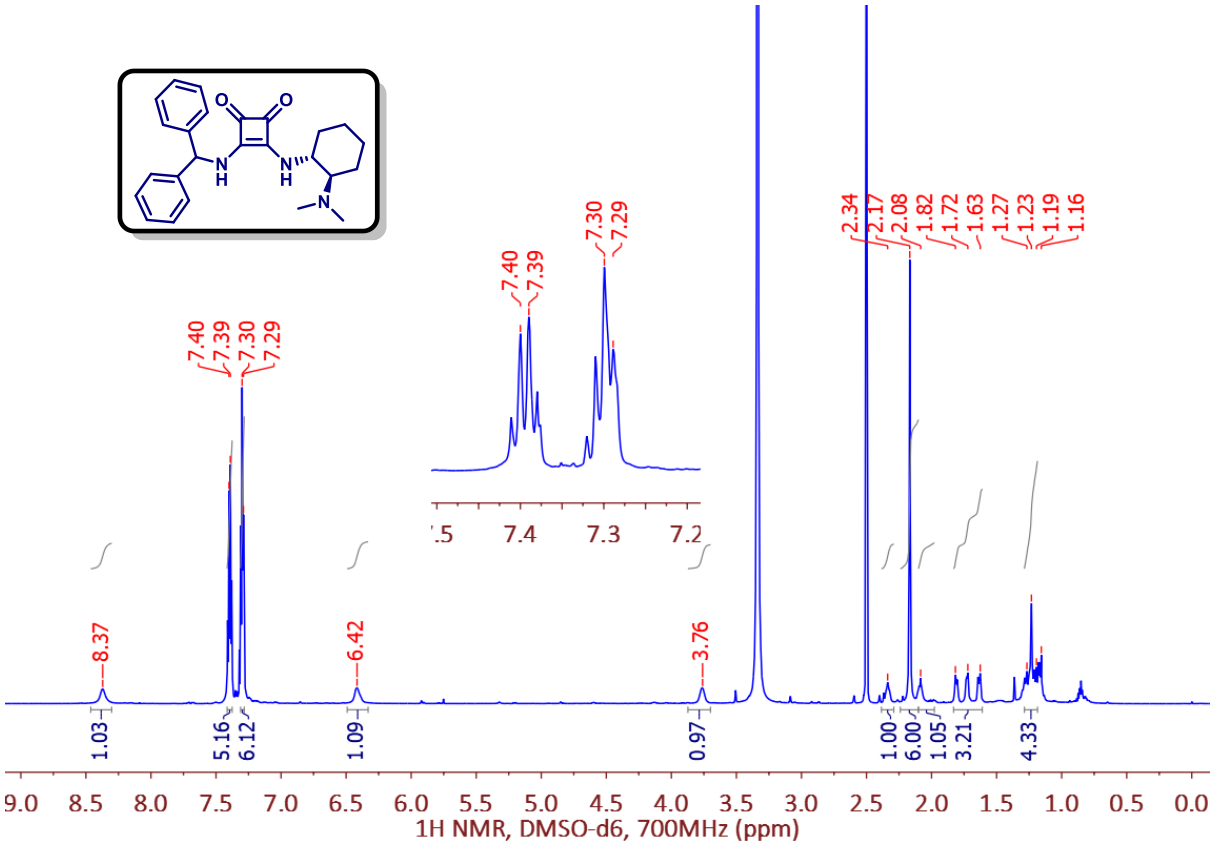

182.42
182.09
168.32
167.27
143.82
139.83
129.12
128.09
125.44
120.39
39.98
39.52 DMSO-d6
66.12
58.25
54.12
39.98
39.52 DMSO-d6
34.70
24.46
24.28
24.46
24.28
21.31
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 75MHz (ppm)

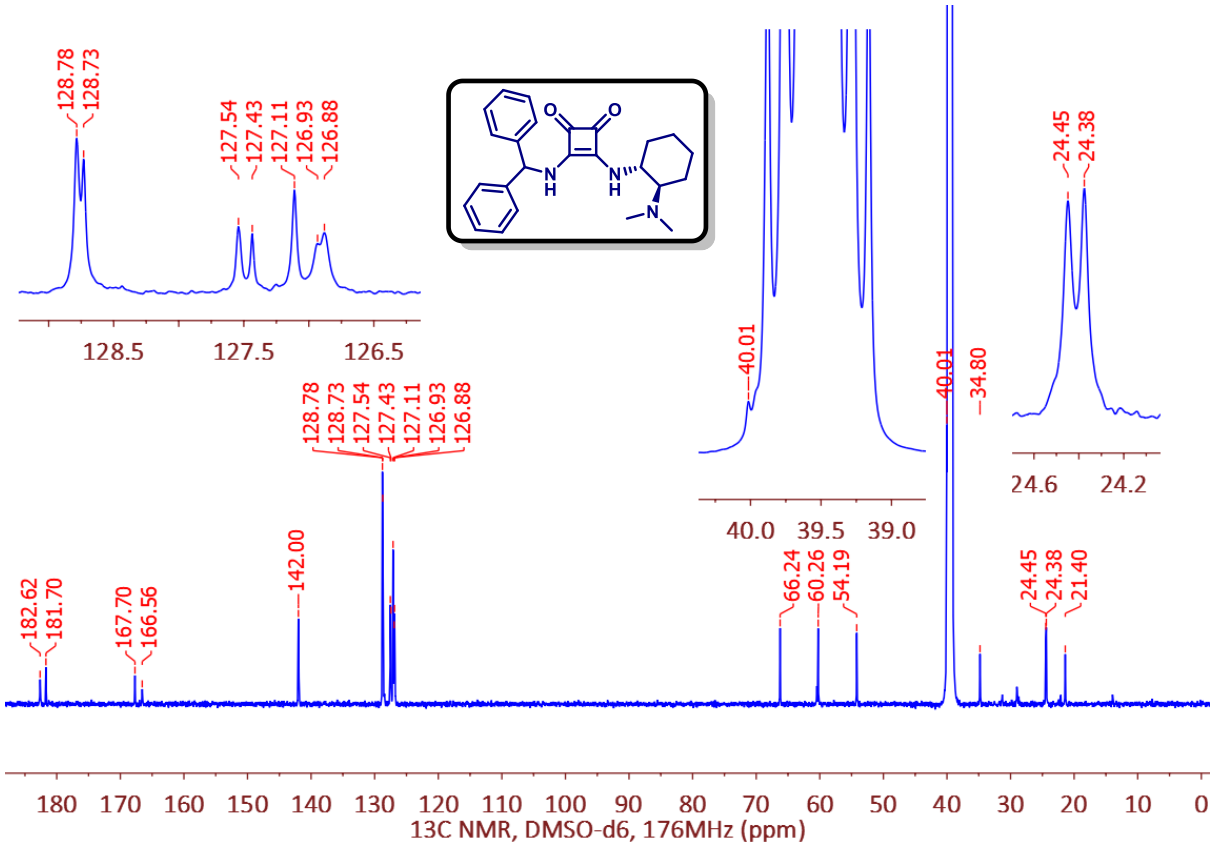

8.41
8.39
7.41
7.39
7.26
7.24
7.23
7.21
6.55
6.54
3.76
3.75
3.10
3.06
2.32
2.30
2.15
2.04
1.80
1.71
1.61
1.22
1.18
1.15
1.05
3.08
6.17
1.04
1.00
2.06
2.14
1.03
6.06
1.06
3.53
4.28
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 700MHz (ppm)

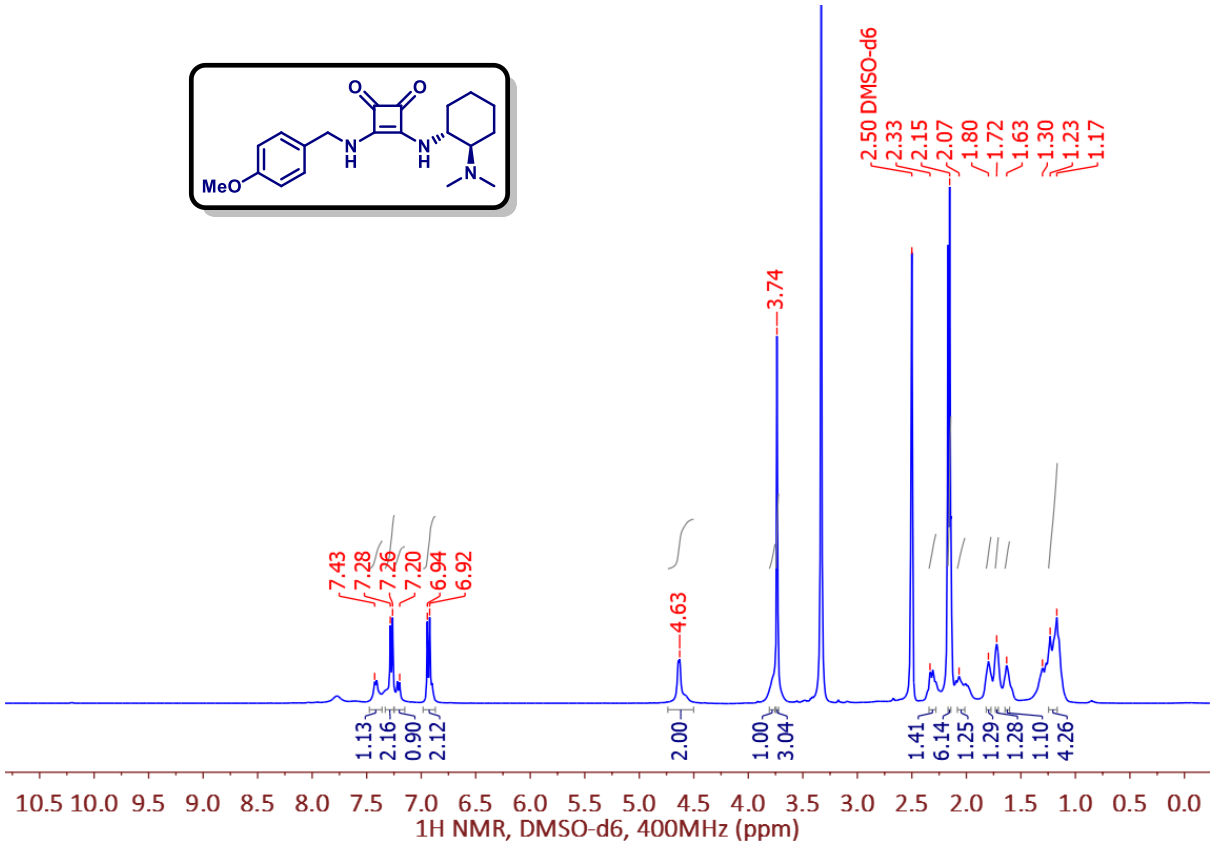

138.83
138.77
138.69
138.26
130.61
130.23
128.86
40.02
34.87
32.19
31.80
24.41
24.39
44 142 140 138 136 134 132 130
40.5 40.0 39.5 39
35 33 31
24.4 24.3
182.31
181.62
167.54
165.80
138.83
138.77
138.69
138.26
130.61
130.23
128.86
128.55
128.12
128.08
126.55
126.49
66.24
60.96
54.16
40.02
34.87
32.19
31.80
24.41
24.39
21.20
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 176MHz (ppm)

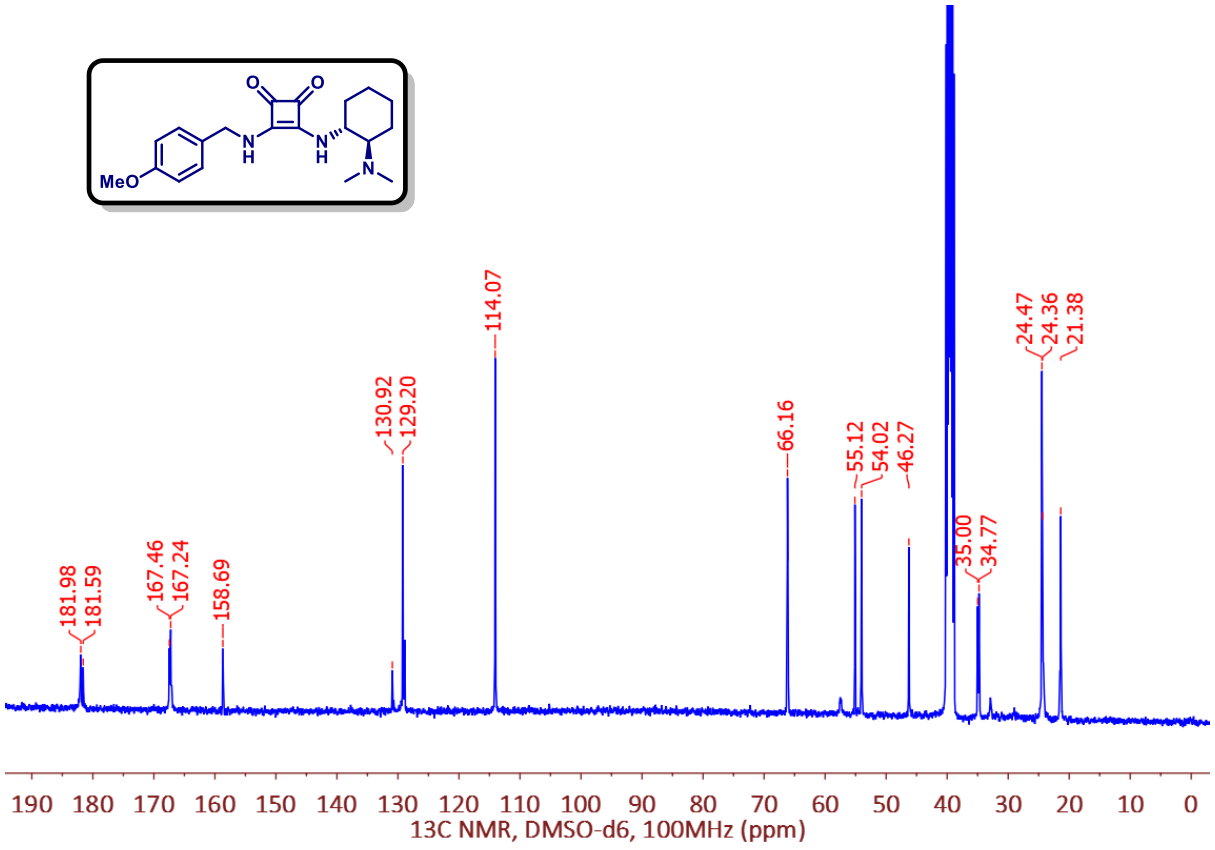

4.73
4.71
4.8
4.7
4.6
2.50 DMSO-d6
2.35
2.31
2.28
2.16
2.06
1.80
1.71
1.61
7.38
7.36
7.30
7.85
4.73
4.71
3.75
1.24
1.18
1.15
1.00
6.07
2.00
1.00
1.00
6.00
1.00
3.00
4.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 300MHz (ppm)

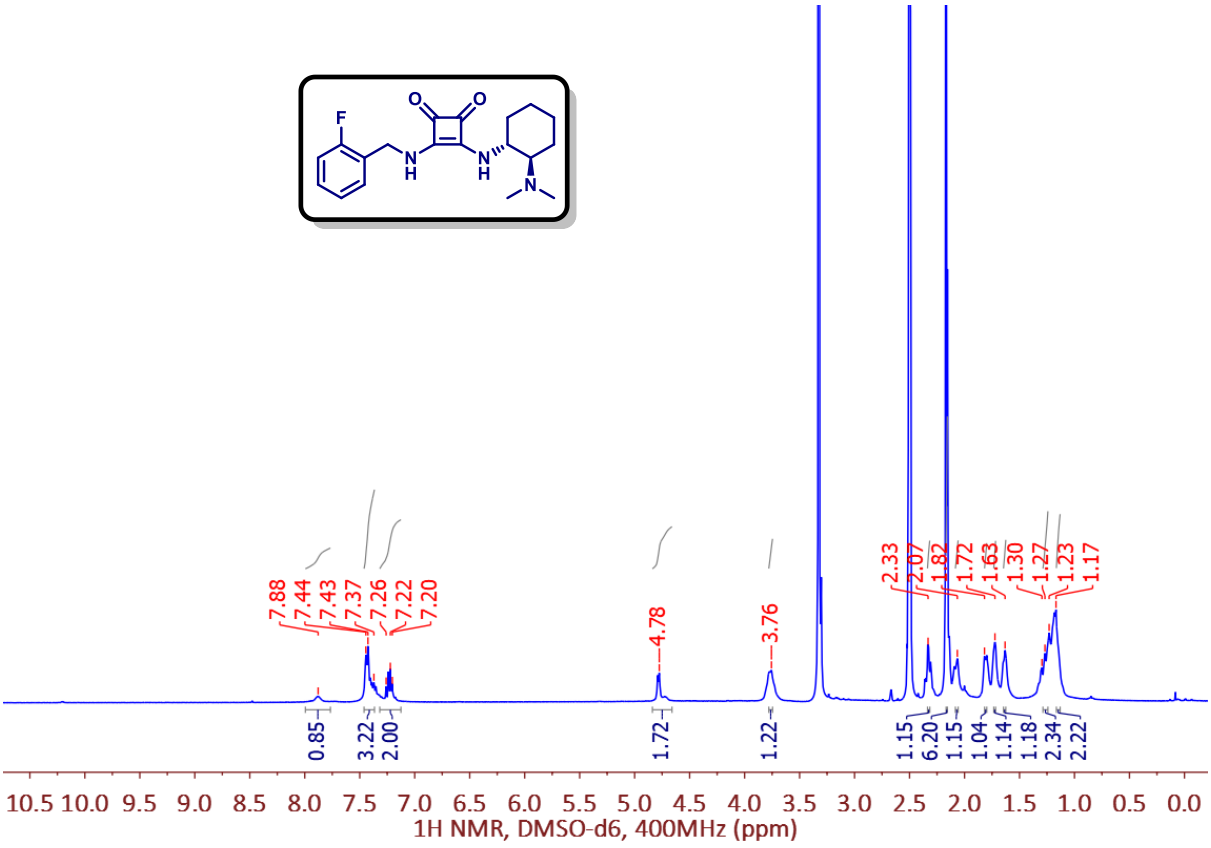

182.24
181.97
182.5
181
128.69
127.74
127.47
129
127
39.95
39.52 DMSO-d6
40.5
39.5
38.5
54.10
46.83
39.95
39.52 DMSO-d6
34.77
66.16
24.49
24.37
21.41
25
24
167.51
167.18
138.94
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 75MHz (ppm)

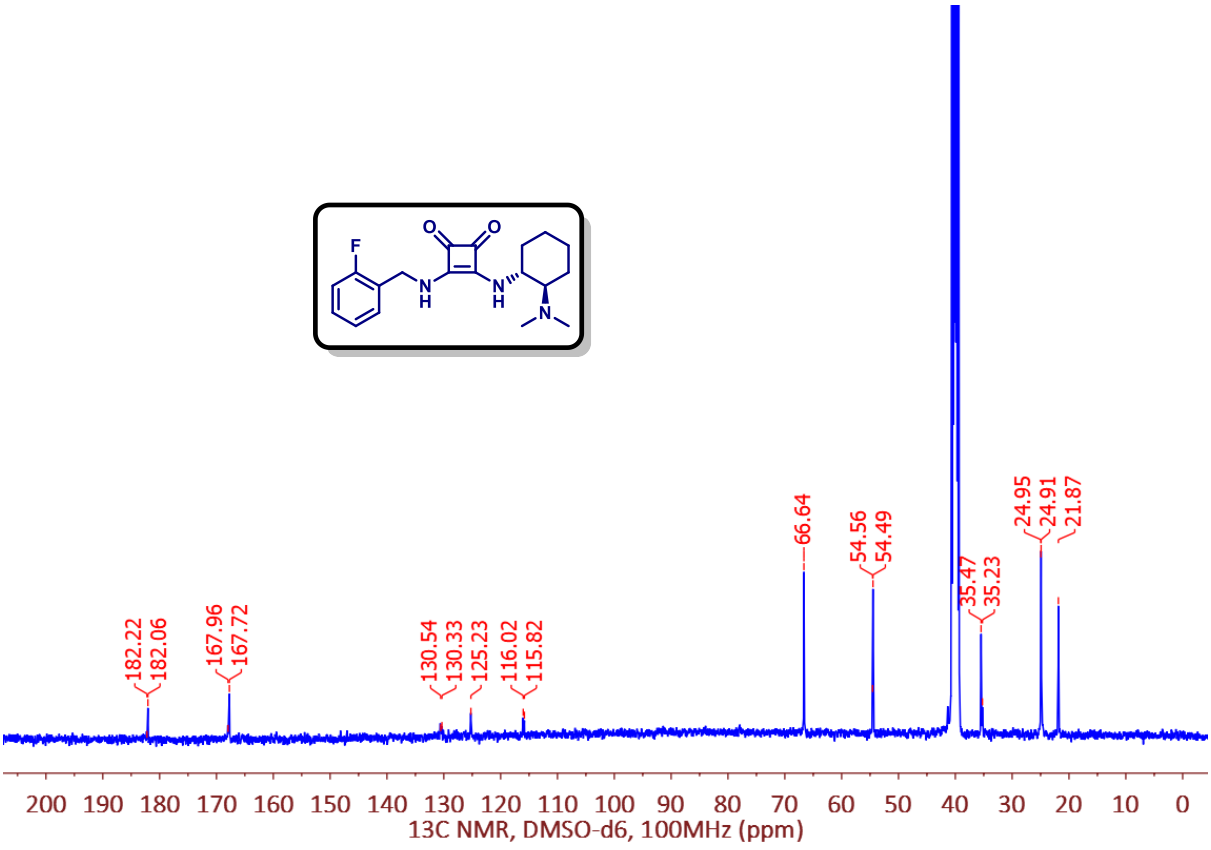

8.37
7.40
7.39
7.30
7.29
6.42
3.76
2.34
2.17
2.08
1.82
1.72
1.63
1.27
1.23
1.19
1.16
1.03
5.16
6.12
1.09
0.97
1.00
6.00
1.05
3.21
4.33
1H NMR, DMSO-d6, 700MHz (ppm)

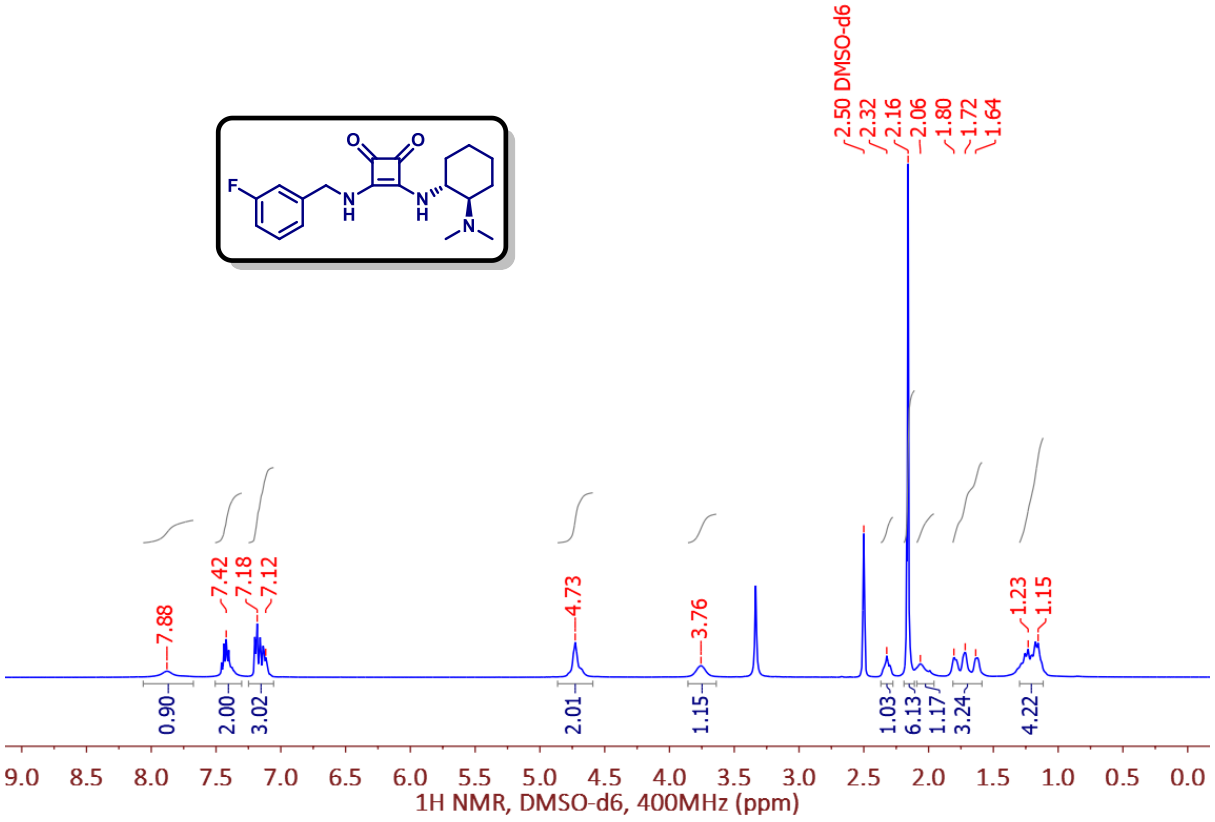

128.78
128.73
127.54
127.43
127.11
126.93
126.88
40.01
34.80
24.45
24.38
182.62
181.70
167.70
166.56
142.00
66.24
60.26
54.19
21.40
13C NMR, DMSO-d6, 176MHz (ppm)

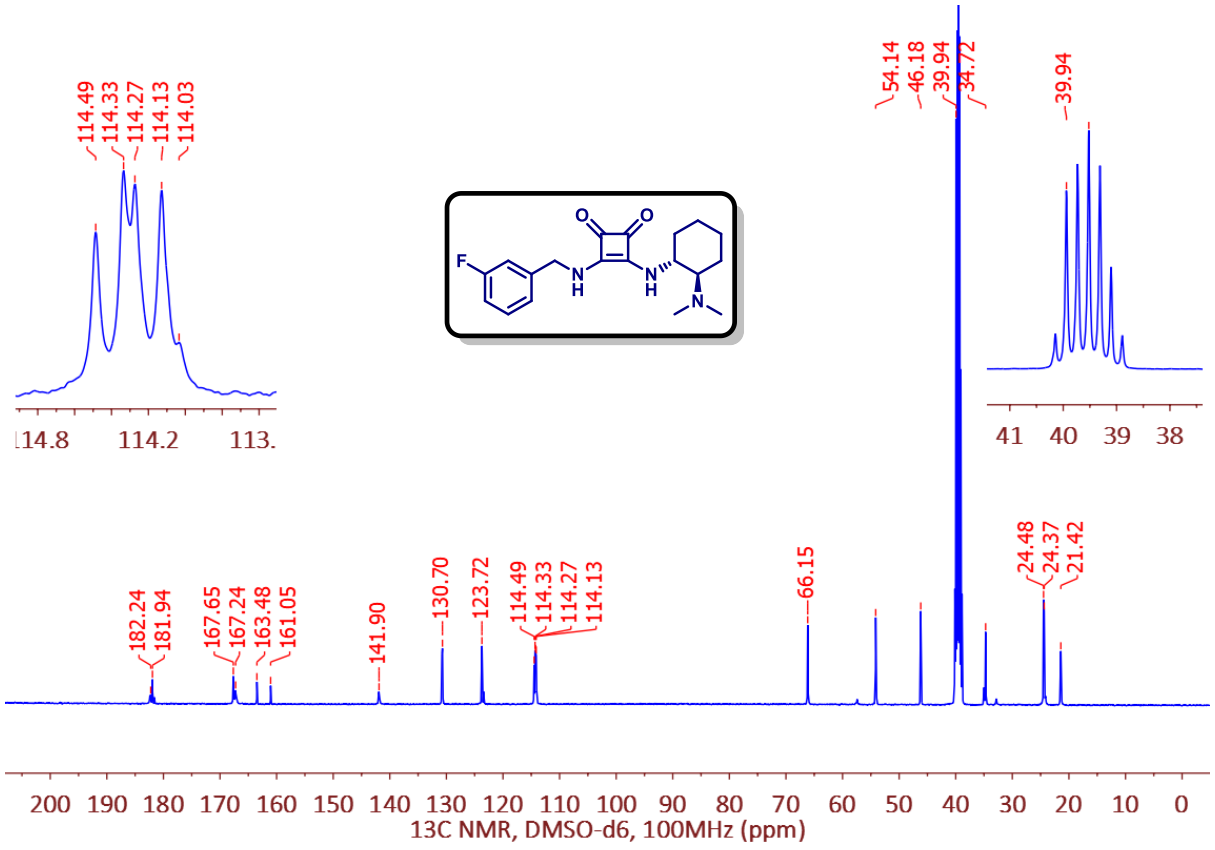

MeO
2.50 DMSO-d6
2.33
2.15
2.07
1.80
1.72
1.63
1.30
1.23
1.17
3.74
7.43
7.28
7.26
7.20
6.94
6.92
4.63
1.13
2.16
0.90
2.12
2.00
1.00
3.04
1.41
6.14
1.25
1.29
1.28
1.10
4.26
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 400MHz (ppm)

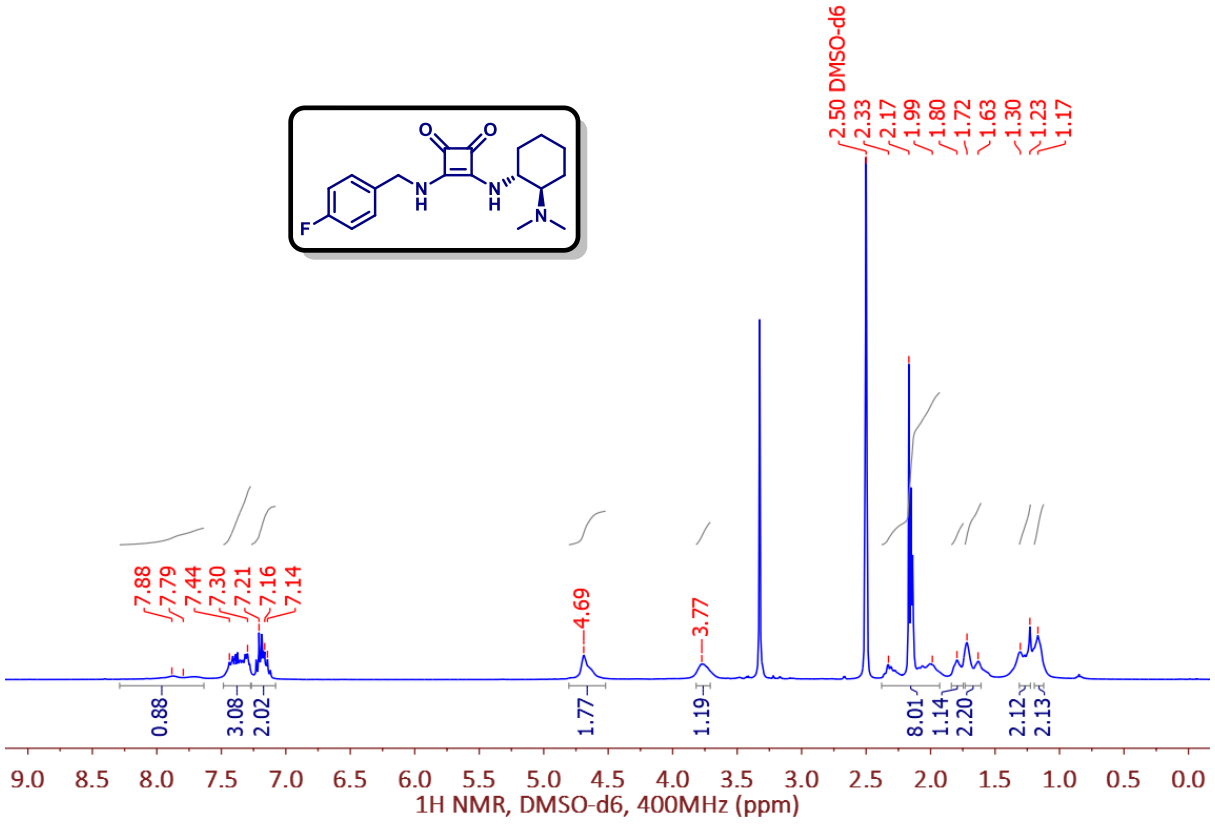

MeO
181.98
181.59
167.46
167.24
158.69
130.92
129.20
114.07
66.16
55.12
54.02
46.27
35.00
34.77
24.47
24.36
21.38
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 100MHz (ppm)

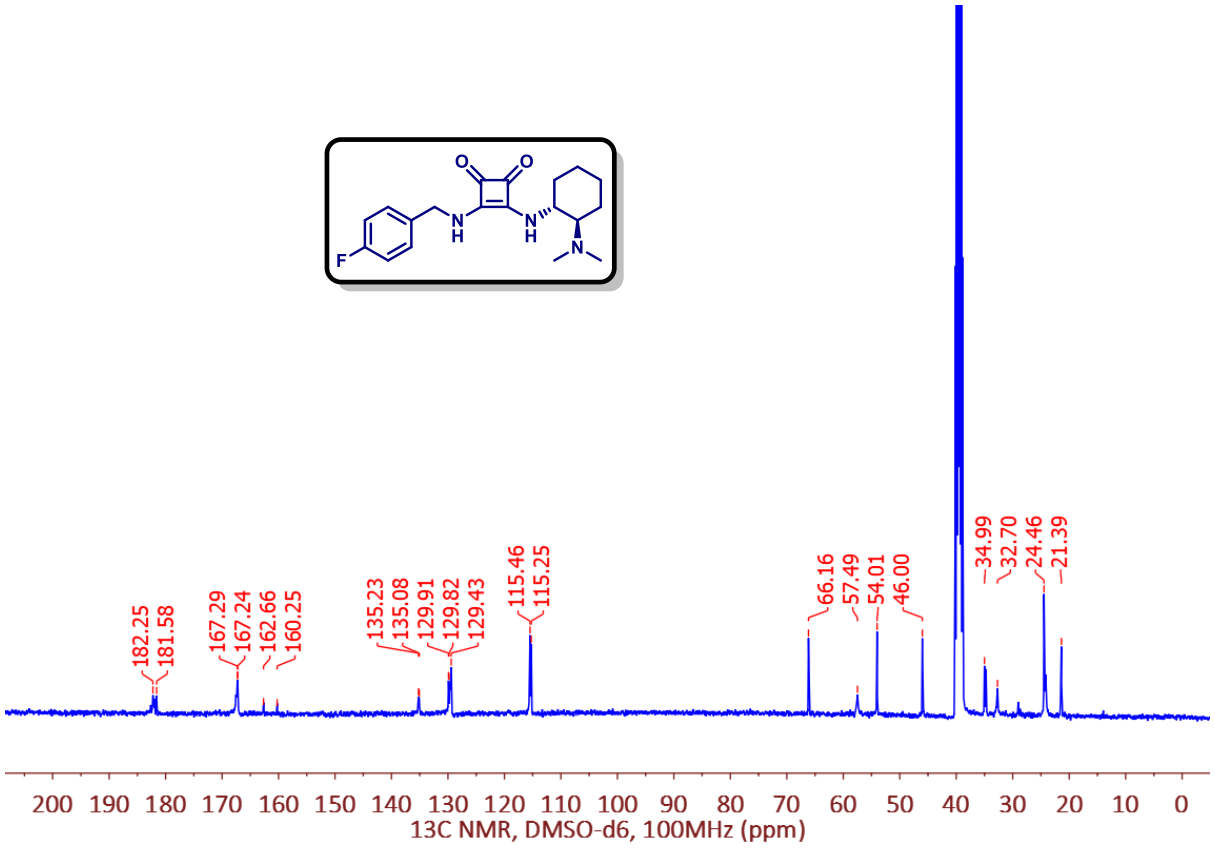

7.88
7.44
7.43
7.37
7.26
7.22
7.20
4.78
3.76
2.33
2.07
1.82
1.72
1.63
1.30
1.27
1.23
1.17
0.85
3.22
2.00
1.72
1.22
1.15
6.20
1.15
1.04
1.14
1.18
2.34
2.22
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 400MHz (ppm)

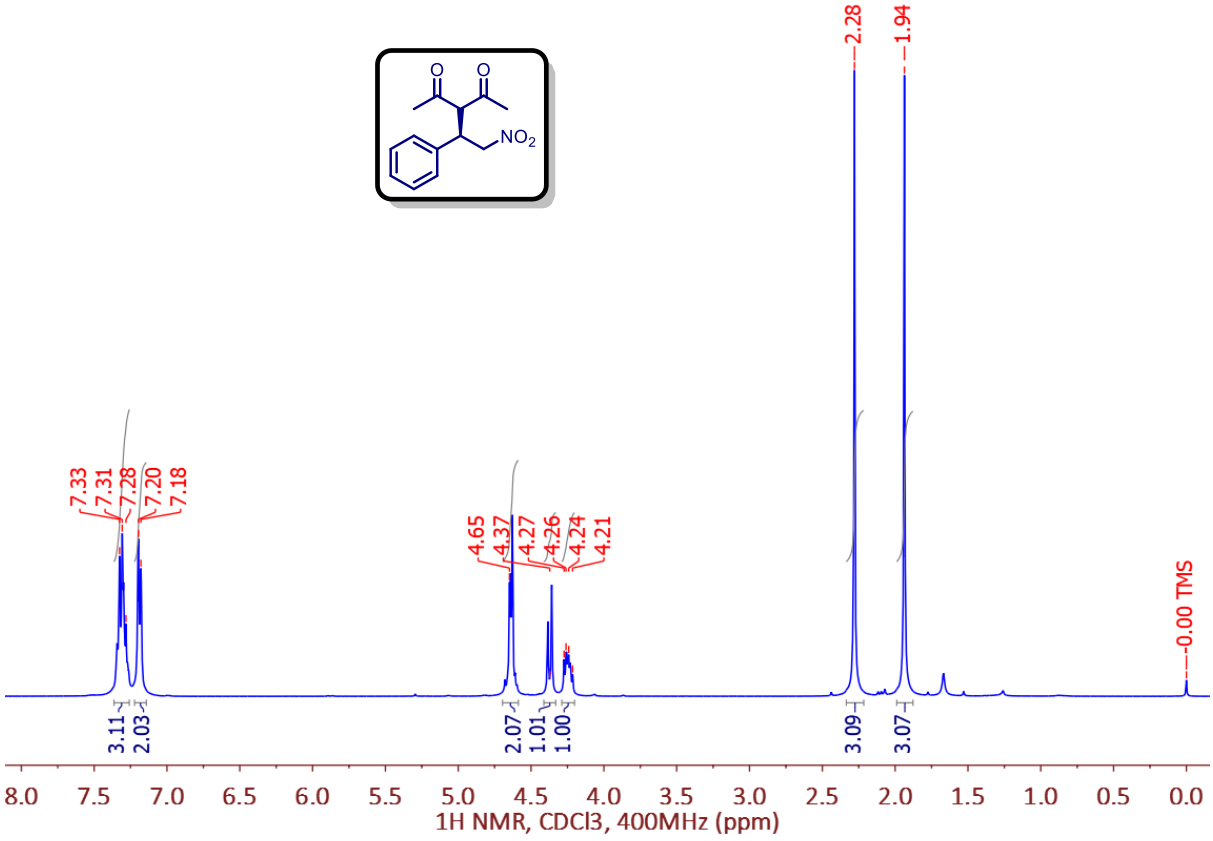

182.22
182.06
167.96
167.72
130.54
130.33
125.23
116.02
115.82
66.64
54.56
54.49
35.47
35.23
24.95
24.91
21.87
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 100MHz (ppm)

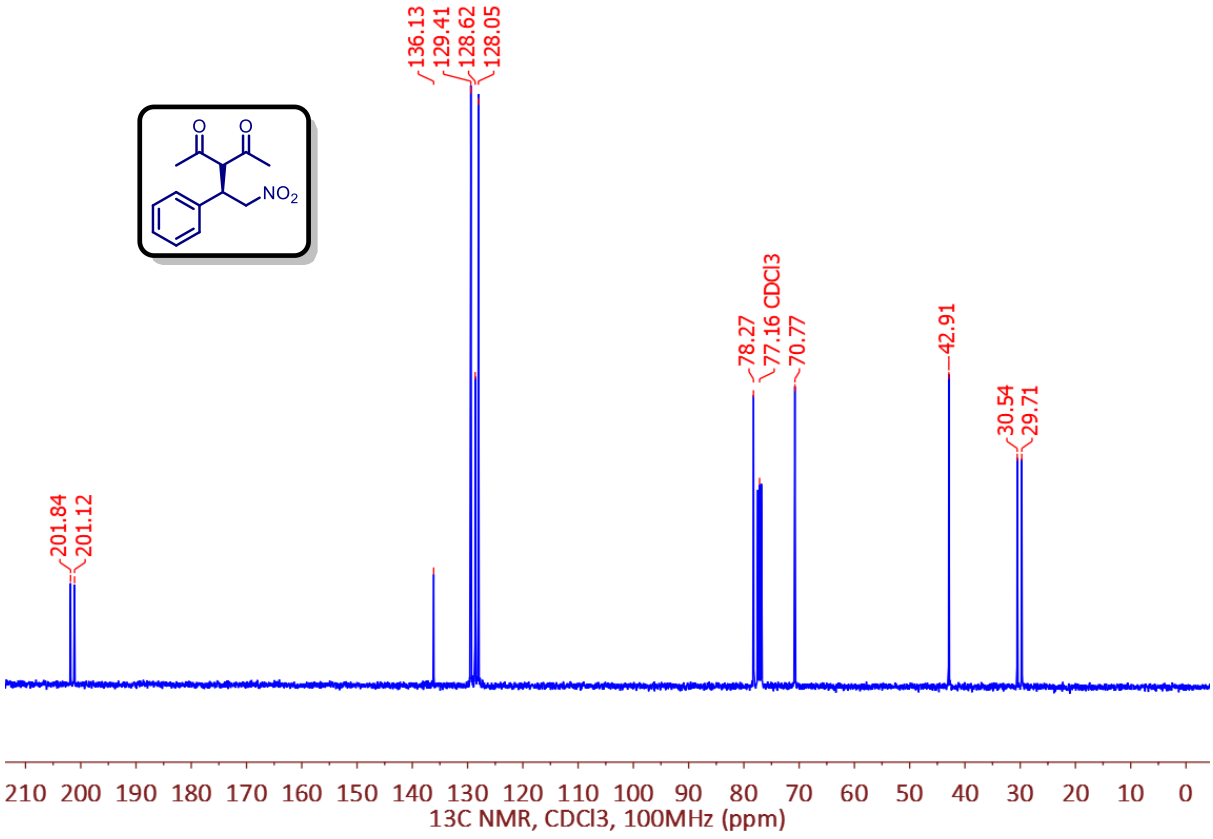

2.50 DMSO-d6
2.32
2.16
2.06
1.80
1.72
1.64
7.88
7.42
7.18
7.12
4.73
3.76
1.23
1.15
0.90
2.00
3.02
2.01
1.15
1.03
6.13
1.17
3.24
4.22
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 400MHz (ppm)

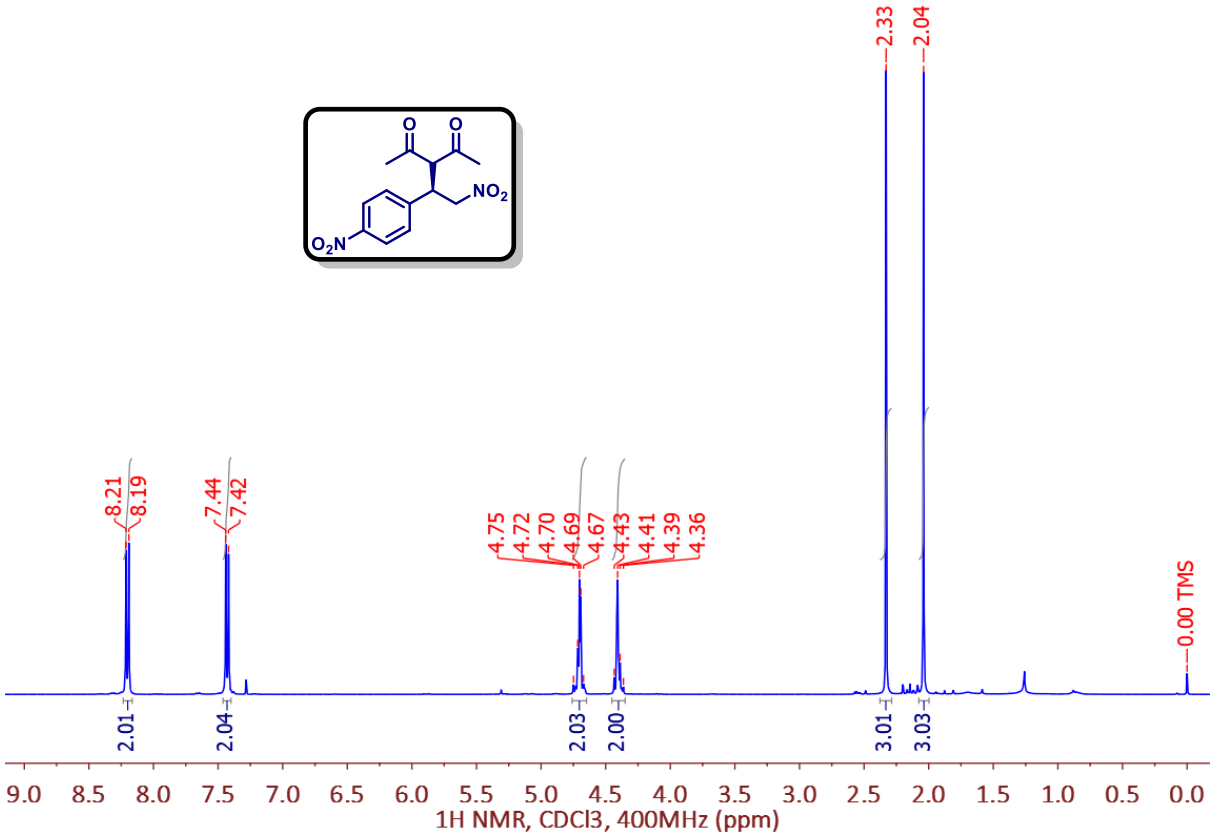

114.49
114.33
114.27
114.13
114.03
14.8 114.2 113.
54.14
46.18
39.94
34.72
39.94
41 40 39 38
182.24
181.94
167.65
167.24
163.48
161.05
141.90
130.70
123.72
114.49
114.33
114.27
114.13
66.15
24.48
24.37
21.42
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 100MHz (ppm)

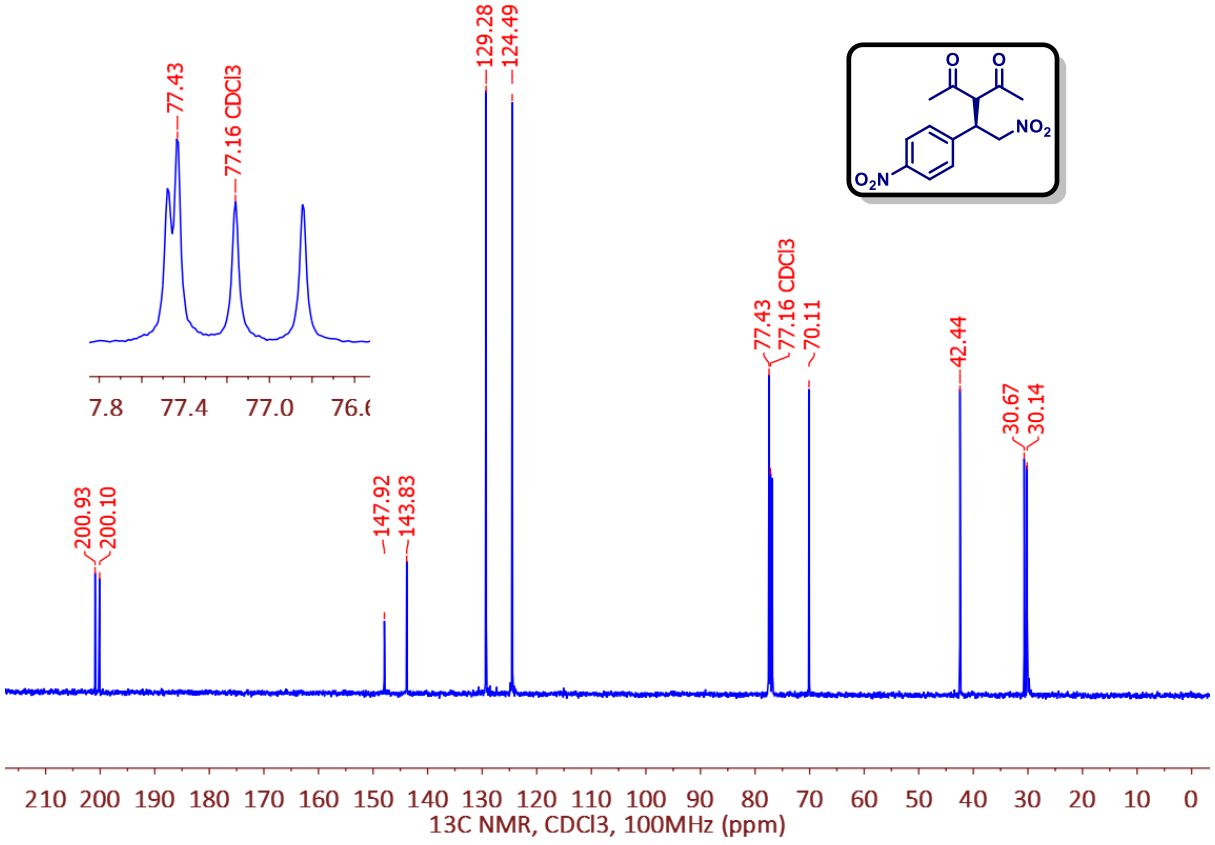

2.50 DMSO-d6
2.33
2.17
1.99
1.80
1.72
1.63
1.30
1.23
1.17
7.88
7.79
7.44
7.30
7.21
7.16
7.14
4.69
3.77
0.88
3.08
2.02
1.77
1.19
8.01
1.14
2.20
2.12
2.13
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, DMSO-d6, 400MHz (ppm)

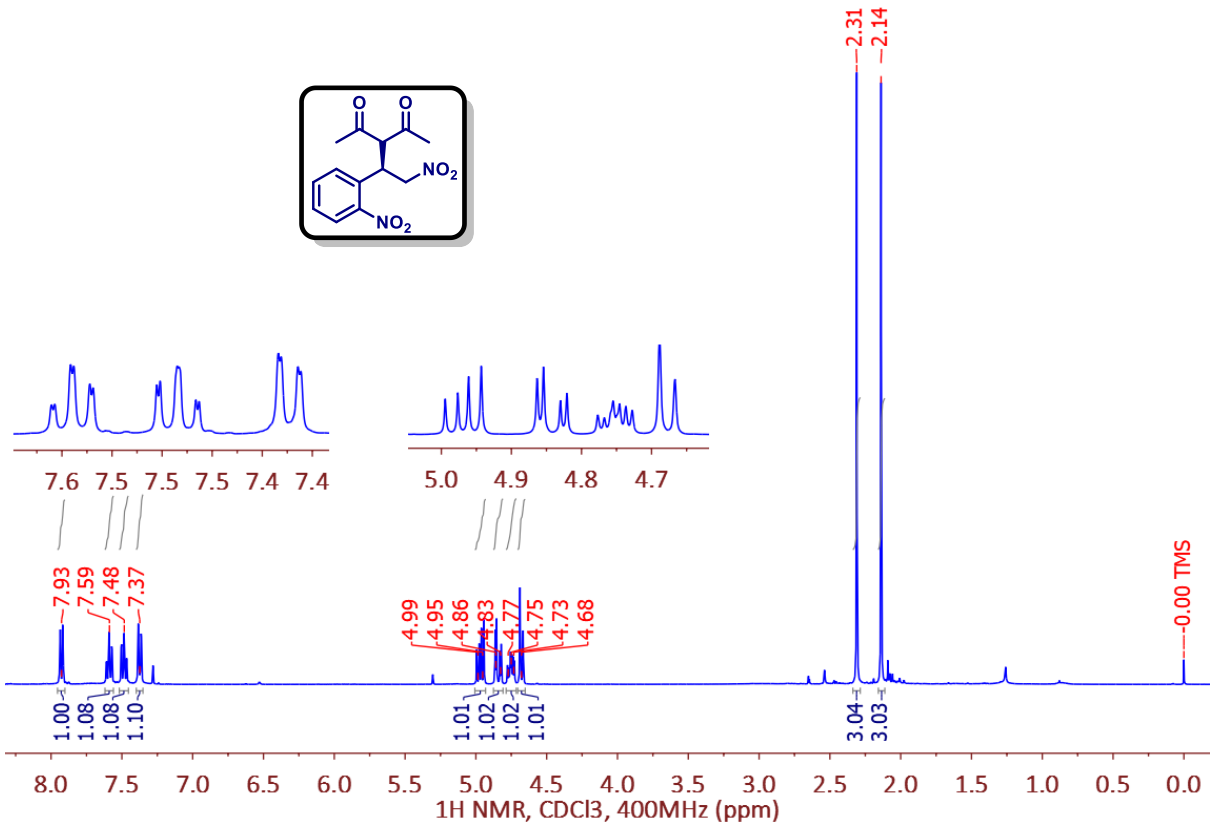

182.25
181.58
167.29
167.24
162.66
160.25
135.23
135.08
129.91
129.82
129.43
115.46
115.25
66.16
57.49
54.01
46.00
34.99
32.70
24.46
21.39
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, DMSO-d6, 100MHz (ppm)

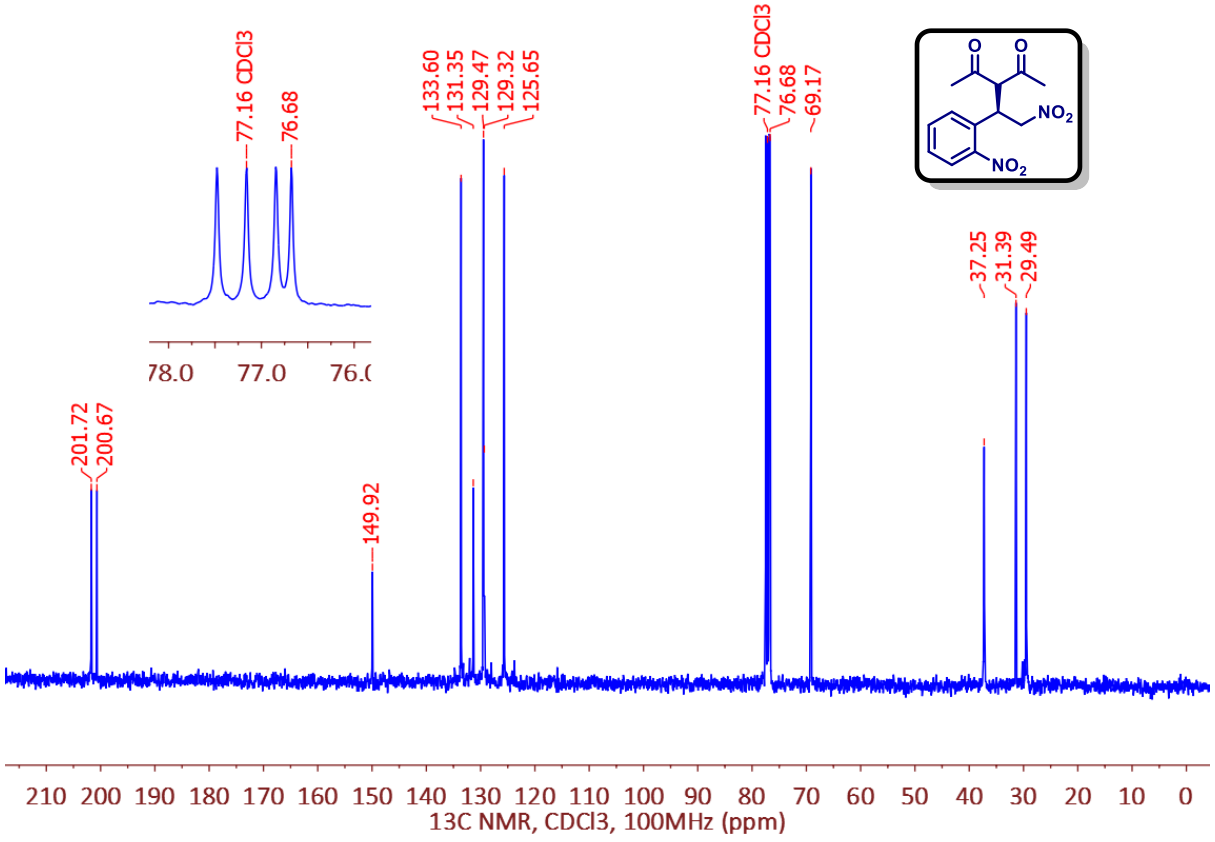

2.28
1.94
7.33
7.31
7.28
7.20
7.18
4.65
4.37
4.27
4.26
4.24
4.21
0.00 TMS
3.11
2.03
2.07
1.01
1.00
3.09
3.07
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)

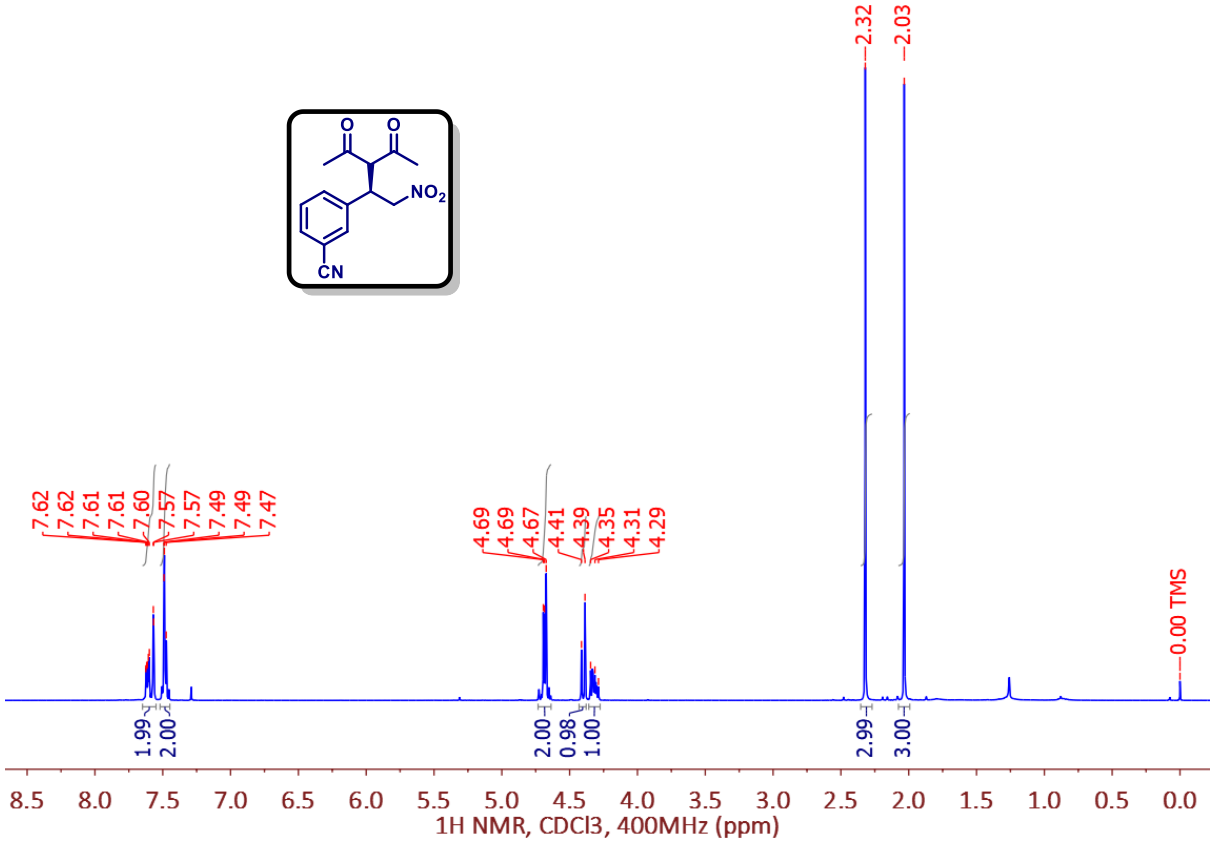

136.13
129.41
128.62
128.05
78.27
77.16 CDCl3
70.77
42.91
30.54
29.71
201.84
201.12
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)

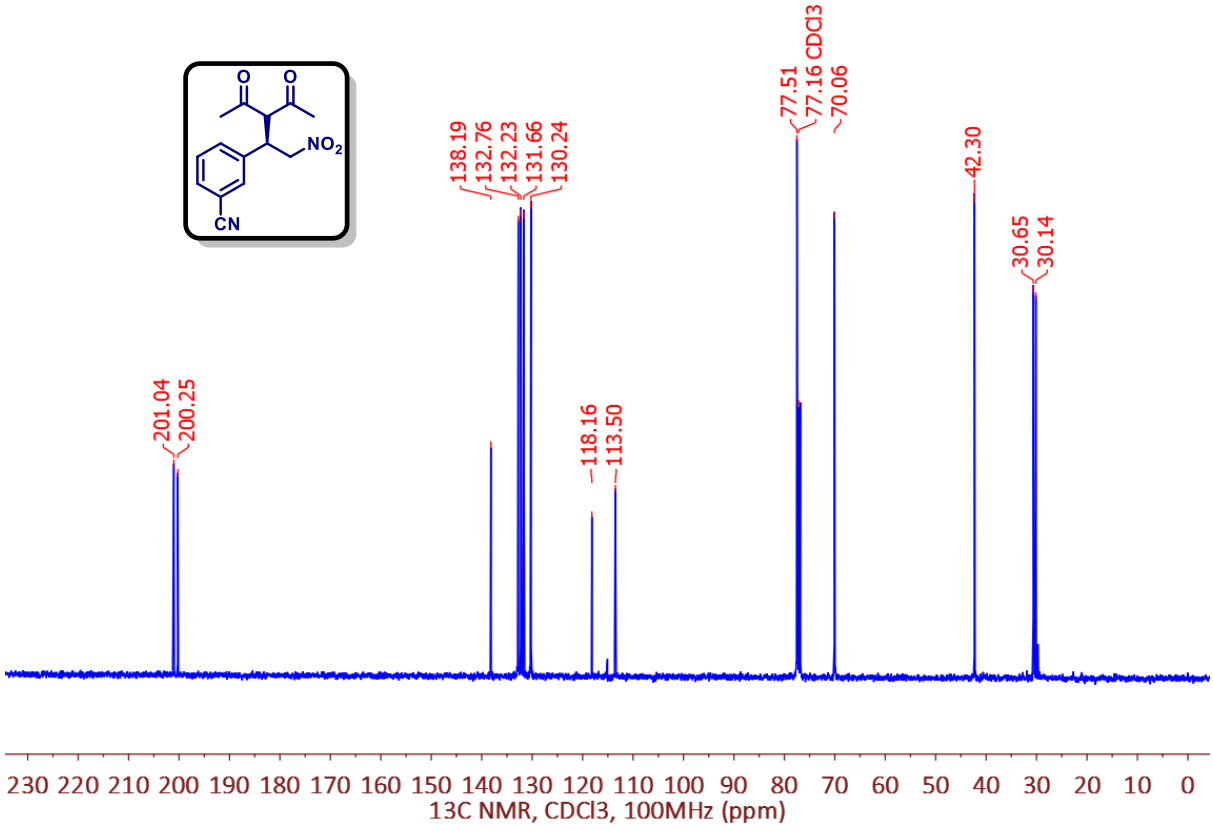

2.33
2.04
8.21
8.19
7.44
7.42
4.75
4.72
4.70
4.69
4.67
4.43
4.41
4.39
4.36
0.00 TMS
2.01
2.04
2.03
2.00
3.01
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)

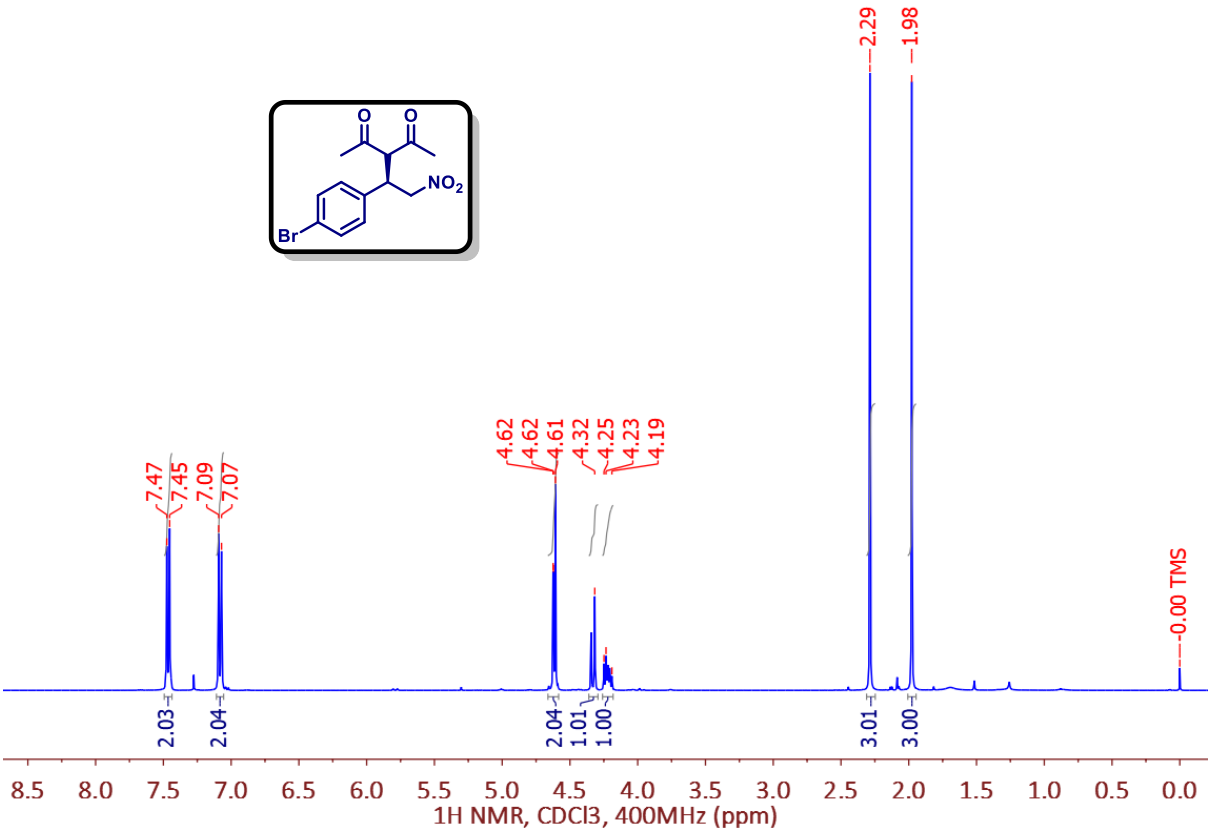

129.28
124.49
77.43
77.16 CDCl3
77.43
77.16 CDCl3
70.11
42.44
30.67
30.14
200.93
200.10
147.92
143.83
7.8 77.4 77.0 76.
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)

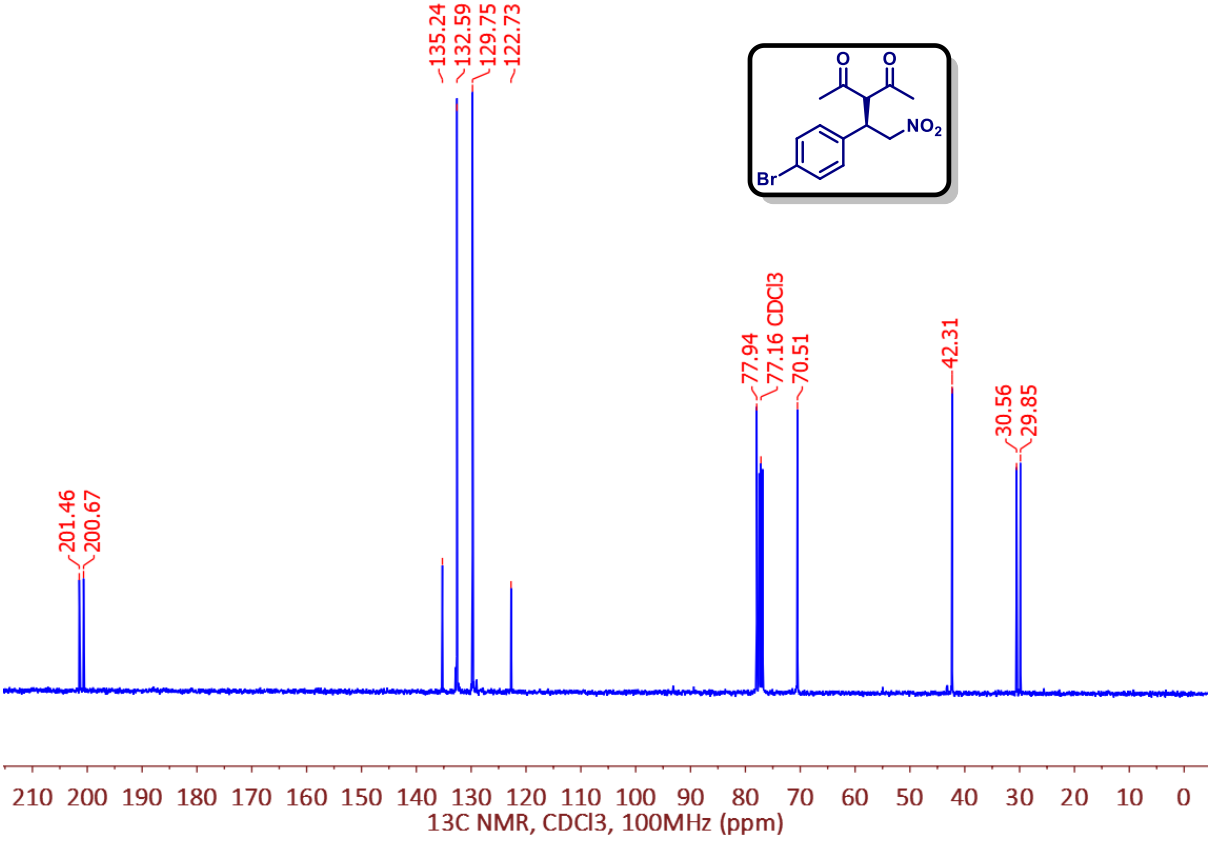

2.31
2.14
7.93
7.59
7.48
7.37
4.99
4.95
4.86
4.83
4.77
4.75
4.73
4.68
0.00 TMS
1.00
1.08
1.08
1.10
1.01
1.02
1.02
1.01
3.04
3.03
1H NMR, CDCl3, 400MHz (ppm)

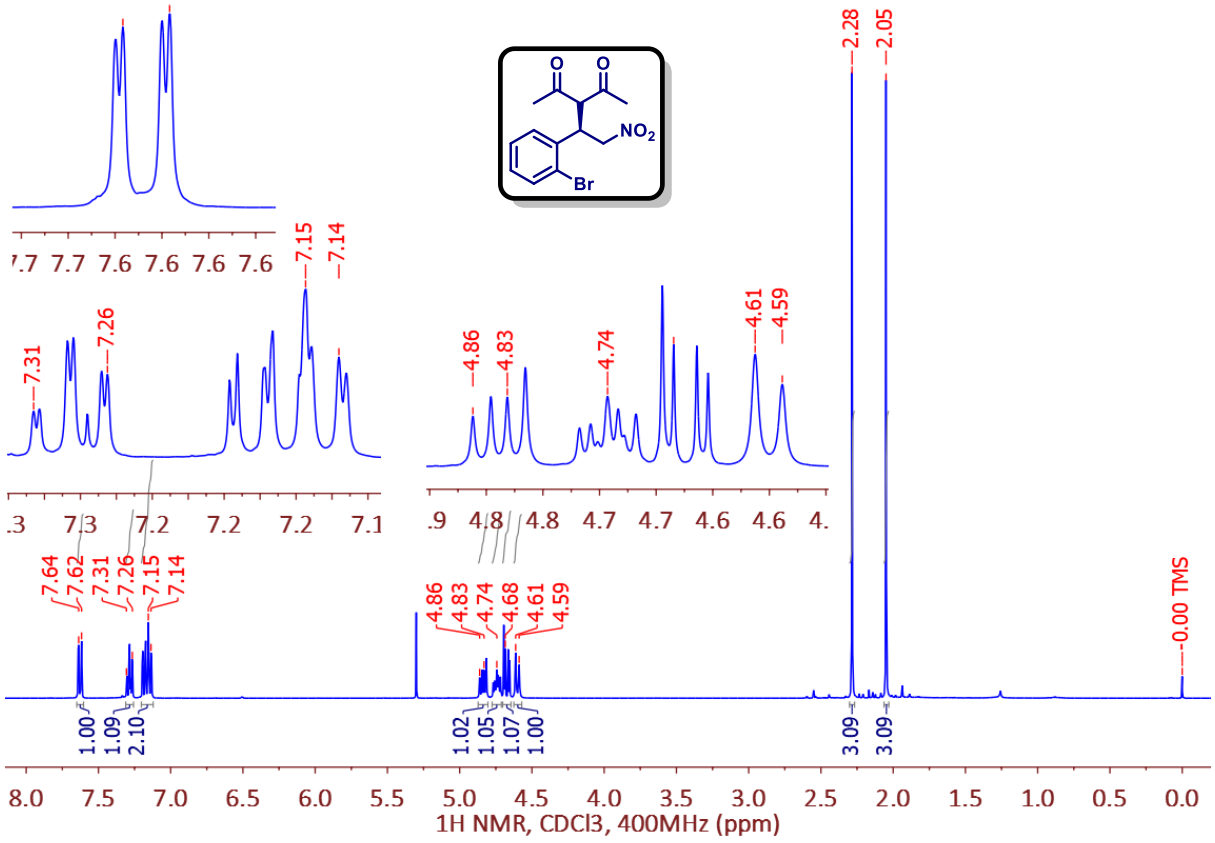

77.16 CDCl3
76.68
133.60
131.35
129.47
129.32
125.65
77.16 CDCl3
76.68
69.17
37.25
31.39
29.49
201.72
200.67
149.92
13C NMR, CDCl3, 100MHz (ppm)

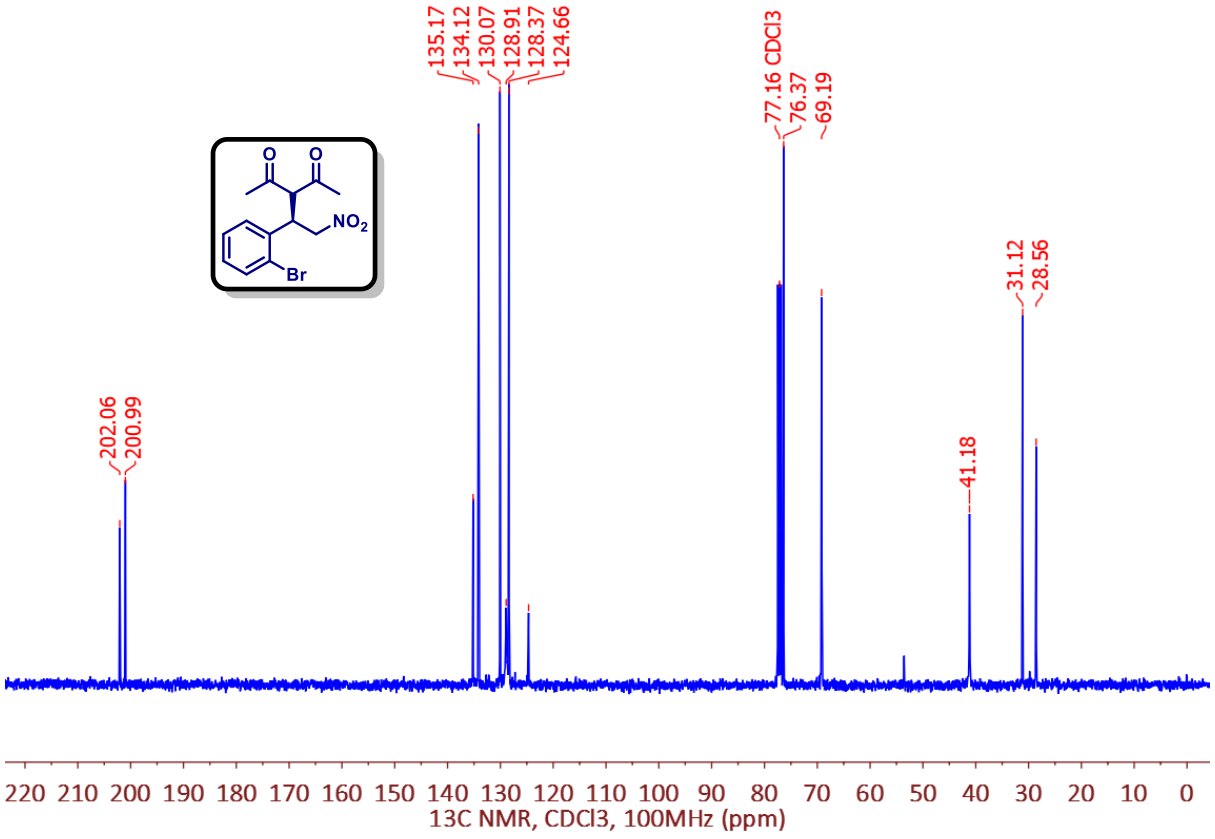

O
O
NO2
CN
2.32
2.03
7.62
7.62
7.61
7.61
7.60
7.57
7.57
7.49
7.49
7.47
4.69
4.69
4.67
4.41
4.39
4.35
4.31
4.29
0.00 TMS
1.99
2.00
2.00
0.98
1.00
2.99
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)

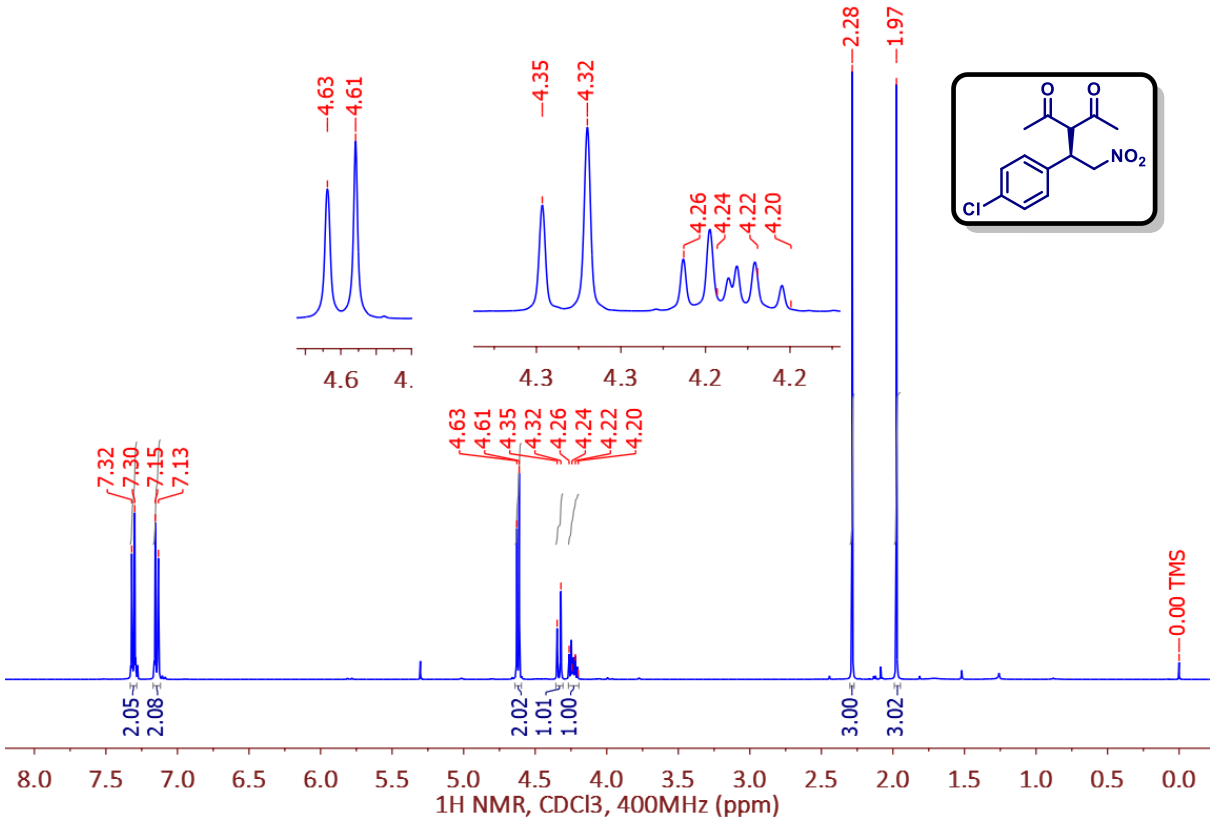

O
O
NO2
CN
138.19
132.76
132.23
131.66
130.24
77.51
77.16 CDCl3
70.06
42.30
30.65
30.14
201.04
200.25
118.16
113.50
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)

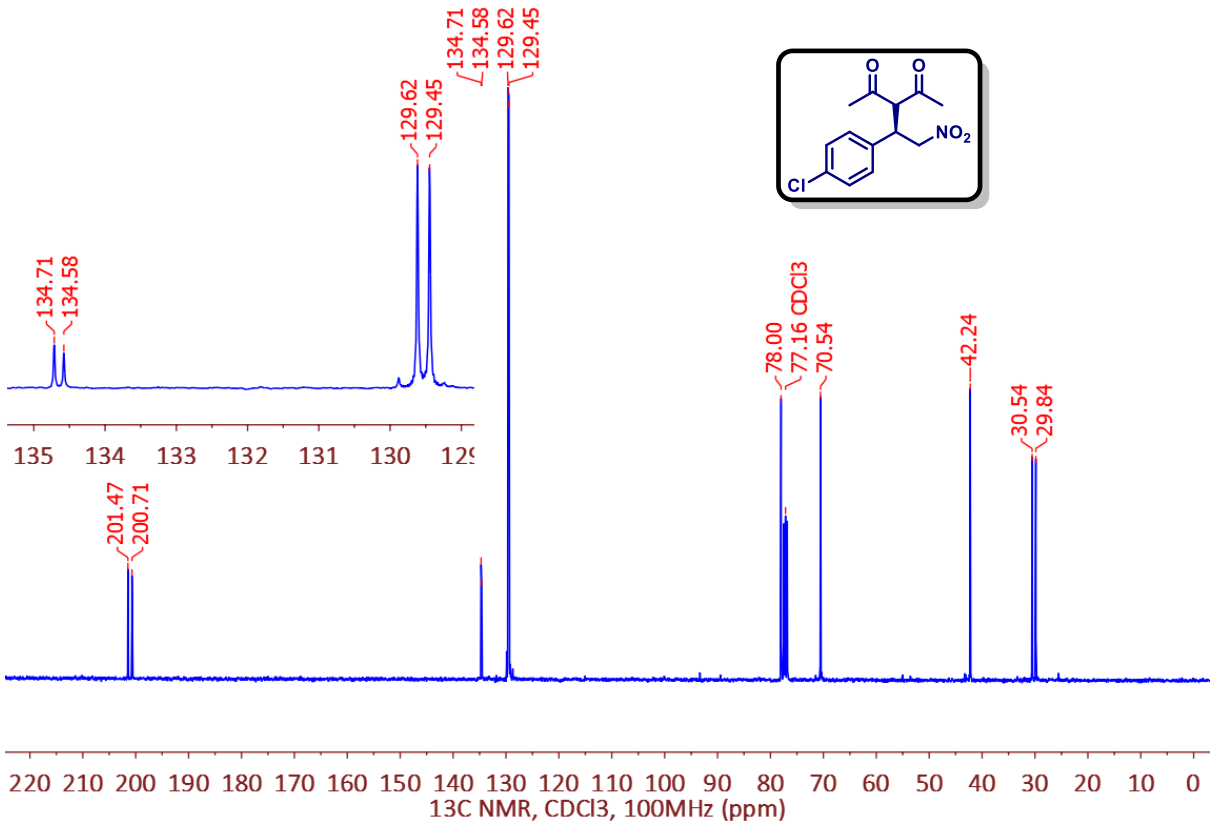

O
O
NO2
Br
2.29
1.98
7.47
7.45
7.09
7.07
4.62
4.62
4.61
4.32
4.25
4.23
4.19
0.00 TMS
2.03
2.04
2.04
1.01
1.00
3.01
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)

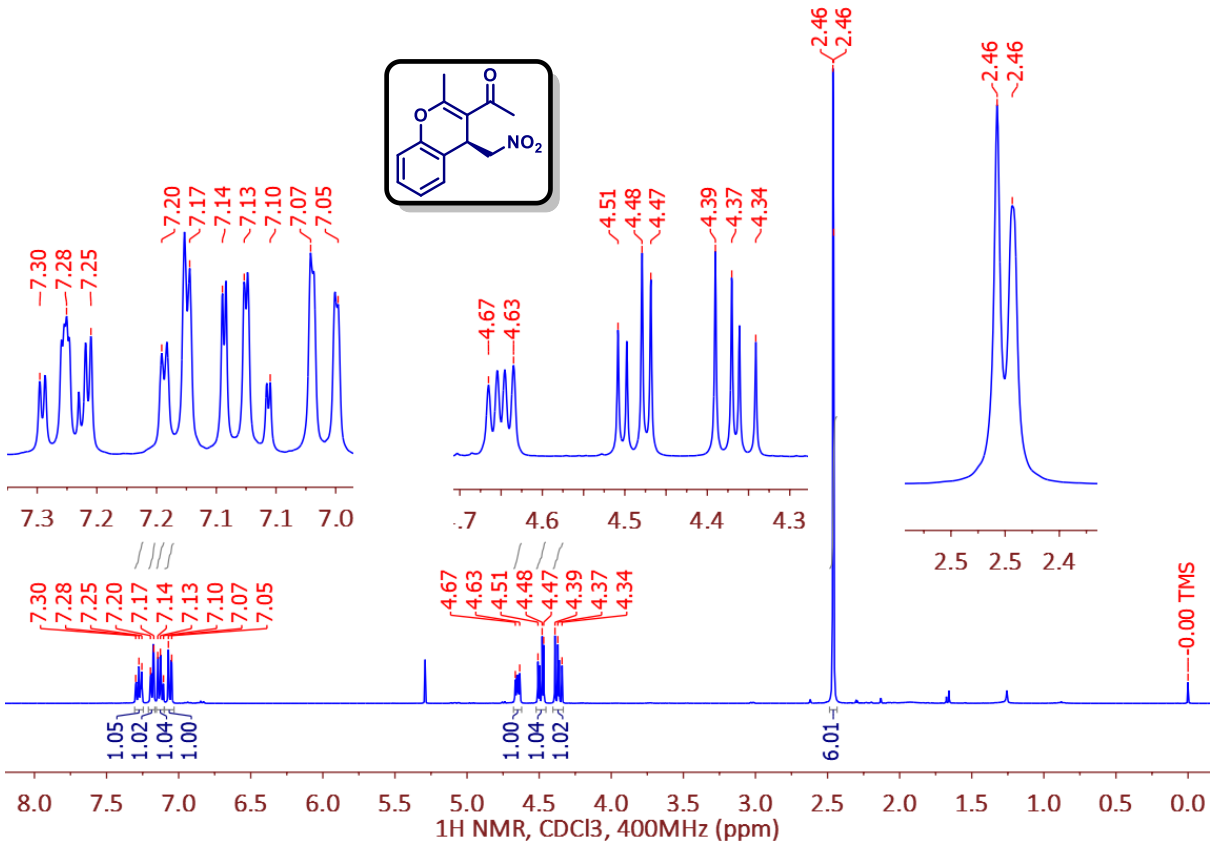

O
O
NO2
Br
135.24
132.59
129.75
122.73
77.94
77.16 CDCl3
70.51
42.31
30.56
29.85
201.46
200.67
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)

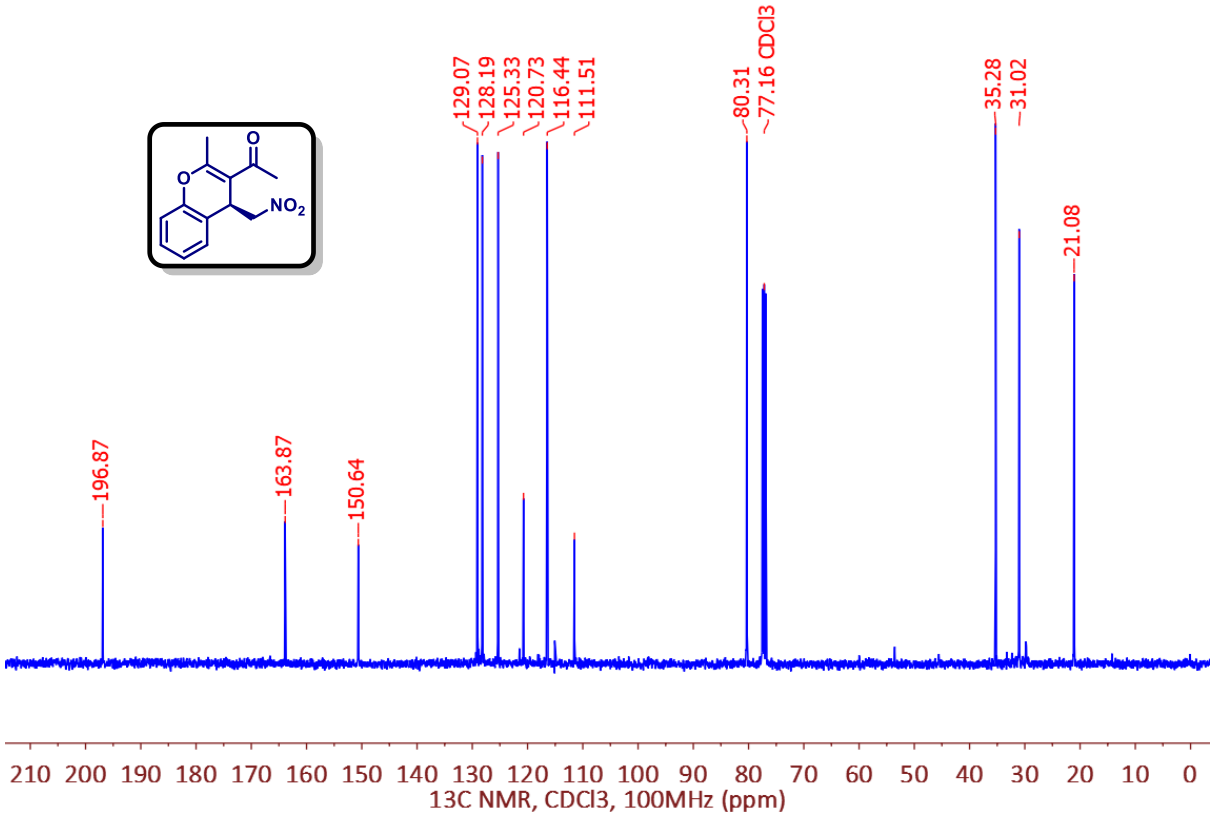

O
O
NO2
Br
2.28
2.05
7.64
7.62
7.31
7.26
7.15
7.14
4.86
4.83
4.74
4.68
4.61
4.59
0.00 TMS
1.00
1.09
2.10
1.02
1.05
1.07
1.00
3.09
3.09
1H NMR, CDCl3, 400MHz (ppm)

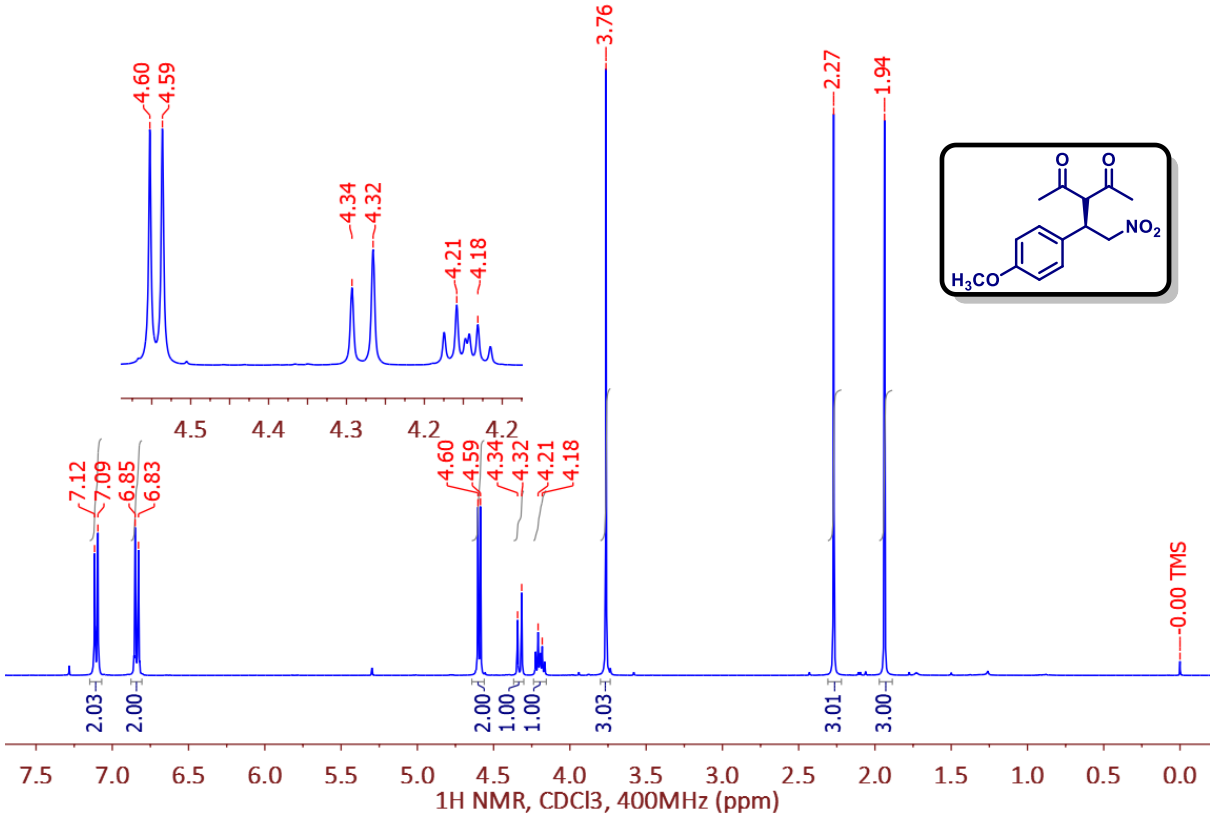

O
O
NO2
Br
135.17
134.12
130.07
128.91
128.37
124.66
77.16 CDCl3
76.37
69.19
31.12
28.56
202.06
200.99
41.18
13C NMR, CDCl3, 100MHz (ppm)

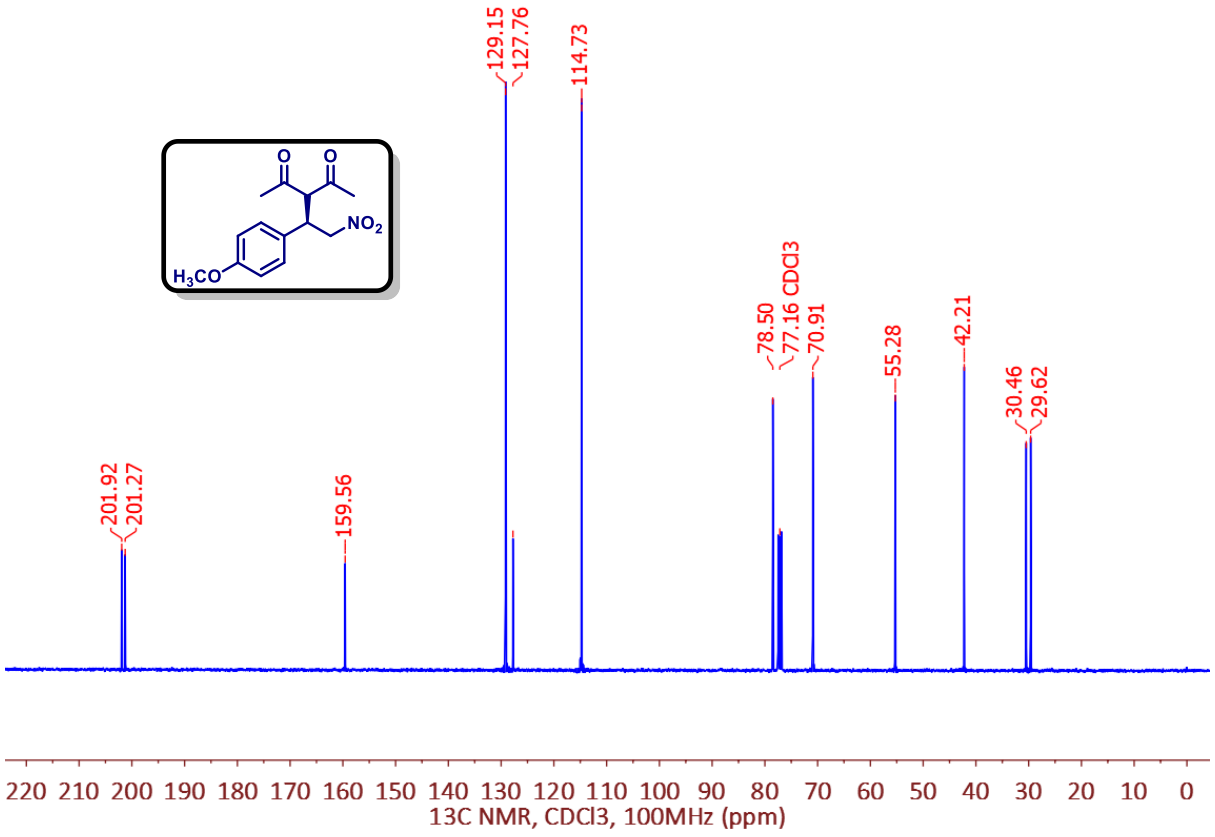

4.63
4.61
4.35
4.32
4.26
4.24
4.22
4.20
2.28
1.97
7.32
7.30
7.15
7.13
0.00 TMS
2.05
2.08
2.02
1.01
1.00
3.00
3.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)
NO2
Cl

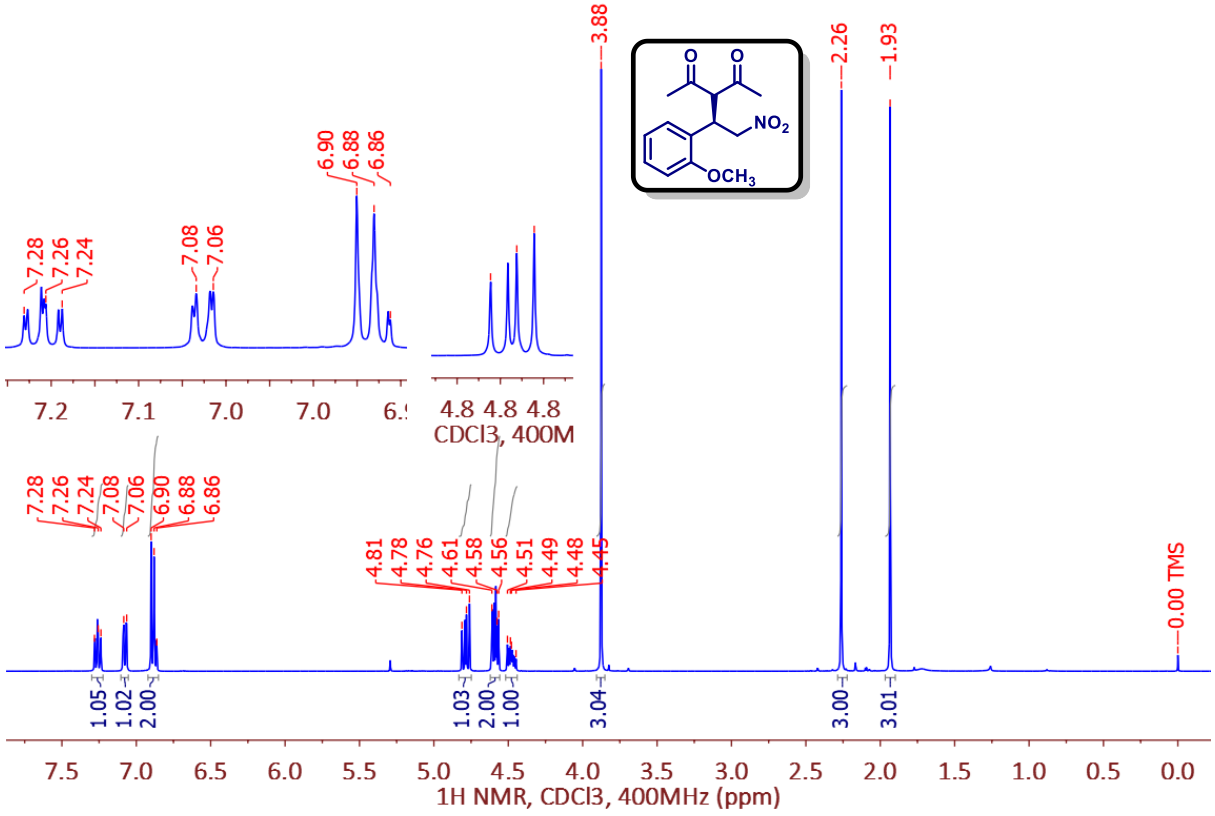

134.71
134.58
129.62
129.45
201.47
200.71
78.00
77.16 CDCl3
70.54
42.24
30.54
29.84
135 134 133 132 131 130
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)
NO2
Cl

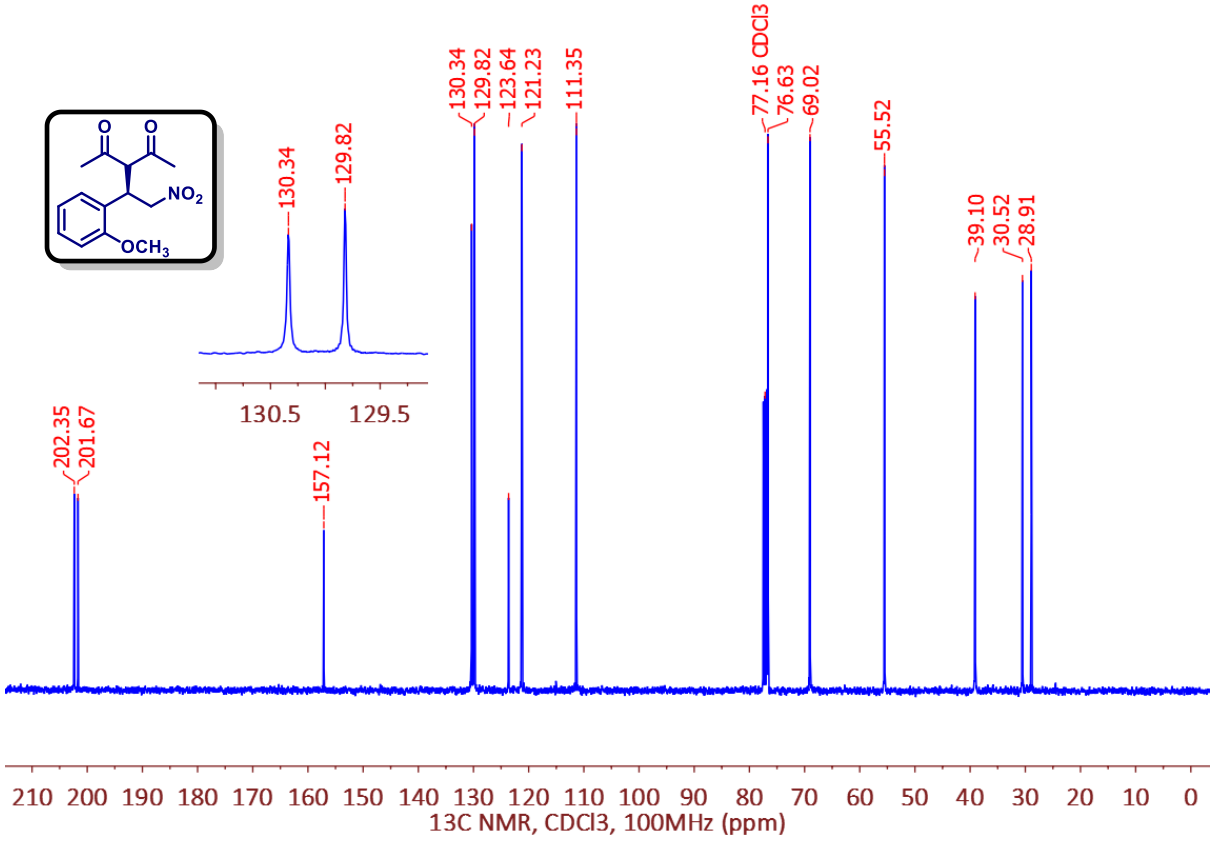

7.30
7.28
7.25
7.20
7.17
7.14
7.13
7.10
7.07
7.05
4.67
4.63
4.51
4.48
4.47
4.39
4.37
4.34
2.46
2.46
0.00 TMS
1.05
1.02
1.04
1.00
1.00
1.04
1.02
6.01
1H NMR, CDCl3, 400MHz (ppm)

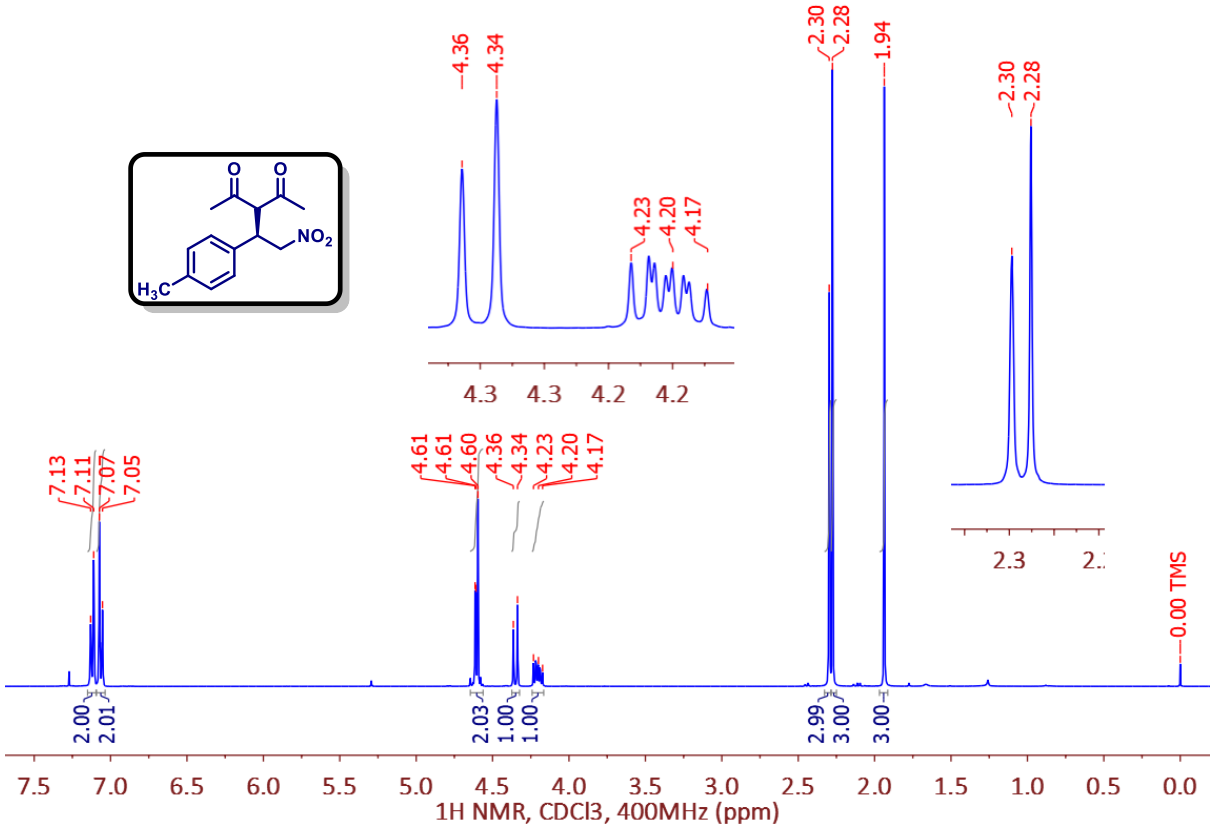

196.87
163.87
150.64
129.07
128.19
125.33
120.73
116.44
111.51
80.31
77.16 CDCl3
35.28
31.02
21.08
13C NMR, CDCl3, 100MHz (ppm)

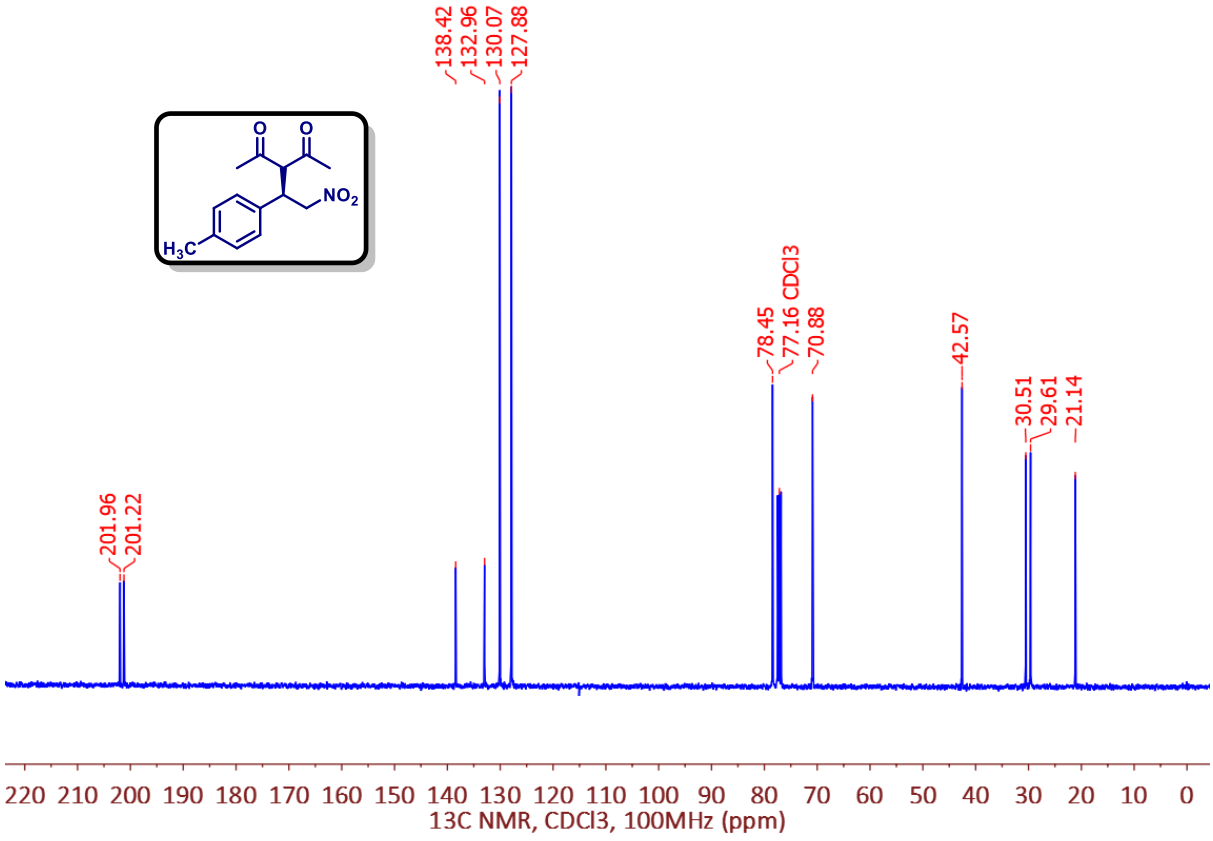

4.60
4.59
4.34
4.32
4.21
4.18
3.76
2.27
1.94
7.12
7.09
6.85
6.83
0.00 TMS
2.03
2.00
2.00
1.00
1.00
3.03
3.01
3.00
O
O
NO2
H3CO
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)

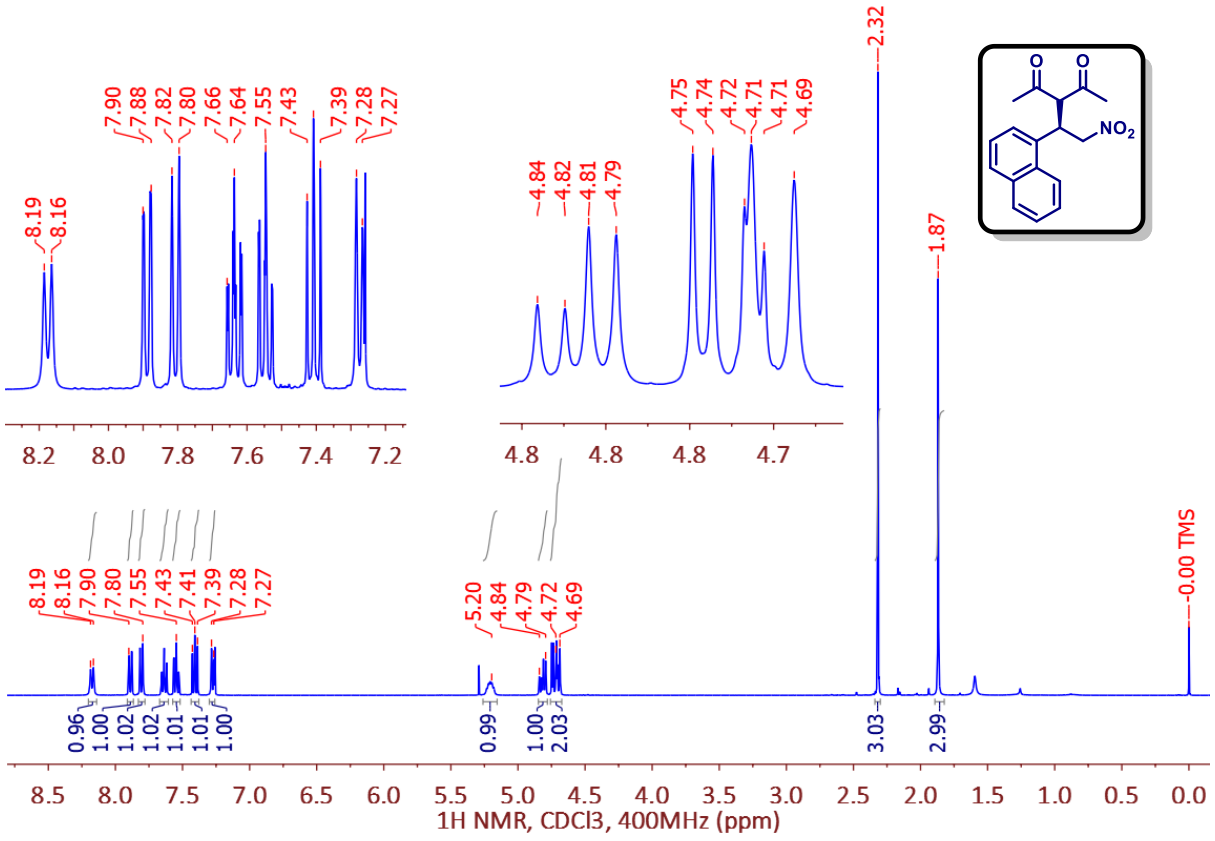

129.15
127.76
114.73
78.50
77.16 CDCl3
70.91
55.28
42.21
30.46
29.62
201.92
201.27
159.56
O
O
NO2
H3CO
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)

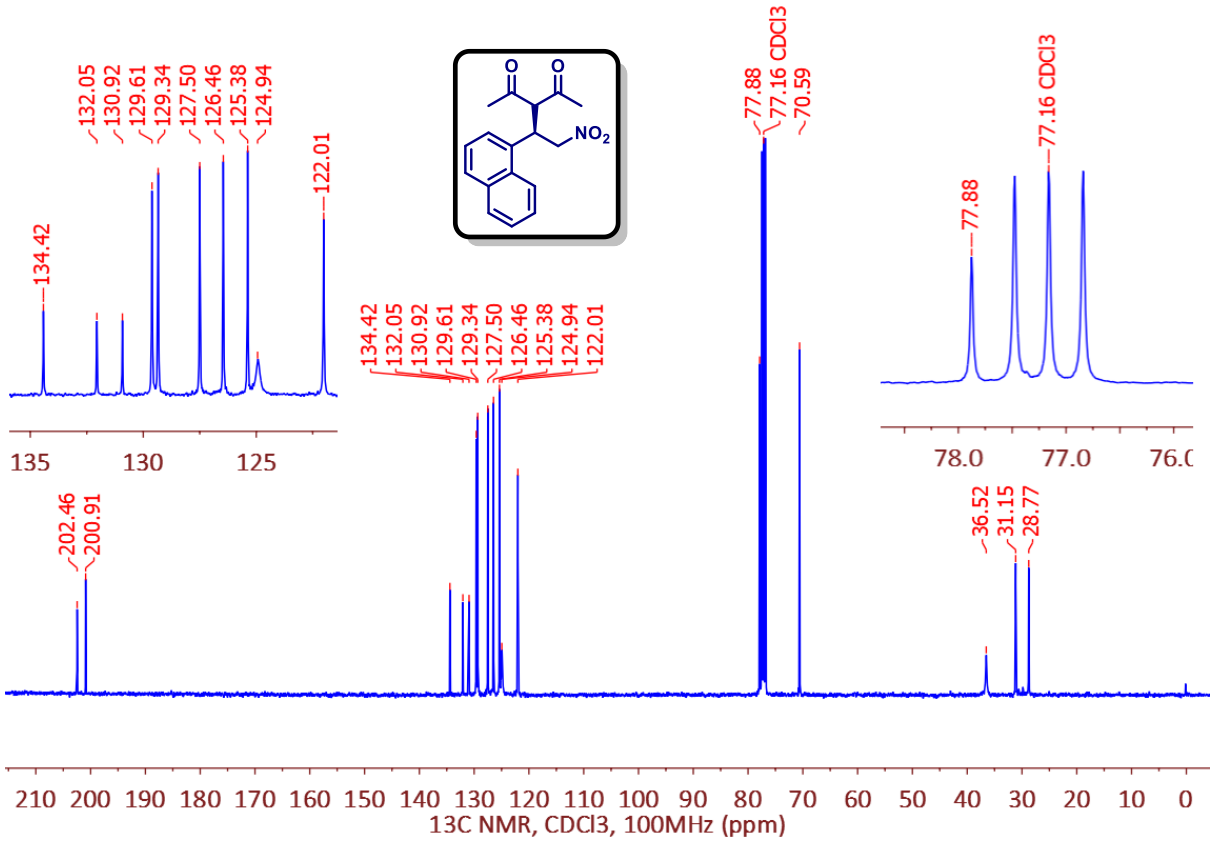

7.28
7.26
7.24
7.08
7.06
6.90
6.88
6.86
4.81
4.78
4.76
4.61
4.58
4.56
4.51
4.49
4.48
4.45
3.88
2.26
1.93
0.00 TMS
1.05
1.02
2.00
1.03
2.00
1.00
3.04
3.00
3.01
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)
7.2 7.1 7.0 7.0 6.
4.8 4.8 4.8
CDCl3, 400M
NO2
OCH3

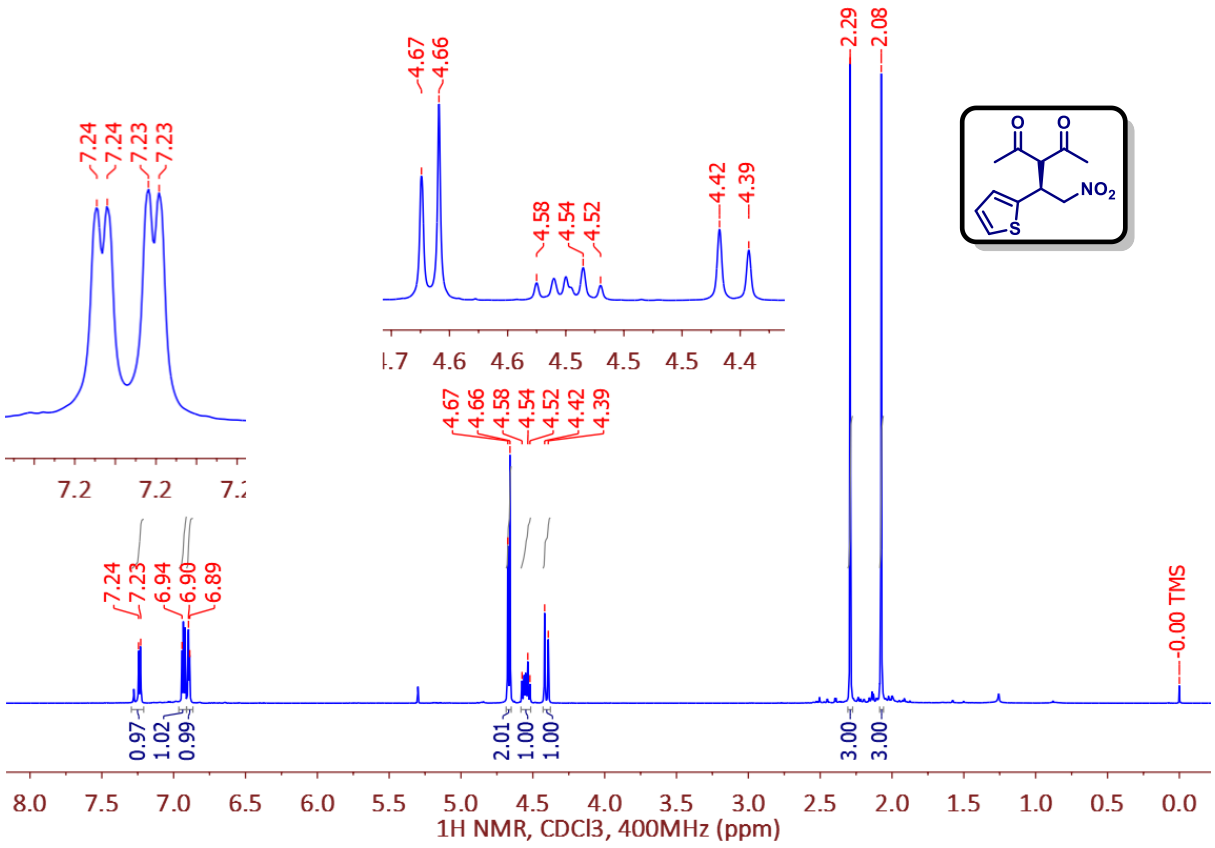

130.34
129.82
123.64
121.23
111.35
77.16 CDCl3
76.63
69.02
55.52
39.10
30.52
28.91
202.35
201.67
157.12
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)
130.5 129.5
NO2
OCH3

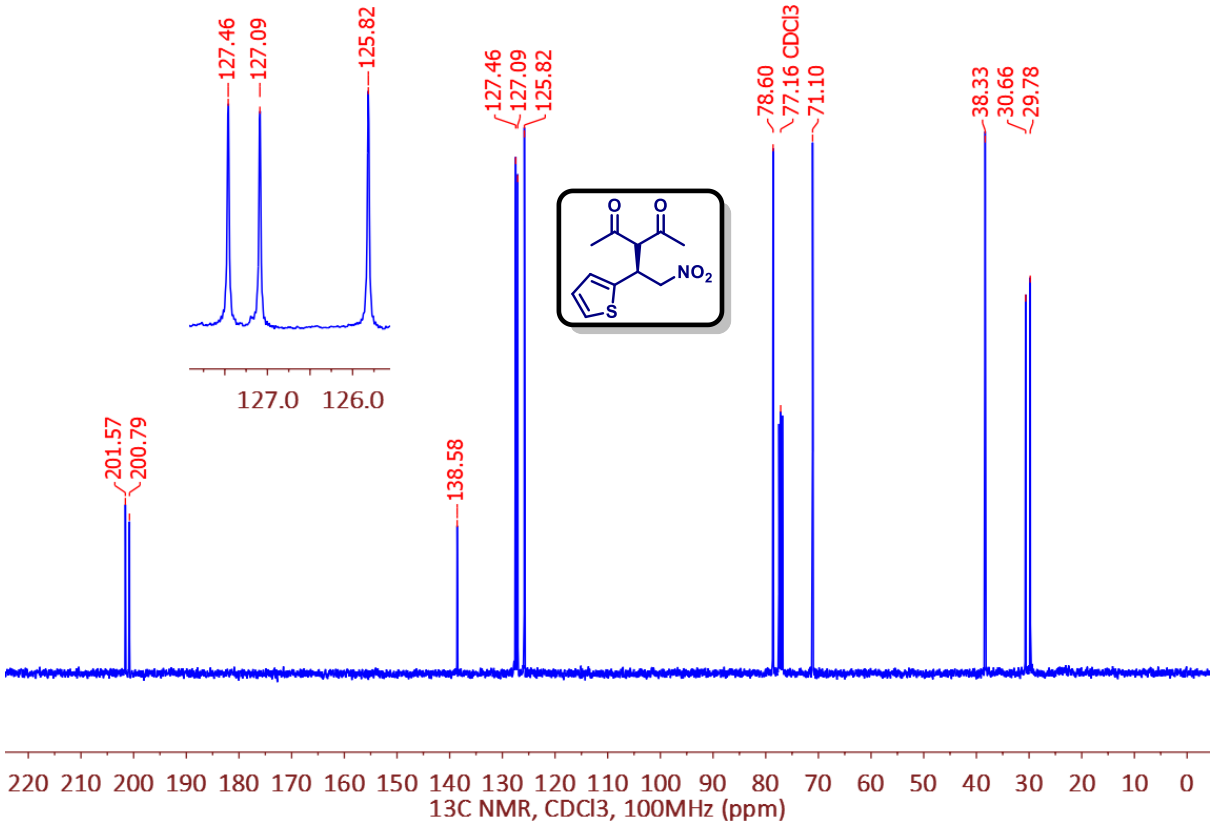

4.36
4.34
4.23
4.20
4.17
2.30
2.28
1.94
7.13
7.11
7.07
7.05
4.61
4.61
4.60
4.36
4.34
4.23
4.20
4.17
0.00 TMS
2.00
2.01
2.03
1.00
1.00
2.99
3.00
3.00
1H NMR, CDCl3, 400MHz (ppm)

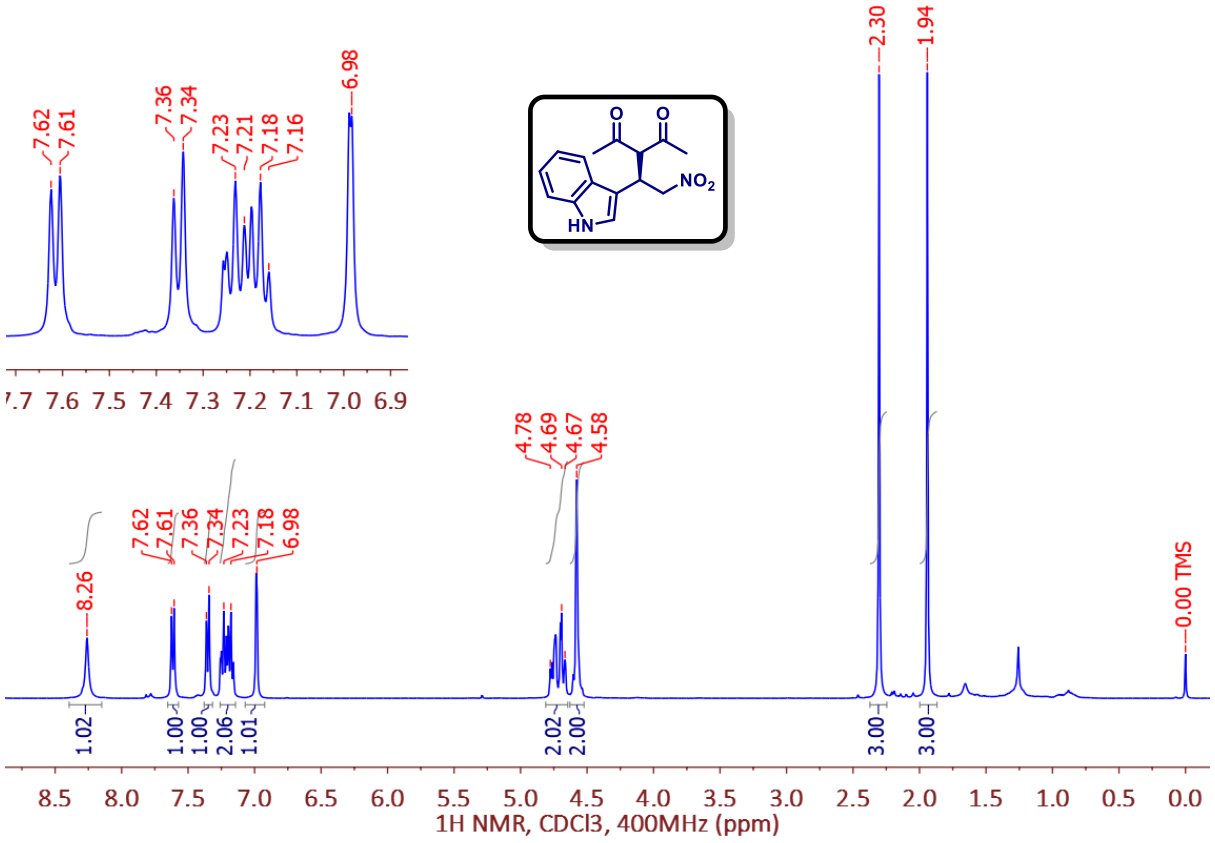

138.42
132.96
130.07
127.88
78.45
77.16 CDCl3
70.88
42.57
30.51
29.61
21.14
201.96
201.22
13C NMR, CDCl3, 100MHz (ppm)

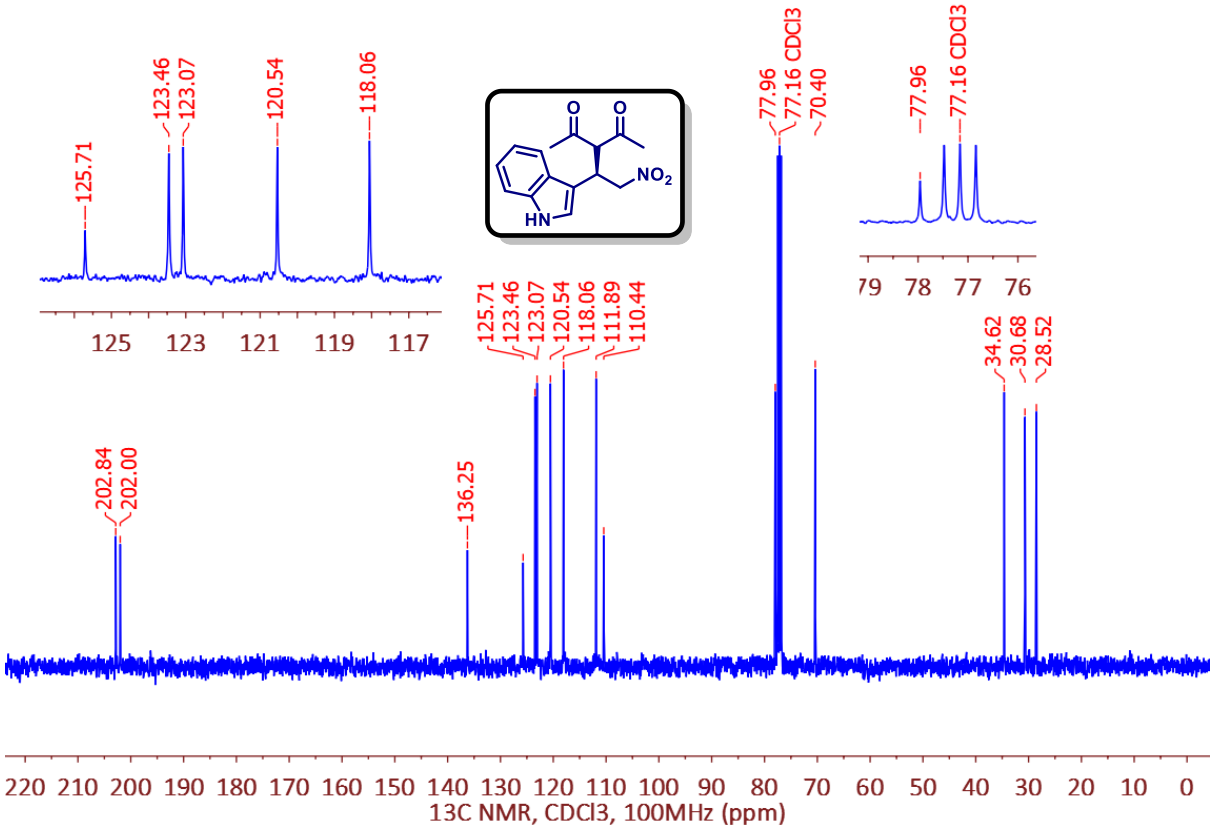

8.19
8.16
7.90
7.88
7.82
7.80
7.66
7.64
7.55
7.43
7.39
7.28
7.27
4.84
4.82
4.81
4.79
4.75
4.74
4.72
4.71
4.71
4.69
2.32
1.87
0.00 TMS
0.96
1.00
1.02
1.02
1.01
1.01
1.00
0.99
1.00
2.03
3.03
2.99
1H NMR, CDCl3, 400MHz (ppm)

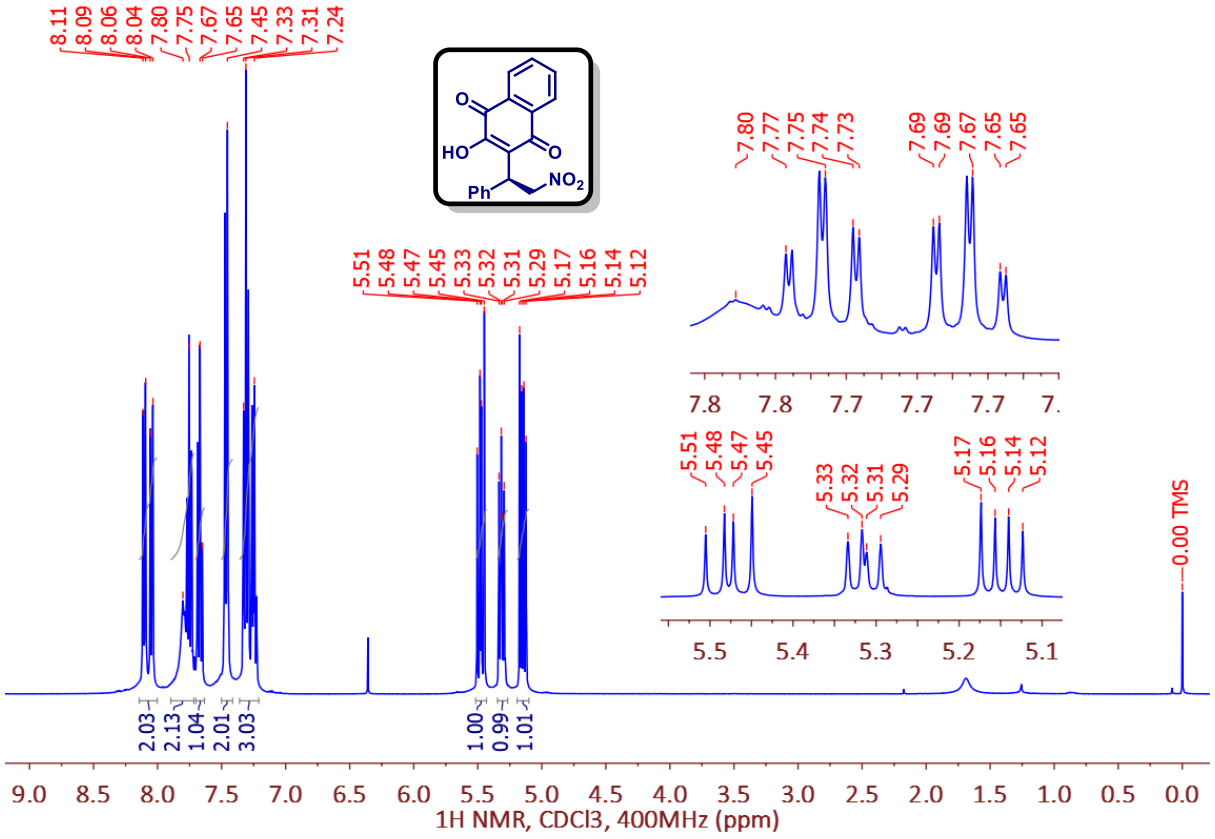

132.05
130.92
129.61
129.34
127.50
126.46
125.38
124.94
122.01
134.42
77.88
77.16 CDCl3
70.59
202.46
200.91
36.52
31.15
28.77
13C NMR, CDCl3, 100MHz (ppm)

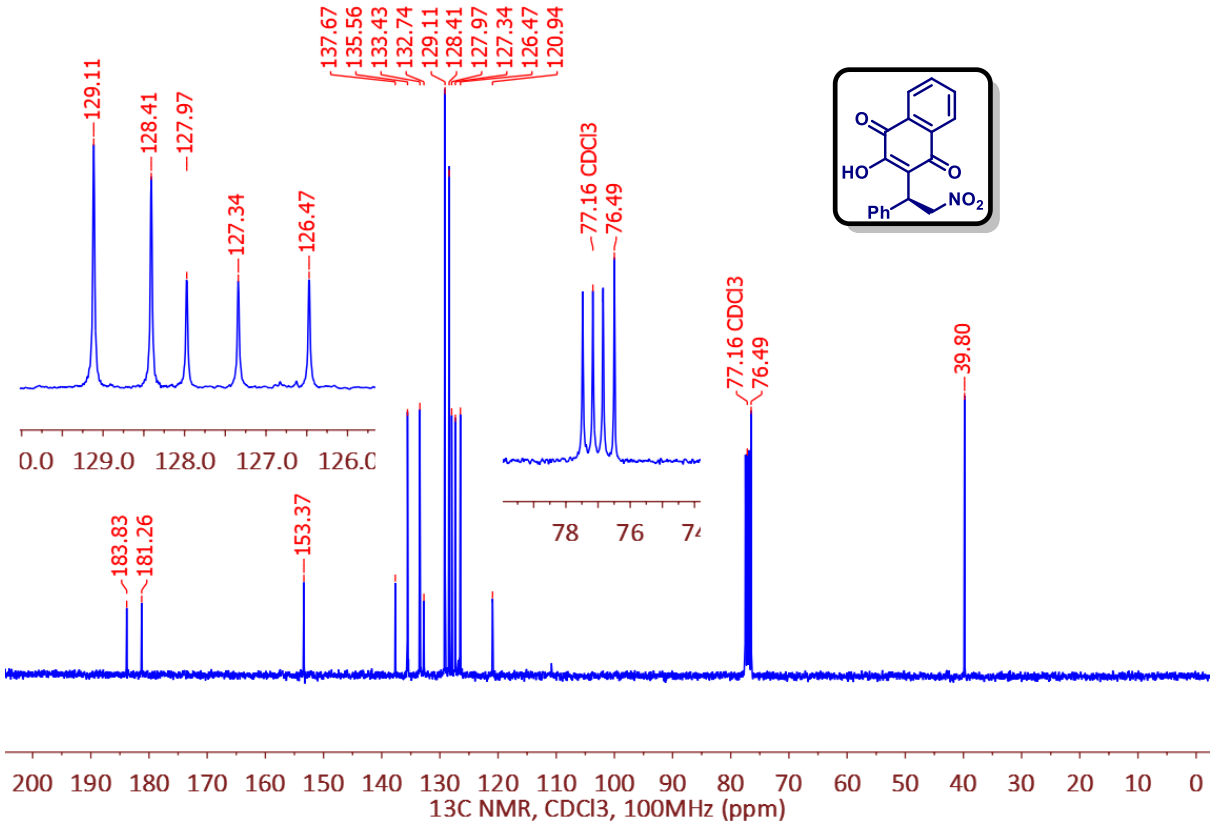

7.24
7.24
7.23
7.23
4.67
4.66
4.58
4.54
4.52
4.42
4.39
2.29
2.08
6.94
6.90
6.89
0.00 TMS
0.97
1.02
0.99
2.01
1.00
1.00
3.00
3.00
1H NMR, CDCl3, 400MHz (ppm)

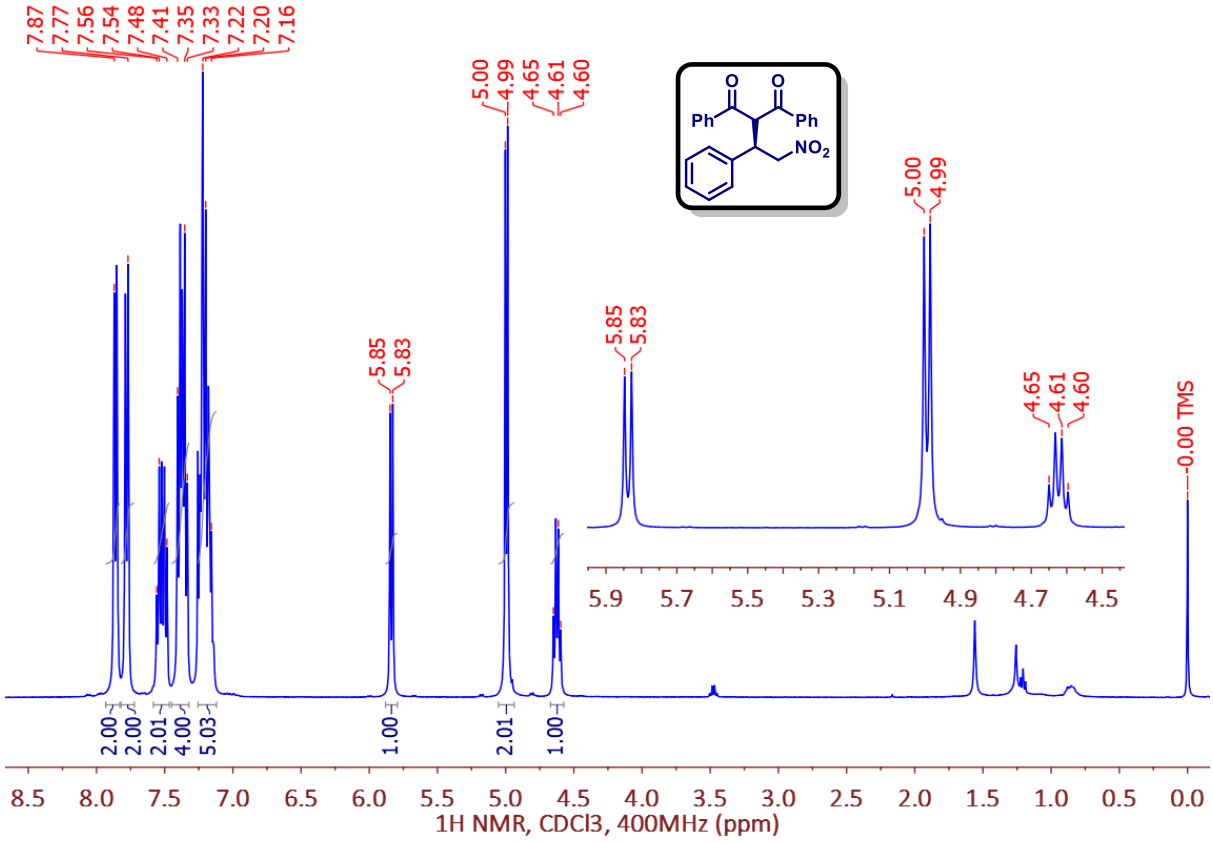

127.46
127.09
125.82
78.60
77.16 CDCl3
71.10
38.33
30.66
29.78
201.57
200.79
138.58
13C NMR, CDCl3, 100MHz (ppm)

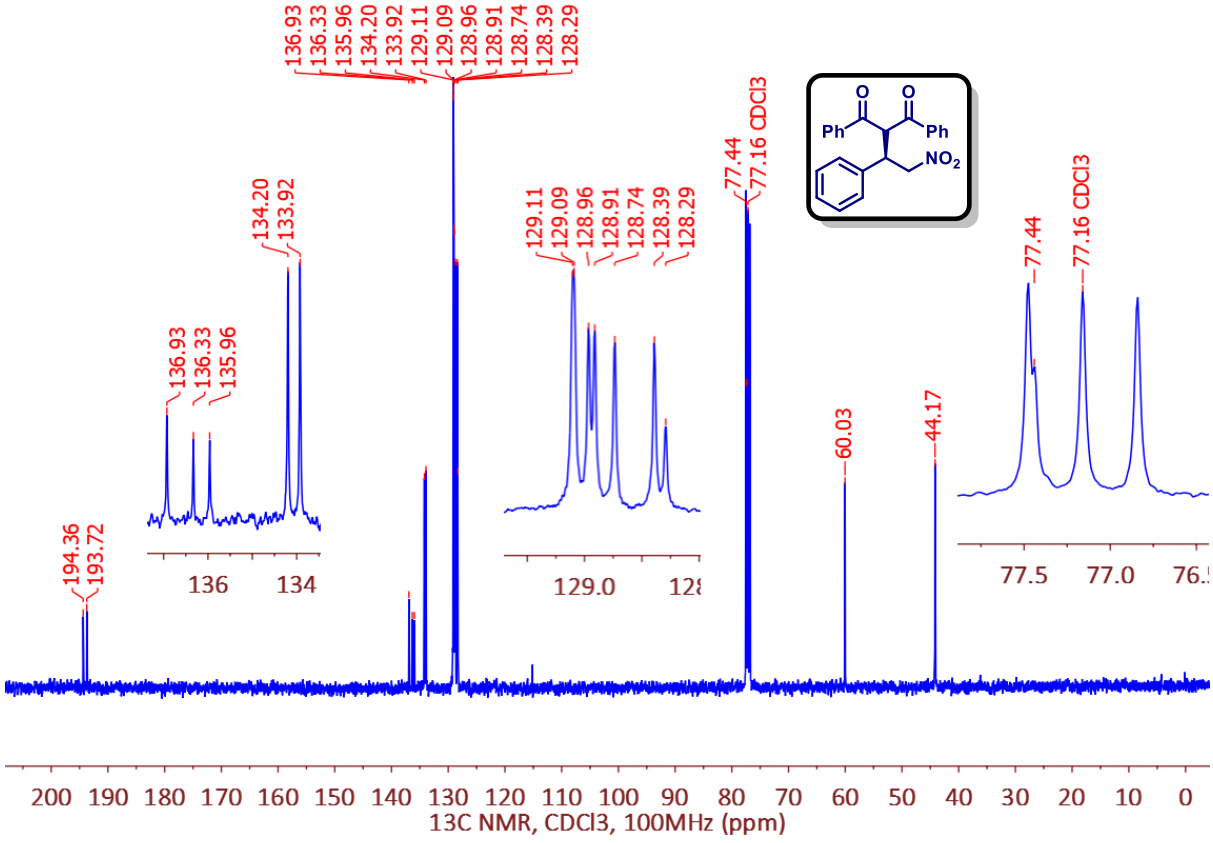

7.62
7.61
7.36
7.34
7.23
7.21
7.18
7.16
6.98
2.30
1.94
4.78
4.69
4.67
4.58
8.26
0.00 TMS
1.02
1.00
1.00
2.06
1.01
2.02
2.00
3.00
3.00
1H NMR, CDCl3, 400MHz (ppm)

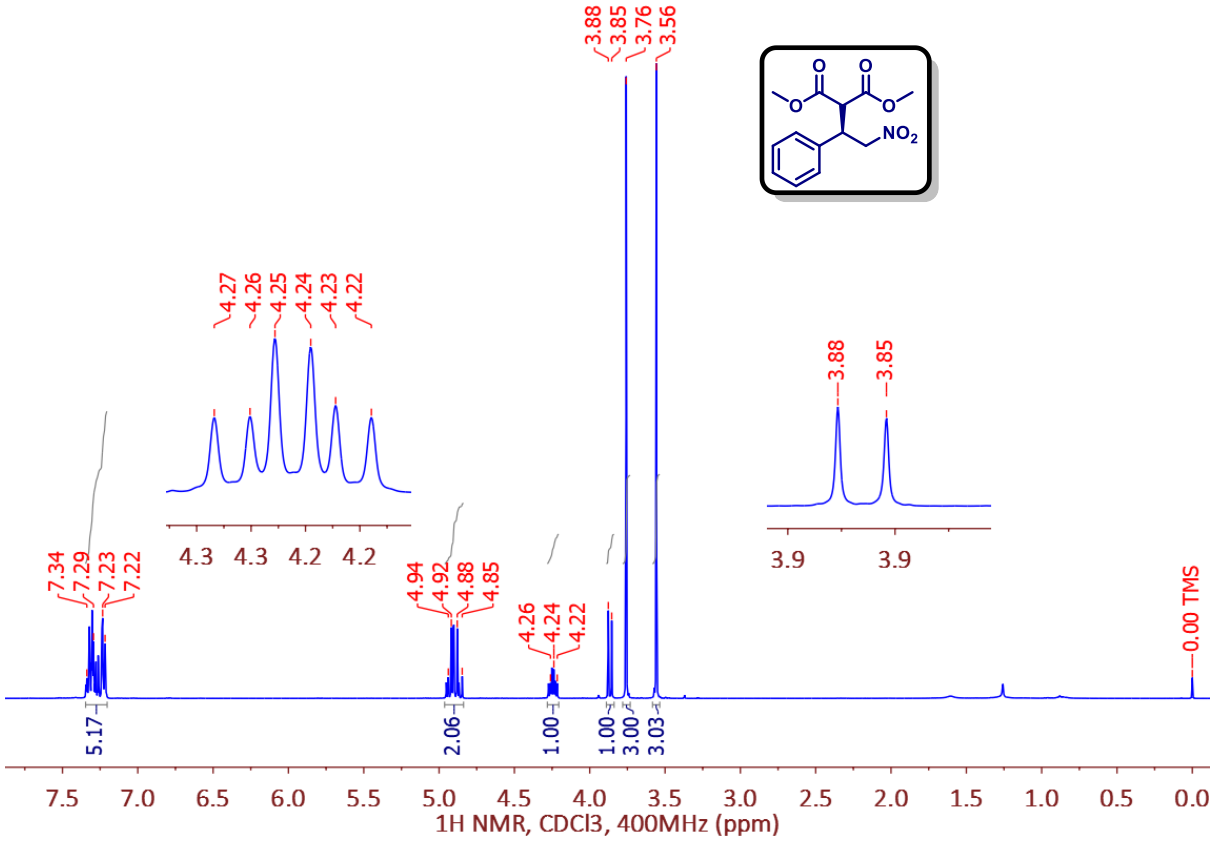

125.71
123.46
123.07
120.54
118.06
77.96
77.16 CDCl3
70.40
202.84
202.00
136.25
111.89
110.44
34.62
30.68
28.52
13C NMR, CDCl3, 100MHz (ppm)

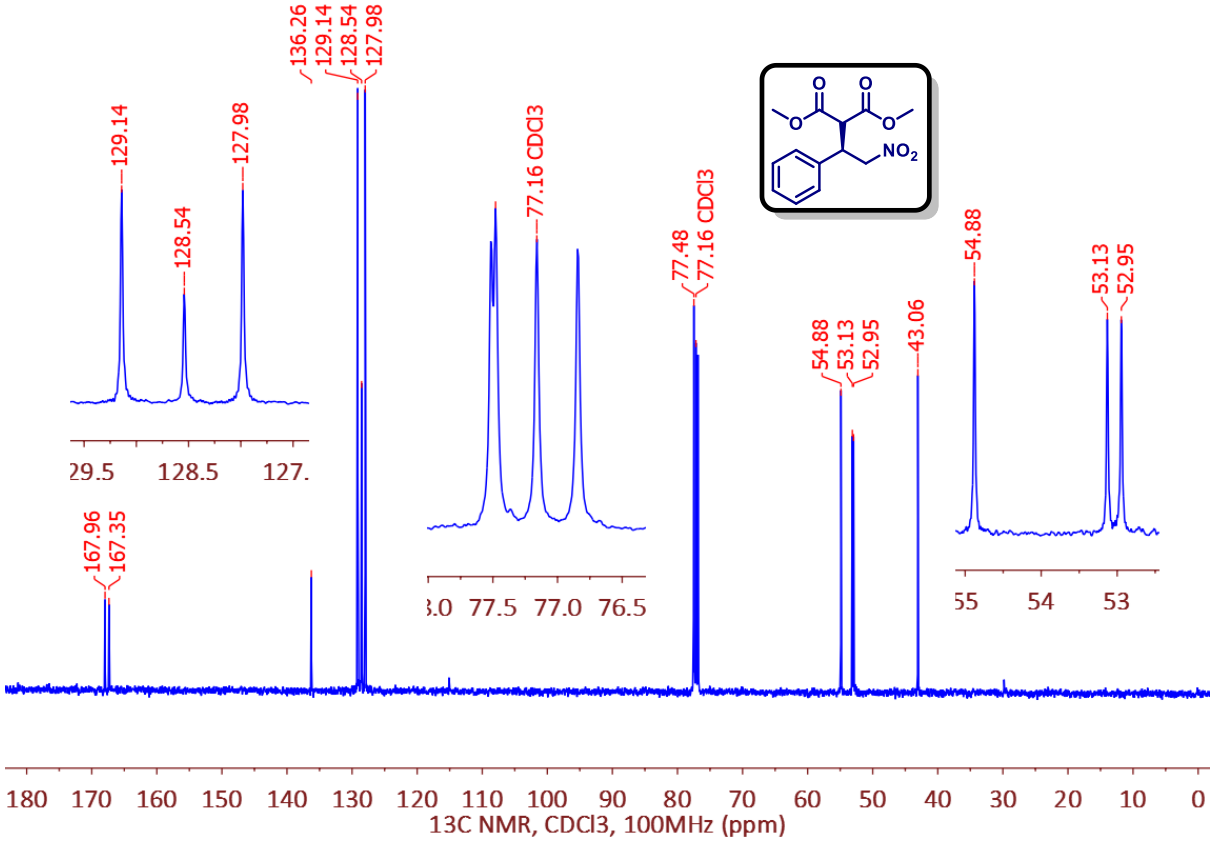

8.11
8.09
8.06
8.04
7.80
7.75
7.67
7.65
7.45
7.33
7.31
7.24
5.51
5.48
5.47
5.45
5.33
5.32
5.31
5.29
5.17
5.16
5.14
5.12
0.00 TMS
2.03
2.13
1.04
2.01
3.03
1.00
0.99
1.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)

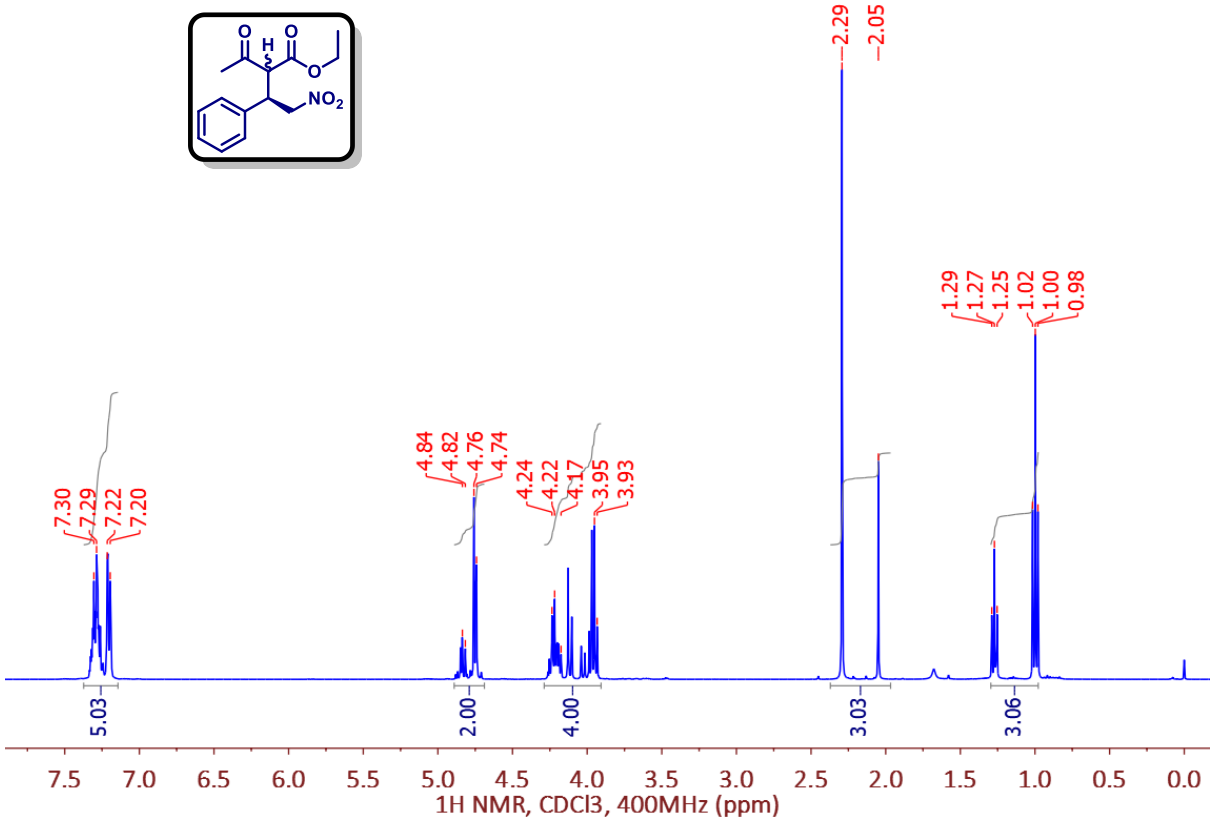

137.67
135.56
133.43
132.74
129.11
128.41
127.97
127.34
126.47
120.94
77.16 CDCl3
76.49
39.80
183.83
181.26
153.37
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)

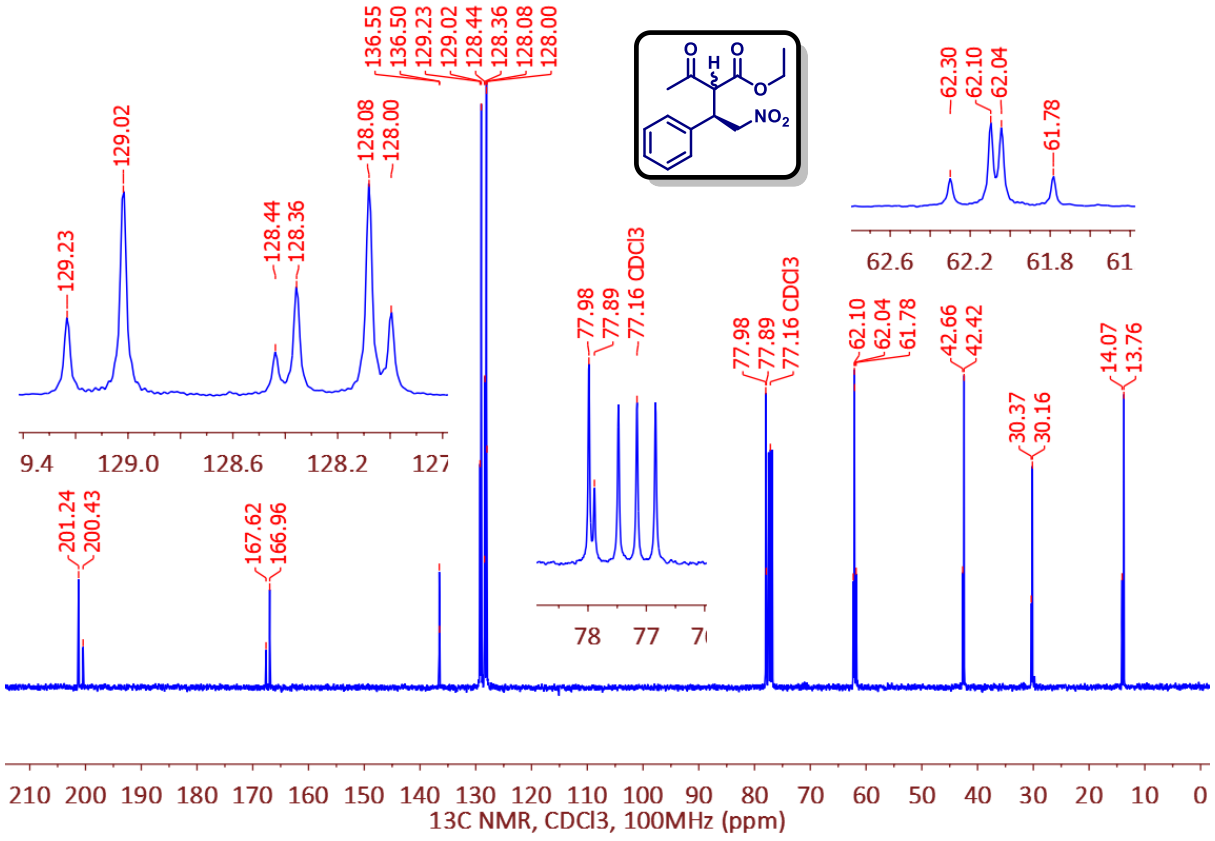

7.87
7.77
7.56
7.54
7.48
7.41
7.35
7.33
7.22
7.20
7.16
5.00
4.99
4.65
4.61
4.60
5.85
5.83
0.00 TMS
2.00
2.00
2.01
4.00
5.03
1.00
2.01
1.00
1H NMR, CDCl3, 400MHz (ppm)

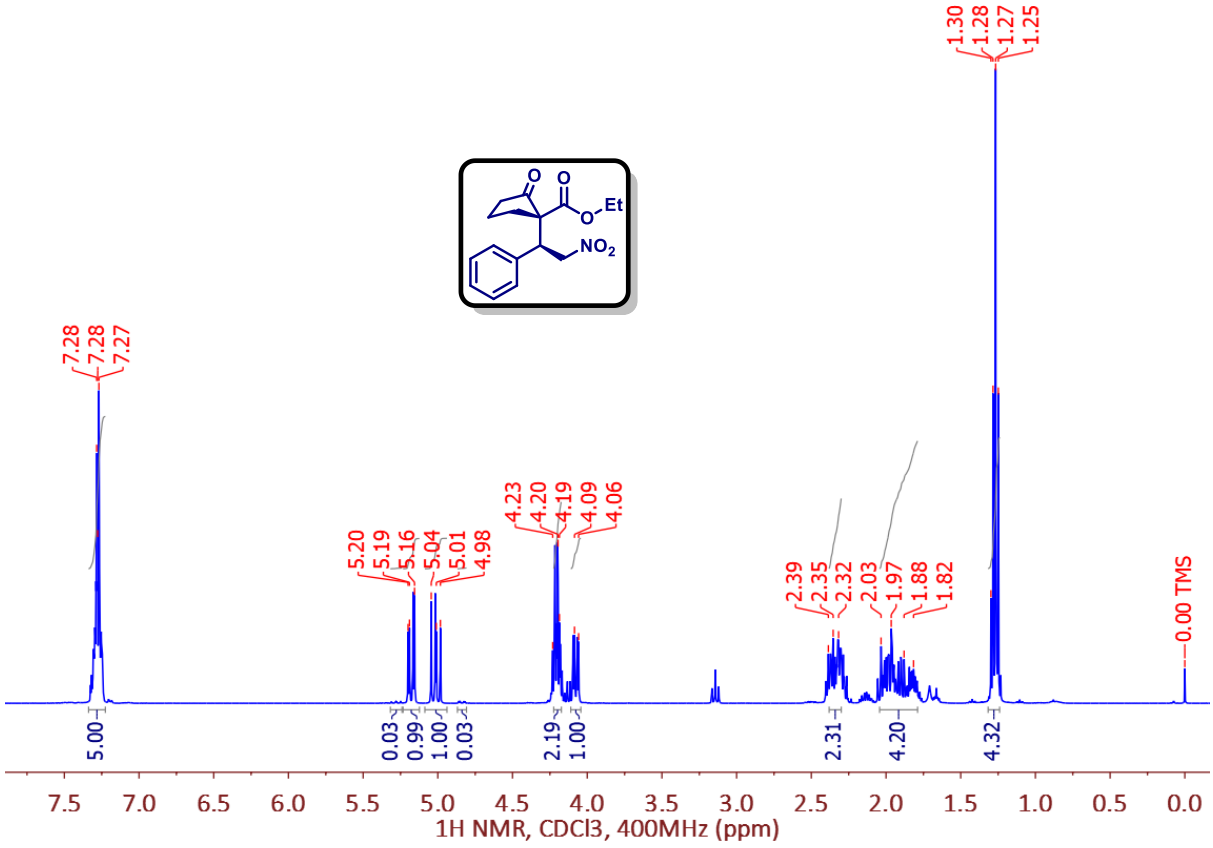

136.93
136.33
135.96
134.20
133.92
129.11
129.09
128.96
128.91
128.74
128.39
128.29
77.44
77.16 CDCl3
60.03
44.17
194.36
193.72
13C NMR, CDCl3, 100MHz (ppm)

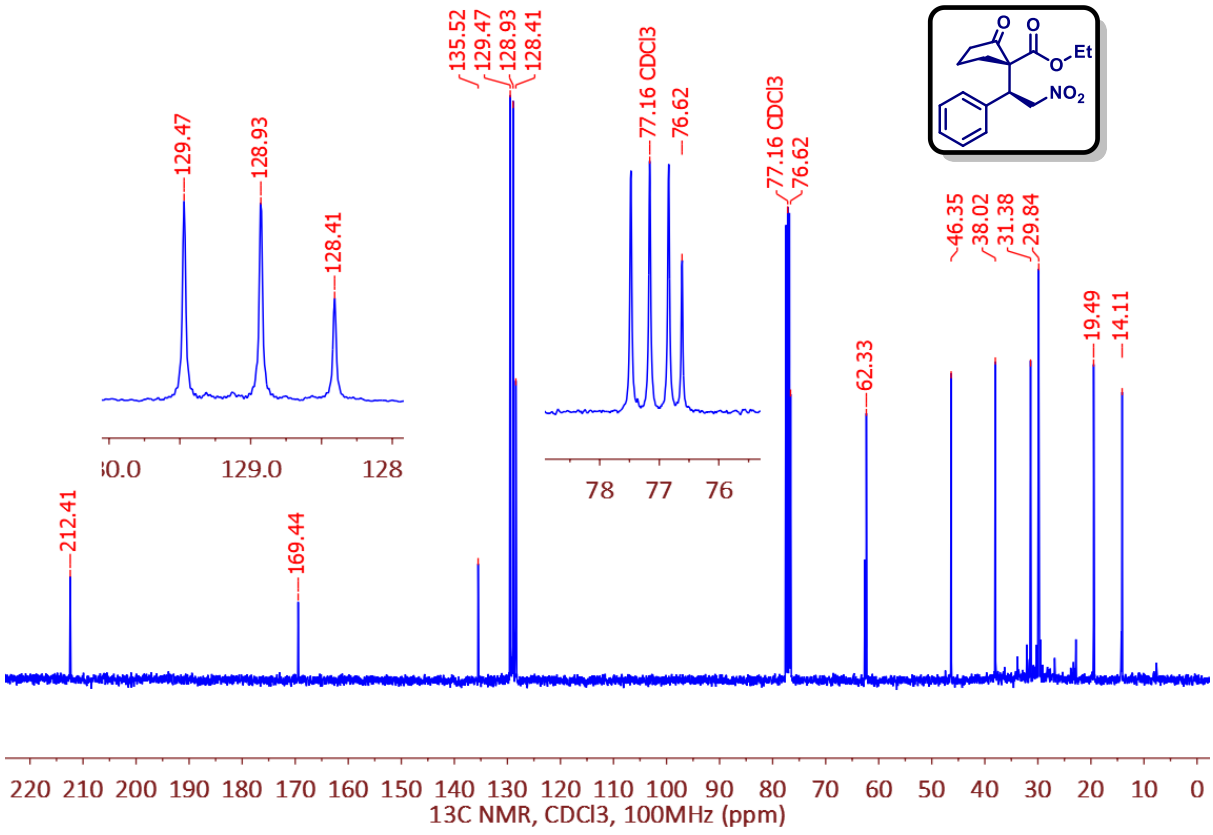

3.88
3.85
3.76
3.56
NO2
4.27
4.26
4.25
4.24
4.23
4.22
4.3 4.3 4.2 4.2
3.88
3.85
3.9 3.9
7.34
7.29
7.23
7.22
4.94
4.92
4.88
4.85
4.26
4.24
4.22
0.00 TMS
5.17
2.06
1.00
1.00
3.00
3.03
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
1H NMR, CDCl3, 400MHz (ppm)


136.26
129.14
128.54
127.98
NO2
129.14
128.54
127.98
29.5 128.5 127.
77.16 CDCl3
3.0 77.5 77.0 76.5
77.48
77.16 CDCl3
54.88
53.13
52.95
43.06
54.88
53.13
52.95
55 54 53
167.96
167.35
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)


7.30
7.29
7.22
7.20
4.84
4.82
4.76
4.74
4.24
4.22
4.17
3.95
3.93
2.29
2.05
1.29
1.27
1.25
1.02
1.00
0.98
5.03
2.00
4.00
3.03
3.06
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
1H NMR, CDCl3, 400MHz (ppm)

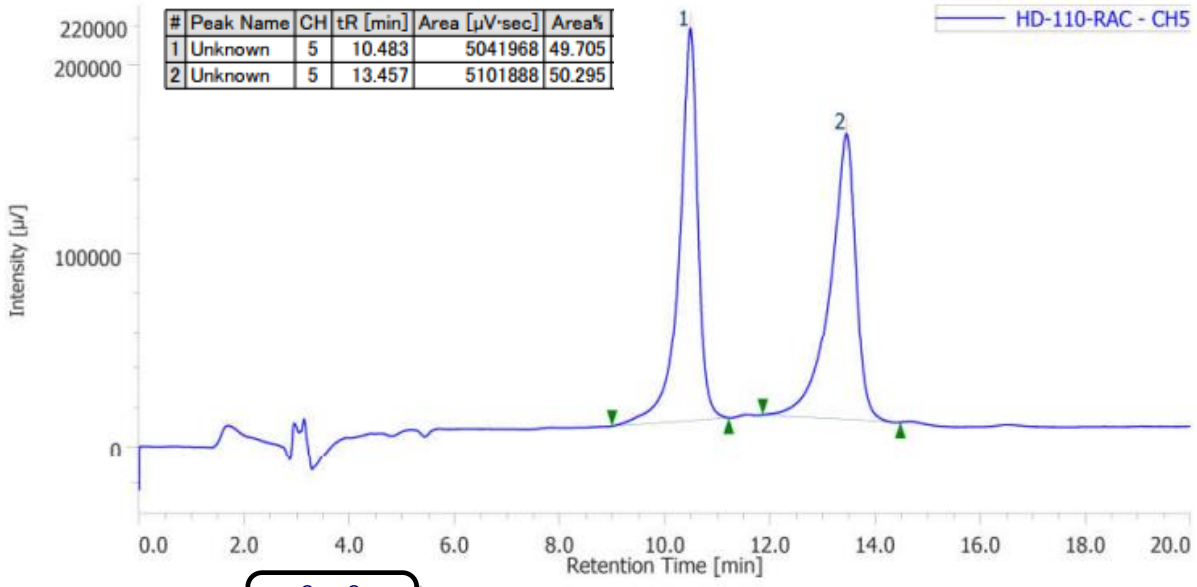

136.55
136.50
129.23
129.02
128.44
128.36
128.08
128.00
129.23
129.02
128.44
128.36
128.08
128.00
9.4 129.0 128.6 128.2 127
77.98
77.89
77.16 CDCl3
78 77 7
62.30
62.10
62.04
61.78
62.6 62.2 61.8 61
201.24
200.43
167.62
166.96
42.66
42.42
30.37
30.16
14.07
13.76
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)


1.30
1.28
1.27
1.25
7.28
7.28
7.27
5.20
5.19
5.16
5.04
5.01
4.98
4.23
4.20
4.19
4.09
4.06
2.39
2.35
2.32
2.03
1.97
1.88
1.82
0.00 TMS
5.00
0.03
0.99
1.00
0.03
2.19
1.00
2.31
4.20
4.32
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
1H NMR, CDCl3, 400MHz (ppm)

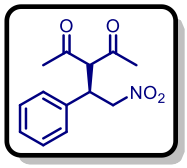

135.52
129.47
128.93
128.41
77.16 CDCl3
76.62
77.16 CDCl3
76.62
46.35
38.02
31.38
29.84
19.49
14.11
62.33
212.41
169.44
129.47
128.93
128.41
129.0
128
78
77
76
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
13C NMR, CDCl3, 100MHz (ppm)

9. CSP-HPLC traces

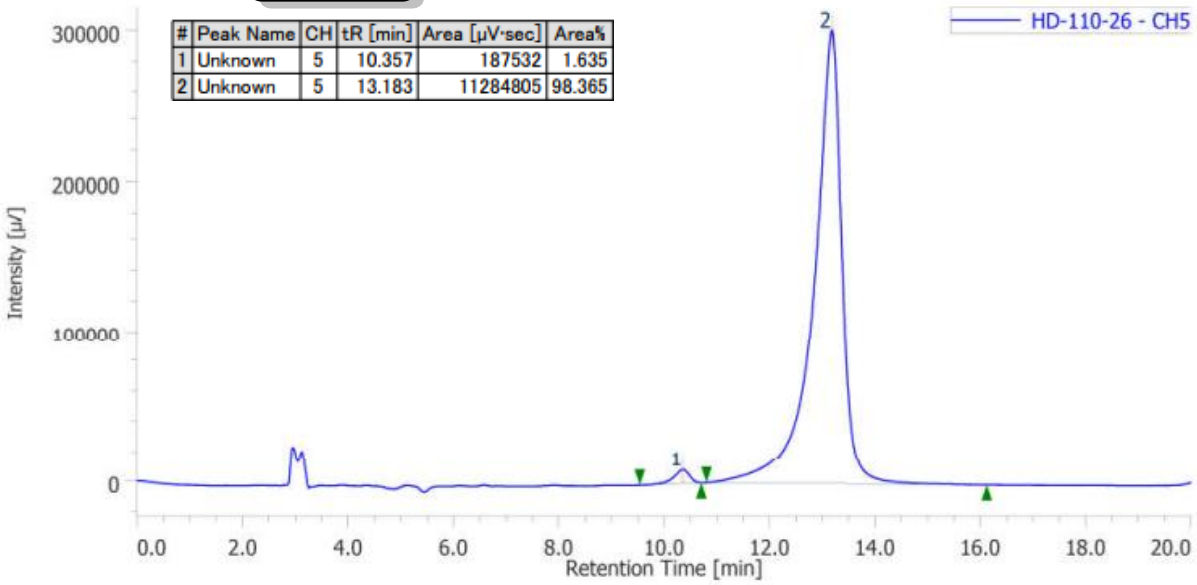
Compound **2a** (97% ee). HPLC: Chiralpak IA, hexane/isopropanol 90:10, 1.0 mL/min, 208 nm.



#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%
1	Unknown	5	10.483	5041968	49.705
2	Unknown	5	13.457	5101888	50.295



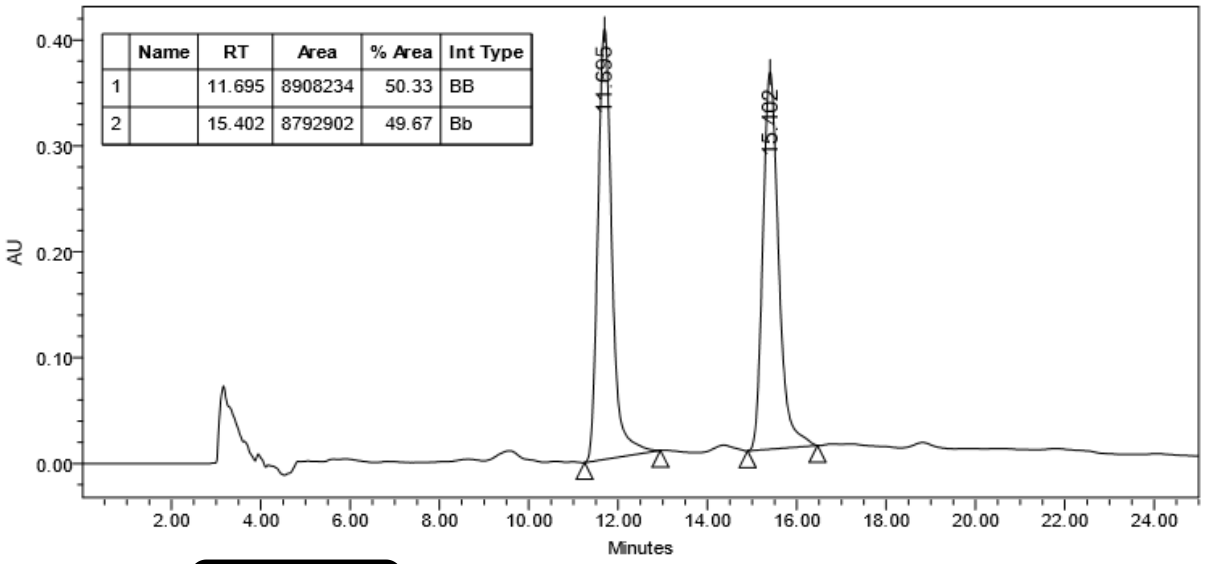
Racemic.



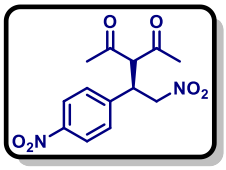
#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%
1	Unknown	5	10.357	187532	1.635
2	Unknown	5	13.183	11284805	98.365

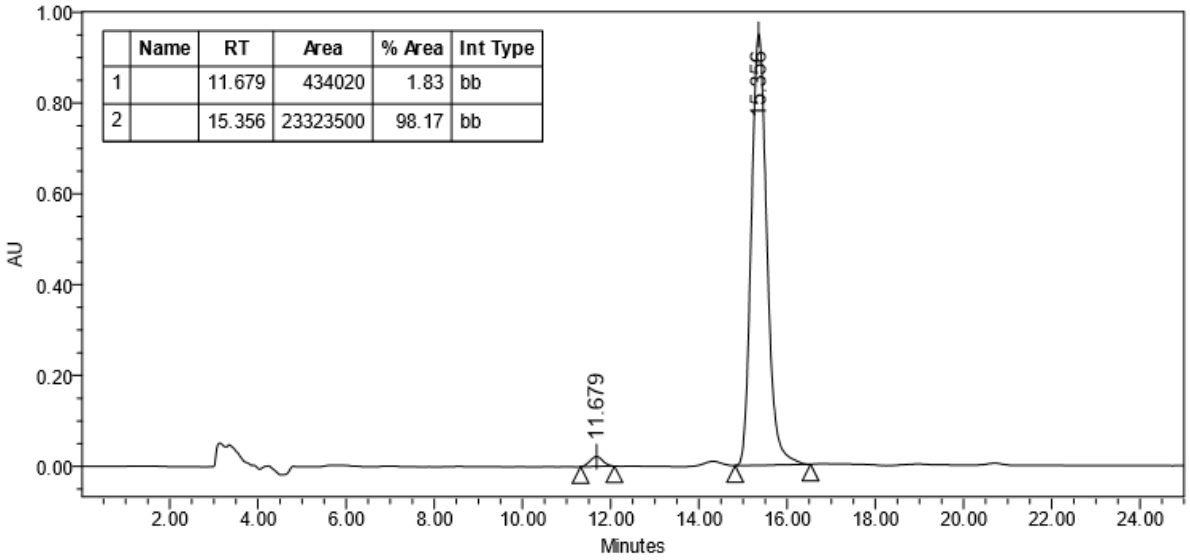
Enantiomerically enriched.

Compound **2b** (96% ee). HPLC: Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm.



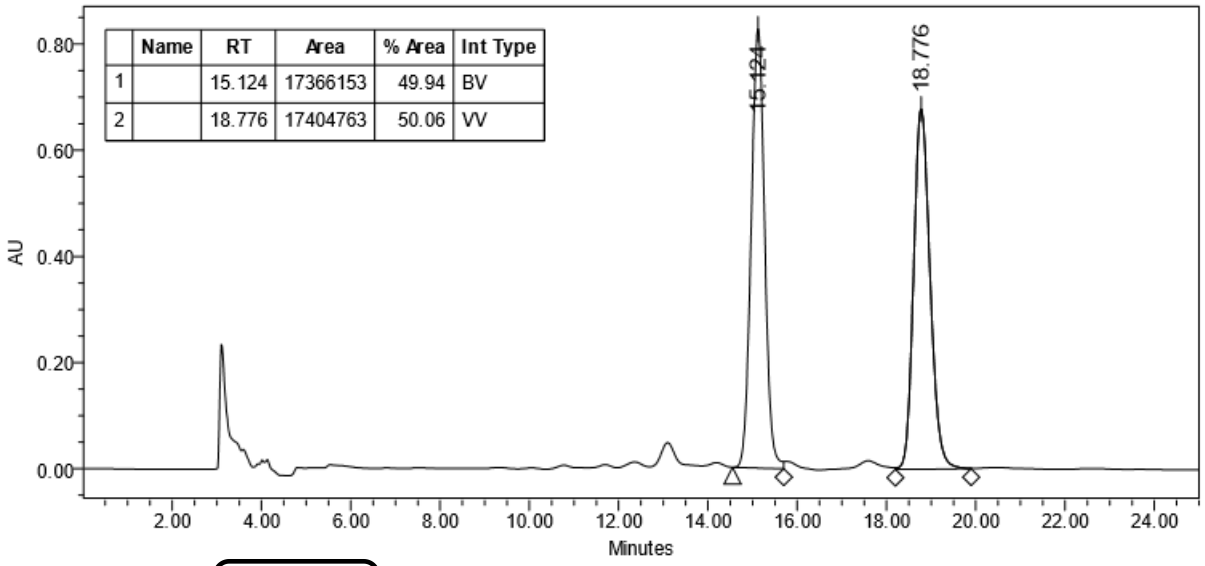
Racemic.



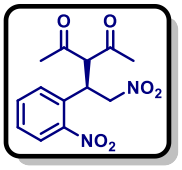


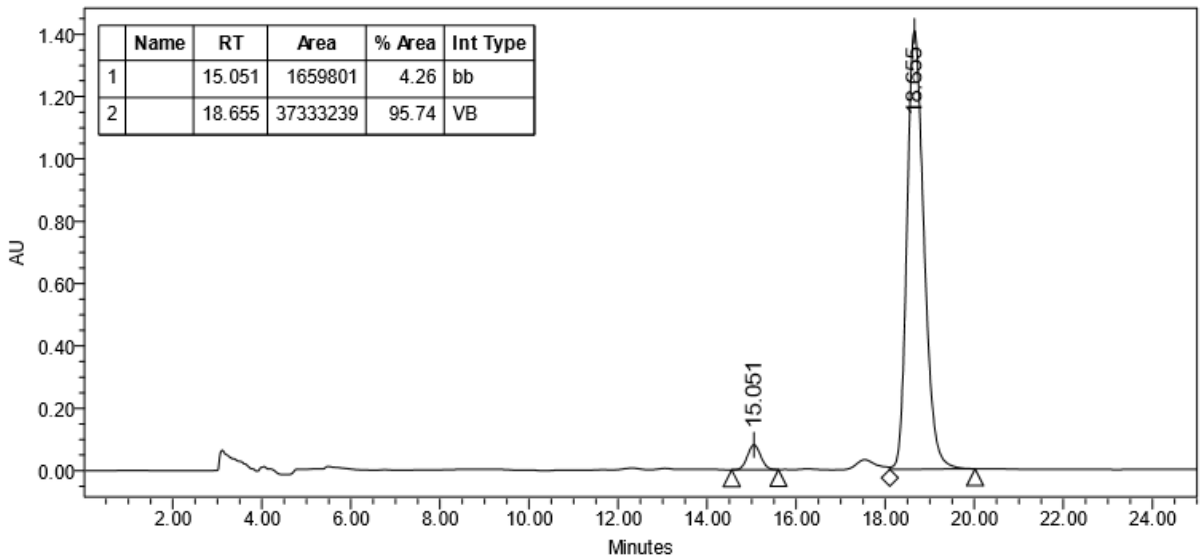
Enantiomerically enriched.

Compound **2c** (91% ee). HPLC: Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm.



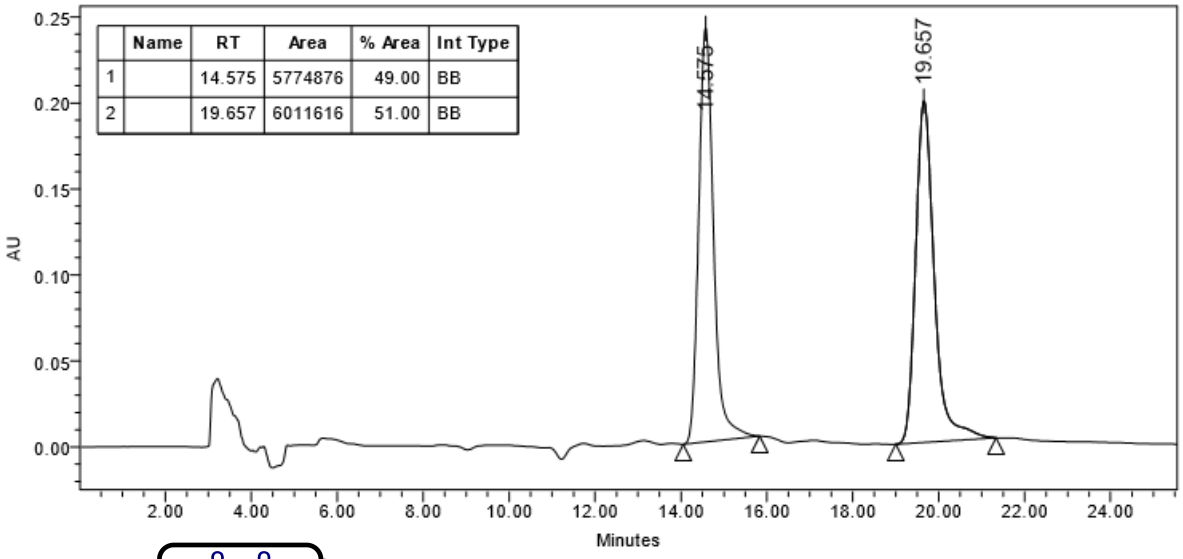
Racemic.



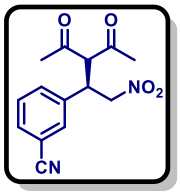


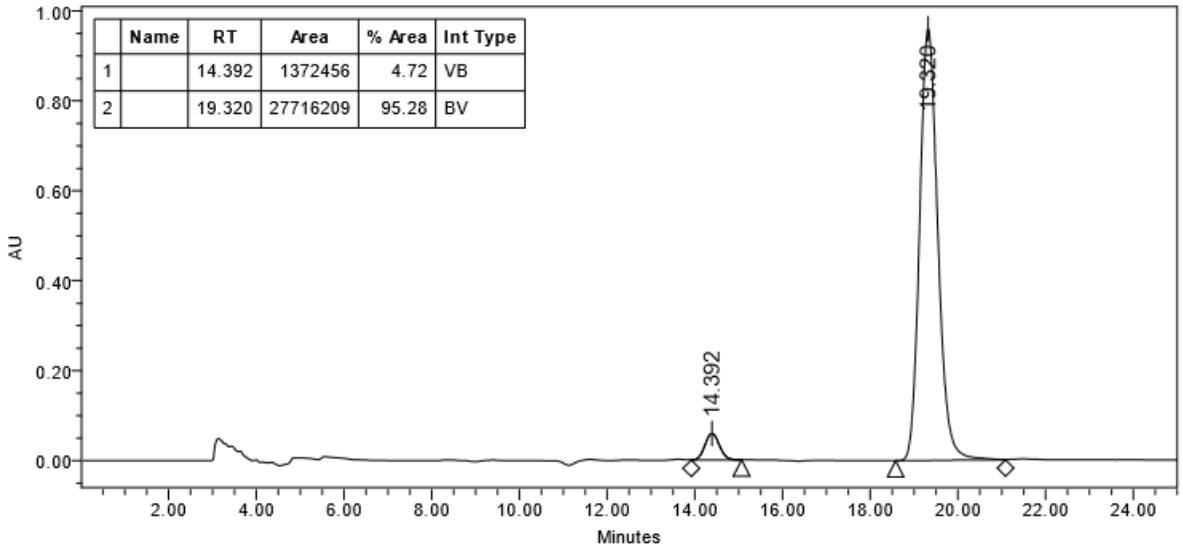
Enantiomerically enriched.

Compound **2d** (91% ee). HPLC: Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm.



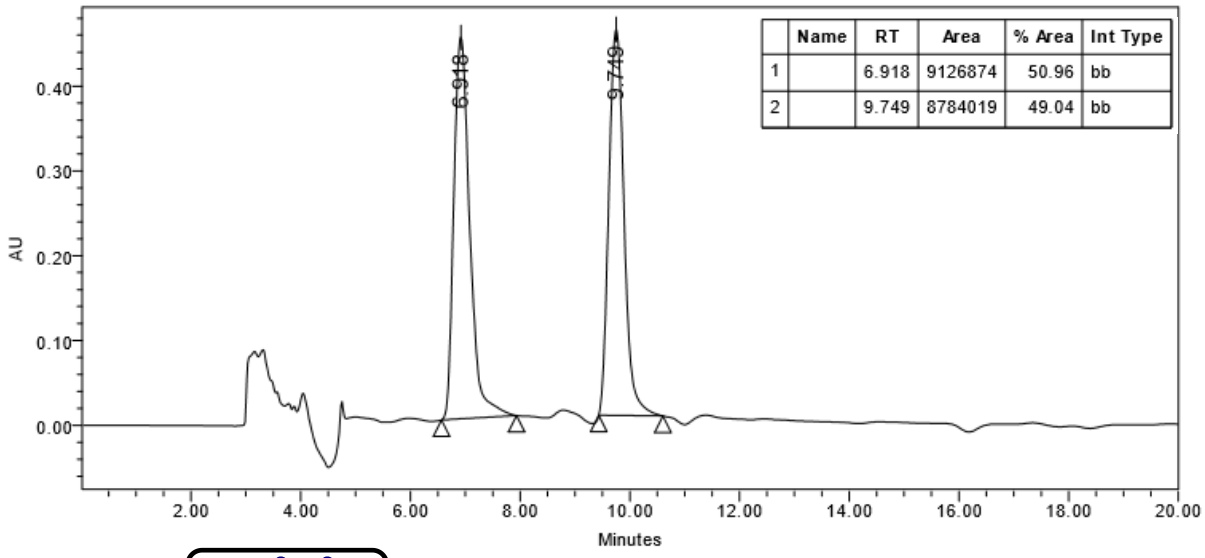
Racemic.



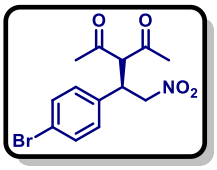


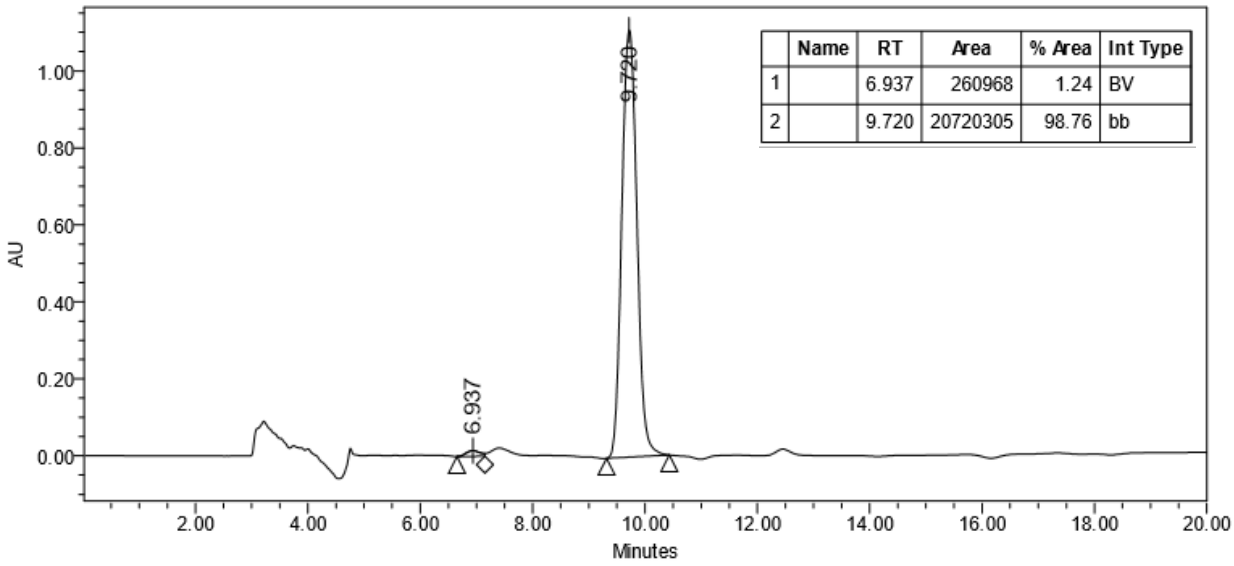
Enantiomerically enriched.

Compound **2e** (98% ee). HPLC: Chiralpak IC-3, hexane/ethanol 85:15, 0.6mL/min, 220 nm.



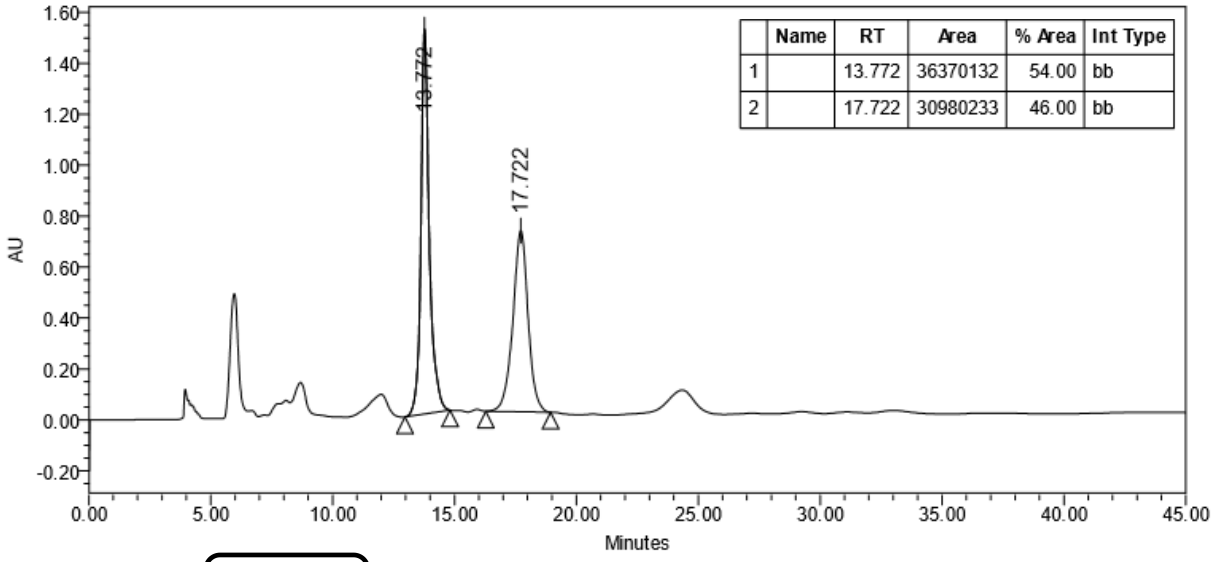
Racemic.





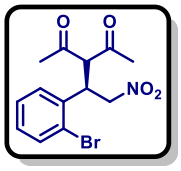
Enantiomerically enriched.

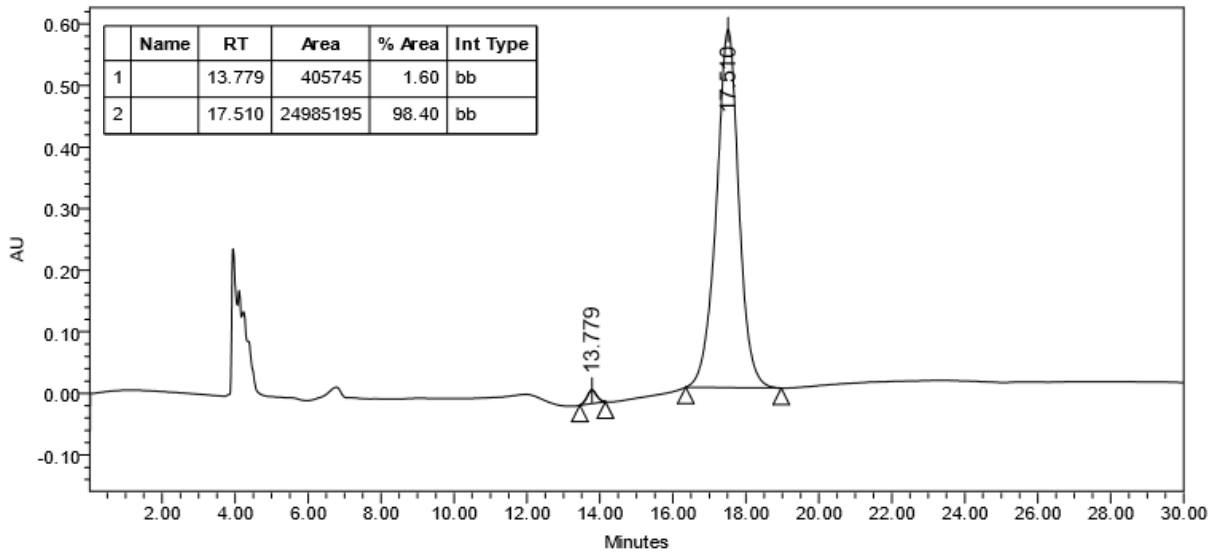
Compound **2f** (97% ee). HPLC: Chiralpak IA, hexane/ethanol 95:5, 0.8 mL/min, 220 nm.



	Name	RT	Area	% Area	Int Type
1		13.772	36370132	54.00	bb
2		17.722	30980233	46.00	bb

Racemic.

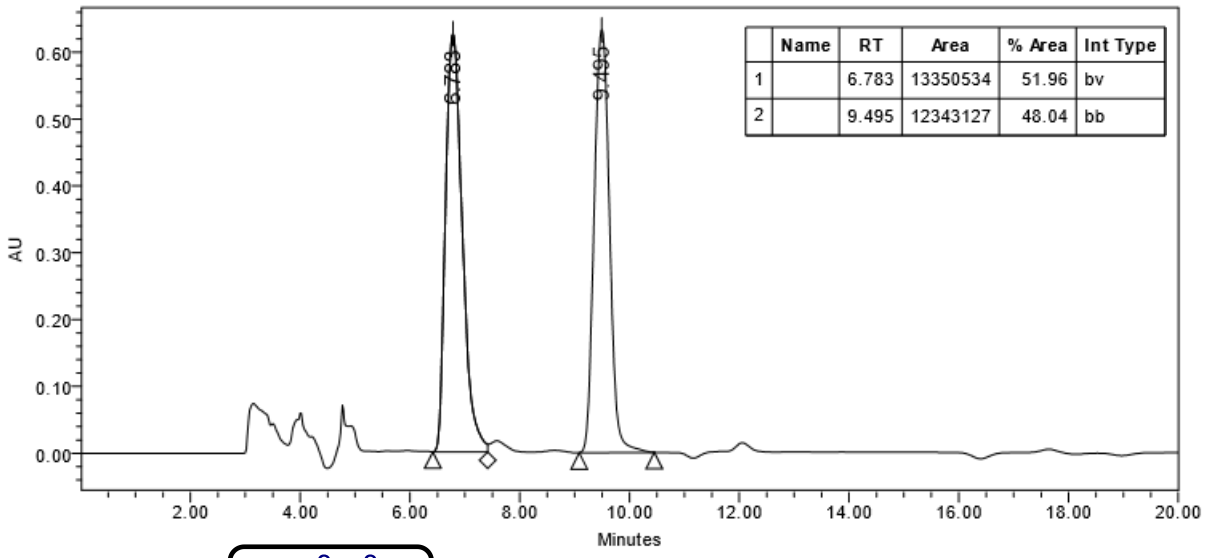




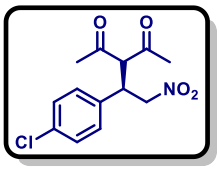
	Name	RT	Area	% Area	Int Type
1		13.779	405745	1.60	bb
2		17.510	24985195	98.40	bb

Enantiomerically enriched.

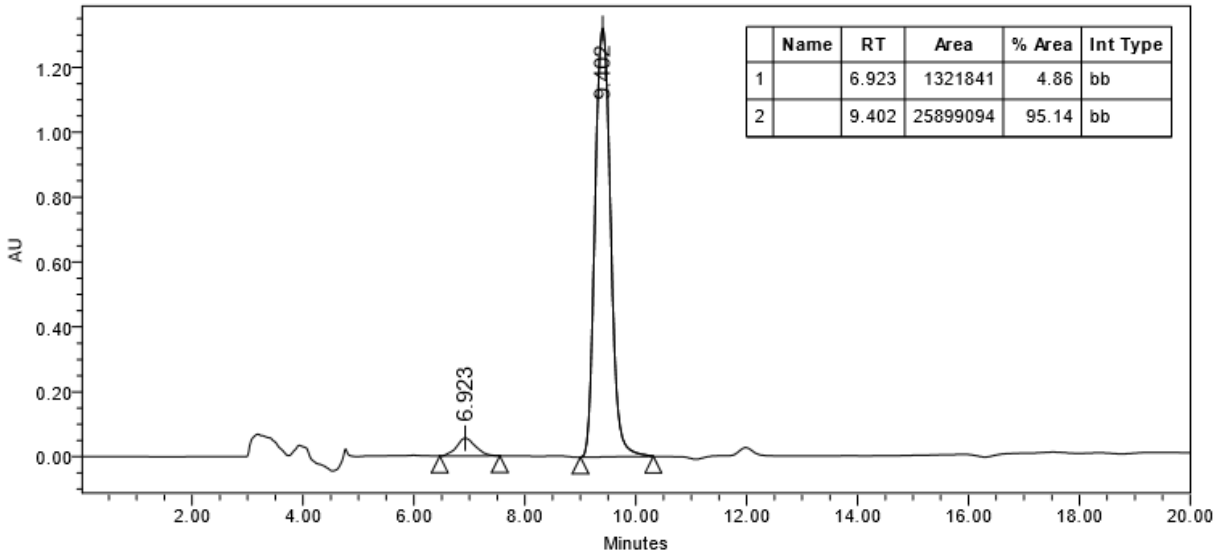
Compound **2g** (90% ee). HPLC: Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm.



	Name	RT	Area	% Area	Int Type
1		6.783	13350534	51.96	bv
2		9.495	12343127	48.04	bb



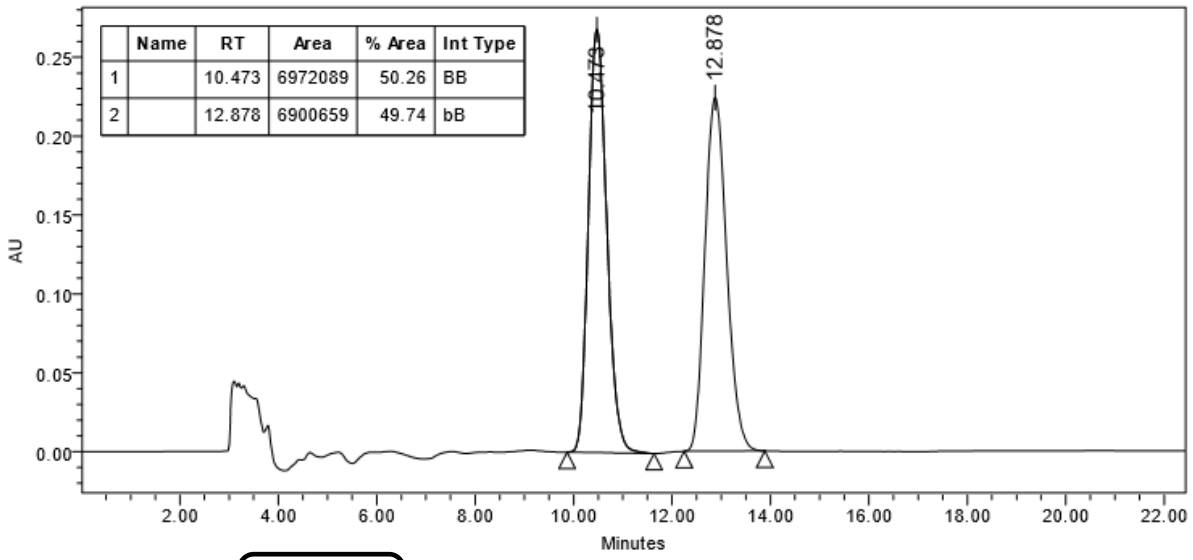
Racemic.



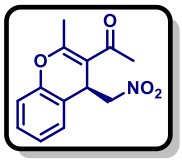
	Name	RT	Area	% Area	Int Type
1		6.923	1321841	4.86	bb
2		9.402	25899094	95.14	bb

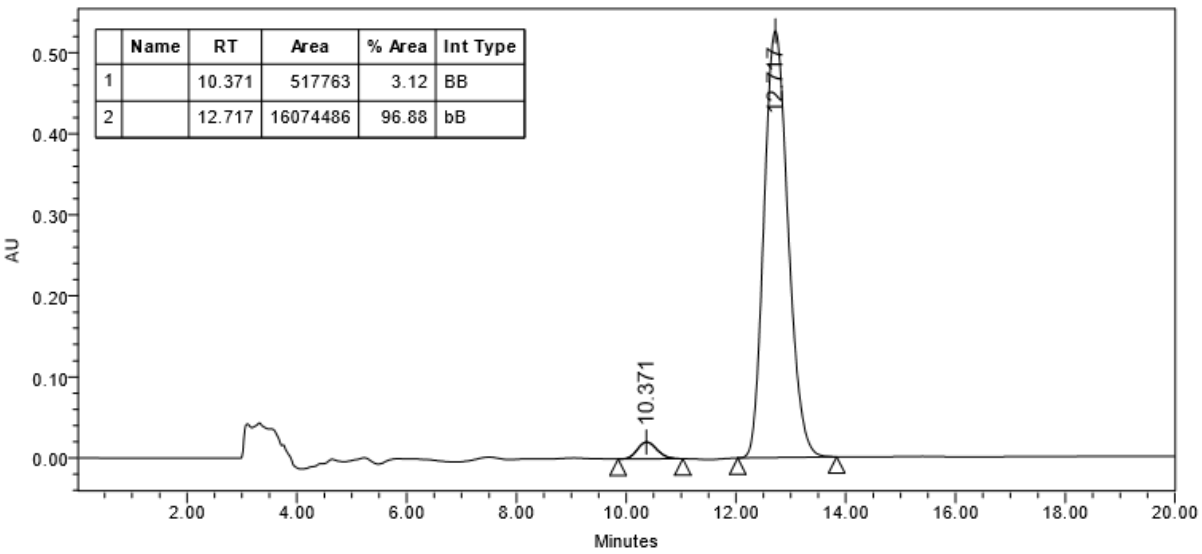
Enantiomerically enriched.

Compound **2h** (94% ee). HPLC: Chiralcel OD, hexane/isopropanol 90:10, 1.0 mL/min, 254 nm.



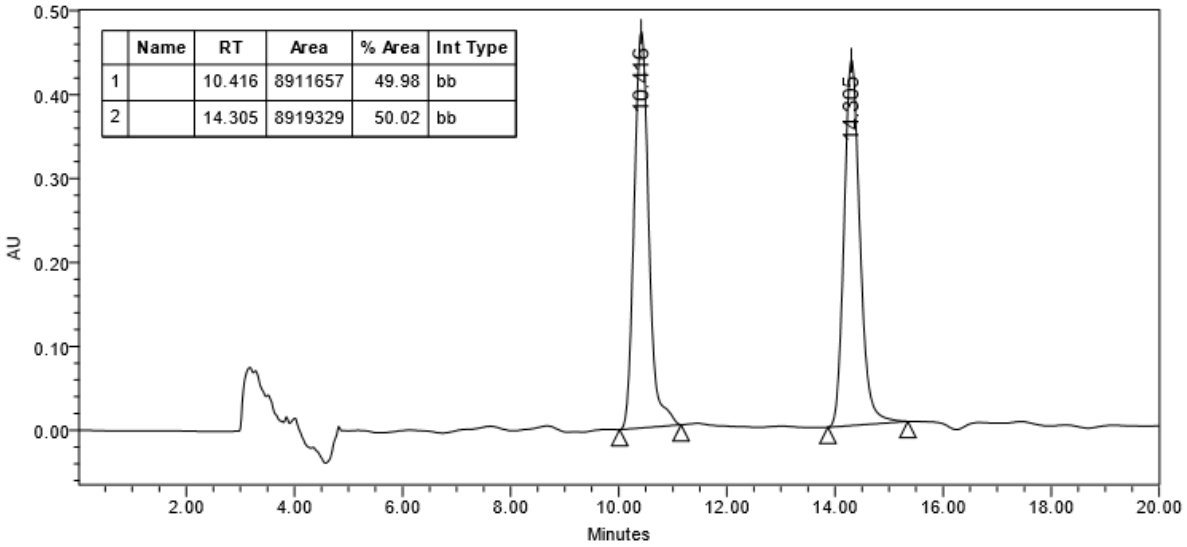
Racemic.



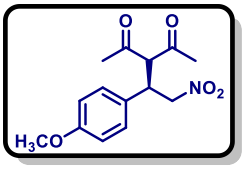


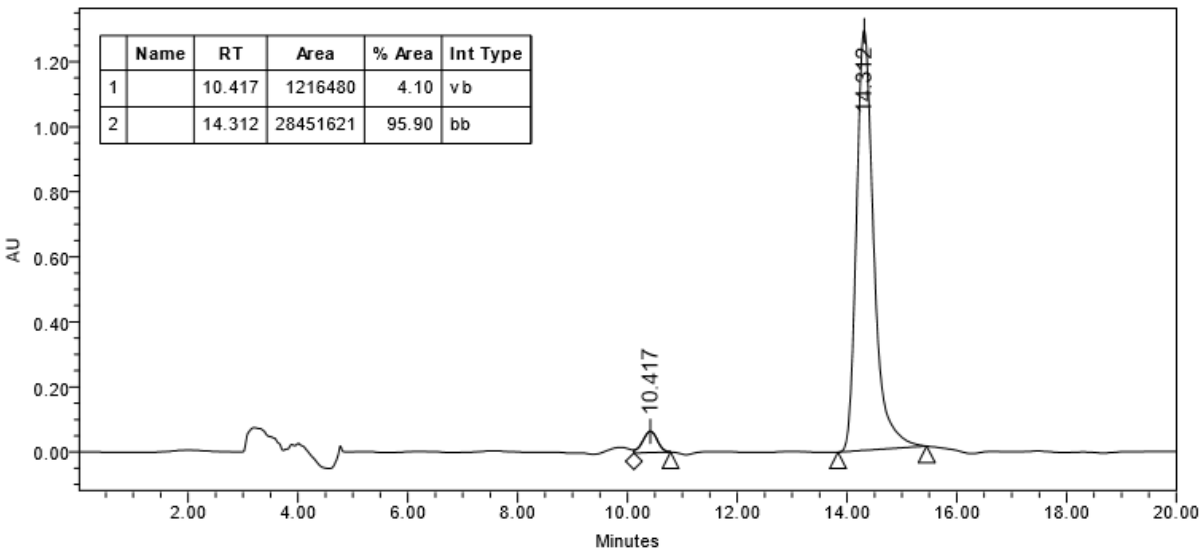
Enantiomerically enriched.

Compound **2i** (92% ee). HPLC: Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm.



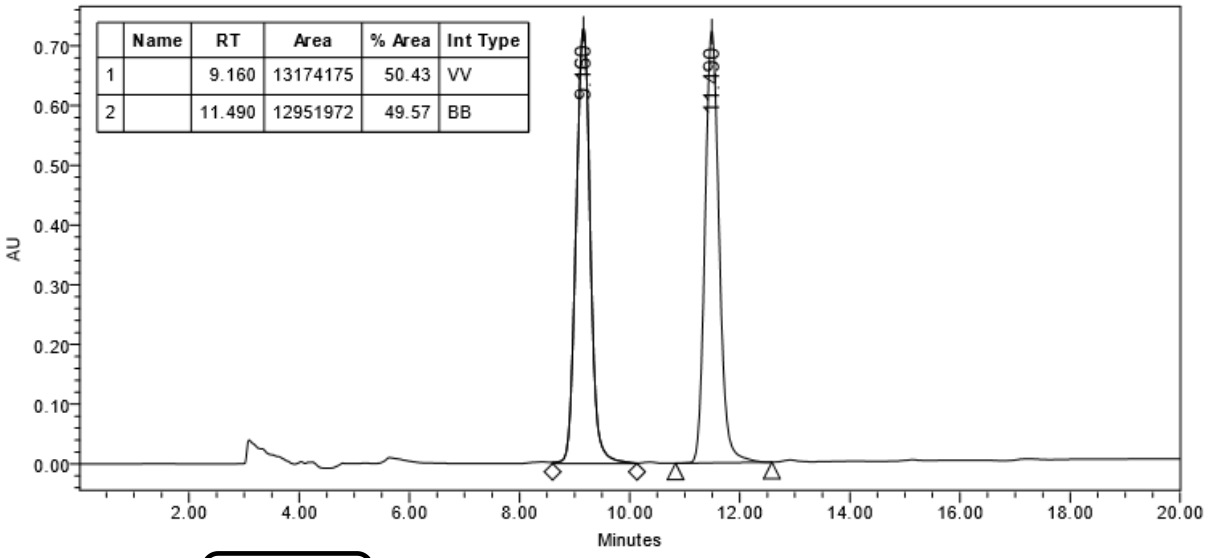
Racemic.



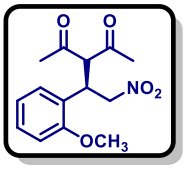


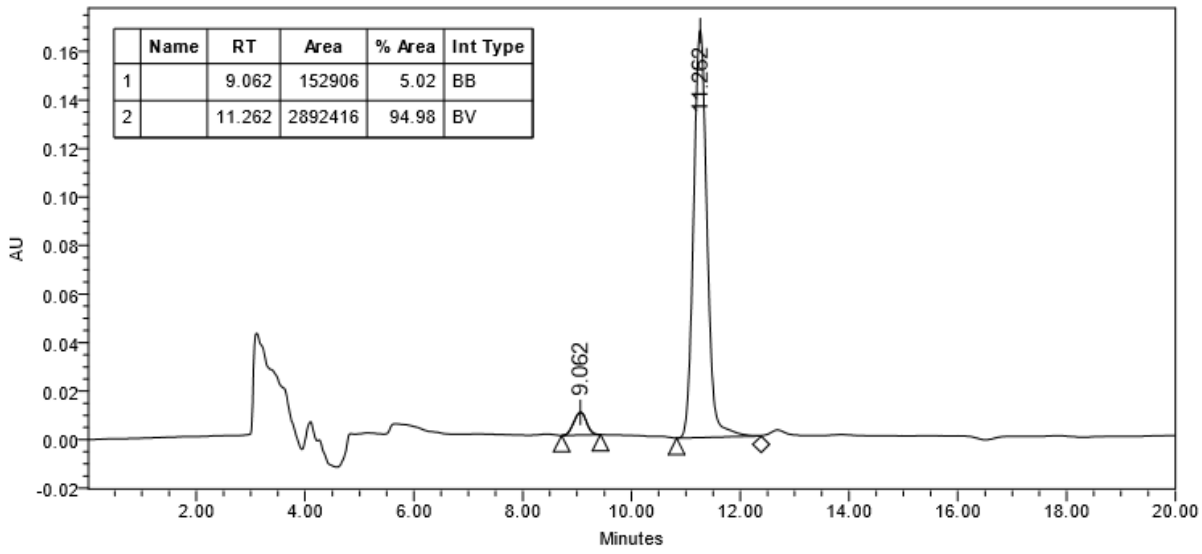
Enantiomerically enriched.

Compound **2j** (90% ee). HPLC: Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm.



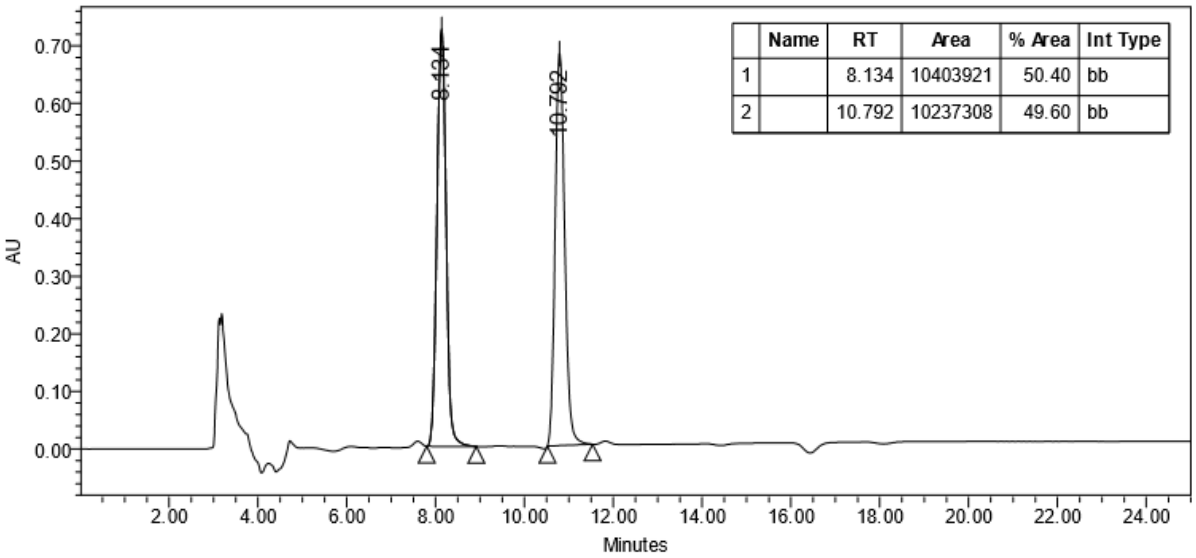
Racemic.





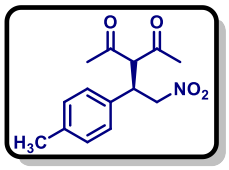
Enantiomerically enriched.

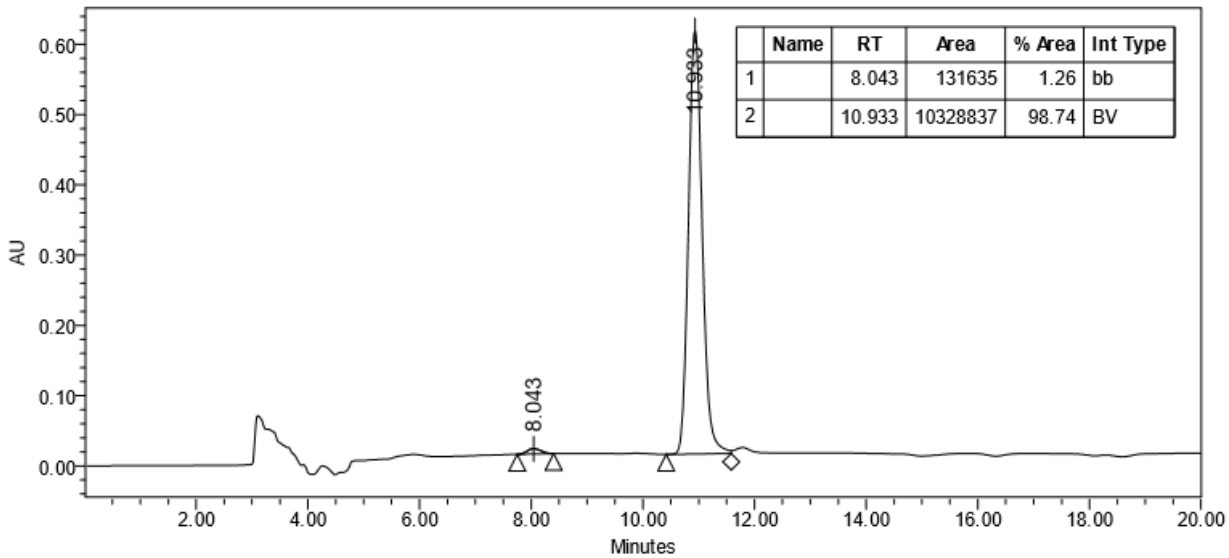
Compound **2k** (97% ee). HPLC: Chiralpak IC-3, hexane/ethanol 85:15, 0.6 mL/min, 220 nm.



	Name	RT	Area	% Area	Int Type
1		8.134	10403921	50.40	bb
2		10.792	10237308	49.60	bb

Racemic.

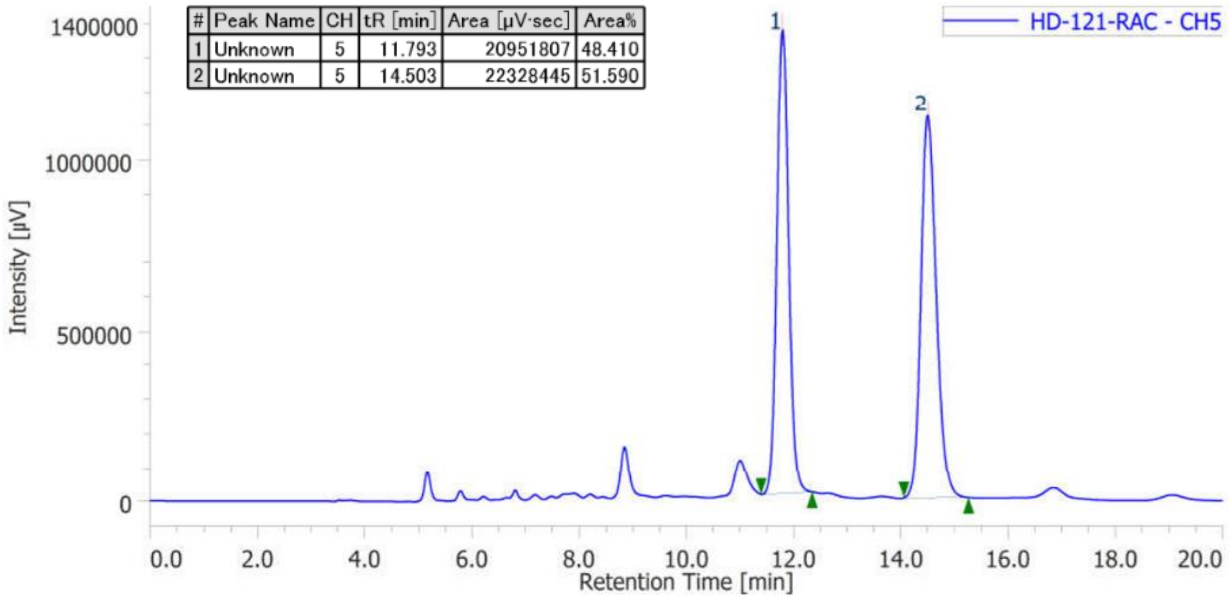




	Name	RT	Area	% Area	Int Type
1		8.043	131635	1.26	bb
2		10.933	10328837	98.74	BV

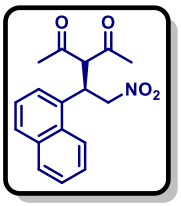
Enantiomerically enriched.

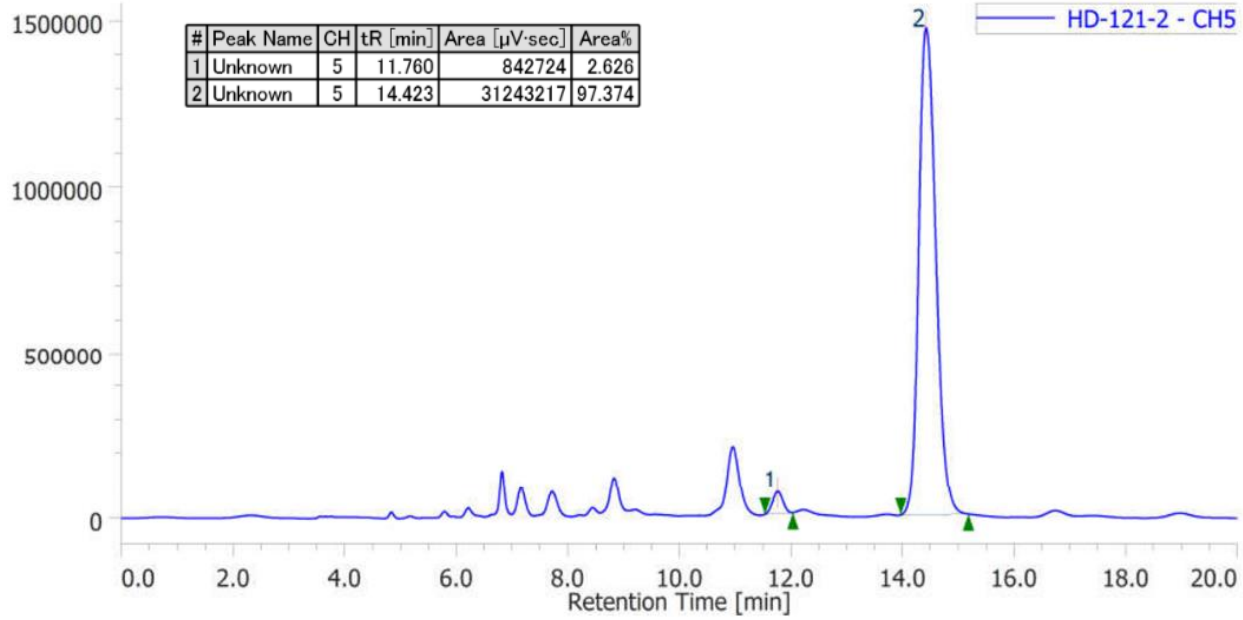
Compound **2l** (95% ee). HPLC: Chiralpak IA, hexane/ethanol 85:15, 0.8 mL/min, 220 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	11.793	20951807	48.410
2	Unknown	5	14.503	22328445	51.590

Racemic.

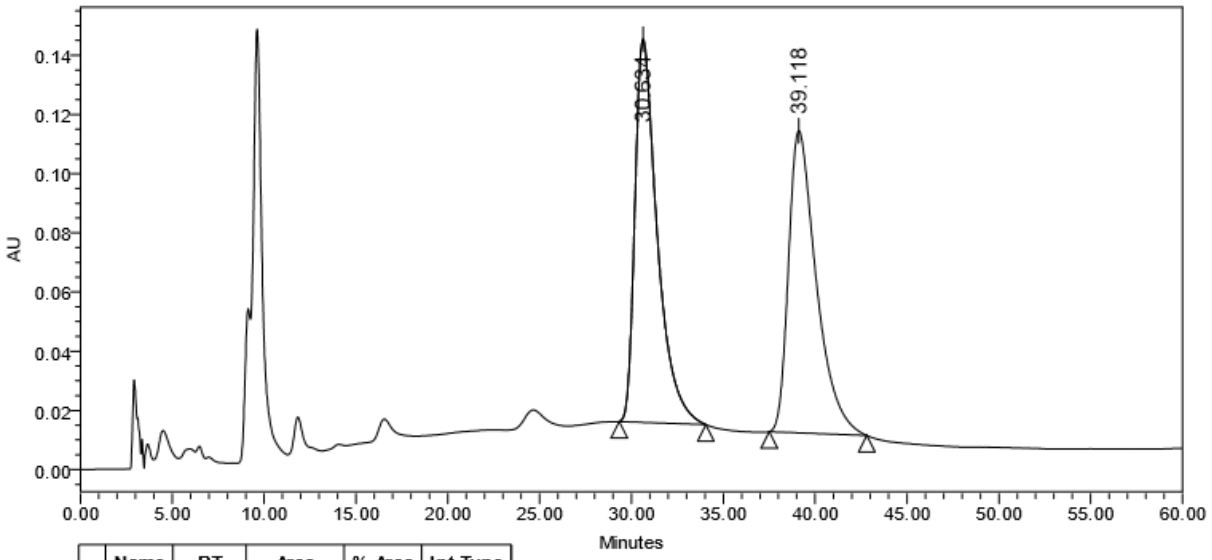




#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	11.760	842724	2.626
2	Unknown	5	14.423	31243217	97.374

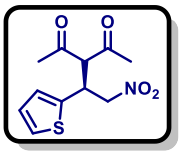
Enantiomerically enriched.

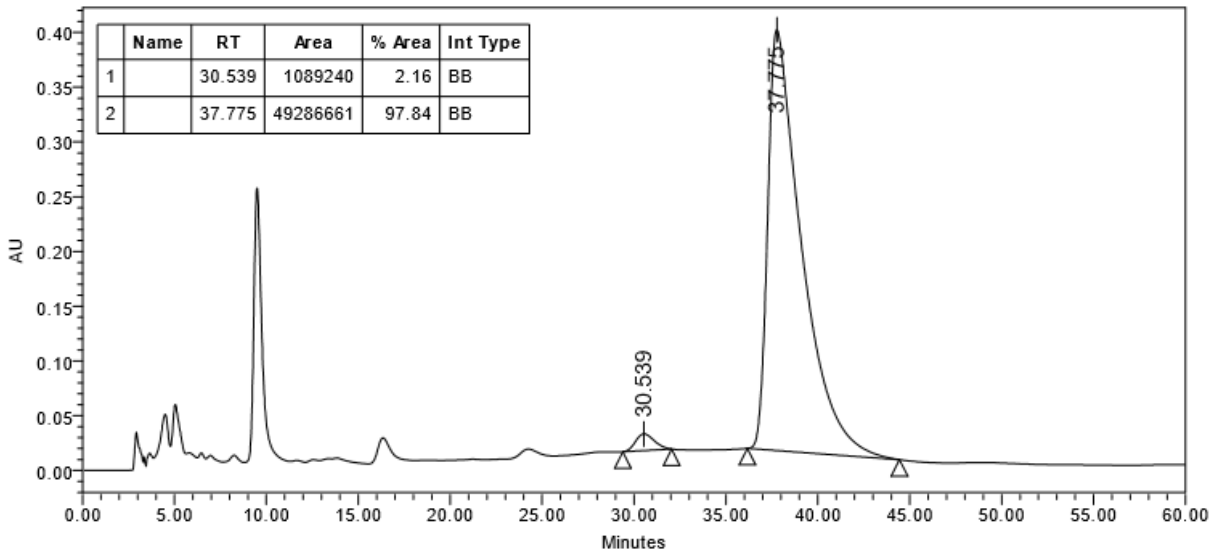
Compound **2m** (96% ee). HPLC: Chiralcel OJ, hexane/ethanol 70:30, 1.0 mL/min, 220 nm.



	Name	RT	Area	% Area	Int Type
1		30.634	10968088	50.50	BB
2		39.118	10749086	49.50	BB

Racemic.

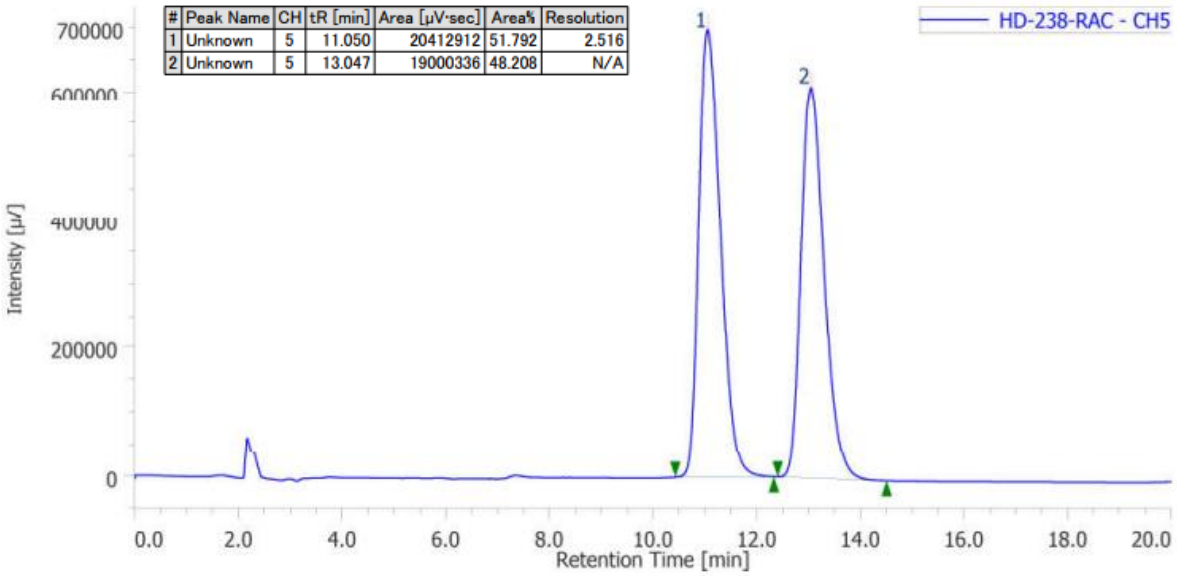




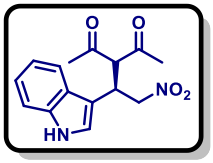
	Name	RT	Area	% Area	Int Type
1		30.539	1089240	2.16	BB
2		37.775	49286661	97.84	BB

Enantiomerically enriched.

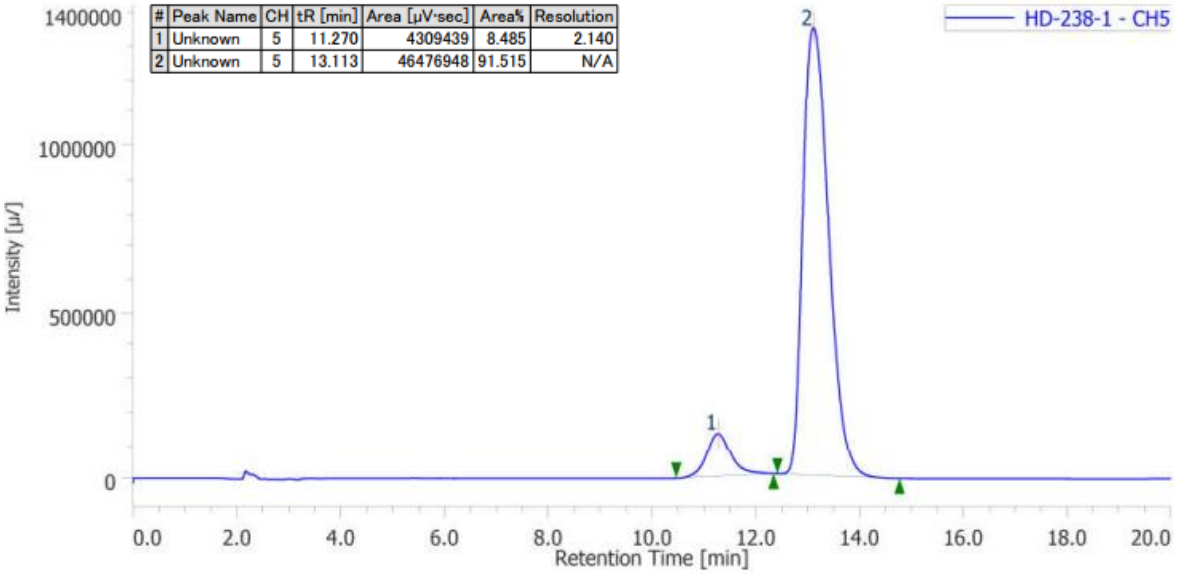
Compound **2n** (83% ee). HPLC: Chiralpak IC, hexane/isopropanol 90:10, 1.0 mL/min, 220 nm.



#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%	Resolution
1	Unknown	5	11.050	20412912	51.792	2.516
2	Unknown	5	13.047	19000336	48.208	N/A



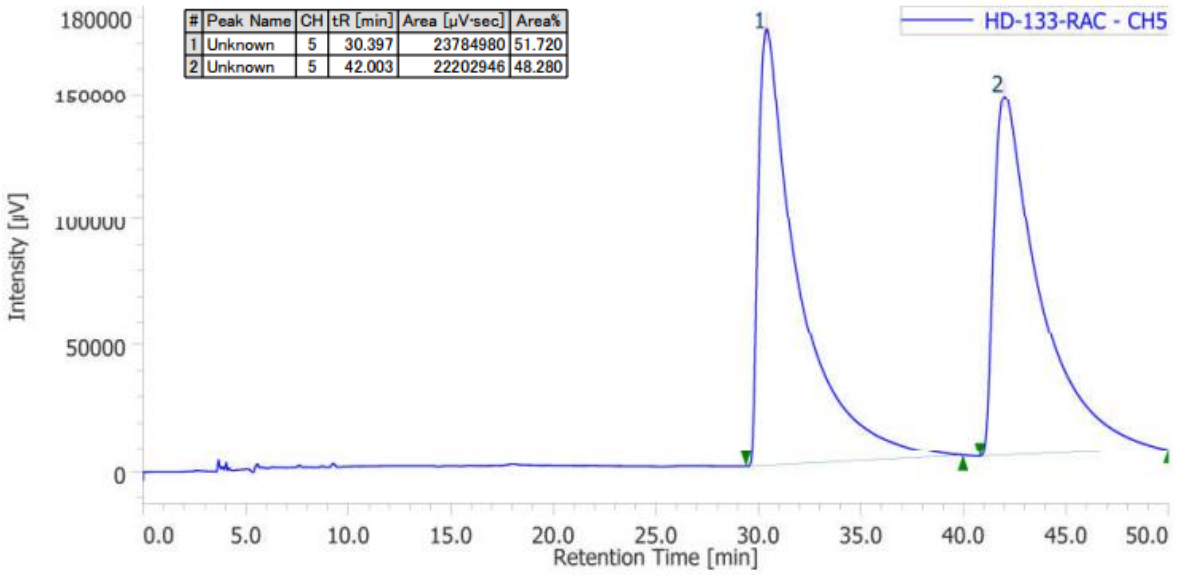
Racemic.



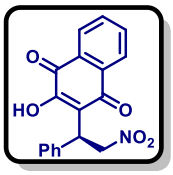
#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%	Resolution
1	Unknown	5	11.270	4309439	8.485	2.140
2	Unknown	5	13.113	46476948	91.515	N/A

Enantiomerically enriched.

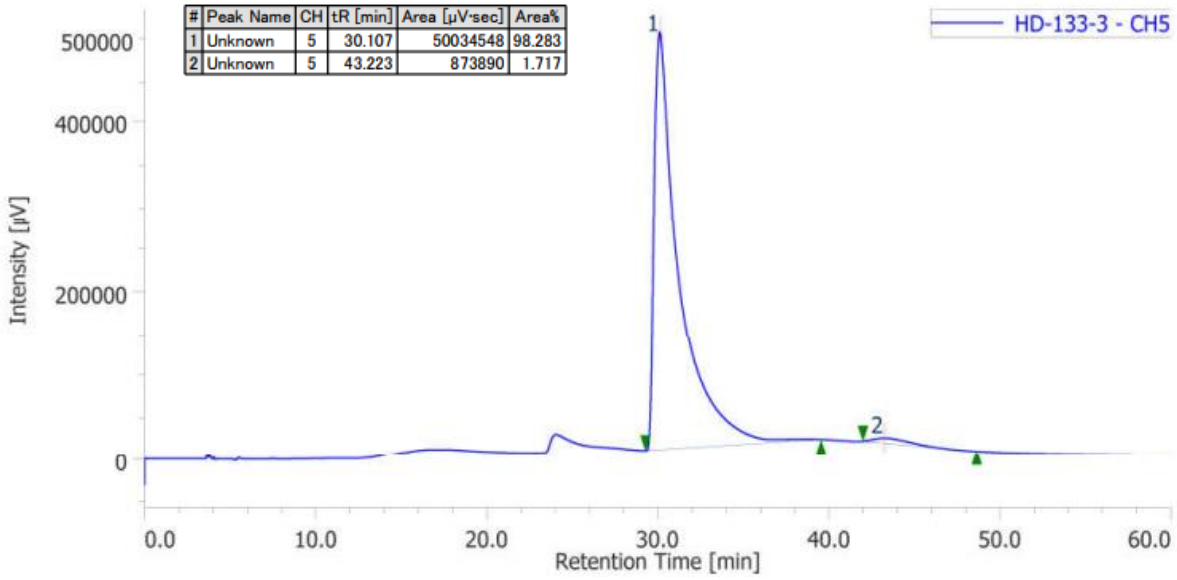
Compound **3a** (97% ee). HPLC: Chiralpak IA, hexane/ethanol 90:10, 0.8 mL/min, 254 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	30.397	23784980	51.720
2	Unknown	5	42.003	22202946	48.280



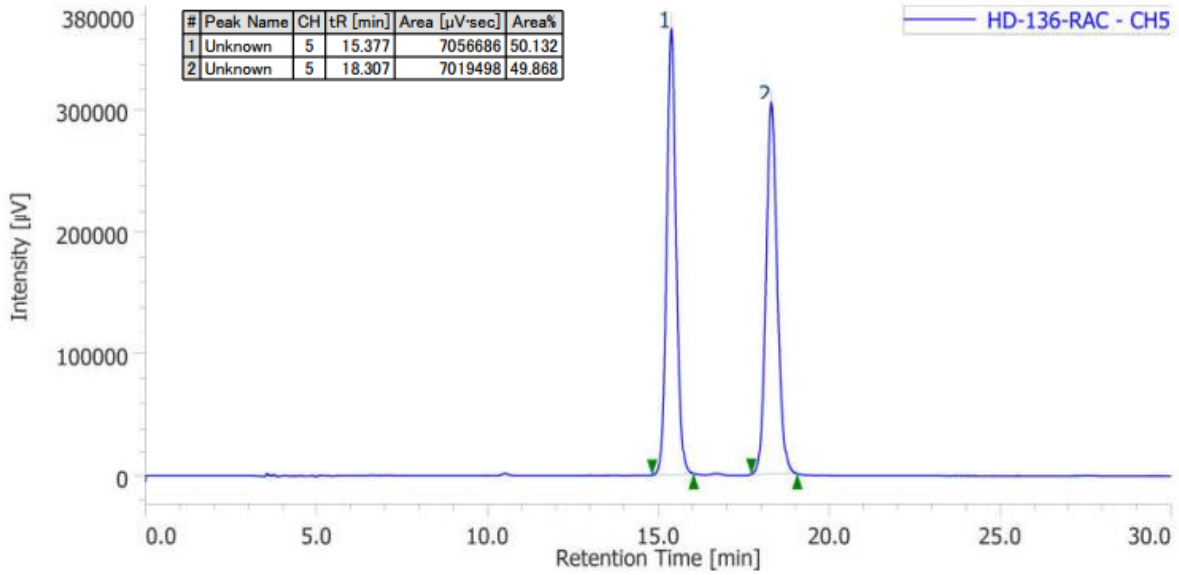
Racemic.



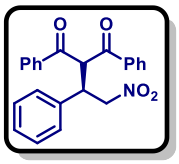
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	30.107	50034548	98.283
2	Unknown	5	43.223	873890	1.717

Enantiomerically enriched.

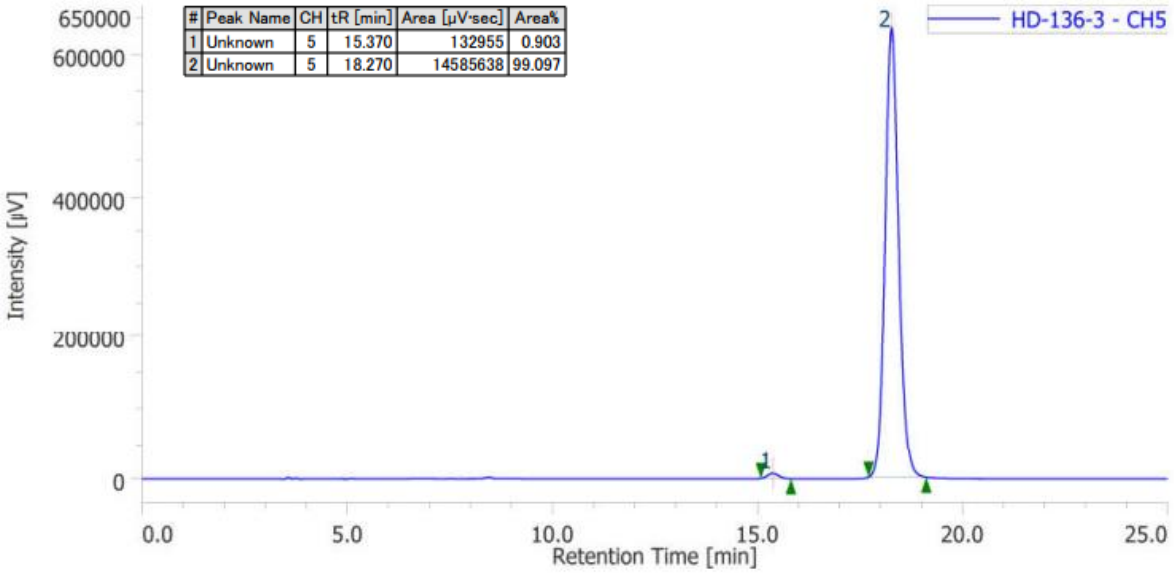
Compound **3b** (98% ee). HPLC: Chiralpak IA, hexane/ethanol 85:15, 0.8 mL/min, 250 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	15.377	7056686	50.132
2	Unknown	5	18.307	7019498	49.868



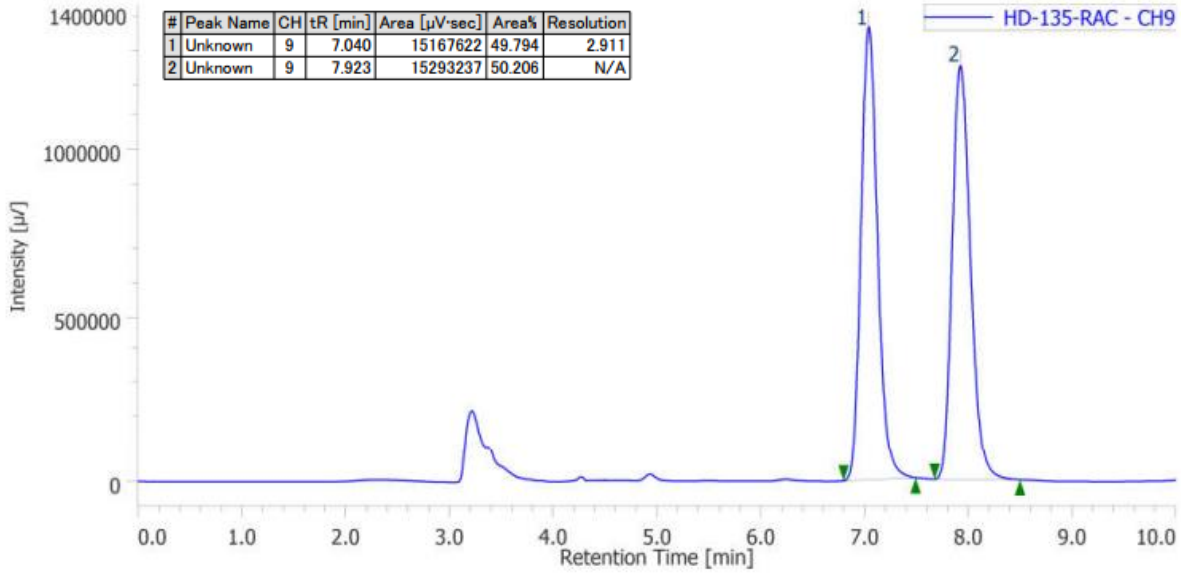
Racemic.



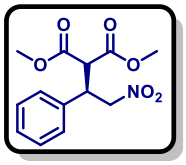
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	15.370	132955	0.903
2	Unknown	5	18.270	14585638	99.097

Enantiomerically enriched.

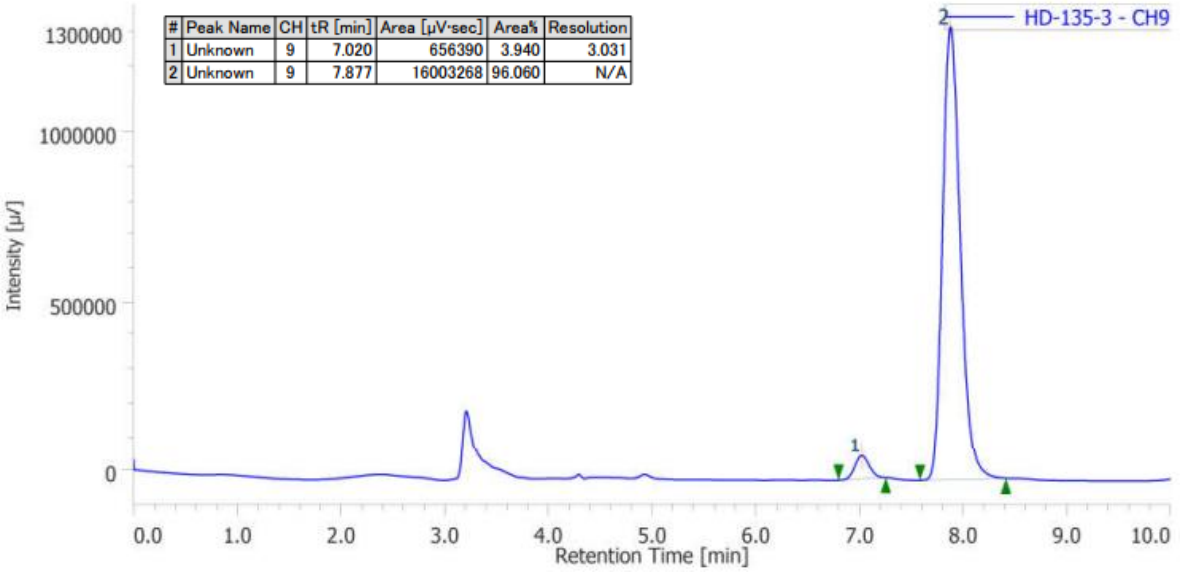
Compound **3c** (92% ee). HPLC: Chiralpak IC, hexane/ethanol 85:15, 0.6 mL/min, 220 nm.



#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%	Resolution
1	Unknown	9	7.040	15167622	49.794	2.911
2	Unknown	9	7.923	15293237	50.206	N/A



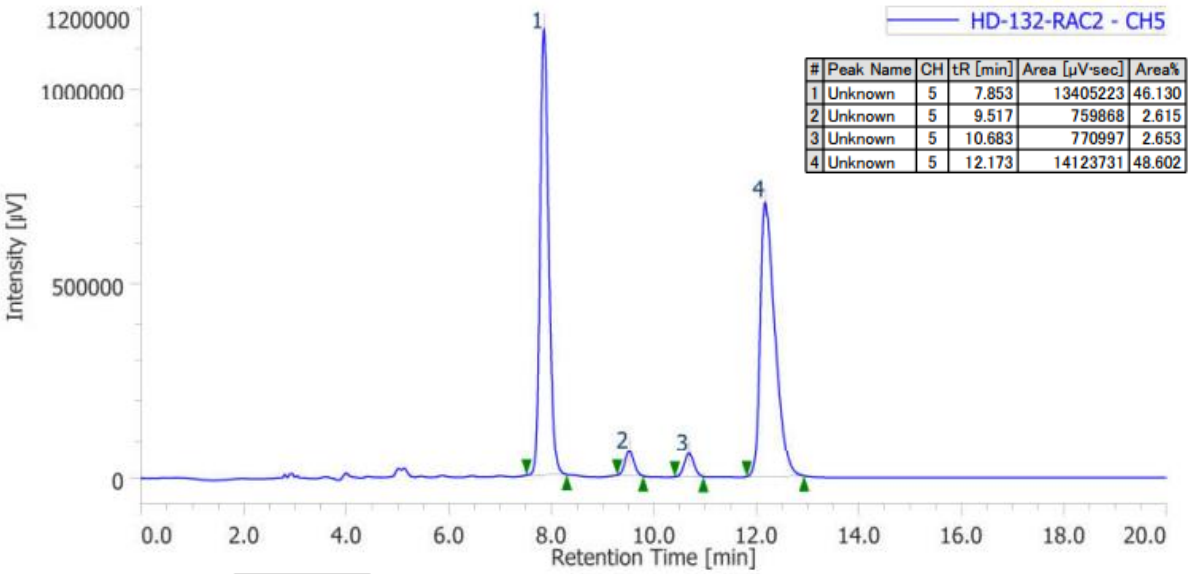
Racemic.



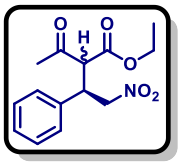
#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%	Resolution
1	Unknown	9	7.020	656390	3.940	3.031
2	Unknown	9	7.877	16003268	96.060	N/A

Enantiomerically enriched.

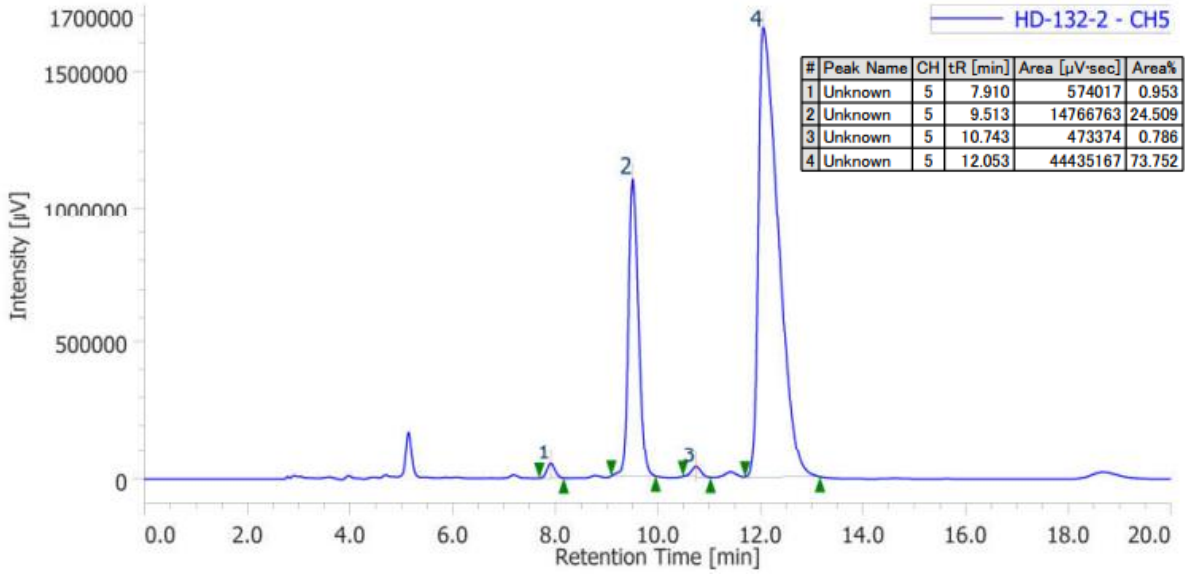
Compound **3d** (75:25 dr; 98, 93% ee). HPLC: Chiralpak IA, hexane/ethanol 85:15, 1.0 mL/min, 220 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	7.853	13405223	46.130
2	Unknown	5	9.517	759868	2.615
3	Unknown	5	10.683	770997	2.653
4	Unknown	5	12.173	14123731	48.602



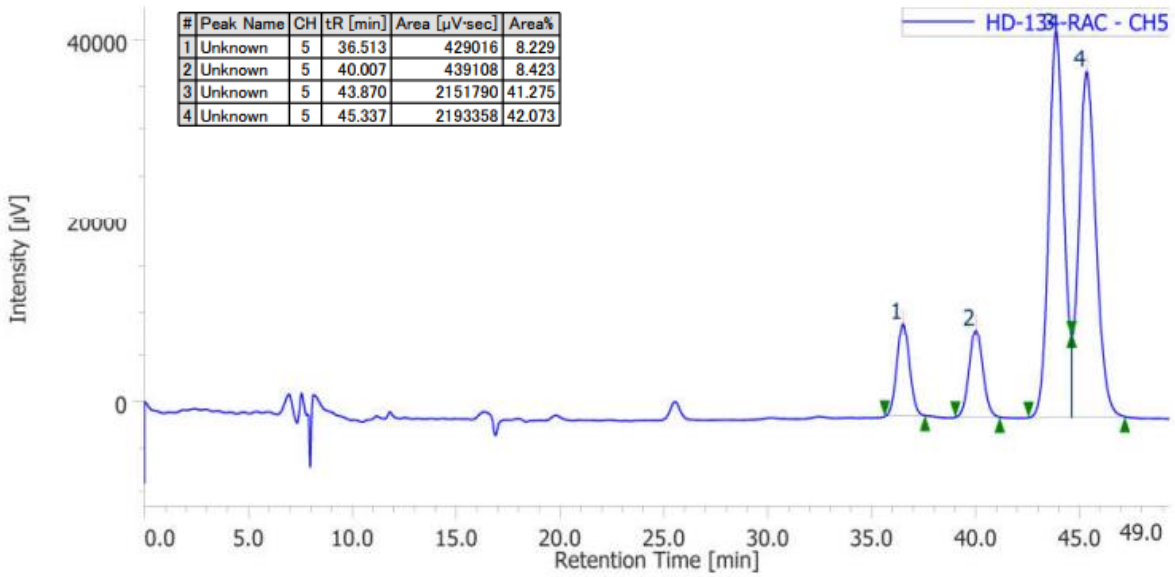
Racemic.



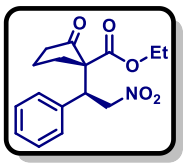
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	7.910	574017	0.953
2	Unknown	5	9.513	14766763	24.509
3	Unknown	5	10.743	473374	0.786
4	Unknown	5	12.053	44435167	73.752

Enantiomerically enriched.

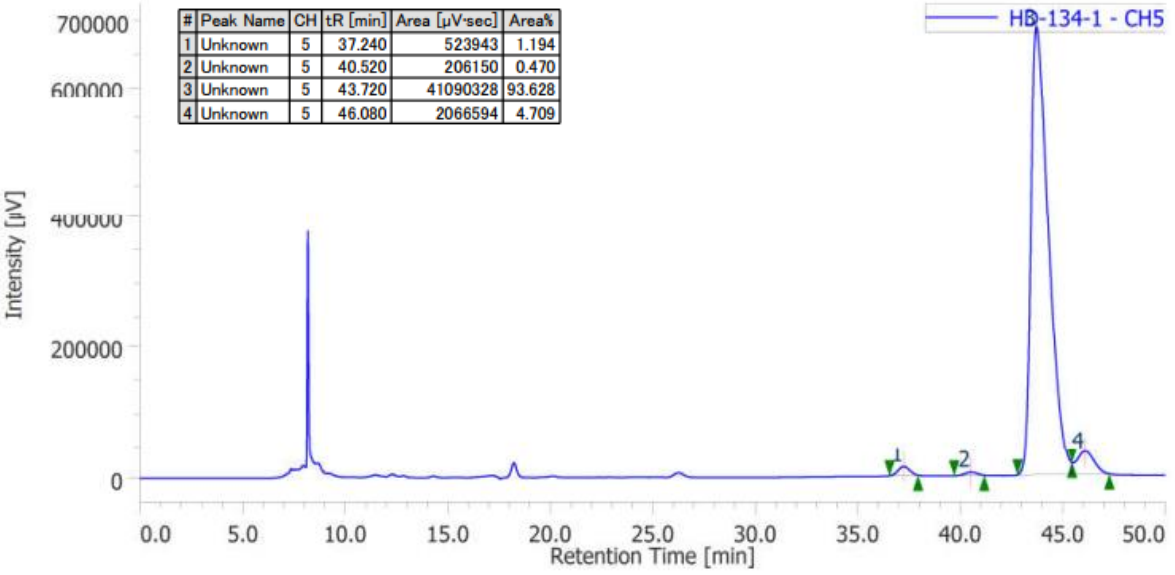
Compound **3e** (97:3 dr; 90, 44% ee). HPLC: Chiralpak IA, hexane/ethanol 97:3, 0.4 mL/min, 220 nm.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	36.513	429016	8.229
2	Unknown	5	40.007	439108	8.423
3	Unknown	5	43.870	2151790	41.275
4	Unknown	5	45.337	2193358	42.073



Racemic.



#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	5	37.240	523943	1.194
2	Unknown	5	40.520	206150	0.470
3	Unknown	5	43.720	41090328	93.628
4	Unknown	5	46.080	2066594	4.709

Enantiomerically enriched.

10. XYZ coordinates and electronic energies of the calculated structures

10.1. Structures for MLR model (B97-D/def2-TZVP approximation)

Benzene (probe)

E(RB97D) = -232.153285 Hartree/Particle

XYZ coordinates

H	2.48697900	0.01017600	-0.00000200
C	1.39875100	0.00569700	0.00000000
C	0.69438800	1.21414700	0.00000100
C	0.70429500	-1.20843000	-0.00000100
C	-0.70428400	1.20845700	-0.00000100
H	1.23467700	2.15881500	0.00000400
C	-0.69442500	-1.21414600	0.00000200
H	1.25223500	-2.14868100	-0.00000100
C	-1.39873100	-0.00572500	0.00000000
H	-1.25226500	2.14866900	-0.00000400
H	-1.23462300	-2.15885200	0.00000000
H	-2.48697400	-0.01012600	0.00000100

1a (A- and B-conformer have the same structure)

E(RB97D) = -1170.104266 Hartree/Particle

XYZ coordinates

C	0.42102700	-1.59650700	0.01730100
C	-0.97432900	-1.50439300	-0.02893400
C	0.41216900	-2.18935100	1.38281000
N	1.40343600	-1.25702800	-0.83594700
C	-1.13059700	-2.08605000	1.32974300
N	-1.85412700	-1.08355600	-0.95731300
O	1.26846700	-2.55149700	2.16678100
H	1.14872000	-0.68797700	-1.63667200
O	-2.07647300	-2.31993100	2.06008000
H	-1.46010600	-0.61655000	-1.76816600
C	-3.16374200	-0.54994800	-0.55345200
C	-3.10146300	0.99267900	-0.41574300
C	-4.23963200	-0.95670500	-1.56989900
H	-3.39911000	-0.99859700	0.41774700
C	-4.49079400	1.53929900	-0.01752400
H	-2.87253400	1.37728500	-1.42482500
C	-5.61688300	-0.39357800	-1.18943000
H	-3.94913300	-0.57262600	-2.56165100
C	-5.56510000	1.13362100	-1.03646500
H	-4.43713800	2.63164700	0.07654800
H	-4.75849600	1.13971100	0.97038200
H	-6.36017900	-0.68153100	-1.94420800
H	-5.93418800	-0.84050700	-0.23533000

H	-6.54567000	1.52124600	-0.72960700
H	-5.32921200	1.58716000	-2.01194400
H	-4.26733600	-2.05091000	-1.63807100
N	-1.98647400	1.42141100	0.43801600
C	-2.18389500	1.17849600	1.86697700
H	-1.22644200	1.31940800	2.38475700
H	-2.92189400	1.86883100	2.32112900
H	-2.51273100	0.15059000	2.04138200
C	-1.58896100	2.80195600	0.19593400
H	-2.35352500	3.54159700	0.51294200
H	-0.66754900	3.01371700	0.75246400
H	-1.38733100	2.94997100	-0.87314200
C	2.79456700	-1.08135000	-0.37975700
C	3.76054000	-1.68703100	-1.40392300
H	2.87313400	-1.65291600	0.55392000
C	5.20721900	-1.36985500	-1.01259100
H	3.54843700	-1.26259700	-2.39855500
H	3.58378300	-2.76751500	-1.45946200
C	5.44305700	0.14452800	-1.07469900
H	5.90948900	-1.88908600	-1.67646700
H	5.39187700	-1.73361700	0.00867500
H	6.42033700	0.40328400	-0.64583000
H	5.47930700	0.45392900	-2.13198900
C	4.35983100	0.94485400	-0.37400500
C	4.60869600	2.28384300	-0.03641400
C	3.10133300	0.38684400	-0.07176100
C	3.64143100	3.06763500	0.59017100
C	2.13155400	1.18292600	0.56035800
C	2.39376300	2.51176400	0.88936600
H	3.85940100	4.10210600	0.84751800
H	1.15825500	0.75947200	0.79579500
H	1.63117400	3.10820900	1.38542800
H	5.58411000	2.70984600	-0.26932500

1b (A-conformer)

E(RB97D) = -1092.713371 Hartree/Particle

XYZ coordinates

C	0.88476000	-1.74142000	-0.33849100
C	-0.50363700	-1.64675000	-0.20771200
C	1.04908700	-2.34419300	1.01035400
N	1.75252400	-1.38880900	-1.30993900
C	-0.48628900	-2.22732100	1.16214200
N	-1.49586700	-1.21436900	-1.00957300
O	1.99568200	-2.71494000	1.68009200
H	1.38195000	-0.77685800	-2.03224900
O	-1.32711900	-2.44166700	2.01470500
H	-1.19726900	-0.76925300	-1.87276200

C	-2.67847000	-0.56933700	-0.41346500
C	-2.45750800	0.96384300	-0.32438900
C	-3.93765800	-0.88525200	-1.22985300
H	-2.78909800	-0.98651500	0.59346600
C	-3.70358800	1.63689000	0.29193400
H	-2.37544200	1.31642000	-1.36732900
C	-5.17581500	-0.19785600	-0.63399900
H	-3.78544400	-0.53349500	-2.26347200
C	-4.96720300	1.31996500	-0.52124300
H	-3.53841900	2.72077400	0.34853100
H	-3.83116200	1.27201800	1.32054700
H	-6.05877800	-0.42129700	-1.24680900
H	-5.36469200	-0.61071300	0.36833300
H	-5.84483800	1.79300300	-0.06080900
H	-4.86335400	1.74631700	-1.53137800
H	-4.07330600	-1.97276400	-1.27034100
N	-1.17772200	1.29006600	0.30955300
C	-1.13562800	1.08807900	1.75601000
H	-0.08903500	1.12119900	2.08341100
H	-1.69636800	1.86460200	2.31375400
H	-1.54315600	0.10825300	2.01999500
C	-0.67055900	2.60713600	-0.04958000
H	-1.27364700	3.43936000	0.37164600
H	0.35644400	2.70861700	0.32170700
H	-0.65522100	2.71378900	-1.14262900
C	3.16462200	-1.08007200	-0.95367200
H	3.43666400	-1.80746400	-0.18212800
C	3.31495800	1.46637400	-1.13926700
C	3.28962200	2.73673200	-0.55816800
C	3.23558700	0.31462800	-0.34341100
C	3.18277400	2.87101100	0.82962200
C	3.12857600	0.45796300	1.04730700
C	3.10337300	1.72764200	1.63034700
H	3.16364000	3.85992200	1.28291900
H	3.06118300	-0.43380700	1.66679000
H	3.02336500	1.82289600	2.71137600
H	3.35691700	3.62156300	-1.18813000
H	3.40552700	1.37620700	-2.22005500
C	4.04546800	-1.28476000	-2.18593400
H	3.71927000	-0.64741000	-3.01877600
H	5.08577600	-1.03142900	-1.95266100
H	3.99260400	-2.32911900	-2.51281200

1b (B-conformer)

E(RB97D) = -1092.710245 Hartree/Particle

XYZ coordinates

C	0.78056600	-1.66563500	-0.16102600

C	-0.61049200	-1.51586100	-0.13393400
C	0.81218500	-2.31816500	1.17654500
N	1.73324600	-1.32819200	-1.04757800
C	-0.72605200	-2.15542300	1.20279600
N	-1.51438100	-1.01897900	-0.99897600
O	1.68967000	-2.74629900	1.90167300
H	1.46396600	-0.71724100	-1.81172200
O	-1.64560200	-2.39095200	1.96535900
H	-1.14096300	-0.52762600	-1.80511800
C	-2.78764600	-0.46656000	-0.51317900
C	-2.66885200	1.06387500	-0.29883600
C	-3.91611800	-0.78557700	-1.50388700
H	-2.99834600	-0.95830700	0.44269400
C	-4.02304400	1.63231800	0.18150200
H	-2.46521300	1.49399700	-1.29486500
C	-5.25792800	-0.19957800	-1.04028400
H	-3.65179700	-0.35983800	-2.48591000
C	-5.14857500	1.31519400	-0.81314300
H	-3.92912100	2.71590400	0.32956500
H	-4.26653500	1.18976600	1.15727200
H	-6.03891300	-0.42471800	-1.77815200
H	-5.55318700	-0.68478600	-0.09787900
H	-6.10285500	1.71779600	-0.44825000
H	-4.93464600	1.81065400	-1.77318400
H	-3.98331300	-1.87333100	-1.62632800
N	-1.50909200	1.41189900	0.53201200
C	-1.66236000	1.10138400	1.95348000
H	-0.68283600	1.18708100	2.44120300
H	-2.36146100	1.78886100	2.46921400
H	-2.01631800	0.07587200	2.08782300
C	-1.07560200	2.79028400	0.34571900
H	-1.80417800	3.53586400	0.72685700
H	-0.12981200	2.94479300	0.88002600
H	-0.90554400	2.98716100	-0.72096300
C	3.15772800	-1.23798900	-0.66131500
C	4.01589300	-1.89594100	-1.74658600
H	3.24496600	-1.82965900	0.25885200
H	3.96501200	-1.32984700	-2.68668000
H	3.65495900	-2.91434400	-1.92411700
C	4.77200100	0.75832000	-0.69113800
C	5.10028500	2.07624700	-0.35656300
C	3.53123000	0.21092800	-0.33321000
C	4.19181000	2.87205500	0.34320700
C	2.62317800	1.02429900	0.36767900
C	2.95072000	2.33837000	0.70397600
H	4.44656900	3.89677400	0.60497500
H	1.65075200	0.63160900	0.65361400
H	2.23460600	2.94630600	1.25293100

H	6.06903600	2.47815700	-0.64650200
H	5.49603800	0.15936300	-1.23583800
H	5.06461100	-1.95062200	-1.43479600

1c (A'-conformer)

E(RB97D) = -1246.286853 Hartree/Particle

XYZ coordinates

C	0.04187200	-1.73406100	0.25727000
C	1.39396800	-1.56034300	-0.04096500
C	-0.31333700	-2.07094700	-1.14733700
N	-0.68708000	-1.60934200	1.38650300
C	1.18369300	-1.84045300	-1.48842700
N	2.48374900	-1.26648700	0.69290000
O	-1.33660500	-2.37238700	-1.72660700
H	-0.23887500	-1.13621500	2.16476600
O	1.89332700	-1.81828200	-2.47605800
H	2.31327300	-1.01013900	1.66018900
C	3.61750400	-0.55220600	0.08695100
C	3.54861100	0.95762800	0.42641500
C	4.95418100	-1.14302000	0.55661400
H	3.53395700	-0.69163100	-0.99608400
C	4.73133500	1.68817100	-0.24791800
H	3.69441400	1.03263100	1.51834200
C	6.14145900	-0.40483800	-0.08070300
H	5.01299600	-1.05940800	1.65392600
C	6.07636600	1.10255000	0.20736200
H	4.67925500	2.75969300	-0.01627800
H	4.63747400	1.58425500	-1.33778100
H	7.08601200	-0.82703800	0.28612500
H	6.11624500	-0.56490600	-1.16899800
H	6.90518800	1.62319200	-0.29042400
H	6.19378300	1.26935500	1.28960000
H	4.97662900	-2.21049900	0.30661700
N	2.21710600	1.52245300	0.16639200
C	1.86820400	1.63177500	-1.25103600
H	0.79789400	1.85593800	-1.33462300
H	2.43059400	2.43313200	-1.76908500
H	2.05715700	0.68714000	-1.76827200
C	2.00609400	2.79117500	0.85194100
H	2.62740200	3.61778500	0.45007000
H	0.95438200	3.08557100	0.74932400
H	2.23300000	2.67886400	1.92055900
C	-2.13761100	-1.37890700	1.28737900
H	-2.51381600	-2.15903700	0.61673800
C	-3.82264800	0.19749700	0.18200400
C	-4.16564900	1.49513900	-0.34157100
C	-2.49698400	-0.02062700	0.68356100

C	-3.18579600	2.52228600	-0.36132600
C	-1.57403100	1.00822900	0.62798900
C	-1.91531100	2.27942100	0.10750100
H	-3.45632200	3.49717600	-0.76325400
H	-0.55153000	0.84638200	0.96129300
H	-1.16201700	3.06326400	0.07635100
C	-5.47647900	1.72279400	-0.83973100
H	-5.71718200	2.70991200	-1.23140600
C	-6.42240100	0.71997700	-0.83674400
H	-7.42155000	0.90639400	-1.22460100
C	-6.08752200	-0.56077100	-0.33740100
C	-4.82429000	-0.81333400	0.15837800
H	-4.59554800	-1.80977400	0.52298400
H	-6.82972200	-1.35608500	-0.35108800
C	-2.74622800	-1.55011000	2.68584400
H	-2.30114500	-0.81956700	3.37640900
H	-3.82423200	-1.36783400	2.65751400
H	-2.55790100	-2.56170500	3.06552600

1c (B'-conformer)

E(RB97D) = -1246.273121 Hartree/Particle

XYZ coordinates

C	-0.24358800	-1.80062600	-0.08612000
C	-1.60856800	-1.50801800	-0.19146800
C	-0.43091800	-2.57543500	1.17103200
N	0.83087900	-1.47701300	-0.82129000
C	-1.94054600	-2.26357300	1.04399300
N	-2.35192000	-0.83679800	-1.09108300
O	0.31347500	-3.15393600	1.94005700
H	0.71613200	-0.78450900	-1.55258700
O	-2.96340900	-2.48482800	1.66677400
H	-1.84138200	-0.30862500	-1.79181300
C	-3.62351100	-0.21275300	-0.69708600
C	-3.39806900	1.26257800	-0.27814200
C	-4.63080400	-0.29897000	-1.85256500
H	-4.00213000	-0.78533500	0.15664600
C	-4.74854600	1.91848000	0.08766500
H	-3.01388600	1.77669000	-1.17628500
C	-5.96392000	0.37449200	-1.49580900
H	-4.19552000	0.19968600	-2.73435800
C	-5.74696000	1.83520200	-1.07516700
H	-4.57662700	2.96281200	0.37878800
H	-5.16787300	1.40161600	0.96186000
H	-6.65226600	0.31543100	-2.34890200
H	-6.43085000	-0.17429300	-0.66420600
H	-6.70132000	2.29785200	-0.79045300
H	-5.35482000	2.40450500	-1.93252400

H	-4.78009800	-1.35346000	-2.11431900
N	-2.34456200	1.38651400	0.73736000
C	-2.73473800	0.94556200	2.07699100
H	-1.83360200	0.86549900	2.69820100
H	-3.43120200	1.64944400	2.57378400
H	-3.20247300	-0.04149300	2.03572600
C	-1.75688000	2.71859700	0.77990200
H	-2.46219900	3.50051700	1.13111700
H	-0.90191300	2.71083400	1.46804400
H	-1.39693100	3.00040300	-0.21843300
C	2.21800300	-1.63700700	-0.32047800
H	2.11690400	-2.17468100	0.63044700
C	4.14470500	0.22619400	-0.20684200
C	4.47307600	1.59437200	0.14946800
C	2.79281000	-0.23204100	0.00671200
C	3.49538900	2.44139600	0.72601300
C	1.89093800	0.64845500	0.59975700
C	2.22695300	1.96796000	0.96206800
H	3.77349800	3.46170000	0.98441800
H	0.87490300	0.32223600	0.80024500
H	1.47216600	2.60215000	1.42104900
C	2.94885800	-2.57500700	-1.29639100
H	3.25411300	-2.06293900	-2.21680500
H	3.82615500	-3.03309000	-0.82924400
H	2.26161000	-3.38716800	-1.55625200
C	5.21676900	-0.55850700	-0.72826700
H	5.06222200	-1.59319200	-0.98499600
C	6.48476400	-0.04485300	-0.91188200
H	7.26581400	-0.69027900	-1.30854500
C	6.78102100	1.29768900	-0.58713700
H	7.78346000	1.69129900	-0.74026900
C	5.78785400	2.09268200	-0.06315700
H	5.99224700	3.12635600	0.21156000

1c (A”-conformer)

E(RB97D) = -1246.289893 Hartree/Particle

XYZ coordinates

C	-0.20282700	2.05716600	-0.09007800
C	1.16539800	1.76205400	-0.07474500
C	-0.18190000	2.57067700	1.30373900
N	-1.16312000	1.90098400	-1.01537800
C	1.32824700	2.24154000	1.32112600
N	2.02226100	1.26056600	-0.98592500
O	-1.02473200	3.00196800	2.07148000
H	-0.92388800	1.36912800	-1.84552500
O	2.25202800	2.28850400	2.11258200
H	1.59654400	0.91816800	-1.84275500

C	3.15092400	0.42567500	-0.54042600
C	2.71603300	-1.06256500	-0.48408400
C	4.35050600	0.60470600	-1.47913000
H	3.42002900	0.77146400	0.46385100
C	3.90874200	-1.94674400	-0.05791700
H	2.45674000	-1.33812500	-1.52114800
C	5.52796600	-0.29086200	-1.06519800
H	4.03667300	0.34334600	-2.50326400
C	5.10517400	-1.76619300	-1.00289900
H	3.58748700	-2.99620100	-0.03019500
H	4.20773500	-1.67057200	0.96268200
H	6.36282400	-0.15734200	-1.76544300
H	5.88448200	0.02363900	-0.07279500
H	5.94654700	-2.39163700	-0.67578000
H	4.82439900	-2.10464100	-2.01266100
H	4.64341200	1.66158900	-1.48672500
N	1.48893600	-1.23410300	0.29711200
C	1.66375800	-1.14148500	1.74468500
H	0.67502800	-1.04646200	2.20853600
H	2.16208100	-2.03357600	2.17440700
H	2.24813500	-0.25443100	2.00505300
C	0.72991000	-2.42333700	-0.06527600
H	1.24479100	-3.37036500	0.20338500
H	-0.23524900	-2.40594600	0.45374500
H	0.54280600	-2.42917300	-1.14747500
C	-2.61197700	1.87724100	-0.68140900
H	-2.68389900	2.18544300	0.36422300
C	-2.87396400	-0.52874100	0.19740400
C	-3.23149800	-1.90459200	-0.04672800
C	-3.09706700	0.43906600	-0.84227400
C	-3.79751000	-2.27321700	-1.29615500
C	-3.66178400	0.02482500	-2.03749100
C	-4.01530500	-1.32562800	-2.26994300
H	-4.06143100	-3.31619400	-1.46336700
H	-3.84600100	0.74953000	-2.82599200
H	-4.45901300	-1.60623500	-3.22285900
C	-3.01528300	-2.87417800	0.96875600
H	-3.29056500	-3.90772400	0.76463400
C	-2.47246100	-2.51948500	2.18558600
H	-2.31112300	-3.27154800	2.95492200
C	-2.12859200	-1.17052100	2.43334200
C	-2.32169400	-0.20276800	1.46717300
H	-2.05549900	0.82002400	1.70538000
H	-1.70982700	-0.88597400	3.39598800
C	-3.35380100	2.92146200	-1.52212300
H	-3.18845300	2.76959000	-2.59597200
H	-4.43141700	2.87540900	-1.32468800
H	-2.98420600	3.91832200	-1.25892900

1c (B”-conformer)

E(RB97D) = -1246.282470 Hartree/Particle

XYZ coordinates

C	0.24917500	-1.83250000	-0.04697400
C	-1.10239400	-1.49753600	-0.20996500
C	-0.04992700	-2.84713900	0.99876100
N	1.38498700	-1.38893300	-0.59894200
C	-1.54265500	-2.49753300	0.79961000
N	-1.75222900	-0.63853600	-1.01003000
O	0.62227200	-3.58779300	1.69184500
H	1.34939700	-0.62812600	-1.26375600
O	-2.61949500	-2.84550200	1.25075200
H	-1.19683800	0.05802900	-1.49428900
C	-3.15123400	-0.25798700	-0.78095100
C	-3.24822600	1.14913000	-0.14197300
C	-3.92967000	-0.30349900	-2.10596000
H	-3.57024100	-1.00241100	-0.09595500
C	-4.73468300	1.52701400	0.05480600
H	-2.82272000	1.85198900	-0.87939100
C	-5.39912800	0.09877000	-1.91620000
H	-3.45019900	0.38815500	-2.81790100
C	-5.50784400	1.48721200	-1.27053100
H	-4.79820200	2.52379300	0.50939500
H	-5.18887100	0.81768000	0.76041400
H	-5.92020900	0.07831200	-2.88224800
H	-5.89130300	-0.64043800	-1.26654500
H	-6.56062500	1.75182500	-1.10438400
H	-5.08986300	2.23978500	-1.95747700
H	-3.85012100	-1.31322100	-2.52679900
N	-2.40690200	1.26912300	1.05630700
C	-2.88846800	0.51769900	2.21637500
H	-2.10158100	0.51115100	2.98127900
H	-3.79820400	0.96092700	2.66774000
H	-3.10273500	-0.51917800	1.94418200
C	-2.14174300	2.65612300	1.41338500
H	-3.04448600	3.20588800	1.75199000
H	-1.41476900	2.68185500	2.23582900
H	-1.71590900	3.18809100	0.55230000
C	2.72079400	-1.76247300	-0.08489200
H	2.57018700	-1.97655900	0.98355600
C	4.95540100	-0.77377500	-0.71243000
C	5.83955200	0.29681700	-0.98158100
C	3.68149800	-0.57449800	-0.20368800
C	5.43017600	1.59513200	-0.78844000
C	3.25568600	0.77627200	0.06940800
C	4.14168300	1.86704300	-0.25904000

H	6.08651400	2.43099500	-1.02448300
H	6.83184200	0.08247500	-1.37236400
H	5.29266700	-1.77994600	-0.93921400
C	3.18518500	-3.07159400	-0.73275600
H	3.36974900	-2.93867500	-1.80612700
H	4.10014200	-3.43972800	-0.25413200
H	2.40292500	-3.82219700	-0.58480500
C	2.03176300	1.10639600	0.72529900
H	1.37572700	0.31900900	1.07597300
C	1.66701900	2.41783000	0.95592300
H	0.72668300	2.62712800	1.45886700
C	2.50953700	3.48294500	0.56110500
H	2.20713800	4.51243300	0.74121700
C	3.72739100	3.20588200	-0.02109800
H	4.40735100	4.01135000	-0.29413900

1d (A'-conformer)

E(RB97D) = -1207.213669 Hartree/Particle

XYZ coordinates

C	0.09262300	-2.27552400	-0.21233300
C	-1.21460800	-1.79952600	-0.07334300
C	0.14402000	-2.76925300	1.18867000
N	0.98486500	-2.26175500	-1.22454200
C	-1.29978500	-2.23588800	1.34623300
N	-2.08335000	-1.19007500	-0.90243200
O	0.98590200	-3.30952000	1.88250900
H	0.75400800	-1.65001000	-2.00331100
O	-2.13584200	-2.14117900	2.22523600
H	-1.70704300	-0.91265900	-1.80447500
C	-3.05100500	-0.22102100	-0.36114200
C	-2.45782400	1.21148200	-0.41486400
C	-4.37185500	-0.28554800	-1.13855600
H	-3.23272300	-0.50746900	0.68049100
C	-3.48406600	2.22331400	0.14144500
H	-2.31885900	1.43929600	-1.48621800
C	-5.38658600	0.73684000	-0.60439900
H	-4.16586000	-0.07576000	-2.20105500
C	-4.80762100	2.15934300	-0.63428000
H	-3.05592300	3.23332000	0.09860200
H	-3.67069200	1.99298700	1.19950100
H	-6.31348600	0.68488700	-1.19032100
H	-5.64420400	0.47488500	0.43280500
H	-5.52885500	2.87444300	-0.21650500
H	-4.62868400	2.45468900	-1.68012000
H	-4.77185100	-1.30486900	-1.07749200
N	-1.12088500	1.26893800	0.18256900
C	-1.09484700	1.19132800	1.64213300

H	-0.06241600	1.00804000	1.96402100
H	-1.44617400	2.12399400	2.12693900
H	-1.71383000	0.36166900	1.99454300
C	-0.32575500	2.39282300	-0.29270500
H	-0.71105000	3.37781400	0.04683900
H	0.70078100	2.28424100	0.07626000
H	-0.30187900	2.39264500	-1.39088800
C	2.44390500	-2.26628700	-0.91124500
H	2.55724900	-2.95631400	-0.06877700
C	3.20785100	0.13233700	-1.35907800
C	3.47137500	1.43835800	-0.93168300
C	2.86136900	-0.87635300	-0.45575700
C	3.38449400	1.75015900	0.43313000
C	2.79027300	-0.54908300	0.90908700
C	3.04889300	0.74272800	1.35279700
H	2.52059400	-1.32232400	1.62518600
H	2.99300600	0.99429000	2.40913700
H	3.73917700	2.19565500	-1.66152900
H	3.28079800	-0.08893600	-2.42218300
C	3.20653300	-2.80377600	-2.12170300
H	3.01802300	-2.19160100	-3.01412400
H	4.28430100	-2.79214300	-1.92412500
H	2.88973300	-3.82999300	-2.33826300
O	3.59778900	2.99359800	0.96093900
C	3.92170100	4.05087600	0.05817400
H	3.11474900	4.20571400	-0.67469500
H	4.03938900	4.94595200	0.67524500
H	4.85999000	3.84062700	-0.47761800

1d (B'-conformer)

E(RB97D) = -1207.210370 Hartree/Particle

XYZ coordinates

C	0.12409100	2.07751500	-0.11686500
C	1.43718000	1.59434100	-0.08721900
C	0.23306800	2.67229000	1.24384900
N	-0.86738300	2.01193600	-1.02220200
C	1.68652900	2.14329700	1.27070500
N	2.20486500	0.92189000	-0.96526800
O	-0.52411900	3.27442700	1.98083900
H	-0.73905700	1.38171000	-1.80736100
O	2.62723500	2.12797200	2.04405400
H	1.73404500	0.56042200	-1.78894800
C	3.30498000	0.06715200	-0.49541100
C	2.82158600	-1.39531900	-0.32187300
C	4.48115800	0.13336300	-1.47988800
H	3.62198500	0.46861900	0.47326300
C	3.99860900	-2.28677800	0.13419200

H	2.52052100	-1.73579400	-1.32783700
C	5.64109200	-0.77146400	-1.03933800
H	4.12540800	-0.18762500	-2.47289400
C	5.16935700	-2.22128200	-0.85646300
H	3.64606100	-3.31963000	0.25178500
H	4.33985800	-1.94463600	1.12096700
H	6.45555100	-0.71917500	-1.77356100
H	6.04162600	-0.39981000	-0.08423800
H	5.99760500	-2.85281700	-0.50839700
H	4.84441400	-2.62165900	-1.82964600
H	4.80835900	1.17611600	-1.57133800
N	1.61260900	-1.47713900	0.50765800
C	1.83817300	-1.25886200	1.93671700
H	0.86775600	-1.11825800	2.42969300
H	2.34851400	-2.11234300	2.42514100
H	2.43172000	-0.35541400	2.09926600
C	0.85731200	-2.70256900	0.28269600
H	1.38753600	-3.61532800	0.62592700
H	-0.09256700	-2.64434100	0.82834500
H	0.63478800	-2.81297900	-0.78674700
C	-2.28053400	2.23774400	-0.64434600
H	-2.23813900	2.79131000	0.30227600
C	-4.30603000	0.66655600	-0.78243800
C	-4.94548500	-0.55249400	-0.52462600
C	-2.98229300	0.90128600	-0.39748800
C	-4.25128000	-1.57500800	0.13456600
C	-2.30099100	-0.14216200	0.26033400
C	-2.91892300	-1.35742300	0.52434300
H	-1.26805200	-0.00635200	0.57119300
H	-2.38655100	-2.15522600	1.03592000
H	-5.97433600	-0.68920900	-0.84187200
H	-4.87087800	1.43977100	-1.29546900
O	-4.77026100	-2.80220900	0.43746800
C	-6.12741500	-3.05572400	0.07257100
H	-6.26356700	-2.98586000	-1.01760900
H	-6.34271400	-4.07372000	0.40898000
H	-6.80839000	-2.34654900	0.56738000
C	-2.94712400	3.12839700	-1.69752400
H	-3.01288800	2.61219800	-2.66506900
H	-3.96028400	3.40663500	-1.38696200
H	-2.36016900	4.04448500	-1.82135800

1d (A”-conformer)

E(RB97D) = -1207.214358 Hartree/Particle

XYZ coordinates

C	0.21237100	-2.26753300	-0.02139700
C	-1.10427600	-1.82139000	0.12969500

C	0.36076400	-2.56138200	1.42812600
N	1.04818200	-2.36289900	-1.07669800
C	-1.09160900	-2.05760400	1.59863900
N	-2.04138400	-1.36095500	-0.72011000
O	1.25952500	-2.97444500	2.13792500
H	0.74844300	-1.87489000	-1.91699000
O	-1.87899500	-1.86567500	2.50651000
H	-1.72620100	-1.19309400	-1.67122000
C	-3.02460700	-0.36801600	-0.25530600
C	-2.51731300	1.06700900	-0.55439300
C	-4.38833300	-0.60325600	-0.91726700
H	-3.12381300	-0.50741100	0.82664900
C	-3.55677400	2.09864800	-0.06273700
H	-2.46973000	1.14694900	-1.65446600
C	-5.42040700	0.43589600	-0.45284400
H	-4.26631300	-0.53567300	-2.01071700
C	-4.92577300	1.86579600	-0.71839700
H	-3.19066100	3.11131700	-0.27628800
H	-3.65512700	2.01010900	1.02819700
H	-6.38044600	0.26017500	-0.95540300
H	-5.59213900	0.30909400	0.62661900
H	-5.65544600	2.59769200	-0.34694500
H	-4.83685000	2.02142900	-1.80503300
H	-4.72533400	-1.62119700	-0.68713200
N	-1.14527200	1.27047800	-0.08118200
C	-1.00403700	1.38627100	1.36851000
H	0.05877900	1.29140000	1.62410500
H	-1.36839000	2.35819800	1.75848500
H	-1.54801100	0.58413400	1.87490400
C	-0.45883900	2.36183700	-0.75933900
H	-0.87157100	3.36204500	-0.50887200
H	0.60014000	2.35007300	-0.47688900
H	-0.52659500	2.22501900	-1.84682900
C	2.51967600	-2.25889600	-0.84646800
H	2.71178600	-2.83333500	0.06550500
C	3.09446800	0.10952600	-1.63109800
C	3.29823400	1.46114300	-1.37534000
C	2.88242400	-0.80510600	-0.58635700
C	3.28956900	1.93585100	-0.05276000
C	2.88991900	-0.32187200	0.72557400
C	3.09234400	1.03390700	1.00277200
H	2.72239000	-1.01577500	1.54642500
H	3.08966300	1.37171500	2.03412000
H	3.46132500	2.16875800	-2.18463000
H	3.10294800	-0.23450600	-2.66361600
C	3.25014000	-2.90306600	-2.02413600
H	2.98671200	-2.41300500	-2.97126300
H	4.33395100	-2.81590700	-1.88815800

H	2.97928800	-3.96203000	-2.09991700
O	3.47011400	3.28288100	0.09742900
C	3.43732700	3.81065800	1.42492100
H	4.23965400	3.37891700	2.04199800
H	3.58737300	4.88886600	1.32150200
H	2.46673800	3.61196900	1.90447800

1d (B”-conformer)

E(RB97D) = -1207.210394 Hartree/Particle

XYZ coordinates

C	-0.00320200	-2.12466300	-0.02712300
C	-1.32429100	-1.66468800	0.01732400
C	-0.04547200	-2.60630600	1.38174400
N	0.95130300	-2.11003800	-0.97308300
C	-1.50561900	-2.09720500	1.42672200
N	-2.14064400	-1.07996300	-0.87989000
O	0.75252900	-3.13192600	2.13363900
H	0.78097500	-1.53814700	-1.79431100
O	-2.41039600	-2.02149100	2.23876500
H	-1.71135500	-0.78512600	-1.75136900
C	-3.23014500	-0.19915600	-0.43414100
C	-2.76657200	1.27985500	-0.42938400
C	-4.45855500	-0.37405000	-1.33813400
H	-3.48716000	-0.50923700	0.58455800
C	-3.93126600	2.19209100	0.01655500
H	-2.53641200	1.52830200	-1.48003300
C	-5.60915500	0.55009800	-0.91290700
H	-4.16724100	-0.14134100	-2.37563600
C	-5.15793600	2.01777100	-0.88999600
H	-3.59398200	3.23671700	0.01693200
H	-4.20464600	1.93735400	1.04985800
H	-6.46369300	0.41886900	-1.58937800
H	-5.94576600	0.26105700	0.09400400
H	-5.97706800	2.66523000	-0.54980600
H	-4.90019800	2.33321700	-1.91322400
H	-4.76934000	-1.42546300	-1.31370100
N	-1.50891900	1.45818600	0.30784600
C	-1.63455000	1.35929100	1.76185000
H	-0.63051400	1.28198200	2.19872400
H	-2.13457000	2.24061400	2.21003200
H	-2.19214200	0.46118900	2.04026900
C	-0.80133900	2.67356800	-0.07091900
H	-1.32428000	3.60242000	0.23923600
H	0.18934700	2.67380400	0.40078500
H	-0.66385600	2.70144300	-1.15986900
C	2.38255800	-2.27808800	-0.63461200
H	2.38819900	-2.79482700	0.33349300

C	4.36456300	-0.65960300	-0.90128500
C	4.96953500	0.57943800	-0.70930100
C	3.05365500	-0.91352300	-0.46290700
C	4.27306600	1.61299200	-0.06532900
C	2.37054400	0.13237700	0.17337900
C	2.96204000	1.38119300	0.37693100
H	1.35172700	-0.01497600	0.52219400
H	2.39725000	2.15898700	0.88026300
H	5.98414200	0.76452000	-1.05341400
H	4.93314700	-1.43765600	-1.40258900
O	4.94566600	2.79375600	0.07872300
C	4.27234600	3.86216100	0.74546500
H	4.00512400	3.57969000	1.77509900
H	4.97802200	4.69738600	0.76069300
H	3.35982600	4.15446000	0.20310100
C	3.03919300	-3.18881000	-1.67667100
H	3.05777000	-2.70760800	-2.66417300
H	4.06993800	-3.42614000	-1.39156900
H	2.47579500	-4.12518000	-1.74686000

1e (A-conformer)

E(RB97D) = -1297.195499 Hartree/Particle

XYZ coordinates

C	-0.11421700	-2.36260300	-0.08323700
C	-1.38051300	-1.78399300	0.04489800
C	-0.04548900	-2.73279800	1.35143000
N	0.74543900	-2.51299100	-1.11732100
C	-1.45060100	-2.10218200	1.50117800
N	-2.23195800	-1.19191700	-0.80759200
O	0.78851600	-3.25930700	2.06604700
H	0.52954300	-1.98036700	-1.95577600
O	-2.25831300	-1.89905200	2.38532200
H	-1.87549300	-1.00790400	-1.74082700
C	-3.16769500	-0.16054900	-0.32890700
C	-2.52492300	1.24478100	-0.46457600
C	-4.48411800	-0.23288100	-1.11334800
H	-3.36127500	-0.37831300	0.72701300
C	-3.52464900	2.32580900	0.00272100
H	-2.35759700	1.39624900	-1.54512900
C	-5.46792800	0.85805800	-0.66470900
H	-4.26110300	-0.10376300	-2.18531900
C	-4.83842900	2.25350200	-0.78797100
H	-3.06050900	3.31491900	-0.10158100
H	-3.73536700	2.17586100	1.07055800
H	-6.38950400	0.79549700	-1.25766900
H	-5.74559300	0.67936600	0.38489800
H	-5.53830000	3.02147700	-0.43301300

H	-4.63579600	2.46678500	-1.84921400
H	-4.91985700	-1.23147700	-0.98766700
N	-1.19825500	1.29731500	0.15869400
C	-1.21020800	1.33860600	1.62086000
H	-0.19351400	1.14631800	1.98575600
H	-1.53621100	2.31900200	2.01971400
H	-1.86647300	0.56147700	2.02179100
C	-0.35602300	2.35684600	-0.38296700
H	-0.71976300	3.37599900	-0.13844400
H	0.65451200	2.25417200	0.02948100
H	-0.29675400	2.26427400	-1.47557600
C	2.20483500	-2.59622500	-0.84110500
H	2.30004100	-3.20668300	0.06262900
C	3.08338000	-0.30093600	-1.54711400
C	3.41882400	1.01866100	-1.25442500
C	2.71037600	-1.19325400	-0.52988800
C	3.37545800	1.44451800	0.07482700
C	2.69191300	-0.74154200	0.79898200
C	3.02230000	0.57598900	1.10922700
H	2.40585400	-1.43079800	1.58978900
H	3.00573800	0.93600900	2.13248000
H	3.70760700	1.71684800	-2.03278700
H	3.11576900	-0.63521300	-2.58127200
C	2.90212000	-3.28916600	-2.01000400
H	2.71674500	-2.76195500	-2.95543500
H	3.98476100	-3.31808200	-1.84275400
H	2.52601700	-4.31290300	-2.11029300
N	3.70031000	2.86188500	0.39199500
O	4.03415400	3.59300000	-0.53777100
O	3.60705700	3.22027400	1.56302400

1e (B-conformer)

E(RB97D) = -1297.192042 Hartree/Particle

XYZ coordinates

C	0.33827700	2.18589900	-0.05020900
C	1.62184100	1.63249000	-0.00220500
C	0.40259400	2.66244400	1.35617400
N	-0.61958400	2.24149100	-0.99653800
C	1.82641100	2.05788700	1.41104100
N	2.39922600	0.98956900	-0.88984800
O	-0.36798000	3.23788900	2.10100400
H	-0.49071200	1.67135600	-1.82592800
O	2.72084000	1.92826400	2.22429000
H	1.96377600	0.72981400	-1.76934600
C	3.42764200	0.03924500	-0.43862500
C	2.85841600	-1.40221000	-0.41626700
C	4.65822100	0.12163200	-1.35270500

H	3.70987600	0.34106000	0.57574700
C	3.96055800	-2.39324000	0.02050500
H	2.59631400	-1.64033100	-1.46169900
C	5.74270200	-0.88166800	-0.93387200
H	4.34189000	-0.09414600	-2.38658800
C	5.18552900	-2.31202200	-0.90103200
H	3.54919500	-3.41068100	0.03090800
H	4.26484800	-2.15414400	1.04880600
H	6.59753800	-0.81468200	-1.61912900
H	6.10938700	-0.61446400	0.06852000
H	5.95860700	-3.01669300	-0.56734000
H	4.89403700	-2.61095200	-1.92007400
H	5.04405700	1.14807500	-1.33620600
N	1.60136700	-1.48450600	0.34078800
C	1.76175100	-1.40106800	1.79351500
H	0.77478100	-1.25343000	2.25041100
H	2.20388100	-2.31803300	2.22921600
H	2.38874000	-0.54714700	2.06322400
C	0.80465400	-2.64989900	-0.02510800
H	1.27407100	-3.61166900	0.26590000
H	-0.16978900	-2.59305400	0.47525200
H	0.63675900	-2.66159500	-1.11004200
C	-2.02890100	2.51065800	-0.64571700
C	-2.63979500	3.45081500	-1.68930400
H	-1.99397100	3.03223900	0.31995200
H	-2.70674600	2.96207200	-2.67082600
H	-2.01243200	4.34327700	-1.77897700
C	-4.11657000	1.03190700	-0.86459500
C	-4.80129700	-0.16443200	-0.65083300
C	-2.79013000	1.19896000	-0.43541000
C	-4.14779200	-1.20851000	0.00117700
C	-2.16064100	0.12396100	0.22000500
C	-2.83021400	-1.07483200	0.44289800
H	-1.13306400	0.21654300	0.55899900
H	-2.34859700	-1.90170200	0.95294100
H	-5.82514900	-0.29493100	-0.98482800
H	-4.63164800	1.83877800	-1.37602800
H	-3.64591100	3.76531300	-1.39158200
N	-4.86517600	-2.49342200	0.22535000
O	-6.03276000	-2.56803000	-0.14812500
O	-4.24511400	-3.40448500	0.76831400

1f (A-conformer)

E(RB97D) = -1766.758578 Hartree/Particle

XYZ coordinates

C	-0.83820700	-2.07132200	-1.35305200
C	-2.05670600	-1.51466500	-0.95481000

C	-0.87157500	-3.11359600	-0.29928100
N	0.05848600	-1.76828600	-2.32186200
C	-2.22693000	-2.51080900	0.14434800
N	-2.81206400	-0.49797200	-1.39856700
O	-0.11964100	-4.00443600	0.05354400
H	-0.07394200	-0.87199300	-2.78297800
O	-3.06098100	-2.70204300	1.00569600
H	-2.39508100	0.09182800	-2.11284700
C	-3.68765500	0.24033400	-0.47323400
C	-2.92615400	1.45236300	0.12446000
C	-4.95746200	0.70018000	-1.20123800
H	-3.95849900	-0.45734700	0.32662800
C	-3.86161900	2.25321100	1.05717000
H	-2.67790500	2.10368000	-0.73142200
C	-5.87386000	1.51542700	-0.27698000
H	-4.66187100	1.32278000	-2.06179900
C	-5.12628200	2.71642200	0.32075100
H	-3.31285500	3.11056700	1.46765700
H	-4.14885400	1.61471200	1.90385200
H	-6.76096300	1.84837500	-0.83108900
H	-6.22641700	0.86761500	0.53958800
H	-5.78126700	3.27316400	1.00391400
H	-4.84314600	3.40646700	-0.48946400
H	-5.47954000	-0.17911600	-1.59764200
N	-1.64280300	1.04988400	0.71029800
C	-1.74803000	0.36397800	1.99865800
H	-0.78033600	-0.09201600	2.23698700
H	-2.01523100	1.04826900	2.82746900
H	-2.49391500	-0.43377800	1.94851700
C	-0.68266700	2.14474700	0.78111200
H	-0.98048900	2.94366800	1.49153100
H	0.28547700	1.74966100	1.10973000
H	-0.55430700	2.59506000	-0.21182000
C	1.49061700	-2.10133900	-2.10312500
H	1.49679700	-3.09284000	-1.63896900
C	2.54824600	0.14430600	-1.51638000
C	2.95781400	1.09299200	-0.57305300
C	2.07149800	-1.10275500	-1.10786600
C	2.89442600	0.80781800	0.78900200
C	2.01231100	-1.39221800	0.26330200
C	2.41705500	-0.44107800	1.19973100
H	3.20190700	1.54547200	1.52240800
H	1.63511500	-2.35785500	0.58838800
H	2.60608700	0.39170300	-2.57295000
C	2.37603500	-0.74538300	2.68336800
C	3.40850300	2.44904800	-1.06795000
F	1.59144400	-1.80479600	2.97812900
F	3.62196000	-1.01485100	3.16322800

F	1.90444800	0.31803400	3.39512200
F	3.96517000	3.21009500	-0.09754700
F	4.31908900	2.34101700	-2.07295400
F	2.35369100	3.15588100	-1.57552800
C	2.20938700	-2.15471100	-3.44965400
H	2.11291000	-1.20478700	-3.99255100
H	3.27645400	-2.35628800	-3.30315600
H	1.77484500	-2.94667400	-4.06871400

1f (B-conformer)

E(RB97D) = -1766.755019 Hartree/Particle

XYZ coordinates

C	0.86499500	2.09394400	0.36535200
C	2.19541000	1.66920800	0.26117400
C	0.94963300	2.26796200	1.83774700
N	-0.13012500	2.28217700	-0.52257000
C	2.42157000	1.80745600	1.72885300
N	2.99078100	1.33086300	-0.76336900
O	0.16652800	2.61072000	2.70434100
H	-0.01146500	1.92663200	-1.46440300
O	3.36397300	1.61482800	2.47231800
H	2.55268300	1.20461800	-1.66946600
C	4.21346500	0.53877200	-0.56875300
C	3.95004800	-0.95459500	-0.88332500
C	5.34073100	1.09046900	-1.45448200
H	4.49433100	0.65019000	0.48374400
C	5.25806000	-1.76096900	-0.71412100
H	3.67306500	-0.99705300	-1.95124900
C	6.63116800	0.27149500	-1.30557500
H	5.00809200	1.05799500	-2.50512900
C	6.37791000	-1.21209300	-1.60867300
H	5.06276500	-2.81692700	-0.93983300
H	5.57448400	-1.70561800	0.33654000
H	7.40784000	0.67578400	-1.96765200
H	7.00088900	0.37074000	-0.27400800
H	7.29791100	-1.79448600	-1.46649600
H	6.08626200	-1.32143000	-2.66502800
H	5.51118300	2.14306700	-1.19752300
N	2.79034300	-1.47140700	-0.14646500
C	3.02385300	-1.67381400	1.28503700
H	2.06269100	-1.87280500	1.77251100
H	3.69526800	-2.53026100	1.49206600
H	3.45441000	-0.77527500	1.73579500
C	2.23372500	-2.67533600	-0.75447700
H	2.91676500	-3.54831900	-0.70110500
H	1.30614400	-2.94426000	-0.23769400
H	2.00259500	-2.48457300	-1.81118300

C	-1.52182700	2.52130300	-0.10207800
H	-1.45321900	2.89224700	0.92889900
C	-3.64981700	1.14071300	-0.47319000
C	-4.35763400	-0.06683500	-0.40676600
C	-2.31674100	1.21252400	-0.06250900
C	-3.74665700	-1.22155200	0.07028700
C	-1.70248000	0.04245000	0.41480000
C	-2.41182300	-1.15426900	0.48590000
H	-4.29363800	-2.15636400	0.12590300
H	-0.66853000	0.06711900	0.74212400
H	-4.15929400	2.02129900	-0.85019000
C	-5.79215900	-0.07721400	-0.89030800
C	-1.73467800	-2.42338900	0.95754900
F	-6.53494200	0.87466900	-0.26198300
F	-6.40885900	-1.26567600	-0.69241600
F	-2.55976500	-3.18869100	1.71557800
F	-0.61994000	-2.18217300	1.68993500
F	-1.35183100	-3.19366700	-0.10527600
F	-5.86005800	0.19501400	-2.22520500
C	-2.13514400	3.61519700	-0.98148800
H	-2.23751000	3.27519600	-2.02122400
H	-3.12612900	3.90387500	-0.61489100
H	-1.48966600	4.49893600	-0.95836000

1g (A-conformer)

E(RB97D) = -1283.162109 Hartree/Particle

XYZ coordinates

C	0.05392900	-1.41254100	0.84260700
C	-1.32011300	-1.45573400	0.59221400
C	-0.13050500	-1.44594000	2.31596900
N	1.14089000	-1.33087000	0.04750500
C	-1.65510200	-1.48605800	2.04222300
N	-2.07071900	-1.47577400	-0.52547100
O	0.61721300	-1.40247800	3.27443500
H	0.97496100	-1.07056600	-0.92027000
O	-2.68802500	-1.47952500	2.68446100
H	-1.56630700	-1.34787500	-1.39791900
C	-3.39614600	-0.83462900	-0.52706000
C	-3.27008100	0.64729800	-0.96843500
C	-4.35706300	-1.59280400	-1.45160700
H	-3.77005100	-0.88423700	0.50152700
C	-4.66582900	1.30854400	-0.99544300
H	-2.89851800	0.62044500	-2.00739000
C	-5.73867600	-0.92297400	-1.49694600
H	-3.92684000	-1.61170500	-2.46645700
C	-5.62636700	0.54887500	-1.92161700
H	-4.56383300	2.35451500	-1.31291000

H	-5.07469100	1.31562200	0.02444100
H	-6.39811100	-1.47291400	-2.18084200
H	-6.19383400	-0.97536700	-0.49649900
H	-6.61589100	1.02501100	-1.91628600
H	-5.24916400	0.59942300	-2.95507100
H	-4.43481100	-2.63194600	-1.10977000
N	-2.24675500	1.35804000	-0.19515600
C	-2.63416500	1.69253200	1.17332300
H	-1.73841000	2.00115400	1.72709400
H	-3.36755700	2.52183900	1.22161200
H	-3.05914800	0.82034900	1.67764500
C	-1.70575500	2.52188000	-0.88444600
H	-2.43507200	3.35355500	-0.98077500
H	-0.83637200	2.89557400	-0.32854300
H	-1.37490200	2.23645100	-1.89183900
C	2.40219300	-0.78098400	0.59027100
H	2.53738500	-1.23375100	1.58106000
C	3.43702000	1.27292800	-0.11318000
C	3.61846400	2.65576200	-0.19939400
C	2.40184800	0.73951300	0.68058600
C	2.74972300	3.49155300	0.51224600
C	1.54538100	1.56721300	1.39638800
C	1.72409200	2.95518600	1.30265300
H	2.87573700	4.57087700	0.45701300
H	0.76314600	1.14907100	2.02398400
H	1.06747800	3.62206500	1.85737000
H	4.41847100	3.07810500	-0.80424400
C	3.56850900	-1.05203000	-0.34174500
C	4.04497000	-2.27145400	-0.80665900
C	4.16536200	0.16225000	-0.73963000
C	5.14522200	-2.27612100	-1.67685500
H	3.57323000	-3.20358700	-0.50161700
C	5.26442100	0.15599400	-1.60270600
C	5.74849700	-1.07277000	-2.06635600
H	5.53637200	-3.22029000	-2.04933700
H	5.73663400	1.08654800	-1.91103600
H	6.60371000	-1.09504100	-2.73865300

1g (B-conformer)

E(RB97D) = -1283.160335 Hartree/Particle

XYZ coordinates

C	0.07190800	-1.35744400	0.66370800
C	-1.30890500	-1.40791900	0.45314400
C	-0.06291700	-1.53852100	2.13290900
N	1.13509600	-1.19388400	-0.15207800
C	-1.59317700	-1.59556700	1.90259000
N	-2.09398200	-1.34516900	-0.63733200

O	0.71464100	-1.58416100	3.06650800
H	0.94073000	-0.89442200	-1.10272600
O	-2.60359300	-1.70330800	2.57141100
H	-1.63423300	-1.09707100	-1.50804700
C	-3.47123900	-0.83877800	-0.53682000
C	-3.50764000	0.68603300	-0.81521500
C	-4.38208500	-1.58909400	-1.51828000
H	-3.80384400	-1.03530000	0.48823500
C	-4.96370700	1.19847400	-0.74859900
H	-3.16145100	0.81092100	-1.85573200
C	-5.82396000	-1.06314000	-1.46811600
H	-3.98185400	-1.45863100	-2.53728000
C	-5.86874400	0.44832800	-1.73588600
H	-4.97673900	2.27730100	-0.95105600
H	-5.34371700	1.05399100	0.27217100
H	-6.44393000	-1.60337600	-2.19528200
H	-6.24393000	-1.26501500	-0.47130000
H	-6.89960800	0.81972600	-1.66367300
H	-5.52591000	0.64434600	-2.76394600
H	-4.34584100	-2.66067400	-1.28774700
N	-2.54437600	1.41597800	0.01873000
C	-2.93660300	1.55823400	1.42060400
H	-2.06971100	1.90620100	1.99706600
H	-3.75635500	2.28944400	1.56417600
H	-3.24907200	0.59503000	1.83248800
C	-2.16644200	2.70401500	-0.54823900
H	-2.99521300	3.44238500	-0.55173000
H	-1.34211900	3.12798800	0.03875100
H	-1.81927600	2.56926300	-1.58102300
C	2.39189300	-0.66491900	0.39367200
H	2.46495000	-1.07747600	1.41205400
C	3.68443200	1.30633600	-0.04238400
C	3.96328000	2.67482300	-0.09463800
C	2.45204100	0.85265700	0.47211000
C	2.97662700	3.57666800	0.32095900
C	1.44994800	1.74710000	0.82678200
C	1.72613500	3.12059200	0.75987700
H	3.17382300	4.64594200	0.28175500
H	0.47673300	1.39046700	1.15695400
H	0.96269200	3.83978400	1.04867800
H	4.91533200	3.03719600	-0.47736900
C	3.65052500	-1.01168100	-0.37321400
C	4.09156000	-2.25097000	-0.81947600
C	4.43325900	0.14946200	-0.54996700
C	5.33822400	-2.32969300	-1.45740000
H	3.48026400	-3.14026700	-0.67850400
C	5.68265000	0.06512300	-1.17052800
C	6.12631100	-1.18269400	-1.62323400

H	5.69964900	-3.28879700	-1.82172500
H	6.29843100	0.95181800	-1.30681300
H	7.09440200	-1.26405000	-2.11313700

1h (A-conformer)

E(RB97D) = -1361.753045 Hartree/Particle

XYZ coordinates

C	-0.09867600	-0.94234200	1.00440500
C	-1.48870700	-1.07203800	0.97307300
C	-0.08589000	-0.51959000	2.42998800
N	0.86683500	-1.10514000	0.07592200
C	-1.63233200	-0.62539000	2.38637600
N	-2.36976600	-1.46676800	0.03688100
O	0.77761200	-0.21834200	3.23046300
H	0.55636500	-1.12988400	-0.88896600
O	-2.57510100	-0.39349900	3.11907700
H	-1.99604100	-1.62227600	-0.89376300
C	-3.74797800	-0.95454700	0.04335200
C	-3.90072900	0.19418000	-0.98416900
C	-4.75343100	-2.07493900	-0.25653100
H	-3.93689600	-0.57458100	1.05296400
C	-5.34641200	0.73695100	-0.93135600
H	-3.75657600	-0.26313300	-1.97876800
C	-6.19520400	-1.54404600	-0.24140600
H	-4.52628500	-2.49939800	-1.24784700
C	-6.36581900	-0.37458800	-1.22262000
H	-5.45550800	1.55798300	-1.65138400
H	-5.53335100	1.15185300	0.06883500
H	-6.89549400	-2.35442100	-0.48188300
H	-6.43585300	-1.19921400	0.77535300
H	-7.38767200	0.02375500	-1.16860400
H	-6.21571900	-0.74003600	-2.25059300
H	-4.62285600	-2.87520400	0.48174300
N	-2.83502900	1.19723400	-0.85338600
C	-2.91113800	2.01259100	0.35977300
H	-1.97497900	2.57433100	0.46596500
H	-3.74786600	2.73793500	0.33636500
H	-3.02819000	1.37882600	1.24321500
C	-2.71420700	2.03844200	-2.03777800
H	-3.57890900	2.71746700	-2.18545800
H	-1.81472600	2.65943200	-1.94812000
H	-2.61416900	1.40919100	-2.93215400
C	2.17640600	-0.48505000	0.29613400
H	2.35216500	-0.59464700	1.37108100
C	4.67046900	1.35201200	0.81909200
H	4.85880600	1.94603800	1.72512200
H	5.45392400	1.63790800	0.10160400

C	3.33888100	1.81836100	0.23324700
C	3.28461300	3.18784100	-0.07608100
C	2.19364600	1.02828400	-0.01463500
C	2.14647800	3.78873300	-0.60639400
C	1.04629500	1.64444800	-0.54283600
C	1.01584200	3.00684000	-0.83901400
H	2.14191800	4.85373000	-0.82828800
H	0.14050400	1.06774900	-0.70887700
H	0.10903000	3.45322100	-1.23997500
H	4.16917000	3.79497500	0.11502900
C	3.28148900	-1.21499500	-0.45516500
C	4.60430000	-1.03853900	-0.00412900
C	3.04069300	-2.02239200	-1.57166900
C	5.64964000	-1.67496000	-0.68261000
C	4.09298000	-2.64875700	-2.24582400
H	2.02677500	-2.19149100	-1.92601900
C	5.40387000	-2.47634300	-1.80002200
H	6.66856000	-1.54026200	-0.32227300
H	3.88397500	-3.27392600	-3.11121600
H	6.22845300	-2.96569700	-2.31390100
C	4.87921000	-0.13343400	1.16850200
H	4.25116000	-0.40498300	2.02764000
H	5.92019000	-0.25820000	1.49071800

1h (B-conformer)

E(RB97D) = -1361.745884 Hartree/Particle

XYZ coordinates

C	-0.05452700	-0.99950400	0.61145800
C	-1.42332100	-1.24377400	0.45634400
C	-0.10136100	-1.23446400	2.07988500
N	0.92245000	-0.64253500	-0.23405400
C	-1.61109500	-1.52395600	1.90380300
N	-2.25467400	-1.26025000	-0.60302200
O	0.71126600	-1.17153000	2.98291800
H	0.67321600	-0.37877500	-1.17945200
O	-2.56284300	-1.81260600	2.60596400
H	-1.87506200	-0.90902200	-1.47669100
C	-3.68730000	-0.97559100	-0.43227200
C	-3.96799500	0.53577100	-0.63331600
C	-4.51031900	-1.81426500	-1.42006200
H	-3.94437900	-1.26623400	0.59222800
C	-5.48209800	0.81306400	-0.49862600
H	-3.68271600	0.75973500	-1.67587000
C	-6.01275900	-1.52009000	-1.30105700
H	-4.17356500	-1.57980800	-2.44345900
C	-6.29755100	-0.02357800	-1.49419000
H	-5.66820800	1.88471500	-0.64666500

H	-5.79725200	0.56616900	0.52454400
H	-6.56951300	-2.11785100	-2.03438700
H	-6.35952500	-1.82688400	-0.30286400
H	-7.36971400	0.18108900	-1.37388500
H	-6.02623000	0.26715700	-2.52122000
H	-4.30189100	-2.87631600	-1.24294000
N	-3.09984100	1.36838400	0.20887000
C	-3.45751500	1.38188700	1.62763600
H	-2.63266100	1.83146600	2.19492300
H	-4.37414300	1.96935000	1.83254200
H	-3.60291700	0.36355700	1.99714000
C	-2.95022700	2.72435500	-0.30173200
H	-3.88883500	3.31573700	-0.26247600
H	-2.20004900	3.25259700	0.30034800
H	-2.60209500	2.69562700	-1.34263500
C	2.23641600	-0.16315000	0.22768200
H	2.23255200	-0.29316700	1.31929300
C	3.46052400	2.11366800	-0.38548900
C	3.32764300	3.49890000	-0.60020500
C	2.30825700	1.36574100	-0.05064600
C	2.12256100	4.17224000	-0.43423300
C	1.11297700	2.07836700	0.19191500
C	1.00785000	3.45232800	-0.00333900
H	2.06437000	5.24518000	-0.60440500
H	0.22760400	1.54631000	0.52645300
H	0.06146500	3.95241100	0.18867700
H	4.21974200	4.06032500	-0.87492900
C	3.33104700	-1.10179700	-0.31851300
C	2.98340000	-2.27790000	-1.00061400
C	4.69153600	-0.87490600	-0.03483600
C	3.94799100	-3.20543600	-1.40240500
H	1.93950500	-2.49253400	-1.20471300
C	5.65001800	-1.81566900	-0.43044900
C	5.29176000	-2.98095100	-1.10927700
H	3.64016000	-4.10599200	-1.92938700
H	6.69646300	-1.61955200	-0.20117300
H	6.05253200	-3.70080800	-1.40359900
C	5.14025800	0.42580500	0.56805500
C	4.87549000	1.56871500	-0.43372500
H	4.61406900	0.63911300	1.50973700
H	6.21164400	0.37570400	0.79483800
H	5.12683000	1.21674900	-1.44548000
H	5.55571300	2.40297300	-0.21885100

1i (A-conformer)

E(RB97D) = -1053.410882 Hartree/Particle

XYZ coordinates

C	-0.89002500	1.82080100	-0.67497400
C	0.48091400	1.67025500	-0.45084100
C	-1.09648000	2.56398800	0.59548100
N	-1.71871200	1.40419900	-1.65682100
C	0.41982000	2.38531100	0.85247000
N	1.49023200	1.10358700	-1.14117900
O	-2.05889000	3.03957900	1.16932100
H	-1.33923400	0.68749200	-2.26864400
O	1.22056500	2.63472900	1.73326300
H	1.21491800	0.60096600	-1.98038700
C	2.57420000	0.42929100	-0.40527100
C	2.21379300	-1.06412400	-0.18626300
C	3.90311200	0.55724600	-1.15940900
H	2.65896200	0.93606800	0.56239400
C	3.35599800	-1.77355000	0.57354400
H	2.16292900	-1.51065700	-1.19457200
C	5.03733700	-0.16773100	-0.41856800
H	3.78238500	0.11792100	-2.16327300
C	4.68863800	-1.64454800	-0.17856600
H	3.09180600	-2.82903600	0.72042300
H	3.45475600	-1.32011700	1.56960900
H	5.97173000	-0.07972500	-0.98795500
H	5.20179900	0.32543200	0.55124300
H	5.49194400	-2.14034600	0.38255400
H	4.60754600	-2.15899600	-1.14896200
H	4.13723400	1.62028200	-1.29287600
N	0.87453700	-1.21844300	0.38755600
C	0.76835800	-0.87993300	1.80487800
H	-0.29362800	-0.79004400	2.06488500
H	1.22076600	-1.64763700	2.46387200
H	1.25008100	0.08050900	2.00827000
C	0.26911900	-2.51430700	0.11221700
H	0.76699900	-3.35275500	0.64387300
H	-0.78264500	-2.49167800	0.42248900
H	0.30799000	-2.72085800	-0.96576900
C	-3.15706300	1.21370000	-1.35169900
H	-3.46701500	2.06240700	-0.73501600
C	-3.65456400	-1.26836900	-1.35142900
C	-3.78733200	-2.49470400	-0.69415700
C	-3.39330600	-0.09598000	-0.62945600
C	-3.66030500	-2.55680200	0.69693600
C	-3.27212400	-0.16431900	0.76614500
C	-3.40565000	-1.38921500	1.42446000
H	-3.76477600	-3.50948200	1.21196000
H	-3.07919900	0.74675800	1.32810100
H	-3.31484400	-1.43196100	2.50796500
H	-3.99594900	-3.39770100	-1.26437900
H	-3.70409100	1.23918700	-2.30130400

H	-3.76290600	-1.21796300	-2.43504700

1i (B-conformer)

E(RB97D) = -1053.409056 Hartree/Particle

XYZ coordinates

C	-0.83431100	1.78275400	-0.48088300
C	0.54171200	1.57133600	-0.34962400
C	-0.92184000	2.52872700	0.80408600
N	-1.74647700	1.42512800	-1.40696700
C	0.60116300	2.29240100	0.94986800
N	1.47578700	0.97305600	-1.11237500
O	-1.82115300	3.04794100	1.43613600
H	-1.45613700	0.72828300	-2.08485500
O	1.47749700	2.52778300	1.76101100
H	1.13421000	0.45580600	-1.91649800
C	2.66761500	0.37302100	-0.49357100
C	2.42751500	-1.13060200	-0.20283900
C	3.88920000	0.55715100	-1.40443600
H	2.83620800	0.90904500	0.44672400
C	3.69673100	-1.75240900	0.42138800
H	2.27590900	-1.60821700	-1.18636900
C	5.14680200	-0.08247100	-0.79779100
H	3.67469100	0.08828600	-2.37891600
C	4.91674800	-1.56986200	-0.49256600
H	3.51768300	-2.81655000	0.62259700
H	3.89119200	-1.26612000	1.38733000
H	5.99718900	0.04501500	-1.48015200
H	5.39942600	0.44201300	0.13593200
H	5.80948400	-2.00768600	-0.02653600
H	4.74671000	-2.11097300	-1.43658500
H	4.04003800	1.62859600	-1.58307400
N	1.18306400	-1.35202800	0.54497200
C	1.24130500	-0.96333600	1.95409400
H	0.22171100	-0.95253400	2.36046300
H	1.84487400	-1.66171800	2.56664500
H	1.65604100	0.04262000	2.05951600
C	0.67269500	-2.70926700	0.40170100
H	1.31258700	-3.47316900	0.89039600
H	-0.32474500	-2.76833900	0.85473500
H	0.58304500	-2.96347100	-0.66263700
C	-3.17650600	1.38800600	-1.06764700
H	-3.33625100	2.14716300	-0.29215300
C	-4.90196300	-0.45392100	-0.94934300
C	-5.36456900	-1.68597500	-0.47873600
C	-3.63955100	0.02671300	-0.57780800
C	-4.56207700	-2.45650300	0.36707500
C	-2.83649000	-0.75531000	0.26603100

C	-3.29682100	-1.98760700	0.73500300
H	-4.91807100	-3.41656900	0.73449900
H	-1.84814000	-0.40468500	0.55378800
H	-2.66764800	-2.58169700	1.39467600
H	-6.34757700	-2.04514600	-0.77645700
H	-5.52688500	0.14424300	-1.61164400
H	-3.75706100	1.67984200	-1.95201500

1j (A-conformer)

E(RB97D) = -1284.363629 Hartree/Particle

XYZ coordinates

C	0.21640000	-0.85460600	1.18526400
C	-1.16414200	-1.03479300	1.08514300
C	0.13048000	-0.31622800	2.56964300
N	1.24518200	-1.05325500	0.33862200
C	-1.40725100	-0.48190000	2.44555500
N	-1.97611400	-1.53083700	0.13186400
O	0.93573500	0.07773500	3.38885900
H	1.02635700	-1.24909300	-0.63228100
O	-2.39982900	-0.22957900	3.10223500
H	-1.53603500	-1.74495300	-0.75768300
C	-3.35032700	-1.02432500	-0.00328300
C	-3.41459200	0.07517700	-1.09332200
C	-4.32248600	-2.16388100	-0.33742300
H	-3.62539800	-0.59900700	0.96785600
C	-4.86134400	0.60590700	-1.20384800
H	-3.17375600	-0.42697500	-2.04658200
C	-5.76109400	-1.64414100	-0.48108300
H	-4.00467900	-2.63479400	-1.28185000
C	-5.84423200	-0.52754400	-1.53259600
H	-4.90537600	1.38973700	-1.97090500
H	-5.14351500	1.06811600	-0.24771900
H	-6.43388600	-2.47110500	-0.74271800
H	-6.09529600	-1.24971400	0.49020500
H	-6.86827200	-0.13599200	-1.59458500
H	-5.59703300	-0.94332400	-2.52195900
H	-4.25746000	-2.92648100	0.44788000
N	-2.37371300	1.09655900	-0.91050500
C	-2.58531900	1.98247500	0.23542000
H	-1.66554300	2.55191100	0.41628200
H	-3.41069300	2.70261500	0.07174700
H	-2.80536800	1.40185400	1.13536400
C	-2.12922200	1.86710800	-2.12354500
H	-2.97555900	2.52778700	-2.40263600
H	-1.24574200	2.50011300	-1.97666400
H	-1.93236000	1.18683900	-2.96278600
C	2.51798700	-0.33764400	0.55070300

H	2.74531400	-0.44745900	1.61794100
C	3.53882000	1.95645800	0.57862700
C	3.52580800	3.32959600	0.33945600
C	2.42920500	1.16082600	0.25845800
C	2.39536200	3.93048100	-0.22633300
C	1.29965400	1.76550800	-0.30344800
C	1.28657000	3.14515600	-0.54337500
H	2.37858500	5.00253200	-0.41023400
H	0.41444800	1.17819000	-0.53832600
H	0.40015500	3.60772900	-0.97217300
H	4.39351600	3.93270200	0.59854000
H	4.41859900	1.48968300	1.01845200
C	3.59581500	-1.04207600	-0.25977300
C	4.34990100	-2.06623900	0.32605700
C	3.80612000	-0.72335400	-1.60775900
C	5.30308800	-2.76169000	-0.42164700
H	4.18506100	-2.31516800	1.37305900
C	4.75244800	-1.42375800	-2.36088900
H	3.24226500	0.09121200	-2.05837500
C	5.50384300	-2.44340100	-1.76879600
H	5.88980600	-3.54937600	0.04641100
H	4.91076500	-1.16621200	-3.40617200
H	6.24741700	-2.98256800	-2.35194000

1j (B-conformer)

E(RB97D) = -1284.361962 Hartree/Particle

XYZ coordinates

C	0.23732100	-1.02202600	0.72917800
C	-1.12861900	-1.27265800	0.55750100
C	0.14850500	-1.13632000	2.21055900
N	1.24674400	-0.74922000	-0.11187000
C	-1.36057900	-1.41298000	2.01876500
N	-1.93256700	-1.38215600	-0.51721100
O	0.94086800	-1.02415300	3.12720100
H	1.03044500	-0.57676300	-1.08668200
O	-2.33708100	-1.61546300	2.71745200
H	-1.52279400	-1.12625200	-1.41019000
C	-3.36083900	-1.04783400	-0.41199300
C	-3.59920300	0.43645100	-0.79071100
C	-4.19016400	-1.97316300	-1.31304700
H	-3.64529600	-1.21284700	0.63296200
C	-5.10678000	0.76369500	-0.70431400
H	-3.30151500	0.52970200	-1.84955800
C	-5.68641900	-1.63285400	-1.24817200
H	-3.83532100	-1.86271700	-2.35103800
C	-5.93339100	-0.16078200	-1.60922800
H	-5.26534500	1.81572800	-0.97467400

H	-5.43645500	0.64137500	0.33666500
H	-6.24966300	-2.29508400	-1.91844800
H	-6.05125000	-1.81940300	-0.22698000
H	-7.00138000	0.08038700	-1.52482400
H	-5.64597400	0.00748000	-2.65898100
H	-4.01004100	-3.01303500	-1.01489900
N	-2.71438700	1.34067800	-0.04498600
C	-3.07229300	1.52061700	1.36204400
H	-2.24162800	2.02027900	1.87684300
H	-3.98006500	2.14106900	1.49725800
H	-3.23371700	0.55318700	1.84485100
C	-2.53619700	2.62730300	-0.70470500
H	-3.45818000	3.24514100	-0.72039600
H	-1.76114700	3.19753500	-0.17737900
H	-2.20606900	2.47273200	-1.74038600
C	2.51670900	-0.15685400	0.36545900
H	2.54157700	-0.35550400	1.44355500
C	3.68903900	2.06101100	-0.16102700
C	3.68485600	3.45532600	-0.26523800
C	2.51761500	1.36363700	0.16599200
C	2.51028900	4.17511100	-0.03587800
C	1.34371600	2.09705900	0.40642100
C	1.33995500	3.48911900	0.30289100
H	2.50654300	5.26003400	-0.11656100
H	0.42400400	1.58043200	0.66914300
H	0.42109900	4.03959600	0.49424700
H	4.60378700	3.97718100	-0.52456100
H	4.61041600	1.51231900	-0.33545300
C	3.67569500	-0.89128100	-0.28483200
C	4.49862700	-1.72052800	0.48386900
C	3.91255000	-0.78339400	-1.66274200
C	5.54374900	-2.43354200	-0.11208200
H	4.31207400	-1.80999200	1.55267100
C	4.95033500	-1.49819600	-2.26269900
H	3.29358800	-0.11965000	-2.26481100
C	5.77019600	-2.32543200	-1.48658800
H	6.17821800	-3.07372800	0.49719000
H	5.12506900	-1.40627400	-3.33276700
H	6.58215500	-2.88001800	-1.95209600

1k (A'-conformer)

E(RB97D) = -1167.911183 Hartree/Particle

XYZ coordinates

C	0.09533100	2.34813800	-0.56757900
C	1.34376300	1.76767500	-0.32713700
C	0.05794800	3.00699100	0.76412300
N	-0.76961700	2.28906300	-1.60331600

C	1.43812800	2.35948500	1.03432600
N	2.16401100	0.97661200	-1.04588700
O	-0.74683400	3.69705900	1.36223900
H	-0.58493000	1.54913600	-2.27480000
O	2.23532600	2.28395100	1.95019400
H	1.78563000	0.64136200	-1.92733800
C	2.98662500	-0.03228700	-0.35683500
C	2.21646400	-1.37658800	-0.26967200
C	4.32425700	-0.22471400	-1.08227600
H	3.17568700	0.35216900	0.65149300
C	3.09002700	-2.43604900	0.43774200
H	2.07547800	-1.70976400	-1.31277000
C	5.18544000	-1.29542500	-0.39506800
H	4.12016900	-0.53112300	-2.12143700
C	4.43001500	-2.62861900	-0.28682900
H	2.53680000	-3.38278200	0.49227500
H	3.27808500	-2.10848700	1.46959700
H	6.12602800	-1.42832800	-0.94530900
H	5.44806500	-0.94741600	0.61525300
H	5.04293700	-3.37378400	0.23768800
H	4.24126200	-3.02012800	-1.29881300
H	4.85005600	0.73690000	-1.12171100
N	0.86920300	-1.19562500	0.27786600
C	0.81814500	-0.94884600	1.71753000
H	-0.18886800	-0.59987700	1.97677900
H	1.03229800	-1.85679100	2.31586100
H	1.53135800	-0.16941600	1.99973400
C	-0.05654500	-2.25376800	-0.10288800
H	0.18502600	-3.23509000	0.35796000
H	-1.06883600	-1.97190500	0.21042800
H	-0.05165300	-2.37602800	-1.19447200
C	-2.21903400	2.48075600	-1.33704000
H	-2.30443000	3.32401800	-0.64529800
C	-3.37912900	0.24440900	-1.57814300
C	-3.84747900	-0.96810800	-1.05936200
C	-2.83395200	1.23041900	-0.75212600
C	-3.76783100	-1.20149000	0.32167900
C	-2.77409600	0.98744100	0.63113400
C	-3.23475300	-0.21034300	1.16444900
H	-2.36251600	1.75044000	1.28799000
H	-3.19208100	-0.40121900	2.23402800
H	-4.26890500	-1.71126600	-1.72860400
H	-2.69628900	2.74549400	-2.28770500
H	-3.44638500	0.41977000	-2.65205000
O	-4.17468000	-2.35096700	0.93924400
C	-4.71561700	-3.38889500	0.12165900
H	-3.97768700	-3.73343600	-0.61922300
H	-4.96696500	-4.20630300	0.80311700

H	-5.62127100	-3.04793500	-0.40283200

1k (B'-conformer)

E(RB97D) = -1167.908969 Hartree/Particle

XYZ coordinates

C	0.14023500	2.17806200	-0.42171700
C	1.42789200	1.64941400	-0.28514600
C	0.20065500	2.86896300	0.89576000
N	-0.80735600	2.08021200	-1.37482100
C	1.62590600	2.28340200	1.04472100
N	2.21308800	0.88359500	-1.06634400
O	-0.56732200	3.55368600	1.54320800
H	-0.66669200	1.36610300	-2.08199200
O	2.51796000	2.27940100	1.87320600
H	1.77325700	0.48880700	-1.89197200
C	3.22555500	0.00203700	-0.46566400
C	2.64297500	-1.41633400	-0.23872300
C	4.47020500	-0.06487600	-1.36151400
H	3.49867600	0.44815500	0.49678300
C	3.72658600	-2.33726400	0.36567000
H	2.40007100	-1.80726600	-1.24209900
C	5.53869800	-0.99961800	-0.77536800
H	4.16782700	-0.43392000	-2.35543400
C	4.96920300	-2.40506900	-0.53326000
H	3.30496100	-3.33861200	0.52208700
H	4.01334100	-1.94663100	1.35183800
H	6.40563400	-1.04410000	-1.44734400
H	5.89104500	-0.58422800	0.18069600
H	5.73067900	-3.05421200	-0.08081800
H	4.69352300	-2.85537200	-1.49977100
H	4.86559800	0.94922900	-1.49550700
N	1.37060700	-1.37559900	0.49326500
C	1.49673200	-1.06746500	1.91780200
H	0.50081500	-0.84148300	2.32003100
H	1.91746700	-1.90904900	2.50264200
H	2.12766800	-0.18722900	2.06693100
C	0.56476900	-2.57255900	0.29022000
H	1.00837500	-3.48309000	0.74400500
H	-0.42374200	-2.42173200	0.74099200
H	0.42908000	-2.75273100	-0.78429300
C	-2.21829300	2.35056600	-1.05537700
H	-2.21755100	3.08204000	-0.23794000
C	-4.30738400	0.92703900	-1.07589500
C	-5.05287500	-0.19598800	-0.69948900
C	-2.98494800	1.10163500	-0.66180700
C	-4.45988200	-1.17879700	0.10610400
C	-2.40209500	0.10362900	0.13896400

C	-3.12563500	-1.02034800	0.51919500
H	-1.36950500	0.20294900	0.46577500
H	-2.67779600	-1.79032000	1.14245500
H	-6.07817800	-0.29612500	-1.04079200
H	-4.77462600	1.68327500	-1.70584000
H	-2.69465700	2.81821900	-1.92662000
O	-5.08435100	-2.31734900	0.53215700
C	-6.44658800	-2.50943000	0.14924600
H	-6.54569000	-2.56466400	-0.94577600
H	-6.75246600	-3.45867100	0.59781200
H	-7.08205600	-1.69470800	0.52856000

1k (A”-conformer)

E(RB97D) = -1167.911767 Hartree/Particle

XYZ coordinates

C	-0.03196800	2.38251900	-0.41114200
C	1.22684500	1.83172200	-0.15369300
C	-0.18460200	2.88109400	0.98080700
N	-0.82856200	2.40776900	-1.50182100
C	1.20415100	2.26272600	1.27000700
N	2.12992500	1.16522300	-0.89819300
O	-1.05639200	3.46554100	1.59745200
H	-0.56398100	1.76235500	-2.24064600
O	1.94310800	2.11218900	2.22489300
H	1.82648700	0.91643100	-1.83541900
C	2.96343000	0.12551000	-0.27063200
C	2.27185900	-1.25785300	-0.39512300
C	4.35687400	0.08906200	-0.91061500
H	3.06085400	0.39710500	0.78617900
C	3.15555300	-2.34474300	0.25574300
H	2.22666300	-1.47510700	-1.47649700
C	5.23139400	-1.00703300	-0.28269300
H	4.24420000	-0.10576900	-1.98976500
C	4.55273200	-2.38165100	-0.38043100
H	2.65869500	-3.31916400	0.16109200
H	3.24972900	-2.12908300	1.32914900
H	6.21436900	-1.02656000	-0.77101400
H	5.40125700	-0.76387300	0.77694500
H	5.17159100	-3.14870900	0.10399300
H	4.45968900	-2.66406800	-1.44084100
H	4.82477100	1.07501000	-0.80262900
N	0.88007600	-1.21271800	0.06116300
C	0.70777900	-1.12949200	1.50932600
H	-0.33322600	-0.85561400	1.72124900
H	0.92478600	-2.08788600	2.02293800
H	1.35480500	-0.35547100	1.93123800
C	0.05095900	-2.26907200	-0.50286400

H	0.31169600	-3.28043600	-0.12477200
H	-0.99824700	-2.07191600	-0.25327800
H	0.14951100	-2.27576900	-1.59648800
C	-2.30018100	2.49111000	-1.30511600
H	-2.47401000	3.25153600	-0.53819400
C	-3.27434300	0.21310900	-1.84527300
C	-3.68081600	-1.06431600	-1.47416200
C	-2.86721800	1.15441000	-0.88641100
C	-3.68497100	-1.43040000	-0.11730800
C	-2.89230900	0.78472900	0.46214000
C	-3.29733300	-0.49465400	0.85420200
H	-2.58775200	1.50561700	1.21749600
H	-3.30564300	-0.74969200	1.90901200
H	-3.99753700	-1.79421500	-2.21512300
H	-2.73922300	2.82718700	-2.25157200
H	-3.27496600	0.48666300	-2.90057000
O	-4.07356400	-2.71291800	0.15151800
C	-4.06844200	-3.13475000	1.51693200
H	-4.76295900	-2.53083900	2.12004700
H	-4.39477100	-4.17835300	1.50808500
H	-3.05842700	-3.06194500	1.94826900

1k (B”-conformer)

E(RB97D) = -1167.909064 Hartree/Particle

XYZ coordinates

C	0.05342300	2.24742000	-0.32815900
C	1.33986100	1.72026900	-0.17543200
C	0.04388600	2.82485400	1.04449700
N	-0.85009300	2.21580600	-1.32738200
C	1.46533800	2.23478100	1.21318700
N	2.16997300	1.02858800	-0.97932100
O	-0.76124800	3.44638000	1.70985400
H	-0.67141800	1.55455300	-2.07632300
O	2.31217800	2.15545700	2.08447400
H	1.77684200	0.70878600	-1.85911800
C	3.15471900	0.09870600	-0.40612800
C	2.57393900	-1.33720900	-0.34908200
C	4.45119600	0.12204200	-1.22760800
H	3.36660700	0.45248500	0.60869200
C	3.62791200	-2.30601300	0.23203100
H	2.39644900	-1.63314400	-1.39760400
C	5.49185800	-0.85881800	-0.66729000
H	4.21293400	-0.15272300	-2.26833500
C	4.92313500	-2.28331600	-0.59201500
H	3.20810100	-3.31969000	0.26795300
H	3.85069400	-2.00846300	1.26605400
H	6.39793500	-0.83670100	-1.28661100

H	5.78204400	-0.53301300	0.34284900
H	5.66258900	-2.96848100	-0.15654200
H	4.71054100	-2.64251900	-1.61116200
H	4.84345700	1.14602500	-1.24130900
N	1.25855400	-1.37113700	0.30350500
C	1.29271500	-1.19146700	1.75457900
H	0.27119000	-1.00868000	2.11255700
H	1.68658600	-2.07931100	2.28763700
H	1.90246000	-0.32416100	2.02148800
C	0.47981500	-2.54830400	-0.05652200
H	0.89895100	-3.49346800	0.34745200
H	-0.53945500	-2.43822300	0.33427000
H	0.42070100	-2.63602200	-1.14933600
C	-2.27708900	2.44382300	-1.04740300
H	-2.32107400	3.13764200	-0.19893900
C	-4.34577100	0.99070200	-1.20498800
C	-5.07602500	-0.15389500	-0.90168000
C	-3.03405700	1.16541700	-0.73702800
C	-4.49914300	-1.16619500	-0.11724500
C	-2.46704800	0.14643600	0.03570600
C	-3.18452400	-1.01171500	0.34887100
H	-1.44783400	0.24387600	0.40178900
H	-2.71575500	-1.77875600	0.95659900
H	-6.09175600	-0.28650700	-1.26596100
H	-4.80311600	1.76778300	-1.81642500
H	-2.72967900	2.94108500	-1.91472300
O	-5.28778700	-2.25491200	0.12892200
C	-4.74232000	-3.30017800	0.93460500
H	-4.47854500	-2.93005600	1.93700000
H	-5.52687100	-4.05789500	1.01298300
H	-3.84768300	-3.73667200	0.46407300

1l (A'-conformer)

E(RB97D) = -1152.642620 Hartree/Particle

XYZ coordinates

C	-0.65660600	1.79176600	-0.58146000
C	0.71771600	1.55176800	-0.51174500
C	-0.63461800	2.72256200	0.57890900
N	-1.63727400	1.33896300	-1.38635700
C	0.88674900	2.44597700	0.66403200
N	1.58349700	0.82134300	-1.24400500
O	-1.47131700	3.37386000	1.17290000
H	-1.41052400	0.56758900	-2.00415400
O	1.82266900	2.75763600	1.37689600
H	1.16571100	0.20973400	-1.93891900
C	2.77140100	0.23459500	-0.60262700
C	2.46169100	-1.20268300	-0.10969400

C	3.95818500	0.22503300	-1.57502900
H	3.01415700	0.87463500	0.25261600
C	3.71941700	-1.81375800	0.54711300
H	2.24461800	-1.79271800	-1.01735500
C	5.20419700	-0.40458200	-0.93373600
H	3.67564100	-0.35308300	-2.47024100
C	4.90807600	-1.82319900	-0.42477600
H	3.49058500	-2.83075500	0.89161900
H	3.97950900	-1.21976000	1.43421100
H	6.03035100	-0.41837300	-1.65654900
H	5.52480800	0.22174500	-0.08772600
H	5.79560700	-2.24748800	0.06340300
H	4.66959600	-2.47233000	-1.28198000
H	4.16021400	1.25294700	-1.89950500
N	1.23938600	-1.24712500	0.69855000
C	1.36771500	-0.67857400	2.03950300
H	0.36406700	-0.53740200	2.45858400
H	1.94205500	-1.33066800	2.72733500
H	1.85603000	0.29864900	1.99767600
C	0.63118800	-2.56837400	0.74805700
H	1.23073000	-3.30912800	1.31828100
H	-0.35198400	-2.49163200	1.22994700
H	0.48966700	-2.95253900	-0.27115100
C	-3.05565100	1.41799900	-0.98990000
H	-3.11718600	2.13470300	-0.16448500
C	-4.51917800	-0.61886800	-1.39624700
C	-4.99417800	-1.88750600	-1.05147700
C	-3.59553700	0.06237500	-0.59153500
C	-4.54394000	-2.50105000	0.12018600
C	-3.16870200	-0.58670500	0.57437500
C	-3.62271400	-1.84745700	0.94485100
H	-4.90814200	-3.48711500	0.39895700
H	-3.26073900	-2.29423500	1.86690200
H	-5.71346800	-2.39155400	-1.69217400
H	-3.64494900	1.80382500	-1.83157100
H	-4.87051700	-0.13298300	-2.30551800
F	-2.27524200	0.03753200	1.37925600

1l (B'-conformer)

E(RB97D) = -1152.640432 Hartree/Particle

XYZ coordinates

C	-0.67982700	1.69314700	-0.42035000
C	0.70096200	1.48292000	-0.35178200
C	-0.69536400	2.52231200	0.81260600
N	-1.64054900	1.28766900	-1.27028500
C	0.83135500	2.28990100	0.89109100
N	1.59407200	0.84608100	-1.13192700

O	-1.55879900	3.09620600	1.44959900
H	-1.40738000	0.55673700	-1.93178600
O	1.75199700	2.58089400	1.63249000
H	1.21236000	0.26456000	-1.87096900
C	2.85162100	0.33138700	-0.56937400
C	2.70304000	-1.16360600	-0.18829400
C	4.00142300	0.52021300	-1.56875200
H	3.05792700	0.92261300	0.32920400
C	4.03741100	-1.69289400	0.38354000
H	2.51495300	-1.70015300	-1.13487400
C	5.32465800	-0.02752900	-1.01307600
H	3.74834800	-0.01104800	-2.50106600
C	5.18811300	-1.50473400	-0.61532900
H	3.92224000	-2.75180100	0.64934400
H	4.26654500	-1.14738700	1.30951200
H	6.12346300	0.10060100	-1.75519000
H	5.60906800	0.55911300	-0.12665600
H	6.12925100	-1.87391700	-0.18628800
H	4.98686500	-2.10472600	-1.51676700
H	4.08916000	1.58589300	-1.81265700
N	1.52061700	-1.39426800	0.64485700
C	1.63262900	-0.91542000	2.02119900
H	0.63450400	-0.92027200	2.47654300
H	2.29772500	-1.54798900	2.64267400
H	2.00800300	0.11126500	2.04301600
C	1.04964700	-2.77036600	0.60698700
H	1.73644000	-3.48631800	1.10631100
H	0.07764800	-2.82831100	1.11350500
H	0.91877900	-3.09084500	-0.43549500
C	-3.06470300	1.43618800	-0.95828500
H	-3.13039000	2.17169100	-0.14644200
C	-5.06805400	-0.09420700	-1.04589900
C	-5.77060400	-1.25693200	-0.72673700
C	-3.77314200	0.15162200	-0.56101500
C	-5.17235600	-2.22734100	0.08166400
C	-3.21050500	-0.84560400	0.24695700
C	-3.88127500	-2.02186400	0.57136800
H	-5.70474200	-3.14168500	0.33273700
H	-3.38779700	-2.74999600	1.20964700
H	-6.77456900	-1.40845800	-1.11536400
H	-5.52601100	0.65483200	-1.69050000
H	-3.58274100	1.85677100	-1.83016500
F	-1.96826300	-0.67305600	0.76748700

1l (A”-conformer)

E(RB97D) = -1152.643901 Hartree/Particle

XYZ coordinates

C	0.64679600	-1.72975800	-0.42829000
C	-0.73075400	-1.58386500	-0.25282600
C	0.83489300	-2.35903500	0.90743700
N	1.49904300	-1.39212900	-1.41987700
C	-0.69152900	-2.17702000	1.11200300
N	-1.72904100	-1.10638400	-1.01954300
O	1.78596600	-2.78569400	1.53034600
H	1.14365500	-0.75499200	-2.12459400
O	-1.51290200	-2.35886800	1.99050800
H	-1.45235100	-0.66254800	-1.88962100
C	-2.91036600	-0.48993100	-0.39702300
C	-2.74300900	1.04895100	-0.32748100
C	-4.18317300	-0.85531000	-1.17306700
H	-2.98168400	-0.90058500	0.61588800
C	-3.99189600	1.67530600	0.33205200
H	-2.71199300	1.39877400	-1.37407500
C	-5.42728300	-0.21215200	-0.54209200
H	-4.07563000	-0.50486600	-2.21258300
C	-5.26948000	1.31201300	-0.43869700
H	-3.86878700	2.76462900	0.38489300
H	-4.07148400	1.30514500	1.36355700
H	-6.31927100	-0.46911500	-1.12793600
H	-5.57099700	-0.62861500	0.46614600
H	-6.14681400	1.75532000	0.05065400
H	-5.21420500	1.73985400	-1.45195100
H	-4.27815200	-1.94735400	-1.20324300
N	-1.45259900	1.43935900	0.25925300
C	-1.34557900	1.20745300	1.70058700
H	-0.29634600	1.32254100	2.00042900
H	-1.95152300	1.91919200	2.29447800
H	-1.65885600	0.19050700	1.95137300
C	-1.08148900	2.80942700	-0.07375200
H	-1.73523500	3.56949400	0.40107900
H	-0.05423100	2.99614100	0.26172700
H	-1.12113700	2.95183600	-1.16175600
C	2.92741800	-1.25927000	-1.13231700
H	3.19928800	-2.06747800	-0.44306500
C	4.66575900	0.42137600	-0.41821900
C	5.11254500	1.60793300	0.14987500
C	3.31323700	0.07853200	-0.51843500
C	4.16556300	2.50482400	0.65239300
C	2.38507800	0.99824300	-0.01137100
C	2.80561600	2.19866300	0.57000900
H	4.49423200	3.43661800	1.10649200
H	2.06820500	2.89175800	0.96688500
H	6.17920900	1.81007800	0.19595400
H	3.48774400	-1.41724000	-2.06110300
H	1.32146400	0.77536000	-0.06452000

F	5.59049800	-0.45357300	-0.90172000

1l (B”-conformer)

E(RB97D) = -1152.643482 Hartree/Particle

XYZ coordinates

C	-0.62094200	1.76351400	-0.36135600
C	0.76142800	1.56918300	-0.28118900
C	-0.67784600	2.46946700	0.94727700
N	-1.55967900	1.41755800	-1.26501000
C	0.85238200	2.25185000	1.03773800
N	1.67895500	1.00728200	-1.08964800
O	-1.56500400	2.95305000	1.62319300
H	-1.28763600	0.74474800	-1.97350600
O	1.75036100	2.47366800	1.82835800
H	1.32044600	0.51177300	-1.90000400
C	2.89692500	0.40474900	-0.52633000
C	2.68361400	-1.10996000	-0.27527800
C	4.08725500	0.63253000	-1.46809200
H	3.08785200	0.91406600	0.42447700
C	3.97877700	-1.73505900	0.28935300
H	2.50664500	-1.55867100	-1.26813000
C	5.37042800	-0.00979400	-0.92069300
H	3.84807800	0.19135900	-2.44971300
C	5.16722400	-1.50878100	-0.65587300
H	3.81827800	-2.80712200	0.46224400
H	4.19806600	-1.27683900	1.26365800
H	6.19764700	0.14973000	-1.62439600
H	5.64571900	0.48837600	0.02097500
H	6.07907900	-1.94986500	-0.23191500
H	4.97372600	-2.02207600	-1.61083000
H	4.21998700	1.71079500	-1.61757500
N	1.46566700	-1.36956800	0.50347000
C	1.56460000	-1.02538200	1.92182600
H	0.55860600	-1.04059900	2.36077700
H	2.19526300	-1.73534600	2.49224300
H	1.97080200	-0.01815200	2.04668100
C	0.96523300	-2.72751400	0.33293500
H	1.62610800	-3.49867800	0.78046200
H	-0.01899500	-2.81133700	0.81063200
H	0.84944400	-2.95059800	-0.73585600
C	-2.97926500	1.37480100	-0.88799200
H	-3.12991600	2.14251800	-0.11967400
C	-4.65961200	-0.52290700	-0.66524000
C	-5.09668900	-1.75439900	-0.18578100
C	-3.40580900	0.01545200	-0.35842000
C	-4.24981700	-2.48871100	0.64673800
C	-2.57620700	-0.74744000	0.47868900

C	-2.98861300	-1.98362400	0.97796500
H	-4.57726400	-3.45078400	1.03379300
H	-1.59081900	-0.36655900	0.73402600
H	-2.32827500	-2.54926000	1.63069500
H	-6.08288800	-2.11485700	-0.46551900
H	-3.58198100	1.64524200	-1.76026800
F	-5.50153700	0.18262600	-1.47055900

1m (A'-conformer)

E(RB97D) = -1152.646097 Hartree/Particle

XYZ coordinates

C	-0.68413900	1.99095900	-0.60316500
C	0.66605700	1.73538000	-0.34820200
C	-0.90560100	2.59563700	0.73468600
N	-1.49540400	1.74679100	-1.65697400
C	0.58954900	2.31671700	1.02122900
N	1.66927500	1.18840000	-1.05826500
O	-1.86995900	3.04563300	1.32631700
H	-1.13067000	1.09408300	-2.34456000
O	1.37004800	2.44258300	1.94455800
H	1.40604700	0.77590300	-1.94862300
C	2.72804400	0.43399000	-0.36594400
C	2.34216100	-1.06628200	-0.28327000
C	4.06992600	0.60777500	-1.08845600
H	2.80353200	0.85300200	0.64337900
C	3.46675100	-1.85923400	0.41870000
H	2.29260000	-1.42085000	-1.32758300
C	5.18398500	-0.19970500	-0.40534600
H	3.95563400	0.26371700	-2.12961400
C	4.80890300	-1.68590700	-0.30652300
H	3.18460700	-2.91896000	0.46864700
H	3.56316200	-1.49860300	1.45204700
H	6.12614900	-0.07475000	-0.95463200
H	5.34445700	0.19933400	0.60745300
H	5.59749400	-2.24539800	0.21403500
H	4.72987800	-2.10717300	-1.32102800
H	4.32143800	1.67471200	-1.12195900
N	0.99570800	-1.25067400	0.26738800
C	0.88973600	-1.04380900	1.71148200
H	-0.17116600	-0.98534100	1.98303100
H	1.34658400	-1.86656200	2.29612700
H	1.36745300	-0.10366400	2.00079900
C	0.38466700	-2.51430900	-0.12337600
H	0.87945400	-3.39950100	0.32875000
H	-0.66592900	-2.51737400	0.19164400
H	0.41889400	-2.62177900	-1.21584900
C	-2.94987300	1.59232700	-1.41741600

H	-3.23983100	2.36615600	-0.70051600
C	-3.61649400	-0.82723700	-1.75775000
C	-3.79998300	-2.12728800	-1.27789800
C	-3.26104200	0.20953500	-0.88430900
C	-3.62569800	-2.41010600	0.07933000
C	-3.09550300	-0.05980600	0.48187800
C	-3.27646000	-1.36304100	0.92978700
H	-3.75907600	-3.41092700	0.48038300
H	-4.08281700	-2.92596900	-1.95999200
H	-3.46723800	1.76683300	-2.36747300
H	-3.75594900	-0.61272300	-2.81626700
H	-2.83453700	0.73004300	1.18114600
F	-3.10087300	-1.62946000	2.24844300

1m (B'-conformer)

E(RB97D) = -1152.645149 Hartree/Particle

XYZ coordinates

C	-0.64569200	1.94794300	-0.39556900
C	0.71473200	1.66524300	-0.23892800
C	-0.75690300	2.56292200	0.95392400
N	-1.53640700	1.72621600	-1.38542400
C	0.74787500	2.24479500	1.13271100
N	1.65398100	1.11172300	-1.02501600
O	-1.66114500	3.05590500	1.60026200
H	-1.25311000	1.08213600	-2.11622900
O	1.59719500	2.35458100	1.99638400
H	1.32845400	0.69177400	-1.88991900
C	2.81469100	0.42493900	-0.43768400
C	2.55217400	-1.09981300	-0.35144100
C	4.07669700	0.70944900	-1.26402600
H	2.94564100	0.83499500	0.56941000
C	3.78861200	-1.80633400	0.24884400
H	2.44730900	-1.44883300	-1.39360400
C	5.30227300	-0.01364600	-0.68623800
H	3.90433900	0.36820100	-2.29801300
C	5.05077000	-1.52478200	-0.57869400
H	3.59615900	-2.88516600	0.30830800
H	3.93960900	-1.44494900	1.27540200
H	6.18351500	0.18854900	-1.30880900
H	5.51442800	0.38851100	0.31575300
H	5.91875000	-2.02635100	-0.13044200
H	4.92221400	-1.94306700	-1.58935000
H	4.24049500	1.79327100	-1.29979500
N	1.27124400	-1.40094200	0.30088400
C	1.26019300	-1.18088100	1.74795100
H	0.22510800	-1.24496200	2.10551800
H	1.85653600	-1.93324200	2.30051500

H	1.64484900	-0.18591900	1.98916300
C	0.77758500	-2.73515000	-0.02372100
H	1.40999400	-3.54776600	0.38995400
H	-0.23187900	-2.85513200	0.38560200
H	0.73184400	-2.85767000	-1.11428300
C	-2.97701600	1.73355000	-1.09875000
H	-3.13370300	2.44787800	-0.28110600
C	-4.79372400	-0.02548800	-1.14709200
C	-5.32764900	-1.25807700	-0.76071000
C	-3.52292400	0.37020700	-0.70953700
C	-4.59847400	-2.11971000	0.06255300
C	-2.78039200	-0.48904400	0.11334400
C	-3.33519000	-1.70917000	0.47961700
H	-4.98691200	-3.08437400	0.37641300
H	-1.78802800	-0.22469100	0.46674300
H	-6.31535000	-1.55488400	-1.10616600
H	-5.36754800	0.63757600	-1.79187000
H	-3.51122200	2.10484100	-1.98203100
F	-2.61304800	-2.53614600	1.28146900

1m (A”-conformer)

E(RB97D) = -1152.643959 Hartree/Particle

XYZ coordinates

C	-0.42860700	1.88887700	-0.48300900
C	0.93140100	1.59472800	-0.35217300
C	-0.47330000	2.63854500	0.80134400
N	-1.36230300	1.58564900	-1.40896600
C	1.03287900	2.30931000	0.94962200
N	1.82799800	0.94170900	-1.11416000
O	-1.34000100	3.21313900	1.43050900
H	-1.11498300	0.87325500	-2.08757800
O	1.92027600	2.48818400	1.76233100
H	1.45885100	0.44990200	-1.92196900
C	2.98180100	0.27129900	-0.49569600
C	2.65566800	-1.21737100	-0.21349300
C	4.21483600	0.38924100	-1.40227200
H	3.17820700	0.79195400	0.44780300
C	3.88541300	-1.91115100	0.41395700
H	2.48224300	-1.68169300	-1.19978100
C	5.43239100	-0.32288100	-0.79443400
H	3.97719300	-0.06301000	-2.37918400
C	5.11724000	-1.79566000	-0.49505200
H	3.64654000	-2.96400200	0.61193400
H	4.10338200	-1.43861800	1.38165600
H	6.29045300	-0.24152000	-1.47416200
H	5.71176100	0.18337400	0.14170200
H	5.98171600	-2.28487900	-0.02701400

H	4.92027300	-2.32349500	-1.44132000
H	4.42668400	1.45109300	-1.57605400
N	1.39660000	-1.37346500	0.52807000
C	1.47013000	-0.99114200	1.93890200
H	0.45121900	-0.93123300	2.34250500
H	2.03727200	-1.71961400	2.55079900
H	1.93389600	-0.00723100	2.04761500
C	0.82196300	-2.70481800	0.38199300
H	1.42565500	-3.49972000	0.86666000
H	-0.17514300	-2.71807600	0.83916800
H	0.71707200	-2.95113500	-0.68279600
C	-2.78638700	1.63303600	-1.06203200
H	-2.90374500	2.41820600	-0.30479400
C	-4.68051600	0.01098200	-0.73438800
C	-5.19796000	-1.16823600	-0.20915000
C	-3.32850800	0.31600400	-0.52837000
C	-4.41960000	-2.06751600	0.51396900
C	-2.52359400	-0.57871000	0.19166500
C	-3.07097500	-1.75713100	0.70656900
H	-4.86419300	-2.97818800	0.90508900
H	-2.44200500	-2.44218500	1.27043000
H	-3.35689800	1.93372900	-1.94994000
H	-1.47074800	-0.36153800	0.35164400
H	-5.33023600	0.67943300	-1.29488800
F	-6.50759600	-1.45412000	-0.41806100

1m (B”-conformer)

E(RB97D) = -1152.643941 Hartree/Particle

XYZ coordinates

C	-0.42656000	1.89376500	-0.48604200
C	0.93277100	1.58493600	-0.37924500
C	-0.43170500	2.67228600	0.78151500
N	-1.38473200	1.58457000	-1.38404300
C	1.07446600	2.33320200	0.89947700
N	1.80285500	0.90214100	-1.14550800
O	-1.27829600	3.26664000	1.42030200
H	-1.16234700	0.85674900	-2.05483700
O	1.98516600	2.52897900	1.68204400
H	1.40865500	0.39229800	-1.93000700
C	2.96796000	0.23874200	-0.54084900
C	2.62893400	-1.23114700	-0.18383100
C	4.16608200	0.29849900	-1.49851300
H	3.20698500	0.79531200	0.37186000
C	3.87203400	-1.92601200	0.41546100
H	2.40194800	-1.72984300	-1.14201800
C	5.39462400	-0.41364800	-0.91351300
H	3.88124000	-0.18613900	-2.44696600

C	5.06586600	-1.86828700	-0.54785200
H	3.62180200	-2.96584800	0.66249800
H	4.14032900	-1.42330000	1.35489700
H	6.22569000	-0.37300800	-1.62948300
H	5.72048600	0.12066500	-0.00851700
H	5.94033600	-2.35749100	-0.09871600
H	4.81941100	-2.42546200	-1.46528200
H	4.38937500	1.34865800	-1.72207200
N	1.40336000	-1.33085400	0.61994000
C	1.55258300	-0.90953400	2.01314900
H	0.55533900	-0.80497200	2.45969400
H	2.12406300	-1.63740700	2.62195300
H	2.04976300	0.06228500	2.07030200
C	0.78329000	-2.64705100	0.54003800
H	1.38444600	-3.44604100	1.02154400
H	-0.19251000	-2.61586100	1.04056800
H	0.62302000	-2.92095500	-0.51099800
C	-2.80335600	1.65960600	-1.01062900
H	-2.89016600	2.44396400	-0.24874200
C	-4.65427200	-0.03935600	-0.80771800
C	-5.16650400	-1.22243900	-0.28347100
C	-3.34973800	0.34663400	-0.47493200
C	-4.42707600	-2.04584300	0.55972400
C	-2.58409400	-0.47167300	0.36944500
C	-3.12335400	-1.65458000	0.87955600
H	-4.86541100	-2.96209000	0.94491300
H	-1.56662300	-0.18864000	0.62515900
H	-2.52606000	-2.27964600	1.53943800
H	-5.27142400	0.56848200	-1.46546000
H	-3.38420500	1.97245800	-1.88734200
F	-6.43013200	-1.58763500	-0.61605500

1n (A-conformer)

E(RB97D) = -1152.645795 Hartree/Particle

XYZ coordinates

C	-0.49372900	2.11138200	-0.57230400
C	0.83839100	1.76303100	-0.33222600
C	-0.64938900	2.75278600	0.75831300
N	-1.33464900	1.90404400	-1.60996900
C	0.82421800	2.36499000	1.02939500
N	1.78894400	1.13564700	-1.04958100
O	-1.56599800	3.28763300	1.35535100
H	-1.02508900	1.21182400	-2.28593200
O	1.62308800	2.44033700	1.94296500
H	1.48336800	0.73968100	-1.93399000
C	2.78760500	0.29959600	-0.36161800
C	2.27310000	-1.16043600	-0.25407000

C	4.12951600	0.34585100	-1.10275000
H	2.91358000	0.72255000	0.64112400
C	3.33257300	-2.04031100	0.44529400
H	2.17855000	-1.52240700	-1.29262200
C	5.17743200	-0.54741000	-0.42146900
H	3.97197300	-0.00023400	-2.13757600
C	4.67560200	-1.99384200	-0.29748200
H	2.95939100	-3.07057400	0.51210000
H	3.47272000	-1.67698200	1.47280200
H	6.11983500	-0.51236200	-0.98326800
H	5.38498300	-0.15086600	0.58373600
H	5.41905900	-2.61321000	0.22165200
H	4.54730400	-2.41963700	-1.30502200
H	4.47309600	1.38606500	-1.15418400
N	0.92362500	-1.21824400	0.31510800
C	0.85313200	-0.98253000	1.75573600
H	-0.19440800	-0.80776800	2.03115300
H	1.22608000	-1.84048700	2.34950100
H	1.42777000	-0.09314000	2.02857800
C	0.19150300	-2.42263900	-0.05349200
H	0.60576800	-3.34585800	0.40315200
H	-0.85033400	-2.32217000	0.27414400
H	0.20157000	-2.54433800	-1.14488300
C	-2.79409700	1.85552400	-1.34867500
H	-3.02170800	2.67622600	-0.66221000
C	-3.56694300	-0.54386500	-1.58392400
C	-3.84153600	-1.80756100	-1.05479900
C	-3.19797600	0.52356300	-0.75445900
C	-3.73909900	-1.98156400	0.32243800
C	-3.11534900	0.31356100	0.63016100
C	-3.38587600	-0.94167100	1.17861800
H	-2.83944500	1.14131800	1.27914700
H	-3.32906800	-1.11957100	2.24911000
H	-4.13306500	-2.64305200	-1.68531000
H	-3.30748400	2.03034000	-2.30110500
H	-3.64699500	-0.38722100	-2.65929100
F	-3.99267500	-3.20697100	0.84751600

1n (B-conformer)

E(RB97D) = -1152.643758 Hartree/Particle

XYZ coordinates

C	-0.39836900	2.01881100	-0.43068000
C	0.94293300	1.65091700	-0.28677200
C	-0.43671200	2.69829100	0.89247200
N	-1.32254800	1.81371800	-1.39152800
C	1.04893500	2.29236600	1.05171200
N	1.82430200	0.99527000	-1.06392600

O	-1.29133600	3.27424000	1.53735700
H	-1.09371200	1.12849400	-2.10393000
O	1.92654100	2.39014100	1.88878600
H	1.45006800	0.56235000	-1.90255900
C	2.93409700	0.24193100	-0.46028900
C	2.52923200	-1.23885300	-0.24557200
C	4.18273800	0.33663200	-1.34800500
H	3.14263100	0.71200000	0.50692400
C	3.71541700	-2.02474700	0.35666400
H	2.33884100	-1.64924200	-1.25239600
C	5.35469800	-0.46531400	-0.76322300
H	3.93361700	-0.05736300	-2.34711600
C	4.96024100	-1.93199400	-0.53688100
H	3.41943400	-3.07151000	0.50339500
H	3.94893200	-1.61006200	1.34698800
H	6.22366500	-0.39699000	-1.43043900
H	5.64890700	-0.01875300	0.19840700
H	5.79335900	-2.48763400	-0.08641700
H	4.74530500	-2.40334000	-1.50872300
H	4.45115200	1.39283800	-1.47068500
N	1.25897900	-1.35954900	0.48255000
C	1.34489300	-1.05359700	1.91087500
H	0.32848200	-0.95351800	2.31313600
H	1.86301300	-1.84430600	2.48810200
H	1.86450900	-0.10525000	2.07097300
C	0.60669100	-2.64464500	0.26594200
H	1.15802900	-3.49814200	0.71184900
H	-0.39315600	-2.62151500	0.71689400
H	0.49522100	-2.82968200	-0.81050200
C	-2.75496200	1.91436900	-1.07684600
H	-2.84842100	2.65211900	-0.27052400
C	-4.66721400	0.26068600	-1.06977500
C	-5.27367200	-0.93303400	-0.66992500
C	-3.36916200	0.58969700	-0.65818400
C	-4.55307600	-1.79863000	0.14678000
C	-2.67098000	-0.31070600	0.16094100
C	-3.25792100	-1.50975100	0.56871100
H	-1.65770600	-0.08214500	0.48179200
H	-2.73039100	-2.21308200	1.20694400
H	-6.27946900	-1.19697300	-0.98490500
H	-5.21540200	0.94797900	-1.71246000
H	-3.28303800	2.30486200	-1.95592600
F	-5.12638700	-2.96409300	0.53829800

1o (A-conformer)

E(RB97D) = -1727.455389 Hartree/Particle

XYZ coordinates

C	0.96739500	1.75029200	-1.84164000
C	2.15449500	1.24530800	-1.30567500
C	1.02557100	2.98910900	-1.02921200
N	0.07307700	1.27418400	-2.74239100
C	2.34677400	2.44181300	-0.43370800
N	2.87243700	0.12807900	-1.50403300
O	0.30192300	3.95810800	-0.88585900
H	0.16950300	0.28910100	-2.97053600
O	3.16846500	2.77390700	0.39582900
H	2.44740400	-0.57576200	-2.10077200
C	3.66515800	-0.44844100	-0.40473200
C	2.80369800	-1.46380200	0.39145000
C	4.92730800	-1.12146400	-0.95880300
H	3.95156600	0.38471600	0.24624300
C	3.64882500	-2.10526100	1.51422300
H	2.54502900	-2.26390600	-0.32359900
C	5.75286700	-1.77817400	0.15752100
H	4.62284900	-1.89135100	-1.68692800
C	4.90571700	-2.78344900	0.95143200
H	3.02960300	-2.82557300	2.06423000
H	3.94701000	-1.32242400	2.22510100
H	6.63529500	-2.26979800	-0.27192100
H	6.11812200	-0.99621500	0.84005500
H	5.49699400	-3.22306800	1.76552700
H	4.60657500	-3.60907800	0.28690000
H	5.52089800	-0.37533600	-1.50078300
N	1.52899500	-0.87509300	0.81636200
C	1.63151200	0.05530900	1.94122100
H	0.69089600	0.61037600	2.02977100
H	1.81640800	-0.45756400	2.90513200
H	2.43400300	0.77765700	1.76914000
C	0.49335800	-1.87223600	1.05863400
H	0.70412200	-2.51909800	1.93538800
H	-0.45901300	-1.36156100	1.24227100
H	0.37844700	-2.51450400	0.17555100
C	-1.33594300	1.71470700	-2.63337000
H	-1.32570400	2.79610200	-2.46923200
C	-2.64859700	-0.23069800	-1.69919800
C	-3.17743000	-0.95198500	-0.62278000
C	-2.02534800	1.00054600	-1.48866600
C	-3.08615800	-0.44786900	0.67299100
C	-1.94138400	1.51418100	-0.18626400
C	-2.46595400	0.78861200	0.88315700
H	-3.48629900	-1.00863300	1.51107400
H	-1.46085500	2.47391400	-0.01887500
H	-1.83263700	1.49641900	-3.58511800
H	-2.72620200	-0.63558100	-2.70637900
C	-2.40524100	1.33266500	2.29611200

C	-3.77704100	-2.31603500	-0.88323200
F	-1.51264100	2.33832100	2.43068500
F	-3.61806300	1.80852700	2.69084200
F	-2.05682000	0.36084300	3.18689500
F	-4.52738400	-2.76837100	0.14838800
F	-4.56417400	-2.31978800	-1.99152400
F	-2.79493700	-3.24218900	-1.09954600

1o (B-conformer)

E(RB97D) = -1727.453312 Hartree/Particle

XYZ coordinates

C	0.86080400	2.22560900	0.16700500
C	2.18311300	1.76998700	0.11985600
C	0.90637800	2.46834500	1.63072800
N	-0.10672700	2.39428400	-0.76061800
C	2.37156200	1.97226500	1.58654200
N	3.00034700	1.36656800	-0.86287100
O	0.10718100	2.86659400	2.45738100
H	0.02522400	1.95237600	-1.66298300
O	3.28782100	1.79403200	2.36450600
H	2.58956800	1.22141500	-1.77895800
C	4.18341500	0.53655500	-0.59521300
C	3.86016300	-0.96044800	-0.82874300
C	5.34911200	0.98771400	-1.48749500
H	4.44762200	0.69748600	0.45527500
C	5.12834900	-1.81209900	-0.59312900
H	3.59621000	-1.05137100	-1.89685700
C	6.59902300	0.12293200	-1.26960800
H	5.03304100	0.91088200	-2.54102000
C	6.28497100	-1.36275400	-1.49638000
H	4.88934000	-2.86943800	-0.76397900
H	5.43147100	-1.71274300	0.45818900
H	7.40367700	0.45590800	-1.93789600
H	6.95578700	0.26271400	-0.23818400
H	7.17584900	-1.97589600	-1.30633100
H	6.00511700	-1.51710100	-2.55028600
H	5.56201200	2.04468500	-1.28623800
N	2.66884800	-1.38363600	-0.08207300
C	2.87844700	-1.52802500	1.36029000
H	1.90397600	-1.65211500	1.84621400
H	3.50125800	-2.40759200	1.61600600
H	3.35187500	-0.63227000	1.77166000
C	2.05986200	-2.58750600	-0.63827100
H	2.70092100	-3.48777700	-0.53848000
H	1.11771300	-2.78905900	-0.11725300
H	1.84464700	-2.43601300	-1.70463900
C	-1.49838200	2.61875900	-0.36193100

H	-1.47319500	3.14464900	0.60059500
C	-3.64321200	1.31495300	-0.62990100
C	-4.41356300	0.15642700	-0.47363600
C	-2.30952400	1.34220000	-0.21973400
C	-3.85597800	-0.98977700	0.08742700
C	-1.74652900	0.18760900	0.34192500
C	-2.51782600	-0.96363600	0.49669300
H	-4.44935700	-1.88918800	0.21042300
H	-0.71029100	0.18997900	0.66486600
H	-4.09176200	2.20210000	-1.07198300
H	-1.97605200	3.27775400	-1.09732300
C	-5.84646700	0.17561300	-0.96231800
C	-1.90346200	-2.22927100	1.05595200
F	-6.53038000	1.23672100	-0.45551800
F	-6.53270000	-0.94297600	-0.63066800
F	-2.77035500	-2.91258000	1.84397900
F	-0.79028000	-1.98879400	1.79156400
F	-1.53648800	-3.07712800	0.04800600
F	-5.89685000	0.29168800	-2.32040000

1p (A-conformer)

E(RB97D) = -1171.314690 Hartree/Particle

XYZ coordinates

C	0.67404100	-1.51032100	0.16951800
C	-0.72260000	-1.57002800	0.17062100
C	0.76678500	-1.84979100	1.61423000
N	1.59116400	-1.21635500	-0.77349800
C	-0.77939200	-1.90261700	1.61920400
N	-1.67130800	-1.40575400	-0.77224900
O	1.67615500	-1.97845100	2.41341500
H	1.23594900	-0.77710500	-1.61830000
O	-1.67323900	-2.07065700	2.42744900
H	-1.33709700	-1.08015700	-1.67482100
C	-2.96779000	-0.81561800	-0.39675100
C	-2.92116100	0.72486000	-0.57396700
C	-4.10233500	-1.41859300	-1.23418500
H	-3.13082400	-1.06218100	0.65815800
C	-4.28456400	1.33693900	-0.18373500
H	-2.78024800	0.89882000	-1.65505300
C	-5.45806800	-0.79476600	-0.86817900
H	-3.89028700	-1.23472100	-2.30024400
C	-5.42429600	0.73378200	-1.01768700
H	-4.24234800	2.42643700	-0.31225400
H	-4.46926600	1.14075400	0.88159000
H	-6.24948900	-1.22622800	-1.49476800
H	-5.69682300	-1.04912900	0.17541400

H	-6.38714900	1.16829300	-0.71745600
H	-5.27098900	0.98981900	-2.07783500
H	-4.11699900	-2.50505900	-1.08552000
N	-1.74875700	1.31114300	0.08058700
C	-1.81926000	1.36606400	1.53916500
H	-0.81772900	1.58488700	1.92999500
H	-2.51147800	2.15042500	1.90538600
H	-2.13979000	0.40304400	1.94605900
C	-1.36214800	2.60185400	-0.47219200
H	-2.09298600	3.40922100	-0.25369600
H	-0.39341100	2.89610800	-0.05074800
H	-1.25512700	2.52177200	-1.56240000
C	2.92392600	-0.70143600	-0.35902500
H	3.17793200	-1.24430300	0.55835400
C	2.74731400	1.75658100	-1.02435800
C	2.52951100	3.09756700	-0.70189600
C	2.78168200	0.77661200	-0.02193500
C	2.33851000	3.47558500	0.63152400
C	2.58742100	1.16248300	1.31053000
C	2.36749800	2.50419100	1.63606800
H	2.21947800	2.78962500	2.67564300
H	2.51104900	3.84844900	-1.48941400
H	2.59949600	0.40071900	2.08736100
H	2.16831400	4.52013200	0.88393200
H	2.90313000	1.47372500	-2.06406500
C	3.98088800	-1.03461300	-1.42868900
H	3.67410200	-0.55982400	-2.37488000
C	4.07254300	-2.55095100	-1.65279600
H	4.38244700	-3.04921100	-0.72380900
H	3.10879300	-2.97311800	-1.95821400
H	4.81720100	-2.77683500	-2.42640500
C	5.34980900	-0.47086600	-1.02056300
H	5.66586200	-0.91066400	-0.06436400
H	6.10444700	-0.72335300	-1.77574100
H	5.32292300	0.61776100	-0.90210100

1p (B-conformer)

E(RB97D) = -1171.307946 Hartree/Particle

XYZ coordinates

C	0.58119000	-1.38245100	-0.02569100
C	-0.81266100	-1.42185100	-0.13666500
C	0.57891500	-2.18571300	1.22707400
N	1.54642400	-0.79975200	-0.74988800
C	-0.96292000	-2.23197500	1.09888800
N	-1.68949200	-0.93438000	-1.03687800
O	1.43712100	-2.57955000	1.99475700
H	1.26669300	-0.19580000	-1.51383900

O	-1.90803000	-2.67824800	1.72387400
H	-1.30301700	-0.30441200	-1.73354200
C	-3.04958500	-0.56427100	-0.61560800
C	-3.10027900	0.93034200	-0.20531800
C	-4.04910400	-0.84729600	-1.74541400
H	-3.29277200	-1.19374400	0.24743200
C	-4.54086600	1.31582500	0.19902600
H	-2.84867500	1.50181100	-1.11567500
C	-5.47729000	-0.44221200	-1.35229200
H	-3.74072500	-0.27739300	-2.63740100
C	-5.53601300	1.03461200	-0.93558400
H	-4.56612200	2.37554300	0.48433500
H	-4.82771900	0.73291600	1.08513100
H	-6.16389600	-0.63620800	-2.18655100
H	-5.80712300	-1.06768000	-0.50922600
H	-6.55372600	1.30454400	-0.62367600
H	-5.28570300	1.66566300	-1.80277800
H	-3.99897900	-1.91178400	-2.00426900
N	-2.06033200	1.26336600	0.77695000
C	-2.31531200	0.76284700	2.12814100
H	-1.39592300	0.85916100	2.71951500
H	-3.11699000	1.32329100	2.64802300
H	-2.58819400	-0.29527300	2.10121100
C	-1.73965000	2.68417700	0.80124600
H	-2.57025200	3.31705500	1.17732100
H	-0.87609300	2.84505200	1.45952600
H	-1.47561700	3.02428600	-0.20886200
C	2.90275200	-0.56101000	-0.21338200
C	4.00677800	-1.36448000	-0.94945100
H	2.86985600	-0.96190700	0.80892000
H	4.31895700	-0.80188400	-1.84228900
C	4.30659400	1.58623000	-0.50917400
C	4.43994300	2.97737500	-0.44300100
C	3.11612900	0.95512500	-0.12054700
C	3.37919700	3.76848300	0.00029400
C	2.04649000	1.76780000	0.30167300
C	2.17816400	3.15510300	0.37018500
H	3.48306900	4.85022700	0.05044000
H	1.10153400	1.31019200	0.58698200
H	1.33756700	3.75726200	0.70855900
H	5.37629300	3.44006100	-0.74834700
H	5.14088800	0.99968800	-0.87855600
C	5.21376000	-1.55071600	-0.01008800
H	6.04657100	-2.02228300	-0.54647600
H	5.56776900	-0.60853600	0.42139400
H	4.92468900	-2.20939100	0.81992900
C	3.50342700	-2.74716000	-1.39102800
H	3.11384600	-3.30120100	-0.52693100

H	2.70461500	-2.67256700	-2.13676900
H	4.33231000	-3.32164300	-1.82356500

1q (A-conformer)

E(RB97D) = -1171.319411 Hartree/Particle

XYZ coordinates

C	0.05876800	-2.00242700	-0.34078700
C	-1.28259500	-1.61228100	-0.41692200
C	-0.18879700	-2.87946300	0.83580000
N	1.15671400	-1.65627200	-1.03005000
C	-1.67333700	-2.45677000	0.73839800
N	-1.96694700	-0.78670700	-1.23361100
O	0.51231800	-3.55929600	1.56192200
H	1.07232600	-0.89097100	-1.68936100
O	-2.70910400	-2.65280800	1.34903600
H	-1.40740700	-0.23713000	-1.87891900
C	-3.14802700	-0.06597100	-0.73439500
C	-2.73815000	1.31922500	-0.17085900
C	-4.18057000	0.09243800	-1.85913800
H	-3.57533100	-0.67982000	0.06618100
C	-3.99241100	2.08606700	0.30509900
H	-2.31408900	1.87765400	-1.02335000
C	-5.41564400	0.87610100	-1.39190700
H	-3.70525800	0.62817600	-2.69742700
C	-5.01549100	2.24696400	-0.82775600
H	-3.69051300	3.06535900	0.69847600
H	-4.45430800	1.53078900	1.13304000
H	-6.12210500	0.99114400	-2.22422600
H	-5.92977600	0.30012200	-0.60788400
H	-5.90110500	2.78605100	-0.46581900
H	-4.57361500	2.85486400	-1.63283300
H	-4.46050000	-0.90286000	-2.22472100
N	-1.65553600	1.21364800	0.81724700
C	-2.06924200	0.68440000	2.11745500
H	-1.17198900	0.43845500	2.69841200
H	-2.66870400	1.40902900	2.70233800
H	-2.65010200	-0.23312300	1.99148100
C	-0.91489200	2.45927500	0.97657900
H	-1.51414700	3.26886000	1.44218900
H	-0.04174700	2.27748200	1.61504900
H	-0.56076500	2.80951000	-0.00188400
C	2.52422800	-1.87283800	-0.50455800
H	2.41973600	-2.45268300	0.41743700
C	4.26362100	-0.12111400	-1.11134100
C	4.86952300	1.12121700	-0.87996400
C	3.22265000	-0.54986400	-0.26039300

C	4.47240600	1.95177300	0.17097800
C	2.80320000	0.27862700	0.80666000
C	3.44002400	1.50816500	1.00458600
H	3.12301300	2.13325800	1.83951600
H	5.67707600	1.44342200	-1.53691500
H	3.08288000	-2.48614100	-1.21772300
C	4.76047300	-0.96927800	-2.26515100
H	5.22051900	-1.90251600	-1.91148800
H	3.94629400	-1.25283300	-2.94610600
H	5.51192300	-0.42270200	-2.84553900
C	1.67346800	-0.11781000	1.72857900
H	0.69886400	0.04866600	1.24869600
H	1.71520600	-1.17629100	2.00907700
H	1.70337300	0.48243400	2.64531100
C	5.12216400	3.29672600	0.39298700
H	4.48919300	4.10715100	0.00192600
H	5.27487100	3.49043000	1.46254900
H	6.09264300	3.35738800	-0.11396100

1q (B-conformer)

E(RB97D) = -1171.315327 Hartree/Particle

XYZ coordinates

C	0.07920900	-1.84577000	-0.21360300
C	-1.28719800	-1.54742000	-0.26405600
C	-0.07197700	-2.67448200	1.01275200
N	1.12824400	-1.45175500	-0.94406900
C	-1.58147300	-2.34220600	0.95474500
N	-2.05084100	-0.82621700	-1.10647100
O	0.69569500	-3.28149800	1.73594800
H	0.98569200	-0.72994600	-1.63981500
O	-2.57845600	-2.55294200	1.62258200
H	-1.55703800	-0.27373900	-1.79984800
C	-3.30503900	-0.21266500	-0.64684300
C	-3.08281300	1.27871400	-0.29095000
C	-4.39803600	-0.34981200	-1.71644100
H	-3.61446800	-0.76406400	0.24740300
C	-4.41294500	1.89671500	0.19554500
H	-2.81126200	1.78139400	-1.23577200
C	-5.71659700	0.28798600	-1.25355800
H	-4.05379900	0.14557800	-2.63894300
C	-5.51260700	1.76045500	-0.86758800
H	-4.25178600	2.95159300	0.45225000
H	-4.72754200	1.38139500	1.11363400
H	-6.47405400	0.19704100	-2.04289500
H	-6.09176300	-0.26489700	-0.37935500
H	-6.45233800	2.19353900	-0.49986700

H	-5.22205500	2.33216300	-1.76292600
H	-4.53610600	-1.41305600	-1.94680000
N	-1.93282100	1.46614200	0.60289500
C	-2.13850700	0.98898400	1.97040100
H	-1.17051400	0.97521100	2.48611700
H	-2.82670100	1.63518300	2.54976700
H	-2.53607700	-0.02953300	1.96904000
C	-1.43471200	2.83557300	0.60122500
H	-2.13456900	3.55866200	1.06824000
H	-0.49130000	2.87379900	1.16019000
H	-1.24180500	3.15975200	-0.43015100
C	2.52575900	-1.73566600	-0.59495500
H	2.49477300	-2.41515200	0.26753200
C	4.66497600	-0.40546600	-0.81509300
C	5.40995900	0.76475700	-0.63252300
C	3.35417800	-0.49202100	-0.28755500
C	4.89253200	1.87083700	0.04672500
C	2.82902000	0.60345200	0.43786100
C	3.60889400	1.75891800	0.58438800
H	2.97815200	-2.28942000	-1.42327300
H	6.42204500	0.81025400	-1.03424700
H	3.20254600	2.58868900	1.16289800
C	1.50257100	0.55228100	1.16964700
H	0.63437600	0.72296700	0.52015600
H	1.35377400	-0.41913900	1.65436500
H	1.48634300	1.32353300	1.94887500
C	5.30639300	-1.55661400	-1.56381200
H	5.29170700	-2.48386100	-0.97576300
H	4.78572800	-1.76821900	-2.50966400
H	6.34947400	-1.32199700	-1.80282400
C	5.69406000	3.14193400	0.19277300
H	5.55244600	3.79647100	-0.68035700
H	5.38491800	3.70553700	1.08166100
H	6.76733000	2.92767500	0.27114200

1r (A-conformer)

E(RB97D) = -1224.232460 Hartree/Particle

XYZ coordinates

C	-0.01467200	-2.31466400	-0.38031800
C	-1.31337700	-1.82233500	-0.21105000
C	0.03208800	-2.87362000	0.99517300
N	0.85713300	-2.27130600	-1.40497600
C	-1.40178200	-2.32490600	1.18302700
N	-2.17324300	-1.16192500	-1.01246600
O	0.87001200	-3.45676000	1.65990900
H	0.60975900	-1.65514800	-2.17309100

O	-2.23558500	-2.26400500	2.06843300
H	-1.79071900	-0.85174100	-1.90139800
C	-3.11357200	-0.19134900	-0.42806800
C	-2.45608800	1.21296100	-0.36454900
C	-4.40936900	-0.14649600	-1.24753500
H	-3.33583900	-0.54144900	0.58617800
C	-3.45686200	2.24311900	0.20402100
H	-2.25206800	1.49580600	-1.41183800
C	-5.39404000	0.89234700	-0.69016300
H	-4.15674400	0.11355700	-2.28882000
C	-4.74937200	2.28489700	-0.62342500
H	-2.97938300	3.23148500	0.23309000
H	-3.69839400	1.96749300	1.23989500
H	-6.30136300	0.91596600	-1.30775300
H	-5.69957800	0.58821200	0.32230100
H	-5.45240400	3.01191500	-0.19517900
H	-4.51577400	2.62428600	-1.64483800
H	-4.85815200	-1.14710100	-1.26054500
N	-1.15308900	1.16319800	0.30151300
C	-1.20532600	1.03150200	1.75517600
H	-0.20667800	0.75359800	2.11310000
H	-1.50765000	1.97177100	2.25965600
H	-1.90155000	0.23947200	2.04456000
C	-0.24857300	2.23069600	-0.09733400
H	-0.57109600	3.23463500	0.25499300
H	0.74494700	2.02693700	0.31788000
H	-0.16486300	2.26020800	-1.19165700
C	2.32060700	-2.35321700	-1.17372900
H	2.46680200	-2.88224200	-0.22720600
C	3.41440700	-0.39261300	-2.32278300
C	3.86714300	0.94309600	-2.36674400
C	2.91523400	-0.96532000	-1.15192200
C	3.83135800	1.74978600	-1.23185200
C	2.88088100	-0.17296300	0.01608500
C	3.34275200	1.17656800	-0.05206100
H	3.45843200	-0.99810700	-3.22763400
H	2.76485900	-2.94447000	-1.98393000
C	2.46675000	-0.40418500	1.36749500
H	2.07501500	-1.32039600	1.78721200
C	2.68091300	0.76869100	2.05085300
H	2.50379500	1.01274900	3.09100000
N	3.20689500	1.72838400	1.20285300
C	3.54518200	3.09250500	1.55737100
H	2.93347700	3.80575000	0.98742600
H	3.35602400	3.23688600	2.62505700
H	4.60540900	3.29363300	1.35271100
H	4.17710500	2.78041900	-1.26166400
H	4.25164400	1.34653600	-3.30071500

1r (B-conformer)

E(RB97D) = -1224.228562 Hartree/Particle

XYZ coordinates

C	-0.06583200	2.12599200	-0.20085600
C	1.25078400	1.64892800	-0.24455700
C	0.19256800	2.94020000	1.01910000
N	-1.14745300	1.92652900	-0.96698600
C	1.65462400	2.44523500	0.94302600
N	1.91478500	0.83352200	-1.08250000
O	-0.48497300	3.65049300	1.73699800
H	-1.09791000	1.23050900	-1.70034800
O	2.69510800	2.60783900	1.55613500
H	1.35817200	0.29146200	-1.73485400
C	3.18369700	0.20132900	-0.70112300
C	2.95169400	-1.23521400	-0.16906900
C	4.13413500	0.18483100	-1.90858600
H	3.61644200	0.82115200	0.09149200
C	4.30770500	-1.89738700	0.16649500
H	2.50463800	-1.80096900	-1.00488600
C	5.46991200	-0.49528500	-1.57763900
H	3.64283500	-0.36035400	-2.73153900
C	5.24314200	-1.91886700	-1.04977200
H	4.13117700	-2.91472400	0.53883800
H	4.78520000	-1.33227100	0.97877200
H	6.11274400	-0.50920700	-2.46747200
H	5.99208500	0.09479200	-0.80959800
H	6.20053200	-2.38708000	-0.78471900
H	4.79223100	-2.53263500	-1.84539600
H	4.29082700	1.21581900	-2.24826400
N	1.95888200	-1.26425000	0.91308000
C	2.43485200	-0.73575600	2.19263300
H	1.57310500	-0.59947100	2.85814400
H	3.15205700	-1.41433400	2.69551700
H	2.90887000	0.23900000	2.05435900
C	1.36452200	-2.58140400	1.09053500
H	2.08569700	-3.34610000	1.44811000
H	0.56153700	-2.51036000	1.83515200
H	0.93341800	-2.92668500	0.14164600
C	-2.50138400	2.31681700	-0.55059800
H	-2.40976000	2.75917000	0.44944700
C	-4.77256700	1.34588700	-0.99908500
C	-5.72811900	0.31041200	-1.00903900
C	-3.46640800	1.15079600	-0.54822600
C	-5.39591400	-0.97180600	-0.58242500
C	-3.09767600	-0.14407800	-0.11054900
C	-4.08417900	-1.17907700	-0.14235700
H	-5.05985600	2.33423300	-1.35460400

H	-2.88512300	3.09976000	-1.21984100
C	-1.89614500	-0.74147300	0.40807400
H	-0.93919100	-0.27446600	0.59711200
C	-2.18747100	-2.06188000	0.65911900
H	-1.55908800	-2.84857200	1.05530000
N	-3.50056300	-2.33407400	0.33071800
C	-4.17054300	-3.61250700	0.46523300
H	-4.52883800	-3.96822900	-0.51061700
H	-3.46283700	-4.34108800	0.87165000
H	-5.02830200	-3.53022200	1.14664900
H	-6.12470500	-1.77869300	-0.59279100
H	-6.73497400	0.51667600	-1.36452900

1s (A-conformer)

E(RB97D) = -1069.445224 Hartree/Particle

XYZ coordinates

C	-0.86600900	1.77262300	-0.49619300
C	0.50602200	1.57750800	-0.32223000
C	-1.01927600	2.46533500	0.81027000
N	-1.74066100	1.43979300	-1.47116300
C	0.50212100	2.24680200	1.00909500
N	1.47698400	1.02497600	-1.07090600
O	-1.95192500	2.94915000	1.42107600
H	-1.41247500	0.78119500	-2.16941300
O	1.34162300	2.46272500	1.86157200
H	1.17874600	0.54061400	-1.91178000
C	2.66098000	0.42659200	-0.43615800
C	2.45185500	-1.09439900	-0.22416300
C	3.90966100	0.68475100	-1.29077700
H	2.78106400	0.92198800	0.53328200
C	3.71383400	-1.70703300	0.42376000
H	2.35365600	-1.53082500	-1.23333500
C	5.16159100	0.05313500	-0.66456700
H	3.74506400	0.25461900	-2.29239400
C	4.96238700	-1.45166100	-0.43245500
H	3.55986200	-2.78338100	0.57283100
H	3.85621000	-1.25745200	1.41616300
H	6.03256300	0.23329100	-1.30784100
H	5.36435100	0.54274700	0.29969600
H	5.84830400	-1.88524100	0.05003200
H	4.84468300	-1.95573900	-1.40447400
H	4.03580200	1.76691400	-1.41581000
N	1.18473500	-1.38657100	0.46198200
C	1.17525400	-1.05168600	1.88747800
H	0.14188300	-1.09715600	2.25391500
H	1.78408000	-1.74952400	2.49446500

H	1.54573600	-0.03574600	2.04698300
C	0.74253500	-2.76033200	0.25232700
H	1.40622200	-3.51223600	0.72593700
H	-0.25882600	-2.88516800	0.68190600
H	0.68876800	-2.97506700	-0.82309600
C	-3.16820600	1.34358100	-1.16044900
H	-3.38890100	2.11611200	-0.41300500
C	-4.94884300	-0.37452100	-0.66333700
C	-5.33899600	-1.60910200	-0.14237700
C	-3.59742800	-0.01138100	-0.62327300
C	-2.69998600	-0.92423900	-0.05854000
C	-3.19616600	-2.13530800	0.43486100
H	-1.63498300	-0.71060100	0.00467600
H	-5.69024100	0.29603500	-1.09545800
H	-3.74444600	1.57822500	-2.06449100
H	-6.38846100	-1.90587900	-0.16777600
H	-2.51238200	-2.85810300	0.88231400
N	-4.48703600	-2.49085600	0.40235300

1s (B-conformer)

E(RB97D) = -1069.445006 Hartree/Particle

XYZ coordinates

C	-0.85607800	1.78057000	-0.48880400
C	0.51893200	1.57035100	-0.35098900
C	-0.95733300	2.51124900	0.80197100
N	-1.76582200	1.43452900	-1.42505500
C	0.56652700	2.28326400	0.95609600
N	1.45958500	0.98106400	-1.11001800
O	-1.86605900	3.01634600	1.43242800
H	-1.47088400	0.75311000	-2.11621700
O	1.43675700	2.52085300	1.77151200
H	1.12889000	0.47010400	-1.92263700
C	2.65550200	0.38845100	-0.49125700
C	2.42182600	-1.11537100	-0.19599300
C	3.87226800	0.57685900	-1.40768900
H	2.82305000	0.92780600	0.44728400
C	3.69778800	-1.73348500	0.41810300
H	2.26259400	-1.59483500	-1.17733600
C	5.13514000	-0.05957900	-0.80908000
H	3.65397700	0.10769500	-2.38122800
C	4.91053300	-1.54781500	-0.50461000
H	3.52285700	-2.79792400	0.62080000
H	3.89868700	-1.24679700	1.38246800
H	5.98078700	0.07132100	-1.49656200
H	5.39206300	0.46440200	0.12373000
H	5.80727800	-1.98439200	-0.04534800

H	4.73499800	-2.08805600	-1.44807400
H	4.01884600	1.64882300	-1.58683300
N	1.18456000	-1.33865000	0.56430900
C	1.26083800	-0.95686000	1.97510700
H	0.24671200	-0.94870400	2.39486300
H	1.87204300	-1.65814900	2.57612800
H	1.67647300	0.04872900	2.07993100
C	0.67596500	-2.69760300	0.42298400
H	1.32747900	-3.46127200	0.89548800
H	-0.31178900	-2.76380800	0.89572400
H	0.56706800	-2.94657600	-0.64074500
C	-3.19162100	1.37572900	-1.07768700
H	-3.36334600	2.12833400	-0.29808100
C	-4.87652200	-0.51156300	-0.93201000
C	-5.25894100	-1.76013800	-0.43343600
C	-3.62711400	0.00968700	-0.58102700
C	-2.81679500	-0.76446500	0.25919700
C	-3.29386800	-1.99971200	0.70246500
H	-3.78432700	1.65566600	-1.95748900
H	-6.22932900	-2.18122200	-0.70069500
H	-2.67901500	-2.61432100	1.36162500
H	-5.54445300	0.04576000	-1.58711000
H	-1.82902500	-0.42275200	0.55846600
N	-4.49110800	-2.50665100	0.37223100

1t (A-conformer)

E(RB97D) = -1085.484012 Hartree/Particle

XYZ coordinates

C	-0.89589400	1.80548500	-0.55910200
C	0.46977000	1.63765400	-0.32766200
C	-1.13220300	2.44713500	0.75986500
N	-1.72268700	1.46270300	-1.57635200
C	0.38387400	2.25356800	1.02914900
N	1.48582500	1.12175300	-1.04070000
O	-2.10727300	2.87992700	1.34158600
H	-1.34018600	0.82559300	-2.26746400
O	1.17056300	2.43978600	1.93539900
H	1.23333700	0.66814300	-1.91343100
C	2.61632400	0.47431400	-0.35452200
C	2.39215900	-1.05758000	-0.28078100
C	3.93552500	0.79110400	-1.07151600
H	2.65084500	0.89259100	0.65709000
C	3.58747600	-1.71621100	0.44387000
H	2.40137800	-1.41696600	-1.32461300
C	5.12592000	0.11315800	-0.37665500
H	3.86587000	0.43427900	-2.11205200

C	4.91156700	-1.40371300	-0.26820400
H	3.42527100	-2.79986400	0.50124600
H	3.63020000	-1.33738300	1.47434800
H	6.05259300	0.33476100	-0.92168300
H	5.23587100	0.53463100	0.63375700
H	5.74927000	-1.87102900	0.26616700
H	4.89000400	-1.83961500	-1.27928600
H	4.06840100	1.87914200	-1.10581000
N	1.06245000	-1.40118600	0.24448500
C	0.89769600	-1.15827500	1.67972700
H	-0.16375200	-1.26473800	1.93361200
H	1.46912500	-1.87400800	2.30161600
H	1.21569700	-0.14416400	1.93762500
C	0.66602700	-2.76781400	-0.09271800
H	1.29815500	-3.53519300	0.39820100
H	-0.37143800	-2.92944600	0.22242700
H	0.73308300	-2.91306800	-1.17957500
C	-3.14363900	1.26214900	-1.28064400
H	-3.44951200	2.06920500	-0.60353000
C	-4.78796700	-0.49659900	-0.48893700
C	-3.45988000	-0.07709700	-0.63748700
C	-2.48999000	-0.95741000	-0.14572000
H	-1.42378800	-0.73486100	-0.21875500
H	-5.60786700	0.12785900	-0.85244700
H	-3.71374800	1.37158200	-2.21201500
C	-4.11110700	-2.40546400	0.52958100
H	-4.37496400	-3.34885100	1.00880600
N	-2.80677800	-2.12340200	0.43979600
N	-5.12939800	-1.65311400	0.08854600

1t (B-conformer)

E(RB97D) = -1085.483520 Hartree/Particle

XYZ coordinates

C	-0.86177500	1.82927600	-0.53325000
C	0.51180800	1.62501500	-0.38317400
C	-0.98159300	2.55484100	0.75795500
N	-1.76769200	1.46467200	-1.46993200
C	0.54304400	2.33756700	0.92665300
N	1.46091200	1.02770400	-1.12472800
O	-1.90227700	3.04260600	1.38498900
H	-1.45657700	0.78845500	-2.15968100
O	1.40159500	2.57333300	1.75332800
H	1.13578600	0.51921000	-1.94153800
C	2.61827800	0.39454900	-0.47003300
C	2.32949100	-1.10519700	-0.20318900
C	3.87376400	0.55752100	-1.33714200

H	2.76606200	0.91787000	0.48079000
C	3.56198500	-1.76151700	0.45851400
H	2.20252800	-1.56998300	-1.19632200
C	5.09397100	-0.11875000	-0.69475600
H	3.68123500	0.10284100	-2.32281600
C	4.81651300	-1.60232800	-0.41185300
H	3.35029200	-2.82200500	0.64506400
H	3.73539600	-1.28707400	1.43422600
H	5.96955800	-0.00616300	-1.34711800
H	5.32779900	0.39099700	0.25192300
H	5.68144700	-2.06632200	0.08040800
H	4.66574000	-2.13104500	-1.36605900
H	4.05681100	1.62652300	-1.49983400
N	1.05336000	-1.30711600	0.49751000
C	1.07758400	-0.94204700	1.91517800
H	0.04832200	-0.93312500	2.29514300
H	1.65838800	-1.65631500	2.53045600
H	1.50048000	0.05748100	2.04833300
C	0.52685800	-2.65916100	0.32395300
H	1.15671600	-3.43435500	0.80650200
H	-0.47735200	-2.71655500	0.76030000
H	0.45581900	-2.89253600	-0.74704300
C	-3.18210200	1.33885600	-1.08779400
H	-3.37474000	2.09741500	-0.31927600
C	-4.74257800	-0.65865000	-0.87610700
C	-3.52817400	-0.03966000	-0.56355300
C	-2.67129500	-0.77459000	0.26774700
H	-3.80966400	1.57107000	-1.95775500
H	-5.45895200	-0.16300500	-1.53600400
H	-1.68475300	-0.39454000	0.53464700
C	-4.19696800	-2.45602200	0.39349800
H	-4.47150000	-3.43338200	0.79198200
N	-5.09207600	-1.86305200	-0.40626500
N	-2.99539700	-1.98095000	0.75073900

1u (A-conformer)

E(RB97D) = -1323.680019 Hartree/Particle

XYZ coordinates

C	0.68733900	1.98821400	0.07725200
C	2.01825800	1.56111400	0.01146500
C	0.84786100	2.52305000	1.45713700
N	-0.35345700	1.91872500	-0.77030700
C	2.31872800	2.04874700	1.38294500
N	2.76394500	0.96578400	-0.93848700
O	0.10934600	3.06027300	2.26034600
H	-0.25123300	1.33215100	-1.59190100

O	3.29662500	2.02378400	2.10800200
H	2.26256200	0.63129200	-1.75556800
C	3.90458600	0.11581700	-0.56436000
C	3.46540100	-1.36759700	-0.47006700
C	5.04412000	0.27620400	-1.58015200
H	4.24622600	0.46340300	0.41665500
C	4.67856100	-2.25083600	-0.10207000
H	3.14593500	-1.65344600	-1.48733900
C	6.24157700	-0.61989300	-1.23049200
H	4.66480600	0.00586200	-2.57938800
C	5.81621500	-2.09138900	-1.12051500
H	4.35755400	-3.29862800	-0.03840600
H	5.03980100	-1.95933700	0.89386800
H	7.03034100	-0.50081900	-1.98465700
H	6.66237100	-0.29372100	-0.26752700
H	6.67235300	-2.71719300	-0.83534800
H	5.47260100	-2.44339600	-2.10587200
H	5.34038200	1.33146300	-1.61719900
N	2.28184700	-1.53423400	0.38224300
C	2.53615500	-1.38895300	1.81518100
H	1.57463000	-1.30475700	2.33787100
H	3.08240700	-2.25254700	2.24341500
H	3.10848500	-0.47913300	2.01495200
C	1.55449300	-2.76570900	0.10542500
H	2.11174900	-3.68041200	0.39699500
H	0.60882800	-2.75722600	0.66146200
H	1.32272300	-2.82907500	-0.96588300
C	-1.74488900	2.09748600	-0.31263100
C	-2.51101800	2.95114700	-1.32594900
H	-1.67562200	2.64620000	0.63540500
C	-3.99325300	2.98034000	-0.95522500
H	-2.39138200	2.51442400	-2.33053900
H	-2.07533600	3.95687100	-1.34617300
C	-4.59365100	1.57284800	-1.05705000
H	-4.54459500	3.66865900	-1.60761700
H	-4.09832000	3.35201100	0.07433200
H	-5.58956500	1.56657700	-0.59577700
H	-4.74974300	1.31796800	-2.11805000
C	-3.73637300	0.49810200	-0.41179600
C	-4.30268700	-0.80053200	-0.17439900
C	-2.41546600	0.74600400	-0.04813600
C	-3.51670500	-1.81053800	0.48138600
C	-1.65422800	-0.26321000	0.60674200
C	-2.18855400	-1.49973700	0.87195700
C	-5.62500200	-1.14554900	-0.57216300
H	-6.24137900	-0.41157400	-1.08254200
C	-6.14246400	-2.40387800	-0.33130100
H	-7.15617600	-2.63982400	-0.64865600

C	-5.36678500	-3.38762900	0.32520000
H	-5.78698700	-4.37314700	0.51434500
C	-4.07885600	-3.09161300	0.72147300
H	-3.46844200	-3.83952200	1.22552100
H	-0.62980600	-0.05091200	0.89973500
H	-1.59946100	-2.25865800	1.38380600

1u (B-conformer)

E(RB97D) = -1323.680002 Hartree/Particle

XYZ coordinates

C	-0.68707900	-1.98047500	0.07070800
C	-2.01900100	-1.55636800	0.00659300
C	-0.84672000	-2.52289200	1.44775900
N	0.35321200	-1.90512500	-0.77716500
C	-2.31931600	-2.05375800	1.37463200
N	-2.76540100	-0.95797900	-0.94078500
O	-0.10746400	-3.06250100	2.24862800
H	0.24816700	-1.31768900	-1.59774700
O	-3.29867500	-2.03868000	2.09795900
H	-2.26462600	-0.61617800	-1.75518200
C	-3.91285000	-0.11831800	-0.56467000
C	-3.48372000	1.36693800	-0.45479800
C	-5.04580800	-0.27729800	-1.58812100
H	-4.25713200	-0.47682700	0.41147700
C	-4.70481000	2.23952300	-0.08745900
H	-3.15902300	1.66348500	-1.46734500
C	-6.25080100	0.60856400	-1.23855000
H	-4.66241400	0.00342700	-2.58294600
C	-5.83496200	2.08160800	-1.11439400
H	-4.39093700	3.28874600	-0.01288800
H	-5.07068500	1.93741800	0.90359900
H	-7.03428400	0.49068300	-1.99838900
H	-6.67537000	0.27225200	-0.28074200
H	-6.69654700	2.70010700	-0.82969300
H	-5.48726500	2.44341300	-2.09476100
H	-5.33521300	-1.33405000	-1.63540500
N	-2.30713300	1.53382200	0.40741100
C	-2.57129000	1.37601600	1.83749300
H	-1.61317400	1.29387800	2.36661100
H	-3.12631300	2.23283900	2.26792800
H	-3.13906200	0.46100900	2.02592700
C	-1.58676000	2.77271000	0.14573400
H	-2.15449900	3.68122600	0.43626500
H	-0.64791200	2.76895400	0.71326600
H	-1.34302200	2.84413800	-0.92240300
C	1.74439500	-2.08073300	-0.32002400

C	2.51430300	-2.94257700	-1.32308700
H	1.67521100	-2.62377600	0.63144100
C	3.98859700	-2.99225500	-0.92311500
H	2.41773800	-2.50309900	-2.32888100
H	2.06630500	-3.94268400	-1.35110900
C	4.61202700	-1.59345700	-1.00727900
H	4.54396500	-3.68621700	-1.56601900
H	4.06649800	-3.36918900	0.10691800
H	5.59208900	-1.60066400	-0.51301800
H	4.80786100	-1.34341500	-2.06275900
C	3.75080400	-0.50159800	-0.39681900
C	4.32520200	0.79489000	-0.16813500
C	2.41806100	-0.72905600	-0.06343000
C	3.53192500	1.82713800	0.44264200
C	1.64834400	0.30336100	0.54359500
C	2.18872000	1.53990600	0.79733900
C	5.66312900	1.11661000	-0.53205800
H	6.28620300	0.36512500	-1.00759200
C	6.18816800	2.37351200	-0.30058100
H	7.21406300	2.59107500	-0.59077400
C	5.40470100	3.37951500	0.31159000
H	5.83086400	4.36380500	0.49365600
C	4.10179800	3.10652500	0.67376800
H	3.48524200	3.87160500	1.14339900
H	0.61295900	0.10979600	0.81019900
H	1.59234500	2.31703200	1.27205900

10.2. Structures for rate-limiting step with catalyst 1a (PCM-(Toluene)-B97-D/def2-TZVP//PCM-(Toluene)-B97-D/TZVP approximation)

trans-β-Nitrostyrene

OPTIMIZATION: E(RB97D) = -513.988222 (Hartree/Particle)
Zero-point correction = 0.132435
Thermal correction to Energy = 0.141782
Thermal correction to Enthalpy = 0.142726
Thermal correction to Gibbs Free Energy = 0.096579
Sum of electronic and zero-point Energies = -513.855787
Sum of electronic and thermal Energies = -513.846440
Sum of electronic and thermal Enthalpies = -513.845496
Sum of electronic and thermal Free Energies = -513.891643

SINGLE POINT: E(RB97D) = -514.013020 (Hartree/Particle)

XYZ coordinates

O	3.83023000	-0.95359700	-0.00027600
N	2.99827400	-0.03352300	0.00014200
O	3.29196300	1.16757100	0.00024900

C	1.59812700	-0.44281000	0.00048200
H	1.48767300	-1.52000200	0.00092200
C	0.60465800	0.46528200	-0.00032600
H	0.89425400	1.51595500	-0.00093900
C	-0.82298100	0.18245900	-0.00027200
C	-1.71916900	1.27366100	-0.00016000
C	-1.35249100	-1.12831400	-0.00022000
C	-3.09879000	1.06492300	0.00011500
H	-1.31997900	2.28650200	-0.00026000
C	-2.72901600	-1.33324900	0.00002200
H	-0.68312100	-1.98511200	-0.00042700
C	-3.60727300	-0.23850900	0.00022500
H	-3.77608900	1.91614400	0.00024200
H	-3.12403500	-2.34685100	0.00005300
H	-4.68256000	-0.40442100	0.00043500

2,4-Pentanodione

OPTIMIZATION: E(RB97D) = -345.700247 (Hartree/Particle)
Zero-point correction = 0.118255
Thermal correction to Energy = 0.126689
Thermal correction to Enthalpy = 0.127633
Thermal correction to Gibbs Free Energy = 0.084685
Sum of electronic and zero-point Energies = -345.581991
Sum of electronic and thermal Energies = -345.573558
Sum of electronic and thermal Enthalpies = -345.572614
Sum of electronic and thermal Free Energies = -345.615561

SINGLE POINT: E(RB97D) = -345.713431 (Hartree/Particle)

XYZ coordinates

O	-1.45246600	-1.42516600	-0.27477200
C	-1.20728900	-0.29267800	0.10138700
C	-2.00911500	0.92027000	-0.31450000
H	-2.53087600	1.32318300	0.56609300
H	-1.32841600	1.70845500	-0.66546300
H	-2.73624700	0.65767000	-1.08848400
C	-0.00001000	0.00016400	1.01220800
C	1.20729200	0.29270500	0.10132100
O	1.45270000	1.42513200	-0.27487800
H	-0.19150700	0.88457600	1.62812400
C	2.00893300	-0.92041400	-0.31441500
H	2.53074800	-1.32321700	0.56619600
H	1.32809400	-1.70857800	-0.66515600
H	2.73600400	-0.65804200	-1.08853400
H	0.19146200	-0.88405500	1.62841100

Catalyst 1a

OPTIMIZATION: E(RB97D) = -1170.067559 (Hartree/Particle)
Zero-point correction = 0.469566
Thermal correction to Energy = 0.495322
Thermal correction to Enthalpy = 0.496266
Thermal correction to Gibbs Free Energy = 0.412804
Sum of electronic and zero-point Energies = -1169.597993
Sum of electronic and thermal Energies = -1169.572238
Sum of electronic and thermal Enthalpies = -1169.571293
Sum of electronic and thermal Free Energies = -1169.654756

SINGLE POINT: E(RB97D) = -1170.113655 (Hartree/Particle)

XYZ coordinates

C	0.42443000	-1.59205600	0.03115900
C	-0.97699800	-1.49716400	-0.02542000
C	0.39826200	-2.18005800	1.39491800
N	1.40863200	-1.24870300	-0.81299700
C	-1.13709000	-2.09596000	1.32281800
N	-1.84542400	-1.07469300	-0.95939000
O	1.24380400	-2.54006200	2.20122200
H	1.15828700	-0.71712600	-1.64025600
O	-2.08582600	-2.36554000	2.04634000
H	-1.44668200	-0.61686300	-1.77378400
C	-3.16660300	-0.54746700	-0.57461000
C	-3.10079200	0.99177400	-0.39266100
C	-4.21073900	-0.92236800	-1.63680000
H	-3.43093200	-1.02083800	0.37689200
C	-4.50153700	1.53670700	-0.03051000
H	-2.83186300	1.40098700	-1.38088300
C	-5.59757300	-0.35733000	-1.29103500
H	-3.88281500	-0.51583100	-2.60758500
C	-5.54020500	1.16642100	-1.10020800
H	-4.44267400	2.62576100	0.09515800
H	-4.80989500	1.11224500	0.93505700
H	-6.31404400	-0.62201500	-2.07982100
H	-5.95256500	-0.82400000	-0.35975300
H	-6.52870800	1.55437500	-0.81949100
H	-5.26395100	1.64133800	-2.05477300
H	-4.24446000	-2.01466700	-1.73212900
N	-2.01469500	1.38843400	0.51652200
C	-2.28244400	1.12667600	1.93288100
H	-1.34727100	1.24312500	2.49591100
H	-3.03157800	1.81987100	2.36377200
H	-2.63415400	0.10072400	2.07222700
C	-1.59240300	2.77165700	0.31611300
H	-2.36590900	3.51286400	0.60641600
H	-0.69863100	2.96520500	0.92252100

H	-1.33583700	2.93298300	-0.73912900
C	2.80461300	-1.07870700	-0.36442100
C	3.76093200	-1.69848800	-1.39103700
H	2.88636300	-1.64224000	0.57323900
C	5.21242500	-1.37228700	-1.02121900
H	3.53664800	-1.28919600	-2.38900200
H	3.58638400	-2.78035800	-1.42701800
C	5.44331200	0.14245100	-1.11002700
H	5.90625200	-1.89927700	-1.68800700
H	5.41250600	-1.72062200	0.00263800
H	6.42840200	0.41027100	-0.70519000
H	5.45434800	0.43670000	-2.17214100
C	4.37119300	0.94870000	-0.39700700
C	4.62528400	2.29135500	-0.07172100
C	3.11624200	0.39331300	-0.07148500
C	3.66584300	3.08025300	0.56349600
C	2.15484900	1.19363500	0.57041200
C	2.42154900	2.52622400	0.88612700
H	3.88726400	4.11707900	0.81007200
H	1.18433400	0.77193700	0.82219600
H	1.66521700	3.12737100	1.38687800
H	5.59723600	2.71606400	-0.32204700

PATH (*R*)

Complex 1

OPTIMIZATION: E(RB97D) = -2029.806996 (Hartree/Particle)
Zero-point correction = 0.728076
Thermal correction to Energy = 0.773419
Thermal correction to Enthalpy = 0.774363
Thermal correction to Gibbs Free Energy = 0.648774
Sum of electronic and zero-point Energies = -2029.078921
Sum of electronic and thermal Energies = -2029.033577
Sum of electronic and thermal Enthalpies = -2029.032633
Sum of electronic and thermal Free Energies = -2029.158222

SINGLE POINT: E(RB97D) = -2029.888142 (Hartree/Particle)

XYZ coordinates

C	1.00192600	2.30691500	-0.46145500
C	2.27945700	1.68889800	-0.40210400
C	1.57956500	3.61848100	-0.03877900
N	-0.22141900	1.89038000	-0.75767600
C	2.93762700	2.93087700	0.02963300
N	2.69755900	0.43451100	-0.61229600
O	1.13038700	4.74017200	0.16953200
H	-0.37754200	0.91190900	-1.04002700
O	4.09515600	3.23791600	0.33836000

H	1.98803100	-0.24162900	-0.97576000
C	4.10487400	0.06278200	-0.61442400
C	4.38843500	-1.03806000	0.43118300
C	4.53888300	-0.44706800	-2.00368000
H	4.69646400	0.95125000	-0.37013600
C	5.87312600	-1.41158500	0.45178800
H	3.78227500	-1.91668800	0.17906000
C	6.01932800	-0.85479400	-2.01782600
H	3.90855000	-1.30722100	-2.27246200
C	6.30550800	-1.91055300	-0.93975300
H	6.06517600	-2.18756000	1.20155000
H	6.46685500	-0.52725900	0.71984400
H	6.29218200	-1.23941800	-3.00869300
H	6.64096300	0.03328900	-1.83044600
H	7.37268000	-2.16354400	-0.91765300
H	5.75543600	-2.83360600	-1.17626800
H	4.34012400	0.34750000	-2.73210000
N	3.86492400	-0.63085900	1.80817000
C	4.49675000	0.60391600	2.38053000
H	3.95863800	0.85100500	3.29932700
H	5.54354800	0.38787400	2.60527100
H	4.41894100	1.42905900	1.67021600
C	3.92719300	-1.75914500	2.79431500
H	4.96949000	-1.94595600	3.06043100
H	3.35899500	-1.45700200	3.67735300
H	3.46497600	-2.63623000	2.33972600
C	-1.38910300	2.78829600	-0.71079100
C	-2.02955600	2.89389700	-2.10569100
H	-1.00389900	3.77699300	-0.43362600
C	-3.41904600	3.53793700	-2.02435200
H	-2.12463100	1.88712000	-2.52534100
H	-1.35700700	3.47628300	-2.74849600
C	-4.34285400	2.65479000	-1.17183400
H	-3.83751000	3.65855700	-3.03223900
H	-3.34592700	4.54032900	-1.57569000
H	-5.33350000	3.11510300	-1.05503400
H	-4.48474400	1.69448400	-1.69095900
C	-3.75387000	2.36880600	0.19361400
C	-4.59785300	2.07874100	1.27733900
C	-2.36012700	2.37425700	0.39736400
C	-4.08539800	1.78158300	2.54142400
C	-1.85106900	2.08343500	1.67246600
C	-2.69960200	1.77893100	2.73889700
H	-4.75928400	1.55264200	3.36501100
H	-0.77358400	2.08455000	1.82335500
H	-2.28273200	1.54825300	3.71759200
H	-5.67589100	2.08624000	1.11685000
H	2.83900000	-0.43786400	1.68366900

O	1.07370700	-0.32692800	1.86991300
N	0.53317000	-1.39316300	1.45157700
O	1.19481500	-2.43361200	1.26980100
C	-0.86285400	-1.34731000	1.23966600
H	-1.27993900	-0.36103100	1.38583600
C	-1.56862700	-2.46007800	0.90861900
H	-1.02645600	-3.39599600	0.79765500
C	-3.01422400	-2.51428000	0.81412100
C	-3.63292500	-3.77236800	0.63794400
C	-3.82944900	-1.36353300	0.90876000
C	-5.02019300	-3.88282900	0.57613700
H	-3.00833700	-4.65974800	0.54827100
C	-5.21537700	-1.47975100	0.84683600
H	-3.38539000	-0.38044900	1.01407000
C	-5.81722400	-2.73488700	0.68483500
H	-5.48244800	-4.85845900	0.44106200
H	-5.82524400	-0.58240000	0.91820500
H	-6.90114200	-2.81788800	0.63436700
O	-2.34536200	-0.27936400	-1.66113900
C	-2.35539200	-1.45858900	-2.06752300
C	-3.68581000	-2.04091600	-2.55629300
H	-4.37458000	-2.10001000	-1.70438800
H	-4.12672800	-1.35460600	-3.29146200
H	-3.58273700	-3.03770700	-3.00186100
C	-1.21929500	-2.33797600	-2.10448200
C	0.11724000	-1.97860900	-1.84209200
O	0.49493100	-0.83748000	-1.43652300
H	-1.39234200	-3.34902200	-2.46620300
C	1.20396300	-3.03063600	-2.06693800
H	0.79559800	-4.00450500	-2.36149100
H	1.88409400	-2.67885700	-2.85622200
H	1.78672900	-3.14693500	-1.14487200

TS*(R)*

OPTIMIZATION: E(RB97D) = -2029.80099 (Hartree/Particle)
Zero-point correction = 0.728348
Thermal correction to Energy = 0.772564
Thermal correction to Enthalpy = 0.773508
Thermal correction to Gibbs Free Energy = 0.651143
Sum of electronic and zero-point Energies = -2029.072642
Sum of electronic and thermal Energies = - 2029.028426
Sum of electronic and thermal Enthalpies = -2029.027481
Sum of electronic and thermal Free Energies = -2029.149847

SINGLE POINT: E(RB97D) = -2029.881487 (Hartree/Particle)

XYZ coordinates

C	1.02721700	2.35493900	-0.38633300

C	2.29022400	1.71051000	-0.34756900
C	1.61756700	3.62582700	0.12723500
N	-0.20063400	1.98710800	-0.73074300
C	2.96435100	2.91536400	0.16493600
N	2.70023800	0.46987300	-0.63646200
O	1.18338500	4.73977100	0.39850800
H	-0.38168000	1.03705300	-1.06730700
O	4.12281200	3.19001700	0.49406700
H	2.02065800	-0.17236300	-1.06720800
C	4.09888800	0.06276200	-0.58126200
C	4.31903600	-1.07916300	0.43680600
C	4.58043800	-0.40066300	-1.97081800
H	4.69132700	0.93259900	-0.28040200
C	5.79703500	-1.48250100	0.49039900
H	3.70221700	-1.93269100	0.13335500
C	6.05107200	-0.84059800	-1.94622800
H	3.94489000	-1.23615100	-2.30063500
C	6.27246900	-1.94175000	-0.89956500
H	5.94788800	-2.28709200	1.21882400
H	6.39823500	-0.62048600	0.81061300
H	6.35308900	-1.19198200	-2.94110400
H	6.68304700	0.02573400	-1.70058000
H	7.33249400	-2.21985500	-0.84750800
H	5.71215200	-2.84264500	-1.19147500
H	4.42666000	0.42550800	-2.67470700
N	3.76365600	-0.71645400	1.80847800
C	4.40577200	0.47177300	2.45451700
H	3.83257100	0.70222700	3.35634200
H	5.43527100	0.21873400	2.72024400
H	4.38547000	1.32627400	1.77643100
C	3.76731500	-1.88645200	2.74520300
H	4.79457100	-2.12421200	3.03010500
H	3.18623700	-1.60055900	3.62536500
H	3.28146500	-2.72296700	2.24085100
C	-1.35456100	2.90012100	-0.63076900
C	-1.96622000	3.13421300	-2.02332800
H	-0.95544200	3.85438200	-0.26738400
C	-3.34858200	3.78901800	-1.91145500
H	-2.06648200	2.17091800	-2.53445600
H	-1.27398600	3.75936400	-2.60161400
C	-4.30118100	2.84818700	-1.15809400
H	-3.74505800	4.00638700	-2.91194300
H	-3.26996000	4.74557700	-1.37312300
H	-5.28543400	3.31478000	-1.01588200
H	-4.45459300	1.94433900	-1.76767000
C	-3.74176200	2.43082300	0.18681500
C	-4.61084600	2.05049000	1.22213400
C	-2.35331200	2.41182700	0.42093400

C	-4.12692900	1.65236600	2.46932700
C	-1.87286600	2.01682700	1.67917500
C	-2.74601600	1.63201100	2.69796900
H	-4.81897300	1.35715000	3.25592600
H	-0.79908100	1.99235100	1.85196400
H	-2.35127600	1.31906000	3.66268800
H	-5.68492600	2.07229400	1.03787500
H	2.72288300	-0.50178400	1.68166700
O	1.07688200	-0.36318800	1.86445800
N	0.53540500	-1.35995600	1.24390600
O	1.25514400	-2.33198200	0.85923800
C	-0.81256300	-1.33487300	1.04164400
H	-1.29965300	-0.42535200	1.35928100
C	-1.47616100	-2.42388600	0.44066500
H	-0.91450900	-3.35562000	0.43477100
C	-2.93469500	-2.58434200	0.63258700
C	-3.49264500	-3.87337300	0.54774400
C	-3.78978400	-1.48986100	0.86033900
C	-4.86796100	-4.06883300	0.69056000
H	-2.83721200	-4.72409500	0.36521300
C	-5.16363500	-1.68662400	1.00134600
H	-3.39271800	-0.48153000	0.91132200
C	-5.71002400	-2.97291900	0.91572800
H	-5.28244800	-5.07310200	0.62541700
H	-5.80688900	-0.82670900	1.17490900
H	-6.78272600	-3.12114800	1.02415900
O	-2.30508100	-0.09287600	-1.78906200
C	-2.41446700	-1.30516200	-1.97871500
C	-3.70266600	-1.90157100	-2.53102200
H	-4.07427200	-2.67863200	-1.84986300
H	-4.45725900	-1.11801600	-2.64949600
H	-3.50814000	-2.38183000	-3.50130400
C	-1.35415700	-2.27973900	-1.66572900
C	0.04741300	-1.94777300	-1.86251100
O	0.48780700	-0.78804200	-1.76169600
H	-1.61003700	-3.31246100	-1.90413500
C	0.97625400	-3.10278100	-2.20850100
H	0.74481600	-3.98475300	-1.59887000
H	0.83606500	-3.37799100	-3.26459900
H	2.01841300	-2.80945700	-2.05137300

Complex 2

OPTIMIZATION: E(RB97D) = -2029.80842 (Hartree/Particle)
Zero-point correction = 0.728772
Thermal correction to Energy = 0.773253
Thermal correction to Enthalpy = 0.774198
Thermal correction to Gibbs Free Energy = 0.651298

Sum of electronic and zero-point Energies = -2029.079649
Sum of electronic and thermal Energies = -2029.035167
Sum of electronic and thermal Enthalpies = -2029.034223
Sum of electronic and thermal Free Energies = -2029.157122

SINGLE POINT: E(RB97D) = -2029.888585 (Hartree/Particle)

XYZ coordinates

C	1.04160700	2.37615300	-0.38600400
C	2.30014300	1.72638600	-0.35891500
C	1.64070000	3.64972000	0.10476900
N	-0.19345500	2.00985100	-0.71035100
C	2.98626800	2.93478200	0.13526500
N	2.70773500	0.48731000	-0.65033700
O	1.21285200	4.76850300	0.36625900
H	-0.38891400	1.05569800	-1.01342600
O	4.14763800	3.20780000	0.44954900
H	2.03501900	-0.17343300	-1.04040900
C	4.09618000	0.05415300	-0.53909800
C	4.26194800	-1.08054700	0.49727300
C	4.61612900	-0.43003600	-1.90741900
H	4.68932200	0.91981500	-0.22823700
C	5.73469800	-1.49758100	0.60309000
H	3.64832200	-1.92768700	0.17176200
C	6.07980500	-0.88668300	-1.83020500
H	3.98097800	-1.26227200	-2.24685500
C	6.25392500	-1.97708800	-0.76375500
H	5.85231500	-2.29649000	1.34367900
H	6.33389900	-0.63911000	0.93707200
H	6.41019600	-1.25269500	-2.81085100
H	6.71306700	-0.02435000	-1.57386600
H	7.30886400	-2.26518300	-0.67309300
H	5.69439900	-2.87579200	-1.06428300
H	4.49558100	0.38945200	-2.62562200
N	3.66054700	-0.70876800	1.84085000
C	4.28219300	0.47767300	2.50176600
H	3.67244600	0.72202900	3.37584100
H	5.29972900	0.22737900	2.81524000
H	4.29632000	1.32632200	1.81685000
C	3.62630300	-1.87332700	2.78018600
H	4.63982900	-2.12463500	3.10308100
H	3.01745900	-1.57933900	3.63883100
H	3.14529300	-2.70489800	2.26171100
C	-1.34526300	2.92567200	-0.60915300
C	-1.94842100	3.17312900	-2.00334600
H	-0.94356900	3.87520900	-0.23660100
C	-3.32669000	3.83642900	-1.89356800
H	-2.05322300	2.21388300	-2.52236500
H	-1.24878900	3.79581800	-2.57506900

C	-4.28985700	2.89396700	-1.15633700
H	-3.71550200	4.06851100	-2.89372900
H	-3.24400100	4.78586700	-1.34370400
H	-5.27003900	3.36772500	-1.01041500
H	-4.45304000	2.00143500	-1.78063900
C	-3.73900300	2.45210400	0.18497300
C	-4.61647600	2.05211700	1.20589000
C	-2.35243900	2.42895200	0.43005900
C	-4.14200300	1.63259300	2.44947600
C	-1.88158600	2.01325000	1.68537000
C	-2.76308800	1.60996800	2.68927600
H	-4.83994300	1.32161200	3.22466400
H	-0.80919500	1.97831500	1.86462900
H	-2.37565100	1.27800700	3.65045800
H	-5.68905600	2.07585800	1.01324700
H	2.59148100	-0.49466500	1.69246100
O	1.06405500	-0.33192900	1.83093000
N	0.50154700	-1.29524800	1.13135700
O	1.24752500	-2.24733200	0.68137500
C	-0.80752600	-1.26197600	0.90650500
H	-1.33470000	-0.40618800	1.29735700
C	-1.45719900	-2.38220700	0.19099300
H	-0.90519300	-3.30192900	0.41935500
C	-2.91757400	-2.58216300	0.56218200
C	-3.43892800	-3.88488700	0.58206500
C	-3.78245100	-1.50481300	0.81064300
C	-4.79384300	-4.11270300	0.84215400
H	-2.77339900	-4.72677100	0.39248900
C	-5.13652100	-1.73044000	1.07349600
H	-3.41280900	-0.48461200	0.79303000
C	-5.64926900	-3.03215400	1.08679200
H	-5.17912700	-5.13071300	0.85846600
H	-5.78756200	-0.88062300	1.26765900
H	-6.70440100	-3.20459400	1.29081000
O	-2.25364700	-0.09283300	-1.75914700
C	-2.37119900	-1.29002300	-1.96293200
C	-3.54951500	-1.87506500	-2.71271700
H	-4.07800100	-2.57353000	-2.04819900
H	-4.22708500	-1.08137500	-3.04109700
H	-3.19496500	-2.45625600	-3.57645800
C	-1.36458600	-2.30583200	-1.43313300
C	0.06401200	-2.02492600	-1.87779200
O	0.50915000	-0.88404300	-1.94609600
H	-1.65064000	-3.30743500	-1.77363500
C	0.87541000	-3.23941800	-2.27044300
H	0.76670800	-4.02135700	-1.50898100
H	0.48782000	-3.63978700	-3.21984800
H	1.92924400	-2.97163300	-2.38935600

PATH (*S*)

Complex 1

OPTIMIZATION: E(RB97D) = -2029.809188 (Hartree/Particle)
Zero-point correction = 0.728159
Thermal correction to Energy = 0.77401
Thermal correction to Enthalpy = 0.774954
Thermal correction to Gibbs Free Energy = 0.646554
Sum of electronic and zero-point Energies = -2029.081029
Sum of electronic and thermal Energies = -2029.035178
Sum of electronic and thermal Enthalpies = -2029.034234
Sum of electronic and thermal Free Energies = -2029.162634

SINGLE POINT: E(RB97D) = -2029.8902 (Hartree/Particle)

XYZ coordinates

C	-0.36437700	2.43224100	0.12649000
C	-1.70235100	1.97561200	0.09495800
C	-0.68507500	3.60458600	-0.72905100
N	0.73131500	1.97149900	0.72027400
C	-2.13117400	3.10156100	-0.75939400
N	-2.30980400	0.89644800	0.59834400
O	-0.04308600	4.53683600	-1.19938300
H	0.61988500	1.14857600	1.33157500
O	-3.19859900	3.44196500	-1.27315600
H	-1.73277100	0.21262200	1.11914500
C	-3.76490200	0.80607100	0.67016100
C	-4.28425900	-0.51620000	0.07608900
C	-4.26822900	0.92323000	2.12281600
H	-4.17738400	1.64257800	0.09580800
C	-5.81387400	-0.53948300	0.06579600
H	-3.89229100	-1.34184700	0.67630000
C	-5.80316100	0.86603100	2.18034200
H	-3.83275200	0.10296100	2.71166100
C	-6.33438300	-0.41117900	1.51066100
H	-6.18307200	-1.47002300	-0.38041400
H	-6.19306700	0.29936700	-0.53362200
H	-6.14162800	0.91693600	3.22309600
H	-6.21425600	1.74441100	1.66070900
H	-7.43152800	-0.41576200	1.50370300
H	-6.00631900	-1.28942000	2.08620000
H	-3.89439600	1.86594000	2.53943600
N	-3.67255800	-0.76194200	-1.29954300
C	-4.04082200	0.25311900	-2.34066600
H	-3.43931100	0.03843900	-3.22621900
H	-5.10524200	0.15050800	-2.56278600
H	-3.81868200	1.25656900	-1.97256400
C	-3.93145900	-2.15549300	-1.79356500

H	-4.99728200	-2.26098900	-2.00649300
H	-3.33837600	-2.29602000	-2.69925800
H	-3.59579400	-2.84338100	-1.01588600
C	2.05961300	2.57740600	0.55824100
C	2.74910000	2.63863300	1.92888300
H	1.89510600	3.60033900	0.19625600
C	4.21968400	3.04019500	1.77593500
H	2.69115000	1.64650700	2.40361100
H	2.20085900	3.33953700	2.56947800
C	4.97156700	1.96088800	0.98531000
H	4.68299100	3.17868700	2.76111700
H	4.28129100	4.00164800	1.24551700
H	5.99203800	2.29065000	0.74840500
H	5.07415500	1.06341800	1.61568000
C	4.26114600	1.56839000	-0.29553400
C	4.97538300	0.89406700	-1.29885400
C	2.89386400	1.84029000	-0.49647900
C	4.36272400	0.50559100	-2.48971000
C	2.28880700	1.46451100	-1.70562900
C	3.01109500	0.80093800	-2.69711900
H	4.93560200	-0.01801700	-3.25289700
H	1.23511000	1.67759900	-1.86384300
H	2.51810400	0.50962500	-3.62244400
H	6.02923200	0.67232200	-1.13292200
H	-2.64938300	-0.69534000	-1.15963600
C	1.46187200	-1.46147800	-0.83176200
C	2.73656100	-1.85978200	-0.26795200
C	3.59512100	-2.80162800	-0.87679400
C	3.13925800	-1.26271900	0.94279600
C	4.80383300	-3.14398700	-0.27802400
H	3.31708700	-3.25995700	-1.82268200
C	4.34232700	-1.61571700	1.54887000
H	2.48673300	-0.53060000	1.40522800
C	5.18022900	-2.55522100	0.93882200
H	5.45882600	-3.86876800	-0.75680000
H	4.62886900	-1.15846300	2.49312100
H	6.12403400	-2.82969400	1.40584200
O	-0.23499500	-0.23360400	2.15051100
C	0.22974700	-1.34100600	2.57214200
C	1.18708800	-1.26526900	3.76352600
H	1.72670500	-2.20362200	3.93639600
H	1.90697400	-0.44981100	3.61287800
H	0.60769700	-1.01864800	4.66526300
C	-0.05087400	-2.61792300	2.04686200
C	-0.94614700	-2.92894300	0.98534100
O	-1.71794200	-2.12082400	0.40810800
H	0.49806200	-3.45023400	2.48060500
C	-0.96066500	-4.38233300	0.49455700

H	-1.98866500	-4.76963800	0.52746500
H	-0.63902000	-4.40018900	-0.55662100
H	-0.30668100	-5.04155700	1.07771600
C	0.87951000	-2.01723800	-1.91597500
H	1.25236500	-2.86405500	-2.47743100
N	-0.37124900	-1.53369500	-2.41878000
O	-0.83398500	-0.45247600	-2.00781400
O	-0.94088100	-2.23358200	-3.27812800
H	0.92635700	-0.66246500	-0.32539000

$TS_{(S)}$

OPTIMIZATION: E(RB97D) = -2029.794159 (Hartree/Particle)
Zero-point correction = 0.727943
Thermal correction to Energy = 0.772581
Thermal correction to Enthalpy = 0.773525
Thermal correction to Gibbs Free Energy = 0.648571
Sum of electronic and zero-point Energies = -2029.066216
Sum of electronic and thermal Energies = -2029.021578
Sum of electronic and thermal Enthalpies = -2029.020634
Sum of electronic and thermal Free Energies = -2029.145589

SINGLE POINT: E(RB97D) = -2029.874714 (Hartree/Particle)

XYZ coordinates

C	0.64107900	2.43760200	-0.43145800
C	1.95402900	1.91655300	-0.39305100
C	1.06197400	3.68943600	0.25642100
N	-0.51584400	1.98943900	-0.90743600
C	2.47562200	3.11324100	0.29985100
N	2.50506400	0.76744800	-0.79491700
O	0.49640200	4.71146600	0.62444900
H	-0.55228000	1.07552200	-1.36904500
O	3.57740000	3.45317700	0.73464900
H	1.93170100	0.01509500	-1.18781400
C	3.94371400	0.52603500	-0.71922200
C	4.27001600	-0.73062400	0.11198200
C	4.54575100	0.36150000	-2.12979800
H	4.40129400	1.40105100	-0.24682400
C	5.78643300	-0.92860700	0.21605900
H	3.80589800	-1.58865900	-0.38620200
C	6.06320300	0.13500000	-2.06737000
H	4.05384200	-0.49049200	-2.61949100
C	6.39517700	-1.08055500	-1.19016200
H	6.01728200	-1.81614500	0.81578200
H	6.23594400	-0.05848700	0.71373600
H	6.46293300	-0.00446400	-3.07987800
H	6.54586300	1.02948900	-1.64584100
H	7.48098300	-1.21178500	-1.10275600

H	5.99102800	-1.99018700	-1.65870400
H	4.30579700	1.26268700	-2.70620600
N	3.59318800	-0.69753600	1.48009200
C	4.00707900	0.44038700	2.36374100
H	3.36356100	0.41316200	3.24659700
H	5.05259100	0.30400000	2.64984200
H	3.87711400	1.38541200	1.83445800
C	3.74365800	-2.00210100	2.20609700
H	4.77112300	-2.10155500	2.56187100
H	3.03522600	-1.99516900	3.03646200
H	3.49718400	-2.81019600	1.51357000
C	-1.78569700	2.69265400	-0.67158600
C	-2.60238000	2.74675400	-1.96928400
H	-1.52007400	3.71878000	-0.38853000
C	-3.96872100	3.38613400	-1.69484500
H	-2.73426300	1.72688100	-2.36063600
H	-2.03760700	3.31567300	-2.71756700
C	-4.77666800	2.51020700	-0.72727600
H	-4.52423900	3.52158400	-2.63157800
H	-3.81824300	4.38328800	-1.25589300
H	-5.68404400	3.03188000	-0.39428100
H	-5.11927300	1.61251900	-1.26824800
C	-3.97989300	2.05629900	0.48251000
C	-4.66007100	1.52647700	1.58974700
C	-2.57060600	2.08131200	0.49477600
C	-3.97075600	1.02037600	2.69179600
C	-1.88393000	1.57814100	1.61069100
C	-2.57200200	1.04310000	2.69972800
H	-4.51949200	0.60651800	3.53585400
H	-0.79759600	1.57759700	1.61612900
H	-2.01725300	0.64320800	3.54592900
H	-5.74936300	1.49964000	1.57207000
H	2.54739100	-0.59091300	1.33046700
C	-1.51253400	-1.60626100	0.43555900
C	-2.91931400	-1.99819300	0.19774200
C	-3.43143200	-3.24110100	0.61520100
C	-3.76797400	-1.11778300	-0.49194100
C	-4.76072400	-3.58264500	0.36347700
H	-2.78209200	-3.94630600	1.13024200
C	-5.09979000	-1.45480900	-0.73783300
H	-3.37840700	-0.15977600	-0.81828500
C	-5.60238300	-2.68837600	-0.31210500
H	-5.14255500	-4.54729100	0.69237800
H	-5.74519600	-0.75332000	-1.26284700
H	-6.63962100	-2.95452900	-0.50566000
O	-0.78243600	-0.46583600	-2.47954500
C	-1.13920500	-1.64394700	-2.33160500
C	-2.20367500	-2.25084000	-3.23024500

H	-2.65880100	-1.47865300	-3.85869200
H	-1.74769100	-3.02277600	-3.86816000
H	-2.97185800	-2.74274400	-2.61956900
C	-0.61280200	-2.51433400	-1.27646600
C	0.82606300	-2.62543800	-1.03705600
O	1.69723300	-1.87082300	-1.49886400
H	-1.13012200	-3.46814800	-1.18048200
C	1.22230500	-3.81155900	-0.16789300
H	2.31196400	-3.88361000	-0.09403400
H	0.78375500	-3.68990100	0.83437500
H	0.81967000	-4.74669400	-0.57868600
C	-0.91282500	-1.98845100	1.65175300
H	-1.33782200	-2.70991700	2.33619100
N	0.24956700	-1.41439800	2.08937400
O	0.86091500	-0.57821200	1.32155300
O	0.71404200	-1.70337600	3.22883800
H	-1.23286200	-0.62159200	0.07392400

Complex 2

OPTIMIZATION: E(RB97D) = -2029.805349 (Hartree/Particle)
Zero-point correction = 0.729391
Thermal correction to Energy = 0.773673
Thermal correction to Enthalpy = 0.774617
Thermal correction to Gibbs Free Energy = 0.652428
Sum of electronic and zero-point Energies = -2029.075957
Sum of electronic and thermal Energies = -2029.031676
Sum of electronic and thermal Enthalpies = -2029.030732
Sum of electronic and thermal Free Energies = -2029.15292

SINGLE POINT: E(RB97D) = -2029.885386 (Hartree/Particle)

XYZ coordinates

C	0.71146300	2.42093000	-0.60625900
C	2.01913400	1.88841800	-0.55066300
C	1.16017600	3.71838000	-0.02786100
N	-0.46664700	1.95987700	-1.01912400
C	2.56967300	3.13282000	0.02799800
N	2.55541000	0.70778400	-0.87547100
O	0.61438600	4.77297600	0.26968900
H	-0.54626900	1.00724500	-1.37832000
O	3.68432100	3.49355200	0.40626800
H	1.96365900	-0.04820700	-1.21519700
C	3.97445800	0.40940400	-0.70072800
C	4.20068300	-0.79207600	0.24325600
C	4.63759400	0.11437000	-2.06126300
H	4.44599000	1.29855700	-0.27054800
C	5.70334200	-1.04148700	0.43130600
H	3.73095000	-1.66995200	-0.21736800

C	6.13899100	-0.16568800	-1.90606400
H	4.13483700	-0.75289200	-2.51270800
C	6.37485900	-1.32212700	-0.92488600
H	5.86703100	-1.88915900	1.10542300
H	6.16239400	-0.15422600	0.88878800
H	6.57991300	-0.39726100	-2.88403000
H	6.63846500	0.73893800	-1.52843000
H	7.44841300	-1.48872900	-0.77105700
H	5.95651600	-2.24878200	-1.34579100
H	4.46393400	0.97773200	-2.71422200
N	3.46417600	-0.63921300	1.56670400
C	3.80349100	0.58939500	2.34834800
H	3.11890000	0.62528800	3.19974100
H	4.83863300	0.52356200	2.69474300
H	3.67201900	1.47510300	1.72779400
C	3.61282300	-1.85189500	2.43533200
H	4.60702300	-1.86077900	2.88841900
H	2.82750300	-1.79781100	3.19261400
H	3.46951300	-2.74221000	1.81873000
C	-1.72388000	2.67128000	-0.73583500
C	-2.61200100	2.69598300	-1.98631500
H	-1.44211700	3.70385200	-0.49652600
C	-3.95130900	3.36318800	-1.65037600
H	-2.77934400	1.66724500	-2.33809800
H	-2.08544800	3.23597300	-2.78245900
C	-4.71390200	2.52828100	-0.61189500
H	-4.55948800	3.48163700	-2.55621900
H	-3.76000600	4.36975800	-1.25054400
H	-5.58430300	3.08084700	-0.23304000
H	-5.11375600	1.62847700	-1.10721800
C	-3.85196900	2.07900800	0.55432200
C	-4.47220000	1.57165900	1.70612400
C	-2.44387100	2.08747700	0.48521500
C	-3.72582000	1.07204300	2.77355100
C	-1.69993300	1.59171300	1.56706400
C	-2.32868500	1.07767000	2.70090900
H	-4.22969300	0.67355700	3.65236700
H	-0.61541500	1.57147600	1.50943700
H	-1.72680600	0.67671800	3.51330800
H	-5.56098000	1.55644700	1.75113300
H	2.39290100	-0.59821700	1.35066400
C	-1.52021300	-1.59868400	0.22777200
C	-3.00281100	-1.92303100	0.12640200
C	-3.51633900	-3.12926900	0.62888400
C	-3.86918500	-1.04879800	-0.54010600
C	-4.87005100	-3.44464800	0.48430500
H	-2.85191300	-3.82264200	1.14257700
C	-5.22374000	-1.36081700	-0.69017100

H	-3.47951400	-0.11341400	-0.92714400
C	-5.73002400	-2.55875300	-0.17689600
H	-5.25473400	-4.37928000	0.88865000
H	-5.88439100	-0.66360100	-1.20249300
H	-6.78498400	-2.80155600	-0.28921700
O	-1.09843700	-0.60743900	-2.50306900
C	-1.21524800	-1.80518300	-2.28347300
C	-1.78413600	-2.76126000	-3.30174600
H	-2.70538700	-3.19936100	-2.88939300
H	-1.99835300	-2.24905400	-4.24425000
H	-1.08206100	-3.59155800	-3.46619800
C	-0.79557700	-2.41376500	-0.94474900
C	0.73782300	-2.54154700	-0.87488700
O	1.50358400	-1.95147500	-1.63103100
H	-1.17583400	-3.44171800	-0.88065800
C	1.22216000	-3.62600300	0.06221100
H	2.31130400	-3.59182800	0.15283200
H	0.73591400	-3.54179100	1.04209500
H	0.93073000	-4.60041800	-0.35716600
C	-1.01165500	-1.80734700	1.61299400
H	-1.61112500	-2.24031900	2.40182800
N	0.14018000	-1.26636100	1.99316100
O	0.88175400	-0.69877700	1.04689900
O	0.56754500	-1.27314200	3.19378600
H	-1.36642100	-0.54563500	-0.03099100

10.3. TS structures for rate-limiting step with catalyst 1g, 1h, 1j, 1p and 1s (PCM-(Toluene)-B97-D/def2-TZVP//PCM-(Toluene)-B97-D/TZVP approximation)

Catalyst 1g

SINGLE POINT: E(RB97D) = -1283.171406 (Hartree/Particle)

XYZ coordinates

C	-0.64518100	-2.86798500	-0.89240600
C	-1.99465500	-2.52207900	-1.06611800
C	-0.98111100	-4.16664600	-0.26068200
N	0.51621200	-2.24331100	-1.16501100
C	-2.46432700	-3.78709100	-0.44191600
N	-2.62483700	-1.46714800	-1.60469600
O	-0.33844500	-5.08903000	0.21884800
H	0.46468200	-1.25896800	-1.41109800
O	-3.55439400	-4.26344400	-0.16330100
H	-2.03537100	-0.68521300	-1.87425900
C	-3.95686300	-1.05957800	-1.12060300
C	-3.81199000	0.04551500	-0.04212400
C	-4.82426100	-0.56845300	-2.28844100
H	-4.42045500	-1.94818600	-0.67954200

C	-5.21031300	0.49081700	0.44348200
H	-3.34957200	0.90713300	-0.55196800
C	-6.20664900	-0.10616700	-1.80068200
H	-4.30949700	0.27317100	-2.77969100
C	-6.07618500	0.98437400	-0.72616500
H	-5.09545300	1.27702200	1.20105900
H	-5.70740900	-0.36114200	0.92809200
H	-6.79819300	0.25832400	-2.65083000
H	-6.74380100	-0.96812500	-1.37686700
H	-7.06834700	1.28459400	-0.36305300
H	-5.60951500	1.87692600	-1.17192700
H	-4.91732200	-1.37443700	-3.02665700
N	-2.86814700	-0.34890900	1.01443400
C	-3.37593100	-1.36686900	1.93540900
H	-2.54033900	-1.74203600	2.54032500
H	-4.14930400	-0.97713900	2.62669400
H	-3.79833700	-2.21004400	1.38110300
C	-2.32820700	0.79222300	1.74805600
H	-3.08277300	1.30342900	2.38191900
H	-1.51647300	0.44623200	2.40136300
H	-1.91680300	1.52569900	1.04206400
C	1.73961800	-2.61044700	-0.42016300
H	1.73627400	-3.70449900	-0.33302200
C	2.99218600	-1.18195100	1.05645900
C	3.27380900	-0.48019400	2.23289400
C	1.81959400	-1.95895800	0.95543500
C	2.36409500	-0.56039300	3.29570700
C	0.91765300	-2.04290900	2.01013900
C	1.19639400	-1.33039000	3.18708100
H	0.01991600	-2.65091900	1.92970000
H	0.50551300	-1.38330900	4.02617200
H	4.17875300	0.11753000	2.32495400
H	2.56628600	-0.02005600	4.21863600
C	2.99613100	-2.09573600	-1.10053100
C	3.44640900	-2.33481000	-2.39384000
C	3.72357200	-1.27097900	-0.21547700
C	4.65156700	-1.74372000	-2.80613500
H	2.87632300	-2.96670900	-3.07263500
C	4.92721700	-0.68844100	-0.62496300
C	5.38370000	-0.93217900	-1.92700900
H	5.02327600	-1.91946900	-3.81358700
H	5.49964000	-0.05590400	0.05094200
H	6.31812300	-0.48548800	-2.26160600

$TS_{(R)}$-1g

SINGLE POINT: E(RB97D) = -2142.937542 (Hartree/Particle)

XYZ coordinates

C	-0.44817300	-2.43914900	-0.32971200
C	-1.79377600	-2.00805800	-0.40106200
C	-0.84369500	-3.80183200	0.10200700
N	0.72450500	-1.86169600	-0.58210900
C	-2.29550900	-3.34282500	0.00308700
N	-2.38571400	-0.84138000	-0.67703400
O	-0.23833900	-4.82453600	0.40335200
H	0.73290800	-0.91301800	-0.96840800
O	-3.40981600	-3.83775500	0.17624100
H	-1.81913000	-0.03763100	-0.95908900
C	-3.83721800	-0.72636500	-0.84190300
C	-4.45695300	0.29617000	0.13648100
C	-4.17177200	-0.32699000	-2.29472500
H	-4.26908600	-1.71294800	-0.64815500
C	-5.97212500	0.40175800	-0.07867700
H	-3.98057600	1.26570700	-0.03719200
C	-5.68388100	-0.19138000	-2.51800700
H	-3.67307600	0.62520200	-2.51143000
C	-6.28226100	0.81616300	-1.52741300
H	-6.40200100	1.13232100	0.61571000
H	-6.43962600	-0.57164400	0.12458800
H	-5.87972300	0.12374900	-3.55107100
H	-6.16775200	-1.16984500	-2.37745700
H	-7.36914400	0.89381100	-1.65778500
H	-5.85450500	1.81175400	-1.71575000
H	-3.74374700	-1.09065300	-2.95542000
N	-4.11430000	-0.02602800	1.59124200
C	-4.59503800	-1.35827400	2.07896000
H	-4.17989800	-1.50706900	3.07930400
H	-5.68671300	-1.34593500	2.12613200
H	-4.25107300	-2.15131900	1.41420400
C	-4.57083300	1.05454200	2.52683800
H	-5.65343700	0.98575600	2.65572400
H	-4.05950400	0.89687900	3.47890000
H	-4.27122100	2.01738800	2.11321400
C	1.99792000	-2.48403000	-0.22606000
H	1.82557000	-3.56827500	-0.16720600
C	3.93316000	-1.62713600	0.91719300
C	4.68841600	-1.17806800	2.00448500
C	2.58525800	-2.00314800	1.09589800
C	4.06838700	-1.07908800	3.25642000
C	1.96698600	-1.90352000	2.33586400
C	2.71939800	-1.42608700	3.42052700
H	0.91886200	-2.16713900	2.46032900
H	2.25176900	-1.32568700	4.39768400
H	5.73100600	-0.89125700	1.88153500
H	-3.05027000	-0.02303700	1.68869600

O	-1.46026800	0.06690500	2.15255400
N	-1.03530300	1.23303900	1.77747100
O	-1.79810100	2.23898100	1.85980800
C	0.23623400	1.32894900	1.30007700
H	0.77344500	0.39287700	1.25934300
C	0.72965600	2.56673300	0.81745300
H	0.19449400	3.43695500	1.19309500
C	2.19314500	2.77966100	0.68007100
C	2.67702500	4.09775700	0.57978200
C	3.11191800	1.72031900	0.59933600
C	4.03621200	4.35146600	0.39245800
H	1.97259600	4.92644900	0.64293800
C	4.47129100	1.97242700	0.40813000
H	2.77746500	0.69193700	0.68234600
C	4.94035800	3.28523700	0.29844800
H	4.39122500	5.37774300	0.31940100
H	5.15961300	1.13443500	0.33914300
H	6.00043300	3.47844200	0.14611600
O	0.19005100	0.62636400	-1.76149200
C	0.68587600	1.76473200	-1.80142500
C	1.98659100	2.01325700	-2.54416300
H	2.60078000	2.76175600	-2.03133600
H	2.54216900	1.07618900	-2.65735900
H	1.74746800	2.40469900	-3.54538100
C	0.09037100	2.89721500	-1.09935600
C	-1.37684600	3.05690900	-1.00991600
O	-2.19145400	2.15867200	-1.23717700
H	0.61298900	3.84251600	-1.24434800
C	-1.84199900	4.46115100	-0.64485700
H	-2.91952300	4.46212000	-0.45582500
H	-1.31035300	4.82001000	0.24634200
H	-1.61308000	5.15415800	-1.46759400
H	4.63683300	-0.71728400	4.11099100
C	3.11803500	-2.17930300	-1.20661400
C	3.11994700	-2.29416600	-2.59140300
C	4.25966500	-1.72621800	-0.51089200
C	4.28902200	-1.95688700	-3.29190700
H	2.22975800	-2.62749900	-3.12159200
C	5.42818600	-1.40519700	-1.20853500
C	5.43246300	-1.52383200	-2.60432300
H	4.30973200	-2.03360600	-4.37716700
H	6.31674200	-1.06230500	-0.68138600
H	6.33156700	-1.27160900	-3.16346300

$TS_{(S)}$-1g

SINGLE POINT: E(RB97D) = -2142.933014 (Hartree/Particle)

XYZ coordinates

C	0.66821100	-2.40782300	-0.05207500
C	2.00059100	-1.98265400	0.14237000
C	1.09072200	-3.53664600	-0.91924300
N	-0.51890500	-1.98819000	0.38619100
C	2.53051600	-3.07599100	-0.70788800
N	2.57176600	-0.96321600	0.79262700
O	0.50925300	-4.42046000	-1.53664200
H	-0.54637700	-1.16473600	0.98977800
O	3.65090400	-3.41957300	-1.08373000
H	1.99439000	-0.25188500	1.24461200
C	4.02465600	-0.79357900	0.82409000
C	4.48108800	0.52534700	0.16521000
C	4.55918500	-0.82759600	2.26951200
H	4.45953400	-1.63458700	0.27496600
C	6.01173100	0.59211000	0.12419000
H	4.08730900	1.35399600	0.75916000
C	6.09171200	-0.71685900	2.29374100
H	4.10705700	0.00390000	2.82866300
C	6.56549700	0.54747000	1.56062300
H	6.34298100	1.51040000	-0.37452400
H	6.40561100	-0.26150800	-0.44414800
H	6.45037500	-0.71311500	3.33088600
H	6.52216800	-1.60185800	1.80191100
H	7.66153300	0.58846900	1.53073100
H	6.21764600	1.43764900	2.10516500
H	4.22716900	-1.76342100	2.73416900
N	3.84656500	0.73003600	-1.20348500
C	4.27880400	-0.25056300	-2.25035700
H	3.63729600	-0.09531600	-3.12119300
H	5.32383500	-0.05775600	-2.50433900
H	4.15956700	-1.26632400	-1.87030200
C	4.02996100	2.13703600	-1.69098200
H	5.07986300	2.29755500	-1.94494600
H	3.38731100	2.26507700	-2.56449200
H	3.71652300	2.81302800	-0.89238600
C	-1.75973700	-2.44163600	-0.24799300
H	-1.55777900	-3.44397800	-0.65176800
C	-3.63369800	-1.27582700	-1.19804000
C	-4.31926800	-0.47998100	-2.12004800
C	-2.26262000	-1.54890200	-1.37626700
C	-3.61046300	0.04787300	-3.20557000
C	-1.55750900	-1.03016400	-2.45450700
C	-2.24239700	-0.21697900	-3.36956600
H	-4.12328700	0.68426600	-3.92435500
H	-0.49253800	-1.21681400	-2.56651500
H	-1.70307400	0.22157000	-4.20635000

H	-5.37416100	-0.25048500	-1.98395100
H	2.79486100	0.61912600	-1.11454300
C	-1.16788300	1.76609500	-0.28727700
C	-2.56621800	2.19204100	-0.03483900
C	-3.07073800	3.43470700	-0.45989400
C	-3.41579700	1.33479100	0.68216200
C	-4.39286400	3.79454300	-0.19223500
H	-2.42799300	4.12738700	-0.99862200
C	-4.73797400	1.69009200	0.94971000
H	-3.03913800	0.37524800	1.02291400
C	-5.23379100	2.92221400	0.51118500
H	-4.76870700	4.75777600	-0.53221900
H	-5.37679900	0.99797900	1.49341300
H	-6.26445300	3.20444800	0.71751000
O	-0.17776800	0.18547200	2.31707500
C	-0.64260200	1.33213200	2.40803600
C	-1.65530400	1.67522100	3.48468200
H	-2.49268300	2.23701900	3.05146800
H	-2.01945400	0.76436100	3.97075300
H	-1.17884100	2.32500100	4.23463400
C	-0.27836700	2.40880700	1.47699900
C	1.14182800	2.68259700	1.20777300
O	2.07911100	1.93299900	1.50956800
H	-0.85791000	3.32274900	1.60370400
C	1.40779800	4.00509700	0.50479500
H	2.47694100	4.23997900	0.52236500
H	1.06539800	3.92147300	-0.53869900
H	0.83668400	4.82207300	0.96309400
C	-0.53046400	2.22251500	-1.46651800
H	-0.89027800	3.04001500	-2.07501900
N	0.58857400	1.61205000	-1.95323800
O	1.11455600	0.63893000	-1.28783800
O	1.09937300	1.99096500	-3.04820900
H	-0.95877800	0.72593900	-0.05529300
C	-2.95765900	-2.49468500	0.68360800
C	-3.05783300	-3.05684600	1.95058600
C	-4.06586100	-1.86718800	0.07350200
C	-4.29361000	-3.00037300	2.61489200
H	-2.19339100	-3.52241500	2.42036000
C	-5.30039300	-1.82856800	0.72862700
C	-5.40434700	-2.40029900	2.00325400
H	-4.39247400	-3.42921000	3.61010600
H	-6.16185700	-1.35356200	0.26351300
H	-6.35691200	-2.37352400	2.52947400

Catalyst 1h

SINGLE POINT: E(RB97D) = -1361.762665 (Hartree/Particle)

XYZ coordinates

C	0.11998000	-2.72312400	0.86975500
C	1.50562700	-2.73389600	1.08895000
C	0.13149700	-4.06195500	0.22979100
N	-0.84581500	-1.81533600	1.11257100
C	1.66064900	-4.06080800	0.43508000
N	2.36444600	-1.88947100	1.67910500
O	-0.71139900	-4.80467800	-0.24893100
H	-0.53333800	-0.87498300	1.32774900
O	2.60605300	-4.77943300	0.14921400
H	1.98981200	-0.99477800	1.97820900
C	3.77883100	-1.83708800	1.27029300
C	4.01066400	-0.64998500	0.30154800
C	4.69776000	-1.71751500	2.49492200
H	3.99525700	-2.77988600	0.75763700
C	5.49502100	-0.62345400	-0.12980200
H	3.81989800	0.26489100	0.88755300
C	6.17553300	-1.65898600	2.07464500
H	4.43499400	-0.80047700	3.04667700
C	6.42508800	-0.50705700	1.08845600
H	5.65800900	0.21276900	-0.82187100
H	5.72441400	-1.54958700	-0.67511800
H	6.81159200	-1.55125700	2.96306200
H	6.44750900	-2.61068200	1.59364500
H	7.47455300	-0.50150500	0.76466100
H	6.23685400	0.45177600	1.59665200
H	4.51344800	-2.56889200	3.16148600
N	3.02645700	-0.63322700	-0.79445800
C	3.20360200	-1.70481800	-1.77884100
H	2.32504700	-1.72907700	-2.43540200
H	4.10330900	-1.56379700	-2.40900100
H	3.28017800	-2.67486400	-1.27919400
C	2.95769600	0.66908500	-1.45311500
H	3.87939300	0.92711000	-2.01357900
H	2.12350000	0.66783600	-2.16530500
H	2.77649700	1.45320500	-0.70603500
C	-2.12117700	-1.90993900	0.39150000
H	-2.32328500	-2.98367600	0.32941400
C	-3.13980300	-1.47306600	-1.94087700
C	-2.99733400	-0.95938400	-3.24242200
C	-2.04023400	-1.37395800	-1.05662400
C	-1.81518500	-0.37146300	-3.68784700
C	-0.84816200	-0.78616200	-1.51653700
C	-0.73006200	-0.28646300	-2.81427500
H	0.02108700	-0.72930700	-0.86668100
H	0.20778200	0.15771300	-3.14032700
H	-3.84557000	-1.03491200	-3.92287900

H	-1.74219800	0.01011000	-4.70446200
C	-3.25698600	-1.24423000	1.15974100
C	-3.04867400	-0.26027100	2.13373300
C	-4.57440800	-1.63201800	0.84020100
C	-4.12839200	0.34274300	2.78830300
H	-2.04259000	0.04554000	2.41080700
C	-5.64758900	-1.02483100	1.50445100
C	-5.43422200	-0.04078500	2.47449100
H	-3.94449700	1.10457300	3.54330800
H	-6.66199700	-1.33505000	1.25644700
H	-6.27984100	0.41862400	2.98264800
C	-4.50613000	-2.09314900	-1.64768600
H	-5.26171700	-1.32581700	-1.87204500
H	-4.66698100	-2.89944100	-2.37783000
C	-4.81243500	-2.65178800	-0.24429500
H	-5.86466000	-2.96099600	-0.23018400
H	-4.21875800	-3.55838400	-0.06575200

$TS_{(R)}$-1h

SINGLE POINT: E(RB97D) = -2221.525504 (Hartree/Particle)

XYZ coordinates

C	-0.25719700	-2.40191600	0.04366700
C	-1.61637600	-2.03633900	-0.10901700
C	-0.61678800	-3.71940400	0.62737200
N	0.90006200	-1.80825600	-0.23344100
C	-2.07979100	-3.33108500	0.44239800
N	-2.24910700	-0.93810600	-0.53733100
O	0.01349500	-4.67666300	1.06212300
H	0.88759700	-0.92472000	-0.74901500
O	-3.17967600	-3.84362700	0.65305500
H	-1.71190200	-0.14221300	-0.89072300
C	-3.69031300	-0.93931600	-0.80181600
C	-4.44119500	0.16264100	-0.02359400
C	-3.95377000	-0.76833900	-2.31313800
H	-4.07910200	-1.91463100	-0.49386200
C	-5.94506600	0.09246200	-0.31984900
H	-4.04118300	1.13317000	-0.33139400
C	-5.45461500	-0.80347900	-2.63183800
H	-3.51941400	0.18771800	-2.63190600
C	-6.20157000	0.26840900	-1.82680000
H	-6.47882000	0.86840400	0.23997200
H	-6.33709400	-0.88354200	-0.00180100
H	-5.61153100	-0.65437100	-3.70791000
H	-5.85818800	-1.79486500	-2.37606100
H	-7.28081400	0.21837600	-2.01929000
H	-5.85684800	1.26573300	-2.13714800

H	-3.42244700	-1.57173400	-2.83759400
N	-4.15386900	0.10159800	1.47381500
C	-4.57712800	-1.16795300	2.14719000
H	-4.20600000	-1.13052600	3.17466800
H	-5.66846700	-1.22422700	2.14317000
H	-4.14985800	-2.02779900	1.62934400
C	-4.71821200	1.28616800	2.20088300
H	-5.80509100	1.19137000	2.25823200
H	-4.27830200	1.29375700	3.20031700
H	-4.41552300	2.18949000	1.67021000
C	2.20362800	-2.37088500	0.17037600
H	2.01331900	-3.41468700	0.44649100
C	4.12165700	-1.46247300	1.61205700
C	4.59542300	-0.82658000	2.76421300
C	2.74561300	-1.65546800	1.41680800
C	3.70105500	-0.37698100	3.74034500
C	1.85740900	-1.22650900	2.41576500
C	2.32916300	-0.58521200	3.56383700
H	0.78740200	-1.36740500	2.28921500
H	1.61962800	-0.24204300	4.31400600
H	5.66570300	-0.67503700	2.89306400
H	-3.09954300	0.18924400	1.61808300
O	-1.56844600	0.44761400	2.18508900
N	-1.14830900	1.57915300	1.70662400
O	-1.90257400	2.59201800	1.71907400
C	0.11952100	1.61990900	1.20991600
H	0.63661900	0.67462200	1.23524300
C	0.63451100	2.79243900	0.61306200
H	0.09736700	3.70411200	0.86854500
C	2.10321900	2.97393200	0.47667900
C	2.59853300	4.24775500	0.13906000
C	3.02094200	1.92049600	0.63675500
C	3.96405200	4.46148300	-0.05166300
H	1.89798200	5.07283700	0.01807300
C	4.38824000	2.13321300	0.44517700
H	2.68436800	0.93091300	0.92836300
C	4.86633300	3.39948000	0.09374000
H	4.32565700	5.45442100	-0.31212000
H	5.07633800	1.30176800	0.57835500
H	5.93186900	3.56198800	-0.05592500
O	0.30046600	0.55017900	-1.71371900
C	0.69820800	1.70769900	-1.92255900
C	1.95934000	1.96727300	-2.72763800
H	2.67011300	2.54870300	-2.12467500
H	2.41188300	1.02129400	-3.03715000
H	1.71713000	2.57176300	-3.61368200
C	0.03192400	2.87885100	-1.35798200
C	-1.43724400	2.95234700	-1.28253800

O	-2.18342200	1.97062200	-1.35027300
H	0.49936300	3.83023800	-1.61157200
C	-2.00597000	4.35805500	-1.13853600
H	-1.45086800	4.92428800	-0.37943700
H	-1.90500900	4.89559300	-2.09304900
H	-3.06283500	4.30694000	-0.86119100
H	4.82519100	-1.79800300	0.85458100
H	4.06940200	0.12990500	4.63007700
C	3.14374600	-2.35392500	-1.02303600
C	3.55106100	-3.55400700	-1.61686100
C	3.59725900	-1.13840500	-1.55638100
C	4.40265400	-3.54335700	-2.72789700
H	3.19788900	-4.49864600	-1.20610100
C	4.44270900	-1.12349900	-2.66732000
H	3.29715300	-0.20155900	-1.09462500
C	4.84991200	-2.32781900	-3.25577000
H	4.71464500	-4.48311400	-3.17965700
H	4.78769700	-0.17348900	-3.07177900
H	5.51192000	-2.31747000	-4.11962900

$TS_{(S)}$-1h

SINGLE POINT: E(RB97D) = -2221.523881 (Hartree/Particle)

XYZ coordinates

C	0.44287500	-2.37460200	-0.50498900
C	1.78933200	-2.01195000	-0.27830400
C	0.82491800	-3.38299500	-1.52814200
N	-0.71817100	-1.98386200	0.01208200
C	2.27866500	-2.97815700	-1.28852600
N	2.39645200	-1.11221000	0.50540100
O	0.21443300	-4.17175200	-2.23850500
H	-0.71144200	-1.28150600	0.75396400
O	3.38483200	-3.28416900	-1.73325800
H	1.84276600	-0.47587900	1.08175600
C	3.85209200	-1.09374300	0.65366600
C	4.46661100	0.27584100	0.30339900
C	4.27243700	-1.46523500	2.08953500
H	4.25600700	-1.84674900	-0.03055700
C	5.99589800	0.19313400	0.35527800
H	4.10665900	1.00738800	1.03090700
C	5.80308100	-1.51358000	2.22199100
H	3.85205400	-0.72018200	2.77991000
C	6.43948600	-0.18633100	1.78043400
H	6.44360900	1.15214400	0.07021600
H	6.34954300	-0.56893300	-0.35255000
H	6.08197500	-1.74332700	3.25828300
H	6.19103400	-2.32729300	1.59137300

H	7.53407400	-0.25330700	1.81652600
H	6.13641500	0.61300700	2.47282500
H	3.82800200	-2.43707900	2.33467700
N	3.94993200	0.80646100	-1.02655900
C	4.34281000	-0.00541200	-2.22343400
H	3.78353200	0.38767800	-3.07588100
H	5.41757300	0.10311900	-2.38666600
H	4.08523200	-1.05264300	-2.05388900
C	4.31005900	2.24979300	-1.22168300
H	5.38479600	2.33310500	-1.39644700
H	3.74038200	2.61532300	-2.07819100
H	4.02161100	2.79319700	-0.31873800
C	-2.01491100	-2.41344000	-0.54000300
H	-1.81477400	-3.32349100	-1.11798100
C	-3.97631500	-1.32367100	-1.75282800
C	-4.50795100	-0.39667800	-2.65380400
C	-2.59464600	-1.36957900	-1.50682900
C	-3.66560700	0.49678200	-3.32418900
C	-1.75541600	-0.48322800	-2.19686400
C	-2.28805400	0.44720000	-3.09476700
H	-4.08078300	1.22824600	-4.01469300
H	-0.68417500	-0.49172500	-2.01814300
H	-1.62108100	1.13892700	-3.60469300
H	-5.58269800	-0.36675400	-2.82424800
H	2.89151800	0.79803500	-1.00909600
C	-0.99343600	2.16997000	-0.18581900
C	-2.36367100	2.69858600	0.03704700
C	-2.60107600	4.06696400	0.25793800
C	-3.45337800	1.81473100	0.02472000
C	-3.89843600	4.53743600	0.46556300
H	-1.76149500	4.75970400	0.28049900
C	-4.75346000	2.28520200	0.22858400
H	-3.28314200	0.76178600	-0.17731300
C	-4.98064500	3.64629600	0.45458700
H	-4.06811900	5.59840200	0.63951200
H	-5.58628100	1.58512100	0.20575300
H	-5.99173400	4.01400000	0.61828100
O	-0.25350100	-0.03222200	2.10365600
C	-0.72136000	1.09415900	2.33568500
C	-1.94751300	1.25769100	3.21709800
H	-1.71821600	1.91643200	4.06657800
H	-2.74599700	1.74507800	2.63929600
H	-2.28729300	0.28343600	3.58058500
C	-0.19318300	2.31654800	1.72489000
C	1.26007000	2.52780600	1.60820000
O	2.12049600	1.65548500	1.77195400
H	-0.72046400	3.22319700	2.01728000
C	1.66770900	3.94749800	1.24446200

H	2.73906600	4.09233800	1.41768400
H	1.44617800	4.10722900	0.17750600
H	1.08916300	4.69106700	1.80651100
C	-0.22197000	2.81533000	-1.18236300
H	-0.44916700	3.79702000	-1.57621600
N	0.86638500	2.21041500	-1.74561300
O	1.23094000	1.04747800	-1.31846700
O	1.49986500	2.78152600	-2.68026500
H	-0.91172500	1.08702800	-0.20356900
H	-4.63895400	-2.00521900	-1.22432200
C	-2.95474100	-2.76574500	0.60185500
C	-3.34614100	-1.78564100	1.52555200
C	-3.44264000	-4.06946200	0.74242800
C	-4.20603000	-2.10495300	2.57760700
H	-2.97538300	-0.76981000	1.42265000
C	-4.31226800	-4.39242800	1.79152000
H	-3.14007400	-4.83199100	0.02628500
C	-4.69477600	-3.41117000	2.71150800
H	-4.49887300	-1.33607600	3.29042100
H	-4.68754200	-5.40933800	1.88972200
H	-5.36911400	-3.66097100	3.52844800

Catalyst 1j

SINGLE POINT: E(RB97D) = -1284.373138 (Hartree/Particle)

XYZ coordinates

C	-0.63667200	-2.89597400	-1.11827800
C	-1.99612200	-2.55562300	-1.09532400
C	-0.85447800	-4.14394000	-0.34408900
N	0.45967400	-2.29344400	-1.61331200
C	-2.34670000	-3.74856300	-0.28050600
N	-2.71308300	-1.54651900	-1.61685900
O	-0.14558800	-5.05290300	0.05581400
H	0.36474100	-1.34084600	-1.94924800
O	-3.36717500	-4.16999400	0.24258100
H	-2.18399900	-0.80646300	-2.06842300
C	-3.93185900	-1.06894100	-0.94011500
C	-3.60503600	0.16758100	-0.06474500
C	-5.02418400	-0.72982500	-1.96481600
H	-4.28355200	-1.88880300	-0.30533800
C	-4.89122600	0.65403800	0.64071600
H	-3.28950600	0.96061000	-0.76366500
C	-6.29716200	-0.21673600	-1.27301500
H	-4.63896300	0.04411200	-2.64811000
C	-5.99055900	0.99466300	-0.37862700
H	-4.65526400	1.52683400	1.26309300
H	-5.25095800	-0.13877100	1.31126100

H	-7.05233900	0.04198100	-2.02683500
H	-6.71866200	-1.02416300	-0.65522600
H	-6.89929400	1.32604000	0.14167100
H	-5.65296200	1.83312400	-1.00794800
H	-5.23709900	-1.62299500	-2.56487600
N	-2.44710700	-0.07225900	0.81395000
C	-2.71102900	-0.99428000	1.92257200
H	-1.75618500	-1.27609300	2.38301500
H	-3.35600900	-0.55015800	2.70561000
H	-3.19017300	-1.90663800	1.55598300
C	-1.85350800	1.16987300	1.30283600
H	-2.50721900	1.72072500	2.00975300
H	-0.91554700	0.94046500	1.82395900
H	-1.62676100	1.83063000	0.45558900
C	1.79650500	-2.63482200	-1.08177000
H	1.86283700	-3.72874600	-1.10951700
C	3.13230800	-2.67698200	1.04553900
C	3.38097800	-2.31118100	2.36898900
C	1.99829300	-2.19934700	0.37119000
C	2.49387100	-1.45796800	3.03838600
C	1.11224000	-1.34906200	1.04343200
C	1.36207400	-0.98191100	2.37246700
H	0.21216900	-0.98567300	0.55153000
H	0.66291100	-0.32798900	2.89023900
H	4.26145800	-2.69496200	2.88094400
H	3.82143700	-3.34084900	0.52534200
H	2.68113000	-1.17506500	4.07238700
C	2.83992500	-2.05560500	-2.02760500
C	3.33702000	-2.83674900	-3.07947100
C	3.26424000	-0.72534300	-1.89990700
C	4.24954400	-2.29793300	-3.99170500
H	3.00576600	-3.86934900	-3.17915300
C	4.17004200	-0.18133700	-2.81641900
H	2.89846900	-0.12497300	-1.06878600
C	4.66540900	-0.96736400	-3.86319200
H	4.63655400	-2.91519100	-4.80024600
H	4.49686400	0.85112500	-2.70733100
H	5.37711700	-0.54748000	-4.57144400

$TS_{(R)}$-1j

SINGLE POINT: E(RB97D) = -2144.138644 (Hartree/Particle)

XYZ coordinates

C	-0.08530900	-2.28186800	-0.80631400
C	-1.48489100	-2.08084400	-0.77833400
C	-0.22872800	-3.75530600	-0.70295800
N	0.97194900	-1.47085100	-0.88946100

C	-1.74102700	-3.53782800	-0.65745500
N	-2.28542900	-1.00668200	-0.78222900
O	0.54485000	-4.70374900	-0.66920300
H	0.78539900	-0.47233200	-0.95816400
O	-2.74753300	-4.23505900	-0.54300600
H	-1.88896100	-0.07416500	-0.92108700
C	-3.73445300	-1.14089400	-0.97278600
C	-4.54023800	-0.38400200	0.10437800
C	-4.14148000	-0.64385200	-2.37546100
H	-3.97525300	-2.20625600	-0.90812400
C	-6.04504400	-0.57546600	-0.12397400
H	-4.28380800	0.67778400	0.04637900
C	-5.64970800	-0.80100800	-2.61292600
H	-3.85119200	0.40963400	-2.46685900
C	-6.44254600	-0.06880600	-1.52181000
H	-6.61546200	-0.03430000	0.63880700
H	-6.29890100	-1.64154600	-0.04231700
H	-5.91381600	-0.41256700	-3.60494800
H	-5.91389200	-1.86934100	-2.59832900
H	-7.52173200	-0.20883500	-1.66360000
H	-6.23860200	1.01014300	-1.58355100
H	-3.56647200	-1.21919800	-3.11127100
N	-4.11716100	-0.78733200	1.51637700
C	-4.24373300	-2.24740500	1.82295000
H	-3.82741500	-2.41041200	2.82039400
H	-5.30111900	-2.52319300	1.80710900
H	-3.69102400	-2.83383800	1.08897600
C	-4.81157300	0.02691300	2.56733300
H	-5.85382000	-0.29058200	2.64246500
H	-4.28813400	-0.14588000	3.51028300
H	-4.72408300	1.07976100	2.29655700
C	2.31378800	-1.94492100	-0.53694900
H	2.33681800	-2.99468300	-0.84793400
C	3.80115100	-2.34215400	1.55645400
C	3.96617700	-2.23355200	2.94958900
C	2.57553100	-1.91607100	0.99144600
C	2.96343200	-1.74906800	3.78815400
C	1.55758400	-1.47117600	1.85157700
C	1.73934100	-1.37567700	3.23138100
H	0.58430700	-1.20789200	1.45438200
H	0.92204800	-1.01614200	3.85292100
H	4.91530400	-2.55193100	3.38136500
H	-3.09014400	-0.52325000	1.63343000
O	-1.60342800	-0.04023200	2.17173400
N	-1.44021100	1.22868400	1.94749900
O	-2.38027900	2.04042600	2.16920500
C	-0.22678000	1.63043700	1.47676700
H	0.47740700	0.83120100	1.32185700

C	0.02010900	2.96875300	1.10580400
H	-0.65225300	3.70307900	1.54537700
C	1.42079000	3.43532400	0.94264000
C	1.66699600	4.81984200	0.87944600
C	2.51167100	2.55580500	0.80594400
C	2.95614300	5.31355000	0.67774100
H	0.83093200	5.51004100	0.98401500
C	3.80247600	3.04880600	0.60096800
H	2.36973700	1.48079000	0.85706600
C	4.03103100	4.42696100	0.53170900
H	3.12375500	6.38801600	0.63359400
H	4.62722900	2.34880800	0.48789900
H	5.03722600	4.80828100	0.36968800
O	-0.07880300	1.16126500	-1.57238800
C	0.07371300	2.39422100	-1.60109400
C	1.19392100	3.02241200	-2.41360400
H	0.84278900	3.92054000	-2.93724800
H	1.99622800	3.33399200	-1.72894200
H	1.59327200	2.29946200	-3.13111800
C	-0.74065600	3.30065900	-0.79901700
C	-2.19046800	3.08483700	-0.66043700
O	-2.75722800	2.01852200	-0.91921700
H	-0.46551100	4.35225100	-0.87914300
C	-2.98638900	4.30273900	-0.21015500
H	-3.98614900	3.99667100	0.11166100
H	-2.47488500	4.82337300	0.60953500
H	-3.07584200	5.01031100	-1.04786000
H	3.13350500	-1.67942900	4.86106300
C	3.40345600	-1.19293700	-1.29785500
C	3.20329900	0.06616600	-1.87698200
C	4.67398500	-1.79798000	-1.39251400
C	4.24504100	0.72825700	-2.53471300
H	2.23342000	0.54935200	-1.83901600
C	5.70742700	-1.12880300	-2.06073300
C	5.50313200	0.13090100	-2.63157700
H	4.06538500	1.70895800	-2.97079000
H	6.68279100	-1.60895700	-2.13214400
H	6.31677500	0.63642700	-3.14855600
C	4.99576100	-2.94741400	0.82053700
H	5.87613100	-2.33002300	1.05391000
H	5.18992900	-3.93379300	1.26652700
C	4.93139700	-3.11502500	-0.70835500
H	5.89220800	-3.52337300	-1.04522100
H	4.16470600	-3.85619700	-0.97023200

$TS_{(S)}$-1j

SINGLE POINT: E(RB97D) = -2144.13378 (Hartree/Particle)

XYZ coordinates

C	-0.30906000	-2.38239600	-0.10029700
C	-1.69592300	-2.12948700	-0.15796000
C	-0.50060600	-3.63564000	0.67159600
N	0.76548700	-1.74046200	-0.56516800
C	-2.00438700	-3.34322100	0.63763700
N	-2.45425800	-1.15046100	-0.66793200
O	0.23954000	-4.49724400	1.12587800
H	0.59858000	-0.85324400	-1.03550000
O	-3.03210500	-3.84338800	1.08903500
H	-2.01520400	-0.35913800	-1.14258500
C	-3.90601200	-1.30744900	-0.77773900
C	-4.67792900	-0.10665700	-0.20179400
C	-4.33766500	-1.51459300	-2.24378200
H	-4.17642600	-2.20435700	-0.21171600
C	-6.18450200	-0.38741000	-0.23280600
H	-4.44987800	0.77389100	-0.80666200
C	-5.85164000	-1.75771700	-2.34233600
H	-4.05526900	-0.62271200	-2.82144900
C	-6.63727700	-0.61106200	-1.68818300
H	-6.73941700	0.45138400	0.20280300
H	-6.40595200	-1.28478400	0.36095100
H	-6.14545700	-1.86912500	-3.39390100
H	-6.09665000	-2.70185200	-1.83349300
H	-7.71406900	-0.82091900	-1.70681100
H	-6.47344800	0.31559800	-2.25796300
H	-3.77722300	-2.36626100	-2.64728500
N	-4.17899300	0.27207500	1.18582900
C	-4.36900200	-0.78252200	2.23313000
H	-3.84744300	-0.44231500	3.13092000
H	-5.43700900	-0.89882400	2.43077500
H	-3.94035700	-1.72418400	1.88462300
C	-4.74003700	1.58644300	1.64100000
H	-5.79812800	1.46584300	1.88308200
H	-4.16541200	1.89837300	2.51587500
H	-4.60674400	2.30582800	0.82934600
C	2.11315400	-2.06601300	-0.08818800
H	2.09704600	-3.14553600	0.09893200
C	3.70467500	-1.51135700	1.89943700
C	3.92715400	-0.80465900	3.09561300
C	2.44864500	-1.37436100	1.26173600
C	2.95027600	-0.00710500	3.68798800
C	1.45992600	-0.59967600	1.89154400
C	1.69645300	0.08370800	3.08338500
H	3.16357400	0.52423600	4.61365900
H	0.47422600	-0.51129300	1.45195300
H	0.90173000	0.67895600	3.52620000

H	4.90048500	-0.90264900	3.57682800
H	-3.13431900	0.44117500	1.14069400
C	0.53056800	2.28412100	0.41082500
C	1.88756500	2.84532400	0.20818600
C	2.14812100	4.22346800	0.31072300
C	2.94672300	1.97586600	-0.10070200
C	3.43832400	4.71725000	0.11218100
H	1.33242500	4.90832100	0.53620200
C	4.23935300	2.46841200	-0.29519400
H	2.76315300	0.90839900	-0.16978900
C	4.48937300	3.84073300	-0.19216300
H	3.62648500	5.78638500	0.19128500
H	5.04579700	1.77643400	-0.52959100
H	5.49460900	4.22791700	-0.34681400
O	-0.18851000	0.53633200	-2.19026100
C	0.15990200	1.72857300	-2.26271500
C	1.26428200	2.15593500	-3.21268700
H	0.95542300	3.03094800	-3.79988100
H	2.14160800	2.45486400	-2.62009200
H	1.53690700	1.33151500	-3.87791200
C	-0.39014600	2.76616900	-1.39303700
C	-1.84036200	2.83165200	-1.13817400
O	-2.64163500	1.91953500	-1.36617100
H	0.05701000	3.74979300	-1.53152900
C	-2.31405000	4.14906400	-0.54215500
H	-3.40687200	4.17335000	-0.48626000
H	-1.89015100	4.25517100	0.46831700
H	-1.94961900	4.99894700	-1.13402000
C	-0.20529500	2.72141700	1.53724100
H	-0.00576000	3.63940700	2.07353100
N	-1.24568200	1.98483800	2.03219900
O	-1.54152100	0.85955100	1.47114200
O	-1.89264300	2.39093200	3.03957000
H	0.44704600	1.22004500	0.21969100
C	3.16609600	-1.78036200	-1.15960100
C	2.93148300	-0.94791700	-2.26256000
C	4.43205300	-2.38488600	-1.01710300
C	3.94000100	-0.69149400	-3.19724400
H	1.96037900	-0.49340100	-2.42656000
C	5.43138600	-2.12750700	-1.96448000
C	5.19691500	-1.28081400	-3.05131900
H	3.73427700	-0.03560100	-4.04100800
H	6.40347800	-2.60411100	-1.84302300
H	5.98426400	-1.09108800	-3.77854800
C	4.87827800	-2.37931300	1.45182300
C	4.72747300	-3.23943900	0.18675700
H	3.94515300	-3.99510800	0.33976000
H	5.66702700	-3.78356700	0.03048300

H	5.74864200	-1.72083100	1.30971700
H	5.13334000	-3.04279600	2.29089900

Catalyst 1p

SINGLE POINT: E(RB97D) = -1171.323299 (Hartree/Particle)

XYZ coordinates

C	0.64038100	-2.94699600	-0.20753100
C	1.99048100	-2.71397900	0.09891600
C	0.97876900	-3.78683900	-1.38274400
N	-0.51503100	-2.53611600	0.34249600
C	2.46031000	-3.54524000	-1.03758100
N	2.62127500	-2.04108400	1.07738000
O	0.34152500	-4.37499800	-2.24575900
H	-0.45231800	-1.79412600	1.03361000
O	3.55074800	-3.85635500	-1.49391000
H	2.02647100	-1.48785900	1.68823400
C	3.92739900	-1.40885300	0.81396900
C	3.71781800	0.02292200	0.24973900
C	4.76222700	-1.37153600	2.10088800
H	4.43432600	-2.02927800	0.06691000
C	5.08627000	0.70678700	0.02561600
H	3.19513600	0.58285200	1.04309000
C	6.11195600	-0.67042400	1.87879800
H	4.19302600	-0.82621600	2.87149000
C	5.91028700	0.74771400	1.32139700
H	4.92212400	1.71965300	-0.36572500
H	5.64270600	0.14710400	-0.73904400
H	6.67430000	-0.63948300	2.82131700
H	6.70770500	-1.25771100	1.16374400
H	6.88085600	1.22843200	1.13859800
H	5.38076700	1.35834500	2.06955200
H	4.90673200	-2.39693400	2.46294500
N	2.81305000	0.01676300	-0.90527100
C	3.41387900	-0.45818900	-2.15219900
H	2.61317700	-0.65551200	-2.87659500
H	4.11089200	0.27796900	-2.60006800
H	3.95336100	-1.39456800	-1.98352300
C	2.12353700	1.28674600	-1.10892000
H	2.79922100	2.10155900	-1.44527500
H	1.34345700	1.15311000	-1.86889800
H	1.64120500	1.60169900	-0.17415300
C	-1.76078400	-2.49666000	-0.47112900
H	-1.69979400	-3.35392000	-1.15066600
C	-2.10893500	0.01926600	-0.74453200
C	-1.99096200	1.19503000	-1.49114200
C	-1.74368400	-1.21746100	-1.29829800

C	-1.50251200	1.14779300	-2.80249200
C	-1.25450800	-1.25671100	-2.61121600
C	-1.13460300	-0.08123100	-3.36043900
H	-0.75354900	-0.12635000	-4.37907500
H	-2.28357400	2.14733600	-1.05217100
H	-0.95882300	-2.21396800	-3.03672200
H	-2.49568400	0.06577400	0.27237700
H	-1.40950600	2.06314000	-3.38392100
C	-2.99348400	-2.68514800	0.43480100
H	-3.00464000	-1.86927400	1.17503100
C	-4.28252300	-2.60927100	-0.39849000
H	-5.15860100	-2.75312000	0.24648900
H	-4.37862100	-1.64561500	-0.91123800
H	-4.28454800	-3.40388800	-1.15800400
C	-2.91895100	-4.02417100	1.18487600
H	-2.91211600	-4.85588300	0.46630500
H	-2.01117900	-4.09478100	1.79503800
H	-3.79297700	-4.14287200	1.83803400

$TS_{(R)}$-1p

SINGLE POINT: E(RB97D) = -2031.083448 (Hartree/Particle)

XYZ coordinates

C	0.47540500	2.52400800	-0.03277300
C	1.75594000	1.91996400	-0.07367200
C	1.03245800	3.78965900	0.51293100
N	-0.75016500	2.12456200	-0.35349400
C	2.40993600	3.14716200	0.43343000
N	2.21123100	0.70985800	-0.42014600
O	0.56266200	4.86642200	0.86548100
H	-0.86305300	1.22657600	-0.83228900
O	3.57190200	3.47812500	0.67915200
H	1.57000400	0.01502200	-0.80868300
C	3.64660800	0.43402200	-0.53309300
C	4.07648600	-0.76079900	0.34496400
C	4.02974000	0.18083300	-2.00645900
H	4.17877800	1.32892300	-0.19666100
C	5.57762800	-1.03871900	0.18894100
H	3.49402600	-1.63794600	0.04558900
C	5.52814900	-0.11084200	-2.16058200
H	3.44211000	-0.66583200	-2.37876900
C	5.93044300	-1.30403300	-1.28461100
H	5.86706300	-1.90178800	0.79838000
H	6.14990700	-0.16981200	0.54282900
H	5.76219100	-0.31119200	-3.21411200
H	6.10965500	0.77327900	-1.85808900
H	7.00621400	-1.50483500	-1.36772600

H	5.39879600	-2.20420700	-1.62611500
H	3.74203700	1.07127500	-2.57880900
N	3.69253700	-0.55014900	1.81170400
C	4.25418200	0.68351800	2.44977600
H	3.83392000	0.74856500	3.45688400
H	5.34174500	0.59309400	2.50446900
H	3.97777800	1.56766900	1.87612000
C	4.01630400	-1.74838900	2.65488300
H	5.09269600	-1.77852500	2.83864400
H	3.46994600	-1.64181300	3.59479900
H	3.66962900	-2.64085100	2.13502200
C	-1.91566200	3.02526700	-0.29153400
H	-1.59305500	3.89286600	0.29621000
C	-4.24807900	1.93643800	-0.06033700
C	-5.22563600	1.31550700	0.72661500
C	-3.01997800	2.31770400	0.49505800
C	-4.97824800	1.04166500	2.07341800
C	-2.77898600	2.03129400	1.85012600
C	-3.74356200	1.39493400	2.63292000
H	-3.53585800	1.17998800	3.67929100
H	-6.17998000	1.04331800	0.27957200
H	2.62919000	-0.46999100	1.85828700
O	0.98968000	-0.46437100	2.19271000
N	0.53485400	-1.54853700	1.65091100
O	1.27267500	-2.57766300	1.59241400
C	-0.73353700	-1.54469300	1.15630300
H	-1.24815800	-0.59788300	1.23486900
C	-1.23684800	-2.68992600	0.48627300
H	-0.70257500	-3.60670500	0.72838800
C	-2.70151300	-2.89569700	0.34154600
C	-3.16435500	-4.19780300	0.07108600
C	-3.64045300	-1.85438700	0.43510300
C	-4.52330100	-4.45755800	-0.10644700
H	-2.44151600	-5.00969400	-0.00104200
C	-5.00178900	-2.11523700	0.25908500
H	-3.32300800	-0.83716000	0.64618500
C	-5.44982600	-3.41114900	-0.01645600
H	-4.86004400	-5.47211000	-0.31114500
H	-5.71100300	-1.29626800	0.33885600
H	-6.51166300	-3.60614200	-0.15380800
O	-0.53304200	-0.35538900	-1.68394600
C	-1.11368800	-1.42418400	-1.93037800
C	-2.42412500	-1.43293600	-2.69856700
H	-2.90437500	-0.45055700	-2.63396400
H	-2.20993100	-1.65179900	-3.75615800
H	-3.09993700	-2.21104500	-2.32648600
C	-0.61607300	-2.71059000	-1.44983200
C	0.83524400	-2.99802900	-1.39214700

O	1.71921600	-2.14370900	-1.48909800
H	-1.20527100	-3.56788700	-1.77218300
C	1.19977800	-4.46144200	-1.17444700
H	0.48936000	-5.14508000	-1.65476100
H	2.21541900	-4.64944100	-1.53856200
H	1.17988500	-4.64740700	-0.09108800
H	-5.73473100	0.54991300	2.68161800
H	-4.45973400	2.13947100	-1.10603100
H	-1.82080000	2.30801100	2.28643100
C	-2.31418500	3.55458000	-1.69150400
H	-2.77050500	2.73044500	-2.26044300
C	-3.32885400	4.70277500	-1.54822200
H	-2.85877300	5.54358100	-1.01953900
H	-3.64392700	5.05731400	-2.53808600
H	-4.22042200	4.40479900	-0.98615200
C	-1.08527200	4.04974800	-2.47128300
H	-0.56597000	4.83437100	-1.90475700
H	-0.37455100	3.23928500	-2.66812200
H	-1.40198500	4.47250700	-3.43343200

$TS_{(S)}$-1p

SINGLE POINT: E(RB97D) = -2031.077889 (Hartree/Particle)

XYZ coordinates

C	0.45073200	-2.43807500	-0.39537600
C	1.78475100	-2.06117700	-0.12172500
C	0.88908600	-3.55336900	-1.27601700
N	-0.73760300	-1.99391600	0.00078900
C	2.32423300	-3.11154000	-1.01649000
N	2.35467500	-1.10131000	0.61466100
O	0.32422700	-4.42835100	-1.92258600
H	-0.75943000	-1.18397400	0.61869400
O	3.45019100	-3.43916600	-1.39298300
H	1.78226800	-0.43784700	1.13933700
C	3.80932800	-0.98436100	0.70494300
C	4.32282300	0.38806200	0.23069800
C	4.31153500	-1.22581900	2.14210200
H	4.23419400	-1.76048300	0.06061000
C	5.85498300	0.39333500	0.20864200
H	3.95380400	1.14859200	0.92318100
C	5.84696100	-1.18565300	2.19669000
H	3.88245000	-0.45555400	2.79807700
C	6.38713000	0.13723100	1.63238700
H	6.23284000	1.35390700	-0.16047300
H	6.21802700	-0.39453300	-0.46542800
H	6.18911000	-1.32534400	3.23013900
H	6.24779600	-2.02194300	1.60469400

H	7.48422600	0.13032100	1.61531600
H	6.07362300	0.96731200	2.28266100
H	3.93512400	-2.19990300	2.47632100
N	3.70768000	0.79303100	-1.10538000
C	4.06759500	-0.09454800	-2.25797200
H	3.44381500	0.20467800	-3.10373700
H	5.12552200	0.04480200	-2.49279200
H	3.87177000	-1.13508300	-1.99450700
C	3.99842500	2.22798300	-1.43018700
H	5.05706600	2.33449100	-1.67553800
H	3.36449400	2.50761800	-2.27355300
H	3.74221900	2.83060100	-0.55561200
C	-1.98264200	-2.38033600	-0.70529300
H	-1.81358700	-3.39830600	-1.07488500
C	-2.81826800	-0.23003200	-1.82035000
C	-2.85496200	0.64370500	-2.90976200
C	-2.15985800	-1.46237800	-1.91218700
C	-2.23883900	0.28878600	-4.11428000
C	-1.55822000	-1.81969100	-3.12810700
C	-1.59613900	-0.94987500	-4.22197400
H	-1.12006900	-1.23817700	-5.15762600
H	-3.36002600	1.60284500	-2.81233400
H	2.65248200	0.74704800	-1.01614300
C	-1.24354500	2.03814600	0.09068200
C	-2.59042200	2.54868600	0.45011400
C	-2.98471000	3.88001100	0.22183100
C	-3.50851300	1.68029600	1.06707400
C	-4.26318500	4.31610300	0.57648300
H	-2.28933600	4.58308600	-0.23033600
C	-4.78935600	2.11049300	1.41692300
H	-3.20717200	0.65648300	1.27372100
C	-5.17351300	3.43320800	1.17005000
H	-4.55112100	5.34847000	0.38724300
H	-5.48475700	1.41505900	1.88279400
H	-6.17066300	3.77456700	1.44025400
O	-0.36481600	-0.08309400	2.29485900
C	-0.71075500	1.05381600	2.64869400
C	-1.63933900	1.25065700	3.83420400
H	-1.07726200	1.71084800	4.66091200
H	-2.44992300	1.94226300	3.56968400
H	-2.04966900	0.29057700	4.16425600
C	-0.28403000	2.26768200	1.93756900
C	1.14733200	2.49289500	1.69123700
O	2.03549300	1.64723500	1.86111500
H	-0.79568000	3.17661700	2.25318900
C	1.49421200	3.88906600	1.19931700
H	2.57807200	4.04297700	1.21613000
H	1.12056500	3.99904900	0.16891200

H	0.99620400	4.65907600	1.80196700
C	-0.57539200	2.62272200	-1.00831900
H	-0.85896700	3.55803700	-1.46969300
N	0.49860700	2.01343300	-1.59999400
O	0.95075100	0.91417100	-1.10467500
O	1.03934800	2.53406600	-2.61715400
H	-1.12920500	0.95921900	0.14566900
H	-1.05047300	-2.77908900	-3.20517400
H	-3.30438800	0.06024100	-0.89523000
H	-2.25886400	0.97156200	-4.96162500
C	-3.16335200	-2.42454300	0.28370000
H	-3.31783800	-1.41193900	0.68441300
C	-4.44495200	-2.86442200	-0.43974000
H	-4.30808800	-3.86881100	-0.86485700
H	-5.28377800	-2.90531800	0.26703800
H	-4.70570500	-2.18071100	-1.25511600
C	-2.85978100	-3.36536900	1.46007500
H	-2.66673300	-4.38170800	1.08852900
H	-1.98143100	-3.03448500	2.02555900
H	-3.71981400	-3.40679300	2.14112600

Catalyst 1s

SINGLE POINT: E(RB97D) = -1069.455637 (Hartree/Particle)

XYZ coordinates

C	1.01878800	2.24126800	-1.01639200
C	2.23011500	1.55733400	-0.75214000
C	1.64345600	3.55901800	-0.71515000
N	-0.19851700	1.86187300	-1.38797300
C	2.94182100	2.80747700	-0.42840700
N	2.57249700	0.26406000	-0.76092000
O	1.25271400	4.72041700	-0.70283200
H	-0.40939000	0.86862000	-1.53174400
O	4.08786900	3.08467700	-0.06558000
H	1.87492400	-0.41242100	-1.09591300
C	3.93170200	-0.20475400	-0.51804500
C	3.99919500	-1.12646100	0.72094600
C	4.46179000	-0.96978800	-1.74754800
H	4.56526900	0.67259000	-0.35277900
C	5.43214800	-1.61506100	0.96329800
H	3.33145800	-1.97839700	0.54777600
C	5.88781000	-1.49180700	-1.52354200
H	3.78394600	-1.81189000	-1.95335100
C	5.95080700	-2.37555900	-0.26992000
H	5.46984300	-2.26580100	1.84412400
H	6.08437700	-0.75204000	1.15422800
H	6.22315200	-2.05271000	-2.40514600

H	6.57063400	-0.63798800	-1.40071500
H	6.97809400	-2.71244400	-0.08342800
H	5.33452000	-3.27402700	-0.42386200
H	4.41788700	-0.29487600	-2.61021000
N	3.39938000	-0.45302800	1.94847900
C	4.10575200	0.78932900	2.39508900
H	3.50467700	1.23798400	3.19029100
H	5.09270500	0.51972200	2.77906700
H	4.19592000	1.48979500	1.56323800
C	3.24109600	-1.40672400	3.09367500
H	4.22350600	-1.66042400	3.49771100
H	2.63649200	-0.90592300	3.85370500
H	2.71279700	-2.28829500	2.72742500
C	-1.30060300	2.80909000	-1.55193300
H	-0.87320100	3.81399200	-1.65516800
C	-3.65199700	2.91147300	-0.61131000
C	-4.51804600	2.95075000	0.48431500
C	-2.27467500	2.80672800	-0.38898100
C	-1.83870000	2.73577400	0.93946600
C	-2.78582600	2.77228100	1.96613400
H	-0.78237300	2.62912700	1.17289100
H	-2.46337300	2.70717200	3.00596600
H	-5.59458600	3.03235200	0.32638900
H	-4.04593400	2.94741700	-1.62503100
H	-1.83702800	2.55632200	-2.47161000
N	-4.11130500	2.88036700	1.76316300

$TS_{(R)}$-1s

SINGLE POINT: E(RB97D) = -1929.224223 (Hartree/Particle)

XYZ coordinates

C	1.02066900	2.22338200	-1.04159400
C	2.23354000	1.54659800	-0.76704100
C	1.64030100	3.54643100	-0.75260900
N	-0.19399000	1.83588600	-1.41310200
C	2.93919500	2.80179900	-0.45056600
N	2.58248700	0.25481700	-0.76593900
O	1.24668200	4.70681300	-0.75723900
H	-0.39962300	0.83963700	-1.54449900
O	4.08226200	3.08626900	-0.08394200
H	1.89046800	-0.42669300	-1.10157100
C	3.94354500	-0.20385900	-0.51305900
C	4.00963600	-1.11947100	0.73093500
C	4.48836900	-0.96911000	-1.73587000
H	4.56987400	0.67846500	-0.34684300
C	5.44391200	-1.59836200	0.98392900
H	3.34725400	-1.97575600	0.55798900

C	5.91793900	-1.47553800	-1.49933900
H	3.82054400	-1.81903000	-1.94249700
C	5.97826200	-2.35686000	-0.24384200
H	5.47980300	-2.24721600	1.86632900
H	6.08804700	-0.72992300	1.17817900
H	6.26750500	-2.03359800	-2.37719800
H	6.58999500	-0.61410300	-1.37042300
H	7.00683800	-2.68480500	-0.04847500
H	5.37111100	-3.26082200	-0.40178300
H	4.44338200	-0.29814200	-2.60154700
N	3.40104000	-0.44250900	1.95180500
C	4.09840400	0.80557000	2.39684400
H	3.48345800	1.26098500	3.17749000
H	5.07973600	0.54270000	2.79951300
H	4.19953900	1.49751000	1.55926300
C	3.23915200	-1.39054700	3.10114000
H	4.21984100	-1.63869400	3.51279300
H	2.62830200	-0.88778200	3.85495000
H	2.71551200	-2.27577100	2.73693400
C	-1.29562100	2.77855500	-1.60252600
H	-0.86865200	3.78198700	-1.72094100
C	-3.65480700	2.88793200	-0.68281700
C	-4.52964400	2.94598500	0.40493700
C	-2.27874300	2.79595000	-0.44733900
C	-1.85287500	2.75463400	0.88560800
C	-2.80830200	2.80794500	1.90381900
H	-0.79763400	2.65959500	1.12866200
H	-2.49394500	2.76672700	2.94736200
H	-5.60532800	3.01849200	0.23700100
H	2.39326700	-0.17707100	1.70397700
O	0.78030400	0.16651000	1.73674100
N	0.15551500	-0.88239300	1.30864000
O	0.77536000	-1.98187300	1.18593400
C	-1.17097000	-0.76044400	1.02172700
H	-1.55859100	0.24210600	1.11769300
C	-1.93953100	-1.87672900	0.63270100
H	-1.48820000	-2.84110500	0.85666400
C	-3.41027800	-1.83550800	0.78844900
C	-4.10844800	-3.04566500	0.95516500
C	-4.13974400	-0.63298500	0.75139000
C	-5.49841300	-3.05686800	1.08871600
H	-3.54997700	-3.98060700	0.97891300
C	-5.52789000	-0.64450600	0.88741100
H	-3.62974900	0.31289800	0.60296100
C	-6.21373900	-1.85366300	1.05438700
H	-6.02258700	-4.00144000	1.22093400
H	-6.07296600	0.29631000	0.86487000
H	-7.29679600	-1.85833000	1.15970400

O	-2.40835500	-0.03542700	-2.16297900
C	-2.66959900	-1.23359500	-2.03929000
C	-4.01528900	-1.79233000	-2.48256900
H	-3.86882200	-2.52084100	-3.29362200
H	-4.49212900	-2.32391200	-1.64840400
H	-4.66286500	-0.98032300	-2.82705200
C	-1.74806300	-2.21999800	-1.44442000
C	-0.30892300	-2.11702900	-1.62479100
O	0.28355000	-1.03002600	-1.75872700
H	-2.12737100	-3.24206500	-1.45385200
C	0.46643300	-3.42569400	-1.64240100
H	0.31865100	-3.92227400	-2.61314100
H	1.53362300	-3.23412600	-1.49701600
H	0.10234200	-4.10492500	-0.86157400
H	-4.04049000	2.89905000	-1.70022400
H	-1.82522400	2.50840400	-2.52126300
N	-4.13267300	2.90487600	1.68802800

$TS_{(S)}$-1s

SINGLE POINT: E(RB97D) = -1929.216762 (Hartree/Particle)

XYZ coordinates

C	0.85486500	2.32104400	-0.83282400
C	2.09175700	1.69915300	-0.55490000
C	1.30395100	3.60464800	-0.22256300
N	-0.27296100	1.93522300	-1.42553200
C	2.62219800	2.90258300	0.11610300
N	2.57471700	0.46992100	-0.76864800
O	0.80930600	4.71314200	-0.07246700
H	-0.38708700	0.97531200	-1.76145300
O	3.66955900	3.17126600	0.70591100
H	1.97209000	-0.20227600	-1.26809100
C	3.98175500	0.14924900	-0.57282400
C	4.15300000	-1.10853400	0.29962400
C	4.70015400	-0.06509600	-1.92153600
H	4.45187100	0.99845800	-0.06622300
C	5.64018200	-1.39580400	0.54088100
H	3.69811600	-1.95984700	-0.22286300
C	6.18864300	-0.37885600	-1.71758000
H	4.20763300	-0.89116600	-2.45612700
C	6.36468000	-1.59883600	-0.80313500
H	5.76699000	-2.28821200	1.16235400
H	6.09128200	-0.54632300	1.07090800
H	6.67151000	-0.55523100	-2.68696300
H	6.68144700	0.49204600	-1.26083500
H	7.42753700	-1.79222100	-0.61299700
H	5.95421000	-2.49100900	-1.29930600

H	4.56551900	0.84251400	-2.52116300
N	3.35242800	-1.01396300	1.59875800
C	3.70745000	0.15689000	2.46717200
H	3.00742700	0.15905400	3.30625300
H	4.73150900	0.03320200	2.82671000
H	3.61252000	1.08221000	1.89735100
C	3.43275600	-2.29003700	2.38684000
H	4.42731600	-2.37509500	2.82822200
H	2.65734600	-2.24871800	3.15104900
H	3.23839000	-3.12682500	1.71033300
C	-1.45645400	2.78922800	-1.42427100
H	-1.13663300	3.83074800	-1.55339600
C	-3.59059100	3.23317900	-0.15416400
C	-4.35414100	3.15578900	1.01180200
C	-2.29387600	2.70165600	-0.15897400
C	-1.83217800	2.12131500	1.02578800
C	-2.67790600	2.08910700	2.13935600
H	-0.84227500	1.67732100	1.08510200
H	-2.33456500	1.62759100	3.06603100
H	-5.36699400	3.56073000	1.02910000
H	2.32775300	-0.89158000	1.35026100
O	0.40265400	-2.09258900	2.93118900
N	-0.08741200	-1.58788600	1.88124200
O	0.59758900	-0.76189600	1.16707100
C	-1.35862200	-1.92805400	1.50000000
H	-1.81569100	-2.67656100	2.13342700
C	-2.04361600	-1.29634900	0.44513200
H	-1.67864000	-0.31969400	0.14311800
C	-3.51182500	-1.47745700	0.39318500
C	-4.11592600	-2.72333000	0.64688000
C	-4.32740500	-0.38400100	0.05882700
C	-5.50172500	-2.86711000	0.57622000
H	-3.49458100	-3.58525500	0.88203100
C	-5.71490400	-0.52696600	-0.00522800
H	-3.86818600	0.57706900	-0.14585600
C	-6.30759100	-1.76740700	0.25114800
H	-5.95538100	-3.83715100	0.77051200
H	-6.33202300	0.33350700	-0.25560300
H	-7.38854200	-1.88024600	0.19706500
O	-2.17279700	-0.06588400	-2.59158200
C	-2.38553800	-1.25989900	-2.35565900
C	-3.61279400	-1.96388100	-2.91432500
H	-3.30490100	-2.78684500	-3.57601800
H	-4.19212700	-2.40437600	-2.09183200
H	-4.23388000	-1.25394600	-3.46922400
C	-1.51719000	-2.07593700	-1.49357500
C	-0.07118900	-1.94155800	-1.53635000
O	0.53454200	-0.96347800	-2.01795900

H	-1.86721600	-3.09214200	-1.31570200
C	0.69800700	-3.12363200	-0.96433000
H	0.58588900	-3.99430600	-1.62599700
H	1.76075500	-2.87912400	-0.87269600
H	0.28647900	-3.40593900	0.01458200
H	-4.00494900	3.69303800	-1.05006600
H	-2.07012000	2.50374000	-2.28364100
N	-3.92241400	2.59199500	2.15393700