Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Design and application of a bifunctional organocatalyst guided by electron density topological analyses

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1. Computational Part

The geometry of all intermediates and transition states were completely optimized with M06-2X/6-31+G(d), PCM-(toluene)-B97-D/TZVP and PCM-(toluene)-B98/TZVP approximations as implemented in the Gaussian 2009 package.[1] 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 energies of all the stationary points obtained by M06-2X/6-31+G(d) method were calculated through the COSMO-(toluene)-RIJCOSX-MP2/aug-cc-pVDZ[2] approximation. This calculation was computed in the ORCA program version 3.0.33.[3] SMD-(toluene)-M06-2X/6-311++G(2d,2p)[4] method was performed with Gaussian 2009 package.

The topological analyses of the electron density determined with methods (M06-2X/6-31+G(d), PCM-(toluene)-B97-D/TZVP and PCM-(toluene)-B98/TZVP) were done following the Quantum Theory of Atoms in Molecules (QTAIM) and the Non-Covalent Interactions (NCI) index employing the AIMAll[5] and NCIPLOT[6] programs, respectively. The QTAIM characterization was done in terms of the properties of electron density $\rho(\mathbf{r})$, the potential energy density $V(\mathbf{r})$, the Laplace field $\nabla^2\rho(\mathbf{r})$, the ellipticity ε, and the Hydrogen Bond energy according to Espinosa estimation $E_{H.}$[7] All topological descriptors taken from the bond critical point. The NCI analysis was done through the relation between reduced gradient, $s(\mathbf{r})$, and $\mathrm{sgn}(\lambda_2)\rho(\mathbf{r})$. Additionally, we determined the volumes of the NCI isosurfaces corresponding to CH···π and NH···O interactions obtained by an in-house modification of NCIPLOT program (J. L. Casals-Sainz).

1.1 Energy profiles

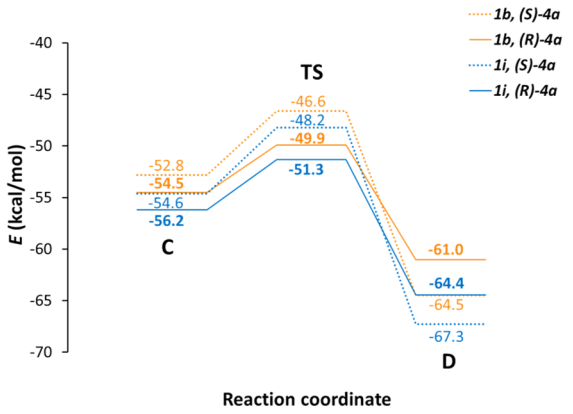
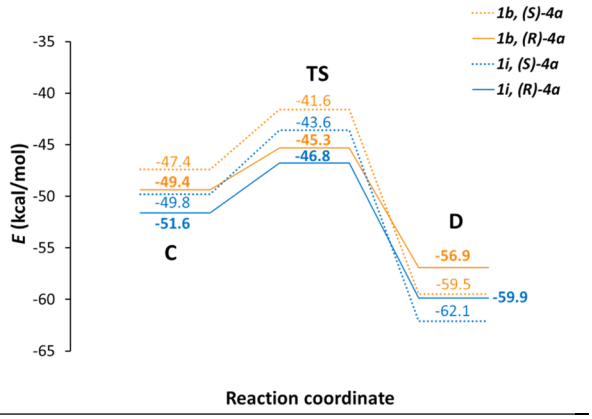
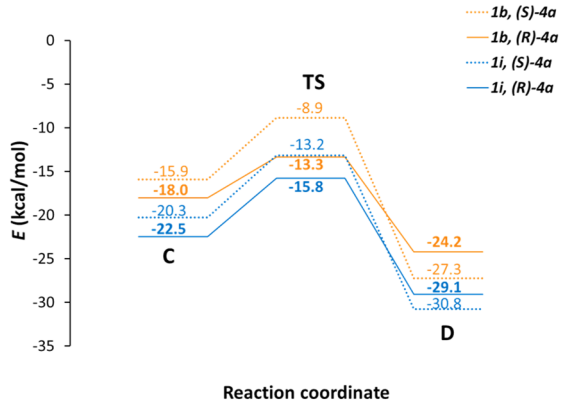
COSMO-RIJCOSX-MP2 Electronic	
COSMO-RIJCOSX-MP2 + ZPE	
COSMO-RIJCOSX-MP2 Gibbs free energy	

Fig. S1. Profiles of relative energies to reactants for the Michael reaction under consideration. The full description of the approximation and basis set is: COSMO-(toluene)-RIJCOSX-MP2/aug-cc-pVDZ//M06-2X/6-31+G(d). The values are reported in kcal/mol.

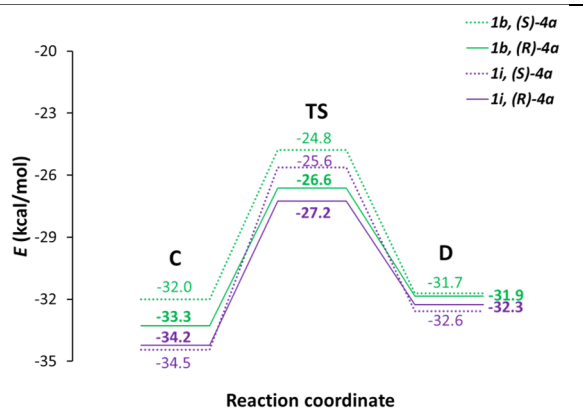
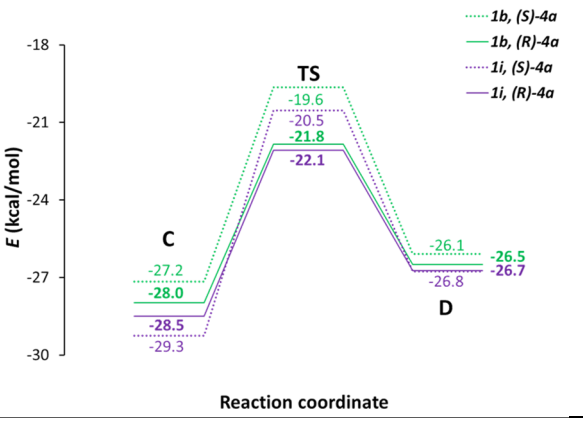
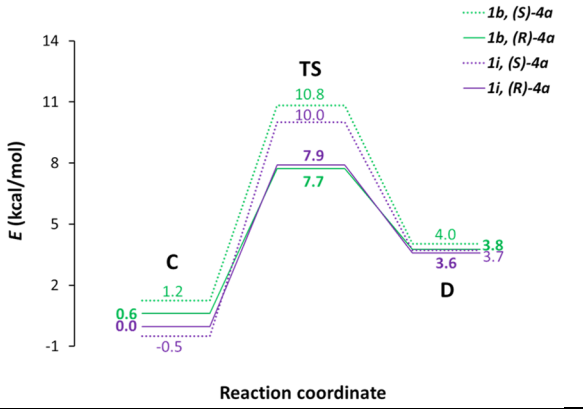
PCM-B97-D Electronic	
PCM-B97-D + ZPE	
PCM-B97-D Gibbs free energy	

Fig. S2. Profiles of relative energies to reactants for the Michael reaction under consideration. The full description of the approximation and basis set is: PCM-(toluene)-B97-D/TZVP. The values are reported in kcal/mol.

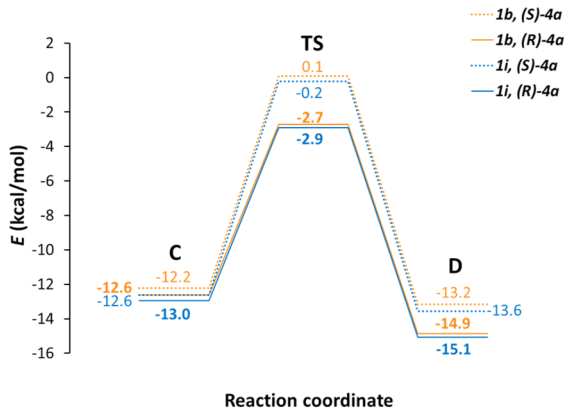
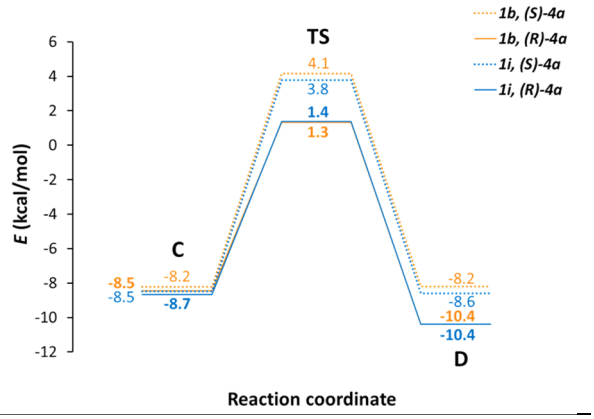
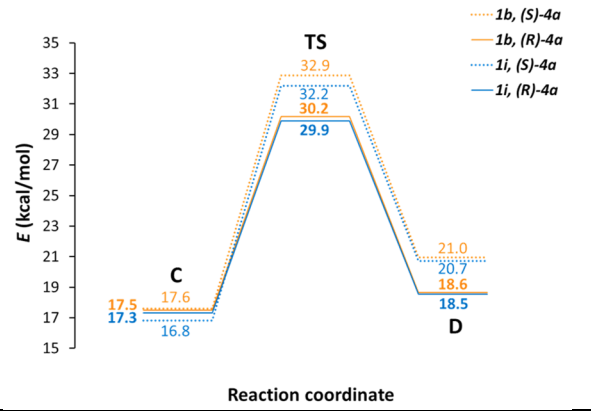
PCM-B98 Electronic	
PCM-B98 + ZPE	
PCM-B98 Gibbs free energy	

Fig. S3. Profiles of relative energies to reactants for the Michael reaction under consideration. The full description of the approximation and basis set is: PCM-(toluene)-B98/TZVP. The values are reported in kcal/mol.

1.2 Activation barriers

Table S1. Theoretical activation barriers in kcal/mol, electronic energy ($E_e^{\ddagger}$), with zero-point energy correction ($E^{\ddagger}$), plus thermal correction at 298.15 K ($E_{298K}^{\ddagger}$), enthalpy ($H^{\ddagger}$), and Gibbs free energy ($G^{\ddagger}$), of the rate-limiting step of the addition of 2,4-pentanedione to β-nitrostyrene with catalysts **1b** and **1i**.

Method[a]		Energy	1b			1i		
			E_a (*R*)	E_a (*S*)	ΔE_a	E_a (*R*)	E_a (*S*)	ΔE_a
1	M06-2X	$E_e^{\ddagger}$	9.1	11.4	2.3	9.5	11.5	2.0
		$E^{\ddagger}$	8.6	11.0	2.4	9.4	11.3	1.9
		$E_{298K}^{\ddagger}$	8.1	10.4	2.3	8.7	10.6	1.9
		$H^{\ddagger}$	8.1	10.4	2.3	8.7	10.6	1.9
		$G^{\ddagger}$	9.2	12.2	3.0	11.2	12.2	1.0
2	SMD-M06-2X	$E_e^{\ddagger}$	9.6	12.1	2.5	9.8	12.2	2.4
		$E^{\ddagger}$	9.1	11.7	2.6	9.7	12.0	2.3
		$E_{298K}^{\ddagger}$	8.6	11.1	2.5	9.0	11.4	2.4
		$H^{\ddagger}$	8.6	11.1	2.5	9.0	11.4	2.4
		$G^{\ddagger}$	9.7	12.9	3.2	11.6	12.9	1.4
3	COSMO-RIJCOSX-MP2	$E_e^{\ddagger}$	4.6	6.2	1.6	4.9	6.4	1.5
		$E^{\ddagger}$	4.1	5.9	1.8	4.8	6.2	1.4
		$E_{298K}^{\ddagger}$	3.5	5.2	1.7	4.1	5.5	1.4
		$H^{\ddagger}$	3.5	5.2	1.7	4.1	5.5	1.4
		$G^{\ddagger}$	4.7	7.0	2.3	6.7	7.1	0.4
4	PCM-B97-D	$E_e^{\ddagger}$	6.7	7.2	0.5	7.0	8.9	1.9
		$E^{\ddagger}$	6.1	7.5	1.4	6.4	8.7	2.3
		$E_{298K}^{\ddagger}$	5.5	6.8	1.3	5.7	7.9	2.2
		$H^{\ddagger}$	5.5	6.8	1.3	5.7	7.9	2.2
		$G^{\ddagger}$	7.1	9.6	2.5	7.9	10.5	2.6
5	PCM-B98	$E_e^{\ddagger}$	9.9	12.3	2.4	10.1	12.4	2.3
		$E^{\ddagger}$	9.8	12.4	2.6	10.0	12.3	2.2
		$E_{298K}^{\ddagger}$	8.9	11.4	2.5	9.1	11.4	2.3
		$H^{\ddagger}$	8.9	11.4	2.5	9.1	11.4	2.3
		$G^{\ddagger}$	12.7	15.3	2.6	12.6	15.4	2.8

[a] The full description of the electronic structure approximations and basis sets are:

1: M06-2X/6-31+G(d)

2: SMD-(toluene)- M06-2X/6-311++G(2d,2p)//M06-2X/6-31+G(d)

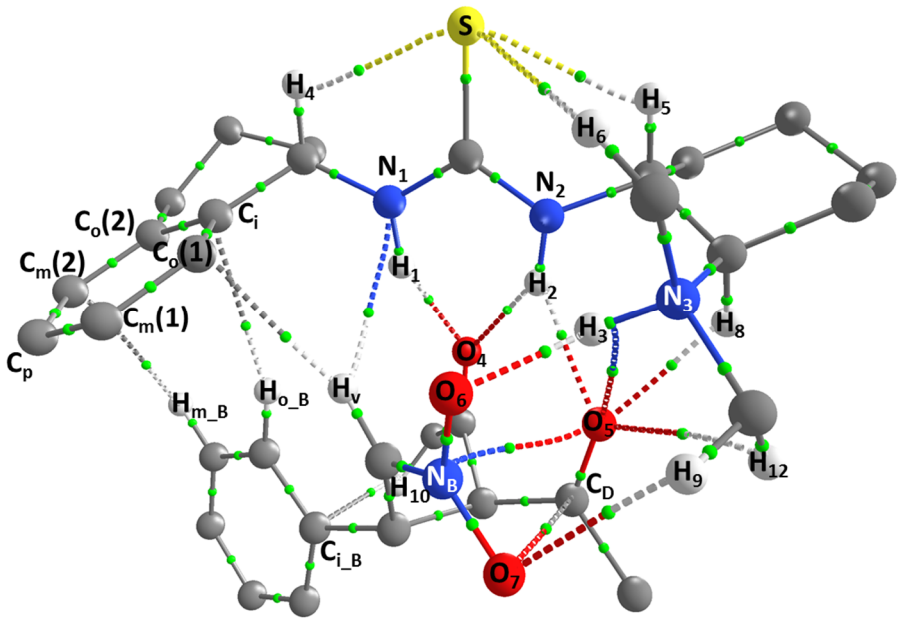
3: COSMO-(toluene)-RIJCOSX-MP2/aug-cc-pVDZ//M06-2X/6-31+G(d)

4: PCM-(toluene)-B97-D/TZVP.

5: PCM-(toluene)-B98/TZVP.

1.3 Quantum Theory of Atoms in Molecules (QTAIM)

Table S2. Selected topological properties and atomic charges with catalyst **1i** computed with the M06-2X/6-31G+(d) approximation.



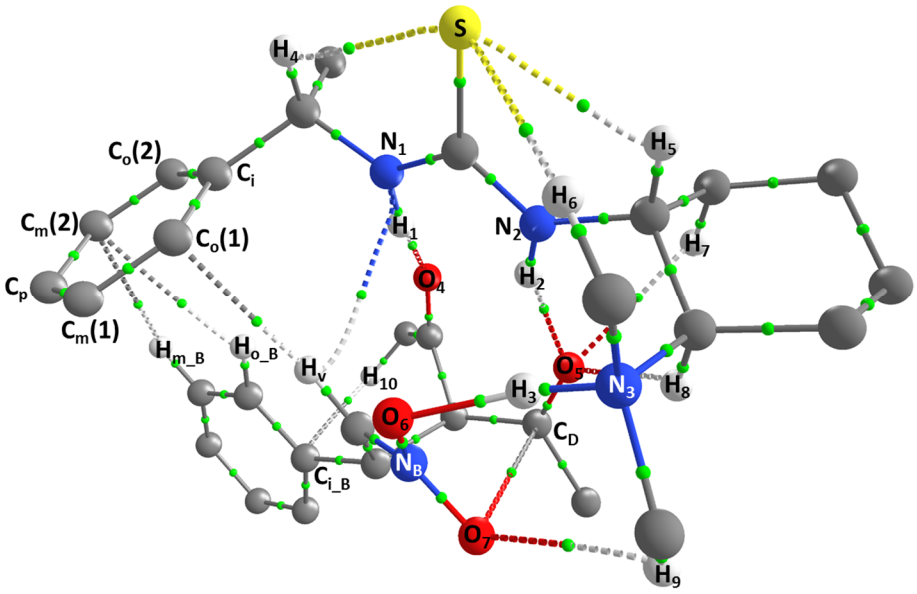
Molecular graphs of the transition state using catalyst **1i**.

Selected topological properties

Interaction	ρ(r)	V(r)	$\nabla^2\rho$	ε	E_H
	a.u.				kcal/mol
$H_1\cdots O_4$	0.0240	-0.0218	0.0944	0.0515	-6.84
$H_2\cdots O_4$	0.0178	-0.0155	0.0640	0.669	-4.86
$H_2\cdots O_5$	0.0163	-0.0140	0.0604	0.1595	-4.39
$H_3\cdots O_5$	0.0110	-0.0089	0.0454	0.7075	-2.79
$H_3\cdots O_6$	0.0328	-0.0288	0.1030	0.1164	-9.04
$H_4\cdots S$	0.0167	-0.0112	0.0565	0.4807	-3.51
$H_5\cdots S$	0.0190	-0.0133	0.0619	0.3011	-4.17
$H_6\cdots S$	0.0085	-0.0042	0.0258	0.1335	-1.32
$H_7\cdots O_5$	0.0170	-0.0137	0.0657	0.1035	-4.30
$H_8\cdots O_7$	0.0090	-0.0062	0.0331	0.1255	-1.95
$H_9\cdots O_7$	0.0078	-0.0053	0.0292	0.6998	-1.66
$H_v\cdots N_1$	0.0063	-0.0034	0.0208	0.7188	-1.07
$H_v\cdots C_o(1)$	0.0098	-0.0056	0.0343	0.2124	-1.76
$H_{o\_B}\cdots C_i$	0.0080	-0.0041	0.0250	1.1340	-1.29
$H_{m\_B}\cdots C_m(2)$	0.0052	-0.0023	0.0158	0.1010	-0.72
$O_5\cdots N_B$	0.0120	-0.0084	0.0443	2.3001	-2.64
$O_7\cdots C_D$	0.0139	-0.0102	0.0489	0.7030	-3.20

Atomic charges	
Atom	**Charge (a.u)**
O_4	-1.233
O_5	-1.242
O_6	-0.709
O_7	-0.668
N_1	-1.309
N_2	-1.306
N_B	0.012
S	-0.076
H_1	0.469
H_2	0.497
H_3	0.535
H_4	0.085
H_5	0.071
H_6	0.106
H_7	0.075
H_8	0.142
H_9	0.066
H_{10}	0.064
C_D	1.067
H_v	0.088
H_{o_B}	0.051
H_{m_B}	0.070
Ph (Thiourea)	
C_i	-0.047
$H_o(1)$	0.088
$C_o(1)$	-0.053
$H_m(1)$	0.057
$C_m(1)$	-0.039
H_p	0.044
C_p	-0.043
$H_m(2)$	0.031
$C_m(2)$	-0.060
$C_o(2)$	-0.031
Sum (Ph thiourea)	**-0.054**

Table S3. Selected topological properties and atomic charges with catalyst **1b** computed with the PCM-B97-D/TZVP approximation.



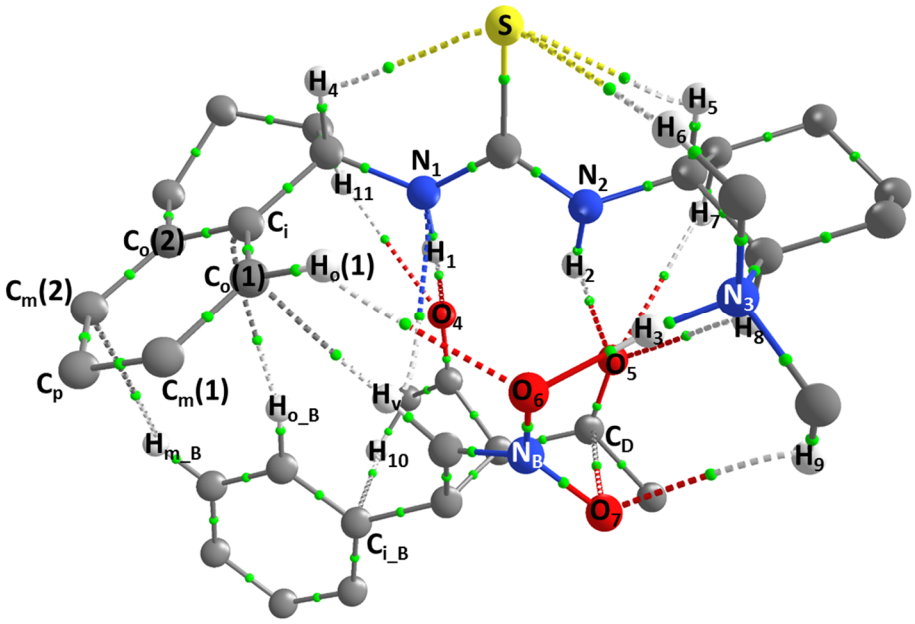
Molecular graphs of the transition state using catalyst **1b**.

Selected topological properties

Interaction	ρ(r)	V(r)	$\nabla^2\rho$	ε	E_H
	a.u.				kcal/mol
$H_1\cdots O_4$	0.0258	-0.0209	0.0985	0.0345	-6.57
$H_2\cdots O_5$	0.0254	-0.0204	0.0973	0.0265	-6.41
$H_3\cdots O_6$	0.0663	-0.0682	0.1157	0.0692	-21.40
$H_4\cdots S$	0.0161	-0.0095	0.0491	0.5700	-2.98
$H_5\cdots S$	0.0164	-0.0097	0.0488	0.4647	-3.03
$H_6\cdots S$	0.0110	-0.0047	0.0277	0.1232	-1.47
$H_7\cdots O_5$	0.0062	-0.0035	0.0256	0.1283	-1.10
$H_8\cdots O_5$	0.0081	-0.0045	0.0315	0.1202	-1.41
$H_9\cdots O_7$	0.0082	-0.0046	0.0308	0.2004	-1.43
$H_{10}\cdots C_{i\_B}$	0.0087	-0.0050	0.0294	0.9357	-1.56
$H_v\cdots N_1$	0.0051	-0.0025	0.0193	1.4229	-0.80
$H_v\cdots C_o(1)$	0.0087	-0.0042	0.0252	0.0436	-1.31
$H_{o\_B}\cdots C_m(2)$	0.0060	-0.0033	0.0216	5.1912	-1.04
$H_{m\_B}\cdots C_m(2)$	0.0051	-0.0025	0.0167	0.5264	-0.79
$C_D\cdots O_7$	0.0092	-0.0050	0.0322	0.2902	-1.58

Atomic charges	
Atom	**Charge (a.u)**
O_4	-1.103
O_5	-1.109
O_6	-0.656
O_7	-0.614
N_1	-1.075
N_2	-1.084
N_B	0.066
S	-0.205
H_1	0.443
H_2	0.444
H_3	0.502
H_4	0.061
H_5	0.047
H_6	0.088
H_7	0.009
H_8	0.052
H_9	0.068
H_{10}	0.045
C_D	0.941
H_v	0.068
H_{o_B}	0.046
H_{m_B}	0.026
Ph (Thiourea)	
C_i	-0.026
$H_o(1)$	0.054
$C_o(1)$	-0.031
$H_m(1)$	0.027
$C_m(1)$	-0.020
H_p	0.020
C_p	-0.022
$H_m(2)$	0.014
$C_m(2)$	-0.024
$H_o(2)$	0.022
$C_o(2)$	-0.031
Sum (Ph thiourea)	**-0.017**

Table S4. Selected topological properties and atomic charges with catalyst **1i** computed with the PCM-B97-D/TZVP approximation.



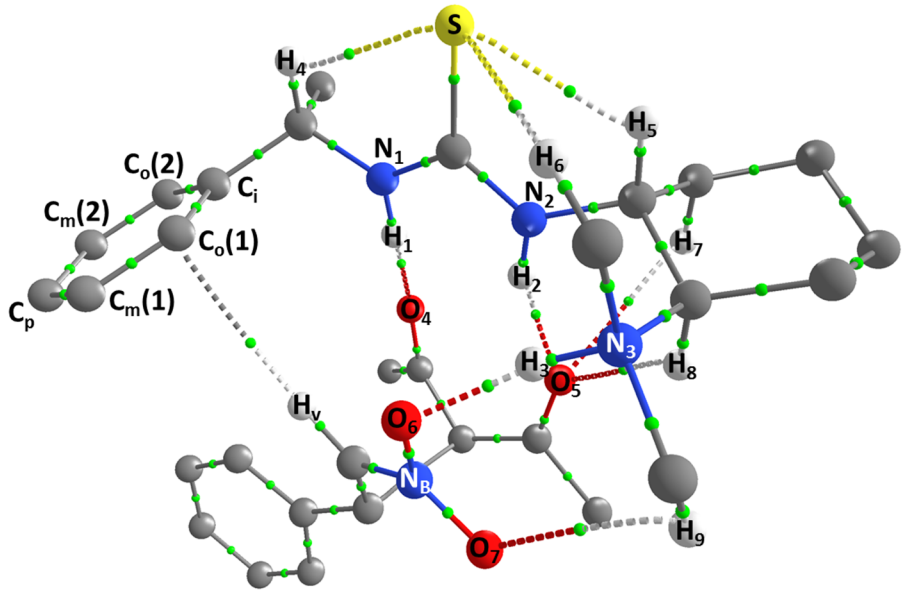
Molecular graphs of the transition state using catalyst **1i**.

Selected topological properties

Interaction	ρ(r)	V(r)	$\nabla^2\rho$	ε	E_H
	a.u.				kcal/mol
$H_1\cdots O_4$	0.0263	-0.0215	0.0994	0.0336	-6.73
$H_2\cdots O_5$	0.0259	-0.0211	0.0989	0.0252	-6.62
$H_3\cdots O_6$	0.0683	-0.0709	0.1164	0.0687	-22.23
$H_4\cdots S$	0.0157	-0.0092	0.0477	0.6072	-2.89
$H_5\cdots S$	0.0160	-0.0094	0.0480	0.5201	-2.96
$H_6\cdots S$	0.0104	-0.0044	0.0262	0.1337	-1.38
$H_7\cdots O_5$	0.0057	-0.0032	0.0234	0.1674	-0.99
$H_8\cdots O_5$	0.0076	-0.0042	0.0292	0.1309	-1.30
$H_9\cdots O_7$	0.0074	-0.0041	0.0277	0.2341	-1.27
$H_{10}\cdots C_{i\_B}$	0.0089	-0.0051	0.0297	1.6854	-1.59
$H_o(1)\cdots O_6$	0.0047	-0.0022	0.0164	0.2189	-0.70
$H_v\cdots N_1$	0.0054	-0.0027	0.0204	1.4711	-0.85
$H_v\cdots C_o(1)$	0.0101	-0.0050	0.0299	0.1284	-1.57
$H_{o\_B}\cdots C_i$	0.0062	-0.0031	0.0192	4.1217	-0.96
$H_{m\_B}\cdots C_m(2)$	0.0048	-0.0023	0.0152	0.3217	-0.72
$O_4\cdots H_{11}$	0.0059	-0.0031	0.0223	0.2587	-0.96
$C_D\cdots O_7$	0.0093	-0.0051	0.0325	0.2527	-1.60

Atomic charges	
Atom	**Charge (a.u)**
O_4	-1.103
O_5	-1.109
O_6	-0.658
O_7	-0.612
N_1	-1.081
N_2	-1.082
N_B	0.064
S	-0.204
H_1	0.442
H_2	0.443
H_3	0.503
H_4	0.058
H_5	0.047
H_6	0.087
H_7	0.007
H_8	0.050
H_9	0.065
H_{10}	0.047
H_{11}	0.005
C_D	0.940
H_v	0.071
H_{o_B}	0.047
H_{m_B}	0.027
Ph (Thiourea)	
C_i	-0.039
$H_o(1)$	0.056
$C_o(1)$	-0.032
$H_m(1)$	0.024
$C_m(1)$	-0.021
H_p	0.018
C_p	-0.023
$H_m(2)$	0.007
$C_m(2)$	-0.030
$C_o(2)$	-0.027
Sum (Ph thiourea)	**-0.067**

Table S5. Selected topological properties and atomic charges with catalyst **1b** computed with the PCM-B98/TZVP approximation.



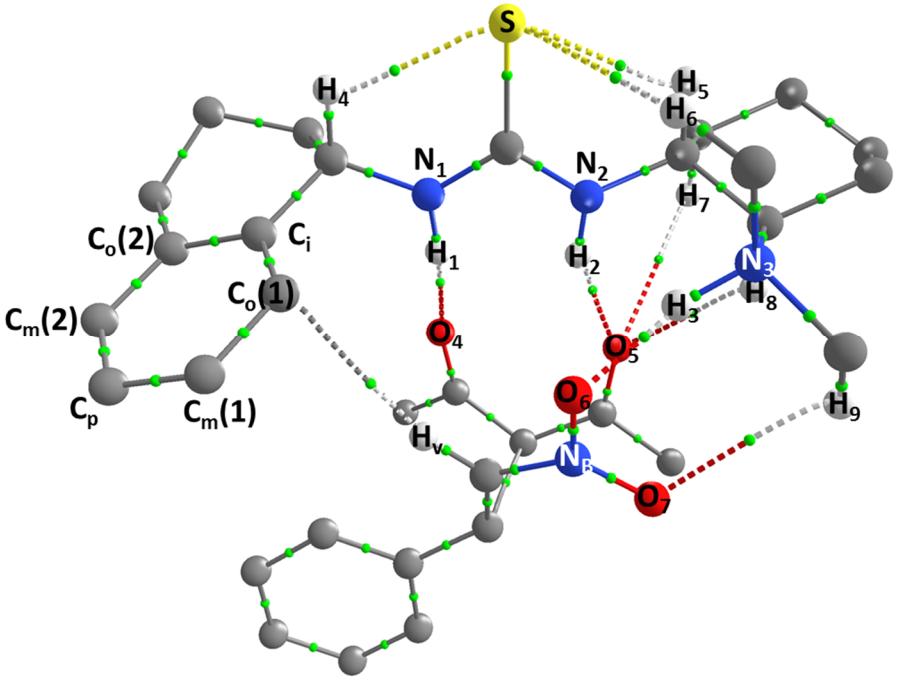
Molecular graphs of the transition state using catalyst **1b**.

Atomic charges	
Atom	**Charge (a.u)**
O_4	-1.174
O_5	-1.178
O_6	-0.632
O_7	-0.574
N_1	-1.157
N_2	-1.158
N_B	0.187
S	-0.200
H_1	0.477
H_2	0.477
H_3	0.512
H_4	0.068
H_5	0.057
H_6	0.100
H_7	0.012
H_8	0.063
H_9	0.069
H_v	0.087

Selected topological properties

Interaction	ρ(r)	V(r)	$\nabla^2\rho$	ε	E_H		
	a.u.				**kcal/mol**	**Ph (Thiourea)**	
$H_1\cdots O_4$	0.0259	-0.022	0.1031	0.0283	-6.90	C_i	-0.024
$H_2\cdots O_4$	0.0465	-0.0456	0.1213	0.0768	-14.31	$H_o(1)$	0.046
$H_2\cdots O_5$	0.0261	-0.022	0.1023	0.0272	-6.90	$C_o(1)$	-0.030
$H_3\cdots O_6$	0.0259	-0.022	0.1031	0.0283	-6.90	$H_m(1)$	0.029
$H_4\cdots S$	0.0179	-0.011	0.054	0.4059	-3.45	$C_m(1)$	-0.029
$H_5\cdots S$	0.0185	-0.0113	0.0541	0.3081	-3.55	H_p	0.025
$H_6\cdots S$	0.0111	-0.0048	0.0283	0.1239	-1.51	C_p	-0.032
$H_7\cdots O_5$	0.0051	-0.0028	0.0201	0.18	-0.88	$H_m(2)$	0.022
$H_8\cdots O_7$	0.0078	-0.0043	0.0294	0.1132	-1.35	$C_m(2)$	-0.030
$H_9\cdots O_7$	0.0059	-0.0032	0.0227	0.3909	-1.00	$C_o(2)$	-0.031
$H_v\cdots C_o(1)$	0.0045	-0.002	0.013	0.2537	-0.63	Sum (Ph thiourea)	**-0.054**

Table S6. Selected topological properties and atomic charges with catalyst **1i** computed with the PCM-B98/TZVP approximation.



Molecular graphs of the transition state using catalyst **1i**.

Atomic charges	
Atom	**Charge (a.u)**
O_4	-1.163
O_5	-1.178
O_6	-0.632
O_7	-0.574
N_1	-1.161
N_2	-1.158
N_B	0.187
S	-0.198
H_1	0.475
H_2	0.476
H_3	0.512
H_4	0.066
H_5	0.056
H_6	0.100
H_7	0.012
H_8	0.062
H_9	0.072
H_v	0.088

Selected topological properties

Interaction	ρ(r)	V(r)	$\nabla^2\rho$	ε	E_H	**Ph (Thiourea)**	
	a.u.				**kcal/mol**	C_i	-0.036
$H_1\cdots O_4$	0.0253	-0.0213	0.1013	0.0269	-6.68	$H_o(1)$	0.049
$H_2\cdots O_5$	0.0261	-0.022	0.1023	0.0259	-6.90	$C_o(1)$	-0.035
$H_3\cdots O_6$	0.0462	-0.0451	0.1211	0.0771	-14.15	$H_m(1)$	0.026
$H_4\cdots S$	0.0179	-0.0109	0.0534	0.4078	-3.42	$C_m(1)$	-0.032
$H_5\cdots S$	0.0185	-0.0113	0.054	0.3108	-3.55	H_p	0.022
$H_6\cdots S$	0.0108	-0.0047	0.0275	0.132	-1.47	C_p	-0.033
$H_7\cdots O_5$	0.005	-0.0027	0.0199	0.1864	-0.85	$H_m(2)$	0.015
$H_8\cdots O_7$	0.0075	-0.0041	0.0284	0.1147	-1.29	$C_m(2)$	-0.035
$H_9\cdots O_7$	0.0064	-0.0035	0.0246	0.2792	-1.10	$C_o(2)$	-0.028
$H_v\cdots C_o(1)$	0.0055	-0.0026	0.0116	0.4212	-0.82	Sum (Ph thiourea)	**-0.087**

1.4 Non-Covalent Interaction (NCI) index

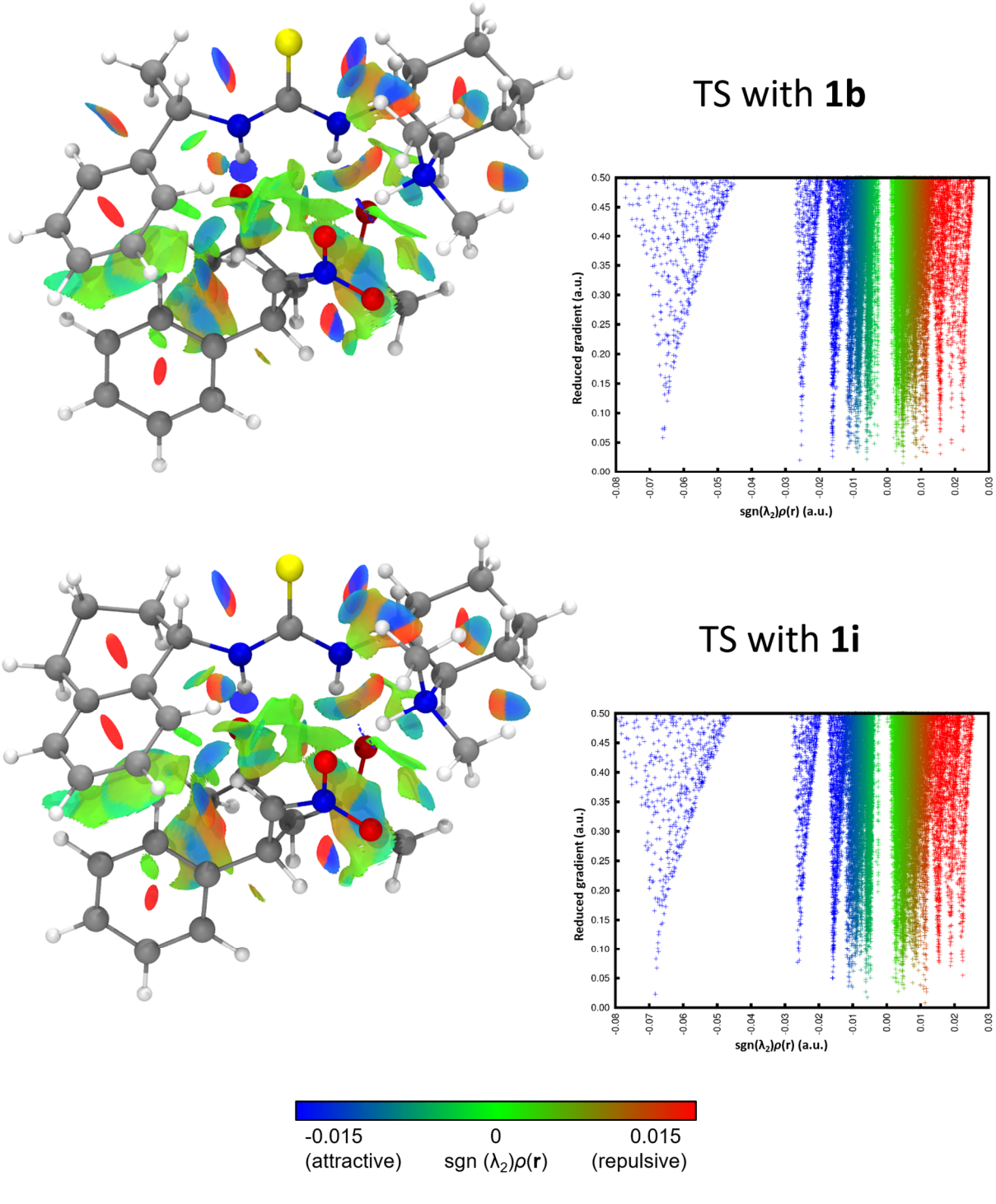


Fig. S4. Non-Covalent Interactions index of the transition states of the studied catalysts **1b** and **1i**. Isosurfaces at reduced gradient 0.5 a.u. (left) and relation between reduced gradient and sgn(λ_2)ρ(**r**) at a density value of $-0.08 < \rho(\mathbf{r}) < 0.03$ a.u. for SCF densities (right). The analysis was performed using PCM-(toluene)-B97-D charge density.

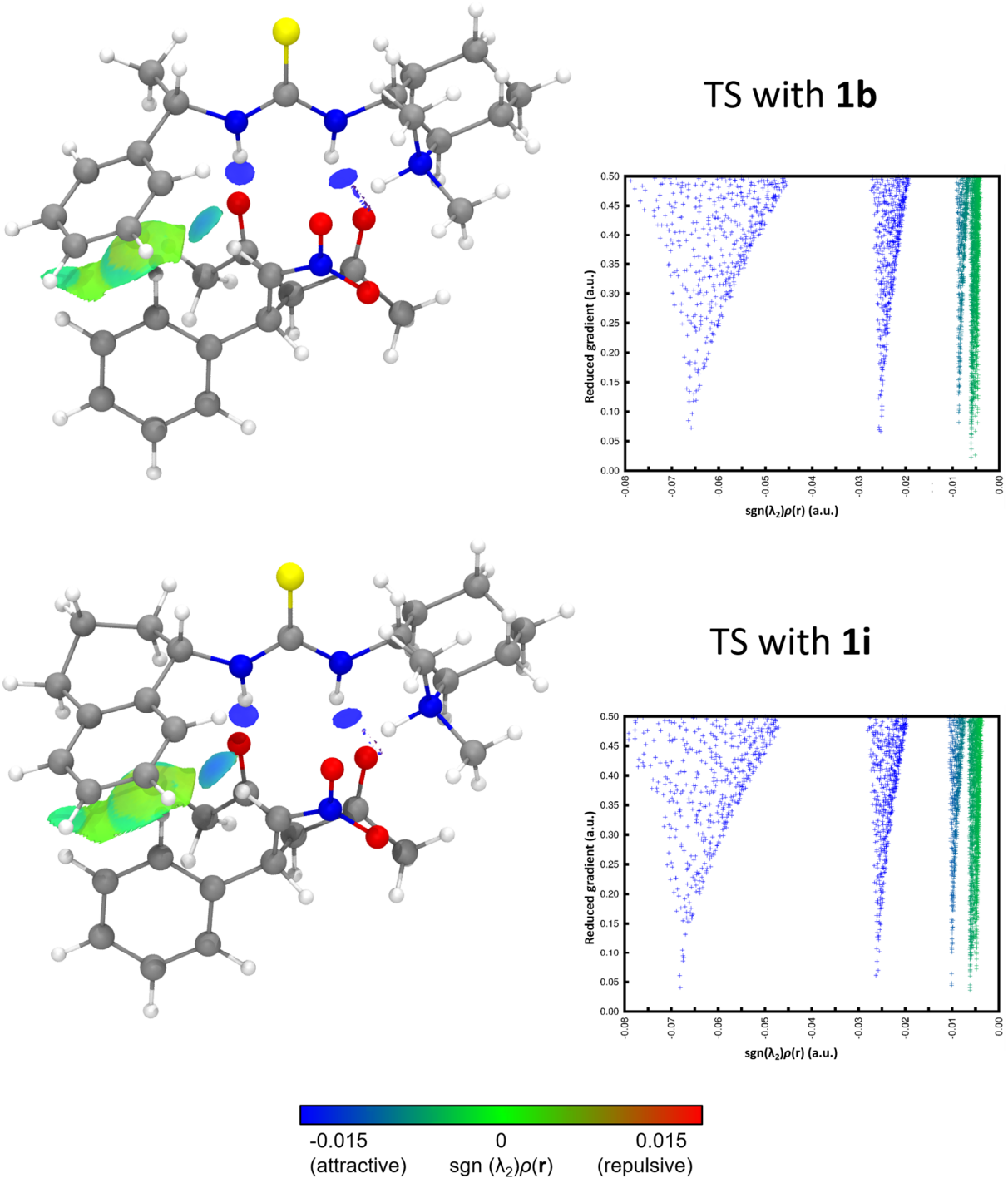


Fig. S5. Selected isosurfaces at reduced gradient 0.5 a.u. (left) and relation between reduced gradient and sgn(λ_2)ρ(**r**) at a density value of −0.08 < ρ(**r**) < 0.00 a.u. for SCF densities (right). The analysis was performed using PCM-(toluene)-B97-D charge density.

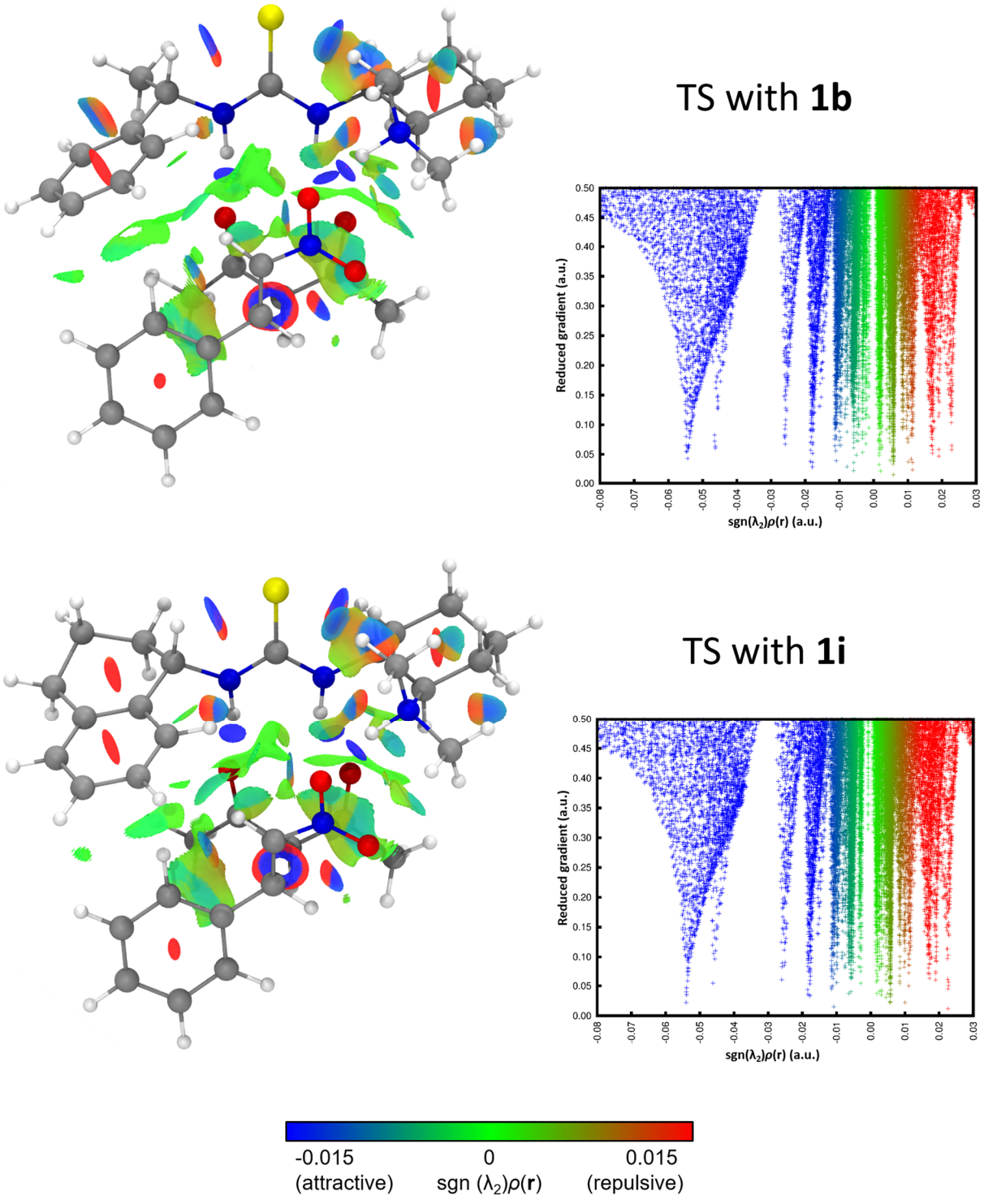


Fig. S6. Non-Covalent Interactions index of the transition states of the studied catalysts **1b** and **1i**. Isosurfaces at reduced gradient 0.5 a.u. (left) and relation between reduced gradient and sgn(λ_2)ρ(**r**) at a density value of $-0.08 < \rho(\mathbf{r}) < 0.03$ a.u. for SCF densities (right). The analysis was performed using PCM-(toluene)-B98 charge density.

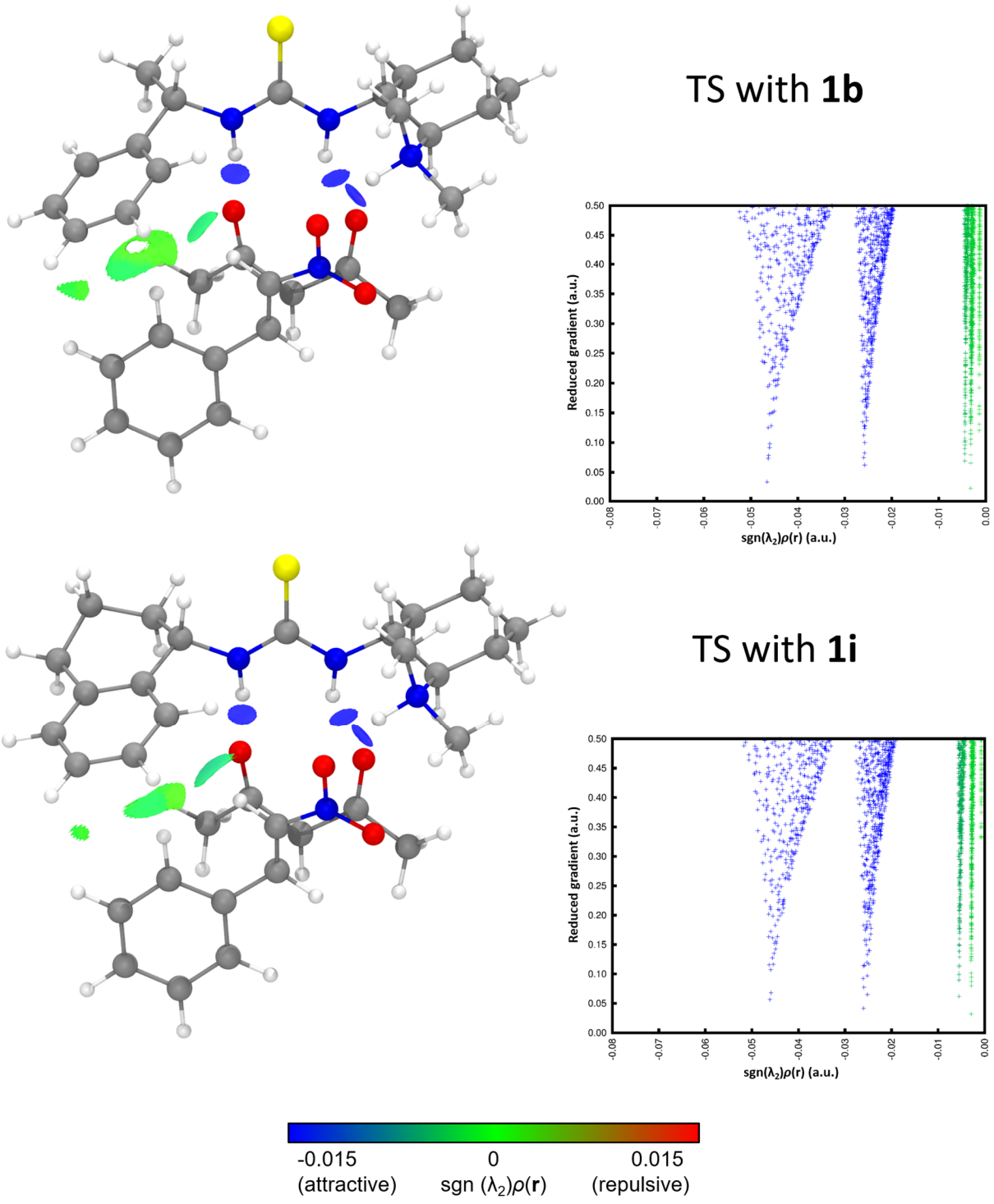


Fig. S7. Selected isosurfaces at reduced gradient 0.5 a.u. (left) and relation between reduced gradient and sgn(λ_2)ρ(**r**) at a density value of −0.08 < ρ(**r**) < 0.00 a.u. for SCF densities (right). The analysis was performed using PCM-(toluene)-B98 charge density.

1.5 XYZ coordinates and electronic energies of the calculated structures

M06-2X/6-31+G(d) approximation

XYZ coordinates and energies of catalyst **1b** were previously reported.[8]

β-nitrostyrene

Zero-point correction= 0.138482 (Hartree/Particle)
Thermal correction to energy= 0.147587
Thermal correction to enthalpy= 0.148531
Thermal correction to Gibbs free energy= 0.102428
Sum of electronic and zero-point energies= -513.807606
Sum of electronic and thermal energies= -513.798500
Sum of electronic and thermal enthalpies= -513.797556
Sum of electronic and thermal free energies= -513.843659
Entropy= 97.033 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -512.7870556 (Hartree/Particle)

XYZ coordinates

O	3.24603500	1.16011700	-0.00014100
N	2.98696300	-0.03207700	0.00000800
C	1.59509000	-0.45868300	0.00002200
H	1.50857400	-1.53617100	0.00011700
O	3.81654000	-0.92835800	0.00015300
C	0.61900800	0.45141300	-0.00004400
C	-0.82006600	0.17634500	-0.00002500
H	0.92336700	1.49640100	-0.00011400
C	-1.70221100	1.26463300	0.00005400
C	-3.07996500	1.06453600	0.00008200
C	-3.59287900	-0.23017000	0.00002700
C	-2.72311500	-1.32345200	-0.00005900
C	-1.34891900	-1.12370200	-0.00008600
H	-1.30039000	2.27487500	0.00009600
H	-3.75009500	1.91864100	0.00014400
H	-4.66679600	-0.39114300	0.00004600
H	-3.12014100	-2.33405800	-0.00011000
H	-0.68551900	-1.98360500	-0.00016300

2,4-pentanedione

Zero-point correction= 0.123392 (Hartree/Particle)
Thermal correction to energy= 0.131736
Thermal correction to enthalpy= 0.132680
Thermal correction to Gibbs free energy= 0.089559
Sum of electronic and zero-point energies= -345.524137
Sum of electronic and thermal energies= -345.515793
Sum of electronic and thermal enthalpies= -345.514848
Sum of electronic and thermal free energies= -345.557970
Entropy= 90.758 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -344.8717319 (Hartree/Particle)

XYZ coordinates

O	-0.97174200	1.23283400	-0.62350900
C	-1.19412700	0.19978300	-0.03309000
C	-0.08254800	-0.59467800	0.65295700
O	1.76898700	-1.14818800	-0.72173900
C	1.28472200	-0.33311900	0.03145800
H	-0.29942100	-1.66556700	0.59542400
C	-2.58242700	-0.38385900	0.07662900
H	-2.63322500	-1.29875000	-0.52505400
H	-2.80377000	-0.66369600	1.11215500
H	-3.31787600	0.33379400	-0.28885900
C	1.97148500	0.95929900	0.38937500
H	1.32730100	1.79734000	0.10370700
H	2.12661200	1.01245200	1.47335400
H	2.93092600	1.02501400	-0.12527300
H	-0.09113800	-0.30231900	1.71256200

Catalyst 1i

Zero-point correction= 0.465667 (Hartree/Particle)
Thermal correction to energy= 0.487652
Thermal correction to enthalpy= 0.488596
Thermal correction to Gibbs free energy= 0.413473
Sum of electronic and zero-point energies= -1303.079210
Sum of electronic and thermal energies= -1303.057225
Sum of electronic and thermal enthalpies= -1303.056281
Sum of electronic and thermal free energies= -1303.131403
Entropy= 158.109 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -1300.783047799 (Hartree/Particle)

XYZ coordinates

C	-2.09552995	1.37788786	-0.02743199
N	-3.40215295	1.85954086	-0.45487999
C	-4.59223395	1.37550386	-0.01163799
S	-4.71858795	0.23299386	1.21639001
N	-5.66836395	1.91865986	-0.64507499
C	-7.04200995	1.71264986	-0.20753899
C	-7.88664795	2.90303686	-0.68904399
C	-9.30639195	2.76677186	-0.11884699
C	-9.94504095	1.45110586	-0.58005999
C	-9.07612295	0.24684486	-0.20713099
C	-7.64759295	0.40769286	-0.73094699
N	-7.19576595	4.17477186	-0.44328899
C	-6.93437095	4.46217186	0.96057001
C	-7.84034695	5.30251186	-1.09511899
H	-7.05656295	1.66984686	0.89160701
H	-7.64258995	0.43225986	-1.83007599
H	-7.01899395	-0.42905914	-0.41374199
H	-9.51843295	-0.67644814	-0.59728899
H	-9.04478895	0.14410086	0.88688201
H	-10.07258295	1.48009286	-1.67196799
H	-10.94729895	1.34947286	-0.14860099
H	-9.26733595	2.78850086	0.97904401
H	-9.92381795	3.61515286	-0.43713999
H	-7.96105395	2.82535886	-1.78658499
H	-3.40988895	2.41699786	-1.30318299
H	-5.53209895	2.84170186	-1.05634999
H	-6.33088895	5.37317286	1.02433901
H	-7.85467395	4.62477286	1.54765501
H	-6.36415595	3.64861086	1.41930701
H	-7.16971095	6.16734086	-1.06851399
H	-8.04300295	5.05685086	-2.14245799
H	-8.79051795	5.59733486	-0.61698299
H	-2.22258595	1.06671786	1.01657901
C	-1.65412895	0.15846186	-0.83803999
C	-1.08225295	2.51305486	-0.07801399
C	-1.46410195	3.79587986	0.33496101
C	0.24197805	2.28731986	-0.48378399
C	-0.56005895	4.85179886	0.33504001
H	-2.48763795	3.95655786	0.66582301
C	1.14212005	3.35927186	-0.47844499
C	0.75391105	4.63259986	-0.07857799

H	-0.87620595	5.83826586	0.66171801
H	2.16899705	3.18148686	-0.79266199
H	1.47234105	5.44741886	-0.08109599
H	-2.34620895	-0.66374914	-0.62929199
H	-1.72629795	0.39318386	-1.91054199
C	0.71984805	0.92014086	-0.93238299
H	0.79217205	0.91375086	-2.02978599
H	1.73577105	0.75274986	-0.55623899
C	-0.21423295	-0.20431714	-0.48916799
H	0.07602505	-1.14592214	-0.96692499
H	-0.12975495	-0.35531114	0.59565001

Product (*R*) obtained with catalyst 1i.

Complex C

Zero-point correction= 0.734887 (Hartree/Particle)
Thermal correction to energy= 0.776166
Thermal correction to enthalpy= 0.777110
Thermal correction to Gibbs free energy= 0.659228
Sum of electronic and zero-point energies= -2162.463827
Sum of electronic and thermal energies= -2162.422548
Sum of electronic and thermal enthalpies= -2162.421603
Sum of electronic and thermal free energies= -2162.539486
Entropy= 248.105 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -2158.531403 (Hartree/Particle)

XYZ coordinates

N	0.29575900	-1.82185800	-0.52554600
C	-0.99918500	-2.09612200	-0.28295900
S	-1.54152700	-3.60096100	0.29298300
N	-1.83773100	-1.04261000	-0.50392000
C	-3.26974900	-1.20649500	-0.65407000
C	-4.02209200	-0.03035000	-0.02657200
C	-5.52702500	-0.27718600	-0.04792200
C	-5.98314700	-0.44663000	-1.50412800
C	-5.21740800	-1.57212000	-2.20441600
C	-3.70482600	-1.35664500	-2.11572200
N	-3.46234200	0.25043500	1.34584700
C	-3.47798200	-0.90843800	2.27910500
C	-4.04763200	1.46230000	1.97478000

O	-0.99980800	0.65187900	2.58394800
N	-0.38461900	1.66884200	2.24842300
O	-0.71112900	2.79040000	2.59507700
C	0.77205900	1.46357800	1.42045000
C	1.48237300	2.51277200	0.99337500
C	-0.34392900	3.00593800	-1.54792500
C	-1.38933600	2.94272000	-0.60502600
O	-1.83707200	1.88755100	-0.08078100
C	2.70196200	2.40544700	0.19170100
C	3.40825500	1.19865400	0.07774200
C	4.56752000	1.13786600	-0.68730300
C	5.03477300	2.27458000	-1.34972900
C	4.34274600	3.48015100	-1.23461700
C	3.18756900	3.54541100	-0.46217600
C	0.35389500	1.87646000	-2.04499300
C	1.46888100	2.10436000	-3.05104500
O	0.12209300	0.68824300	-1.71971700
C	-2.03235200	4.24652700	-0.15786600
H	-3.54076400	-2.12880700	-0.12871300
H	-3.40772100	-0.45760000	-2.67427300
H	-3.16302800	-2.20558100	-2.54634900
H	-5.53004500	-1.64408300	-3.25173800
H	-5.46894900	-2.53156100	-1.73097000
H	-5.81733500	0.49766200	-2.04104100
H	-7.06065400	-0.64114200	-1.52856900
H	-5.77438100	-1.18698800	0.51589700
H	-6.06608100	0.55770700	0.41383600
H	-3.78441200	0.88405400	-0.58211500
H	0.49891200	-0.92267400	-0.97542200
H	-1.41693000	-0.17233300	-0.86815100
H	-3.07090700	-0.57038700	3.23195000
H	-4.50765000	-1.24812000	2.40564900
H	-2.85395100	-1.71066700	1.87800100
H	-3.38809700	1.76126300	2.79153400
H	-4.07978500	2.25486800	1.22692000
H	-5.04498500	1.22781900	2.35152600
H	-0.05787900	3.98227800	-1.92463200
H	-1.57550300	5.12826600	-0.61431400
H	-3.09761400	4.22972600	-0.41778800
H	-1.95631700	4.32065900	0.93249300
H	2.38969200	1.64529500	-2.67307600
H	1.20774700	1.59788300	-3.98654900
H	1.65418800	3.16236300	-3.25261700
H	-2.47183800	0.49027700	1.16441100

H	0.93437800	0.41926600	1.19180600
H	1.13756400	3.50957200	1.26031000
H	3.07173300	0.31288000	0.61039400
H	5.11345400	0.20066300	-0.75167200
H	5.94085300	2.22358800	-1.94670700
H	4.70344500	4.36783900	-1.74592100
H	2.63839100	4.48031800	-0.37588000
C	1.40029200	-2.76119200	-0.42693400
H	0.96747600	-3.71837000	-0.11649800
C	2.05621500	-2.92784800	-1.79825200
C	2.39209600	-2.31381700	0.64021500
C	1.89641300	-1.85508300	1.86727500
C	3.77862300	-2.36223900	0.43115500
C	2.75324400	-1.40484300	2.86549900
H	0.81888400	-1.84209500	2.02618800
C	4.63155900	-1.90747600	1.44516800
C	4.13263800	-1.42158100	2.64884000
H	5.70735200	-1.93654400	1.27898800
H	4.81380800	-1.06509400	3.41619700
H	1.34785900	-3.42952000	-2.46611600
H	2.25946000	-1.93374700	-2.22518100
C	3.36305400	-3.70468000	-1.66994600
C	4.36773200	-2.88370800	-0.86414200
H	3.17402400	-4.66200900	-1.16554300
H	3.77410700	-3.93696700	-2.65815900
H	5.26579400	-3.47190000	-0.64137200
H	4.69830600	-2.03320100	-1.47888100
H	2.34828300	-1.03961100	3.80520900

TS

Zero-point correction= 0.734822 (Hartree/Particle)
Thermal correction to energy= 0.774958
Thermal correction to enthalpy= 0.775902
Thermal correction to Gibbs free energy= 0.662122
Sum of electronic and zero-point energies= -2162.448817
Sum of electronic and thermal energies= -2162.408681
Sum of electronic and thermal enthalpies= -2162.407737
Sum of electronic and thermal free energies= -2162.521517
Entropy= 239.470 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -2158.523655 (Hartree/Particle)

XYZ coordinates

C	-1.18474300	2.89792800	-0.20402700
N	-0.14184200	1.89093900	-0.32286700
C	1.17807400	2.09476900	-0.16198100
S	1.83362000	3.55978900	0.38809900
N	1.94103700	1.00180600	-0.45711400
C	3.38047100	1.06767800	-0.60521900
C	4.05349500	-0.16182400	0.01127200
C	5.56953500	0.00688400	0.01577000
C	6.05342900	0.16146300	-1.43324000
C	5.35750000	1.33123800	-2.13495300
C	3.83346900	1.20425000	-2.06222800
N	3.46054300	-0.44033700	1.36652400
C	3.61287500	0.65811100	2.36044700
C	3.89620200	-1.74339400	1.93450900
O	0.99023300	-0.69590600	2.52645000
N	0.39198100	-1.68257300	2.01232000
O	0.81039700	-2.84179800	2.18841300
C	-0.72120800	-1.43811700	1.25101500
C	-1.34009200	-2.49405900	0.58410100
C	-0.26851300	-2.84858800	-1.22206400
C	1.07319400	-2.93076700	-0.68112000
O	1.77369600	-1.93567900	-0.45295500
C	-2.71670500	-2.35278600	0.05094000
C	-3.30874800	-1.10379400	-0.17603500
C	-4.59376700	-1.02130000	-0.70673800
C	-5.30722800	-2.17887600	-1.01484700
C	-4.73163400	-3.42766900	-0.77763700
C	-3.44675900	-3.51011100	-0.24950000
C	-0.69086800	-1.69299800	-1.99379700
C	-1.75477500	-1.91234100	-3.04959600
O	-0.23965700	-0.55716900	-1.81194600
C	1.60337600	-4.31801400	-0.37700300
H	3.70776100	1.96483400	-0.06959600
H	3.48976100	0.32803900	-2.63062200
H	3.34745000	2.08739000	-2.49040400
H	5.68395300	1.39081000	-3.17885200
H	5.65840100	2.27250500	-1.65414800
H	5.84556300	-0.76921700	-1.97927700
H	7.13975000	0.29987600	-1.44343300
H	5.85238800	0.90015300	0.58866900
H	6.05801500	-0.85673300	0.48133700
H	3.78344900	-1.04766700	-0.57234000
H	-0.41596800	1.01499900	-0.77086300

H	1.46495500	0.17502800	-0.84159700
H	3.08934300	0.34784500	3.26479200
H	4.67478700	0.81118400	2.56127000
H	3.15357900	1.56965500	1.97045600
H	3.20482800	-1.99975200	2.73867100
H	3.82804200	-2.49446300	1.14718700
H	4.91879300	-1.64983400	2.30479600
H	-0.71293900	-3.79710100	-1.52114400
H	0.81423000	-4.96806800	0.01302500
H	1.99123400	-4.77170100	-1.29724400
H	2.40401800	-4.25326700	0.36097600
H	-1.29471600	-2.37459900	-3.93167800
H	-2.54190300	-2.58451900	-2.69218900
H	-2.18745200	-0.95163300	-3.33606500
H	2.43753300	-0.52688000	1.22042000
H	-0.97866800	-0.39476200	1.16954400
H	-1.09061700	-3.48679700	0.95098000
H	-2.77686200	-0.18666100	0.06599300
H	-5.03879300	-0.04311100	-0.86840500
H	-6.30922300	-2.10895900	-1.42817300
H	-5.28361100	-4.33550300	-1.00357700
H	-2.99465800	-4.48388500	-0.07061300
H	-0.71794100	3.77046500	0.26504000
C	-1.68864800	3.28654300	-1.59617300
C	-2.29593700	2.39196500	0.70636600
C	-1.94473500	1.78559600	1.91894400
C	-3.65055200	2.52846500	0.36835500
C	-2.91554200	1.27624300	2.77354900
H	-0.89028700	1.69329600	2.17638500
C	-4.61879200	2.01885400	1.24236200
C	-4.26343400	1.38682900	2.42859200
H	-2.62060000	0.78894800	3.69847900
H	-5.67045300	2.12096100	0.97857400
H	-5.03182100	0.98714800	3.08417400
H	-0.89618500	3.84148700	-2.10975400
H	-1.87499000	2.37052300	-2.17736400
C	-4.08192700	3.20874800	-0.91530400
H	-4.34950700	2.44234100	-1.65894800
H	-4.99288300	3.78924200	-0.72777500
C	-2.97978500	4.09253900	-1.49549300
H	-3.27724200	4.47299100	-2.47851200
H	-2.82118400	4.96353600	-0.84512800

Complex D

Zero-point correction= 0.734787 (Hartree/Particle)
Thermal correction to energy= 0.774926
Thermal correction to enthalpy= 0.775870
Thermal correction to Gibbs free energy= 0.661806
Sum of electronic and zero-point energies= -2162.475478
Sum of electronic and thermal energies= -2162.435340
Sum of electronic and thermal enthalpies= -2162.434396
Sum of electronic and thermal free energies= -2162.548460
Entropy= 240.068 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -2158.544514 (Hartree/Particle)

XYZ coordinates

N	0.34787600	1.79824100	-0.45007300
C	1.67270000	1.85819100	-0.23674500
S	2.49336800	3.27603900	0.21289900
N	2.30172200	0.66468900	-0.39978500
C	3.72985000	0.44793000	-0.41371400
C	4.07808700	-0.75542900	0.47360400
C	5.58503600	-1.01704600	0.47631600
C	6.08594200	-1.24873000	-0.95374000
C	5.74170900	-0.06479900	-1.85793400
C	4.23853700	0.21063600	-1.84038000
N	3.50091900	-0.58756200	1.84845300
C	3.91505000	0.64026300	2.56970300
C	3.68706900	-1.79078900	2.69155000
O	0.95234700	-0.40408100	2.08599600
N	0.41809400	-1.29241700	1.29182600
O	1.18433000	-2.21376100	0.81971100
C	-0.85128300	-1.22856900	0.99790400
C	-1.49504300	-2.32370700	0.21761500
C	-1.22048300	-2.28753000	-1.33686600
C	0.27058800	-2.29819700	-1.67596600
O	0.85231200	-1.28752400	-2.02049900
C	-3.00155800	-2.35106800	0.42371700
C	-3.75505700	-1.17425300	0.51657700
C	-5.14259600	-1.23219900	0.63500300
C	-5.79863100	-2.46198500	0.65397200
C	-5.05646000	-3.63849300	0.56105600
C	-3.66850400	-3.57905700	0.44811900
C	-1.94233900	-1.10428800	-1.96636100
C	-3.04240900	-1.42590800	-2.94515900

O	-1.66929200	0.03842900	-1.66234700
C	0.94196300	-3.64698900	-1.67218400
H	4.20367300	1.35526700	-0.02449600
H	3.68931100	-0.63710200	-2.27553200
H	3.98987200	1.09588300	-2.43541100
H	6.07996000	-0.25715200	-2.88202100
H	6.27895500	0.82798000	-1.50802500
H	5.62079500	-2.16085400	-1.35417100
H	7.16709400	-1.42419100	-0.93843000
H	6.11237400	-0.15302100	0.90428700
H	5.82476500	-1.88773800	1.09638100
H	3.54854400	-1.63431600	0.07811300
H	-0.06314900	0.91305400	-0.75424700
H	1.74904900	-0.09782900	-0.79105300
H	3.40064400	0.64088800	3.53298200
H	4.99634600	0.64069200	2.73030600
H	3.60371700	1.52358800	2.00680900
H	2.99807100	-1.71209400	3.53472400
H	3.41899600	-2.66986100	2.10415200
H	4.71712800	-1.84948100	3.05125000
H	-1.64859500	-3.21811800	-1.73407300
H	0.63997700	-4.22710700	-0.79664300
H	0.64829200	-4.19523600	-2.57645100
H	2.02439300	-3.51102700	-1.66631700
H	-3.49485900	-0.50497400	-3.31551600
H	-2.64370000	-2.01321200	-3.78089900
H	-3.80076700	-2.04051400	-2.44285300
H	2.39835700	-0.49945200	1.77573800
H	-1.39231200	-0.40930100	1.44444400
H	-1.07042000	-3.27580500	0.56452800
H	-3.26917300	-0.20080800	0.48528900
H	-5.70562900	-0.30574000	0.71182200
H	-6.88007000	-2.50453600	0.74629600
H	-5.55615100	-4.60291400	0.58431800
H	-3.09201800	-4.50048700	0.38379200
C	-0.58153700	2.91748800	-0.41090400
H	-0.03233000	3.74902100	0.04468300
C	-0.99426200	3.31515900	-1.83096300
C	-1.76273100	2.58604200	0.49340500
C	-1.50134500	2.04091400	1.75597700
C	-3.08559700	2.86211700	0.11945500
C	-2.53594100	1.75231000	2.64000800
H	-0.47132700	1.81350300	2.02732700
C	-4.11863200	2.56816700	1.01911100

C	-3.85568300	2.01566300	2.26823700
H	-5.14503300	2.78805300	0.72902400
H	-4.67257100	1.79496300	2.95034300
H	-0.13581400	3.79094200	-2.31788400
H	-1.23786300	2.40692600	-2.39580000
C	-2.21312400	4.23323300	-1.80526800
C	-3.40654600	3.47417000	-1.22707000
H	-2.00253400	5.11826300	-1.18901900
H	-2.44505400	4.59102400	-2.81452700
H	-4.27973500	4.13023400	-1.13007300
H	-3.68951200	2.67242200	-1.92531600
H	-2.31404200	1.31889300	3.61148300

Product (*S*) obtained with catalyst 1i.

Complex C

Zero-point correction= 0.735206 (Hartree/Particle)
Thermal correction to energy= 0.776381
Thermal correction to enthalpy= 0.777326
Thermal correction to Gibbs free energy= 0.660169
Sum of electronic and zero-point energies= -2162.460423
Sum of electronic and thermal energies= -2162.419248
Sum of electronic and thermal enthalpies= -2162.418304
Sum of electronic and thermal free energies= -2162.535461
Entropy= 246.577 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -2158.528873 (Hartree/Particle)

XYZ coordinates

C	-1.35302600	2.91753200	-0.12699600
N	-0.26873200	1.99826200	-0.42621300
C	1.02982000	2.18328700	-0.12803300
S	1.62071900	3.58747500	0.62837300
N	1.82886100	1.12806800	-0.45698400
C	3.26898200	1.24701400	-0.56029000
C	3.95996700	-0.02194600	-0.05616100
C	5.47301300	0.16932100	-0.01895700
C	5.97199300	0.49234200	-1.43450400
C	5.26426100	1.71830700	-2.01635100
C	3.74394800	1.54757600	-1.98574200
N	3.36090900	-0.43870900	1.26530800

C	3.37002700	0.60846700	2.32209000
C	3.92290900	-1.71806000	1.77096000
C	-1.36944400	-1.72234900	0.76858900
C	0.21740800	-2.74627800	-1.93012900
C	1.20865300	-2.83180500	-0.93867500
O	1.71293600	-1.85853400	-0.31280600
C	-2.56912700	-2.06530900	0.00495400
C	-3.36045000	-1.02251500	-0.49002900
C	-4.53252300	-1.29855700	-1.18934900
C	-4.90916500	-2.61903800	-1.42371900
C	-4.10851400	-3.66636100	-0.95873400
C	-2.94661400	-3.39255000	-0.24765300
C	-0.43353000	-1.54843400	-2.31965800
C	-1.54914500	-1.67765000	-3.34541300
O	-0.17991900	-0.40682300	-1.86678600
C	1.71456100	-4.21289900	-0.54787400
H	3.56309200	2.09172600	0.07211700
H	3.43182300	0.72943600	-2.65056600
H	3.24039700	2.45882500	-2.32589900
H	5.60620600	1.89808500	-3.04133200
H	5.53573600	2.60738900	-1.43033100
H	5.78696100	-0.37618100	-2.08178100
H	7.05593600	0.64726100	-1.41258100
H	5.73532700	0.99467700	0.65703300
H	5.97263100	-0.73380800	0.34835400
H	3.70377600	-0.85770500	-0.71760800
H	-0.50300200	1.16937400	-0.98106600
H	1.38060600	0.31528300	-0.90965400
H	2.91053400	0.17911700	3.21250900
H	4.40304200	0.89572800	2.52873800
H	2.79023900	1.47336000	1.99239000
H	3.25668700	-2.09044400	2.55106600
H	3.94499400	-2.42969500	0.94523500
H	4.92212000	-1.53943400	2.17214300
H	-0.12556300	-3.66860500	-2.38914900
H	1.58672600	-4.34363100	0.53375800
H	1.20379400	-5.02346000	-1.07376100
H	2.78865300	-4.27859200	-0.75853200
H	-2.00644100	-0.70048300	-3.51434900
H	-1.15440000	-2.06398700	-4.29179300
H	-2.31397500	-2.37992500	-2.99264700
H	2.37308600	-0.64932200	1.03308800
H	-3.05742700	0.00605100	-0.31010300
H	-5.14564500	-0.47980200	-1.55534800

H	-5.81707100	-2.83715700	-1.97873000
H	-4.38761000	-4.69615200	-1.16161900
H	-2.30767900	-4.20848000	0.08020200
H	-0.90249400	3.76279600	0.40413000
C	-1.98157200	3.42698800	-1.42444600
C	-2.37309700	2.25280300	0.79002600
C	-1.91200000	1.45958900	1.84824100
C	-3.75380800	2.41018600	0.59666300
C	-2.79959200	0.79669600	2.68783100
H	-0.83920400	1.34507500	1.99342600
C	-4.63736700	1.73912100	1.45115800
C	-4.17380400	0.93052700	2.48268300
H	-2.42070400	0.17304200	3.49324900
H	-5.70852700	1.85220000	1.29229000
H	-4.87842900	0.41045400	3.12548300
C	-0.76841700	-2.53757400	1.64154200
H	-1.03644900	-3.55341000	1.89779700
N	0.42323000	-2.10350800	2.32039100
O	0.73926000	-0.91661300	2.30690500
O	1.07011600	-2.96535200	2.90251400
H	-0.93850300	-0.73503000	0.61315800
H	-1.24518800	4.04477700	-1.94923500
H	-2.21317500	2.57016400	-2.07592800
C	-4.30664400	3.25400700	-0.53414700
H	-4.67005600	2.58617200	-1.33002500
H	-5.18121600	3.81099200	-0.17784800
C	-3.26181300	4.20013300	-1.12275300
H	-3.65199100	4.67361200	-2.02994200
H	-3.04347700	5.00447100	-0.40714700

TS

Zero-point correction= 0.734905 (Hartree/Particle)
Thermal correction to energy= 0.775024
Thermal correction to enthalpy= 0.775968
Thermal correction to Gibbs free energy= 0.661321
Sum of electronic and zero-point energies= -2162.442431
Sum of electronic and thermal energies= -2162.402312
Sum of electronic and thermal enthalpies= -2162.401368
Sum of electronic and thermal free energies= -2162.516015
Entropy= 241.295 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -2158.518671 (Hartree/Particle)

XYZ coordinates

C	-0.91551100	3.02283300	-0.02643900
N	0.10122200	2.07141200	-0.44182700
C	1.39836000	2.09105800	-0.09339500
S	2.09451700	3.33331600	0.83126100
N	2.10529800	1.00686900	-0.53226400
C	3.55342700	0.94907200	-0.50673600
C	4.05059500	-0.42796200	-0.05525700
C	5.56181400	-0.40263400	0.15188400
C	6.23682200	-0.04397700	-1.18014400
C	5.72257700	1.28896300	-1.73115300
C	4.19620200	1.29578400	-1.85328200
N	3.26957300	-0.88310500	1.14859800
C	3.34048400	0.02147000	2.33047900
C	3.56127200	-2.28646200	1.54028600
C	-1.49911100	-1.79165600	0.27824300
C	-0.54301800	-2.40965200	-1.53699200
C	0.78432400	-2.69837500	-1.03807000
O	1.71592100	-1.88626100	-0.98886200
C	-2.90011600	-1.89398100	-0.19511800
C	-3.57387900	-0.72374900	-0.55631700
C	-4.89168400	-0.77850600	-1.00596800
C	-5.54497500	-2.00410900	-1.11211100
C	-4.87643200	-3.17822400	-0.75681500
C	-3.56436000	-3.12253300	-0.29833400
C	-0.81898100	-1.24071800	-2.35031500
C	-1.91259400	-1.36393500	-3.39082400
O	-0.22910700	-0.16309900	-2.20841800
C	1.01397300	-4.09395300	-0.48552400
H	3.87814500	1.70148200	0.21961300
H	3.86426400	0.57053000	-2.61012400
H	3.83411100	2.28256400	-2.16079900
H	6.18190000	1.49437100	-2.70403800
H	6.02857400	2.10142700	-1.05753100
H	6.03501600	-0.84275000	-1.90728800
H	7.32256000	-0.00782500	-1.04151400
H	5.83169200	0.34631800	0.90859400
H	5.92527900	-1.37555800	0.50176000
H	3.79970000	-1.16986800	-0.82023800
H	-0.20693700	1.30652000	-1.04395700
H	1.61083700	0.30863100	-1.10092600
H	2.69280100	-0.40279100	3.09805100
H	4.37457400	0.07024800	2.67727200

H	2.97551600	1.01383700	2.05526300
H	2.76775700	-2.61107900	2.21967500
H	3.56224800	-2.90013400	0.63839100
H	4.53016800	-2.32822100	2.04142000
H	-1.14587500	-3.28532800	-1.76226400
H	1.11036000	-4.03297200	0.60604100
H	0.20031400	-4.78527200	-0.71548200
H	1.95350000	-4.48814400	-0.88503200
H	-2.30577400	-0.37409000	-3.63294200
H	-1.48485100	-1.80468200	-4.29993000
H	-2.72330600	-2.01580900	-3.04952200
H	2.27471000	-0.88816900	0.85446000
H	-3.06549900	0.23444500	-0.46806900
H	-5.40599500	0.14160600	-1.27035900
H	-6.56990200	-2.04854300	-1.46881200
H	-5.37904600	-4.13759500	-0.84024700
H	-3.04272500	-4.04103000	-0.03668900
H	-0.40138600	3.76870300	0.58928900
C	-1.51566000	3.72217900	-1.24595600
C	-1.97631800	2.33550000	0.82596700
C	-1.57814000	1.36423600	1.75291800
C	-3.33555400	2.66560900	0.71160400
C	-2.51060300	0.70516100	2.54659500
H	-0.52542100	1.10292800	1.83558000
C	-4.26258200	2.00118600	1.52376200
C	-3.86393500	1.02456900	2.42967300
H	-2.17966600	-0.05840200	3.24564300
H	-5.31792400	2.25256400	1.42959000
H	-4.60427000	0.51227700	3.03766500
C	-1.08850100	-2.54311800	1.38397500
H	-1.55151200	-3.45134900	1.74091600
N	0.04022800	-2.17962900	2.07595000
O	0.63557400	-1.10497700	1.78955000
O	0.46498400	-2.91124700	2.98866900
H	-1.04300600	-0.80625900	0.19505100
H	-0.73381700	4.31966900	-1.72678100
H	-1.84526000	2.96579500	-1.97483300
C	-3.82607200	3.68960000	-0.29268800
H	-4.28793500	3.15984800	-1.13989200
H	-4.62087400	4.29303700	0.16128300
C	-2.70363400	4.58090000	-0.82112100
H	-3.06496400	5.18533600	-1.66003200
H	-2.38272000	5.27907000	-0.03609600

Complex D

Zero-point correction= 0.735737 (Hartree/Particle)
Thermal correction to energy= 0.775569
Thermal correction to enthalpy= 0.776513
Thermal correction to Gibbs free energy= 0.663616
Sum of electronic and zero-point energies= -2162.471700
Sum of electronic and thermal energies= -2162.431868
Sum of electronic and thermal enthalpies= -2162.430924
Sum of electronic and thermal free energies= -2162.543821
Entropy= 237.612 cal mol^{-1} K^{-1}

Single-point COSMO-RIJCOSX-MP2/aug-cc-pVDZ= -2158.54902 (Hartree/Particle)

XYZ coordinates

C	-0.72642700	2.83207600	-0.43082000
N	0.29562700	1.84524900	-0.74559600
C	1.58893300	1.91785800	-0.37965000
S	2.27413100	3.27550600	0.37702500
N	2.30745900	0.80068700	-0.66355700
C	3.73653500	0.66005900	-0.50168600
C	4.07830200	-0.66243900	0.19958900
C	5.59083600	-0.79161900	0.39251400
C	6.31868600	-0.69232100	-0.95337400
C	5.97306100	0.60743800	-1.67804700
C	4.46114000	0.74007400	-1.85105700
N	3.30737200	-0.82961800	1.48367400
C	3.37588800	0.30712500	2.43673100
C	3.62433200	-2.10423900	2.17471300
C	-1.65196100	-1.53805600	0.10986200
C	-1.03921700	-2.21255600	-1.17088700
C	0.48635100	-2.38264400	-1.21191500
O	1.19656700	-1.68714500	-1.91751100
C	-3.15901800	-1.69417400	0.03996100
C	-3.95642900	-0.60248900	-0.30675100
C	-5.34077100	-0.73731000	-0.40650300
C	-5.94328900	-1.96983800	-0.16503300
C	-5.15401300	-3.06841900	0.17863900
C	-3.77166400	-2.92973800	0.27786900
C	-1.47599000	-1.37992300	-2.37390600
C	-2.14758900	-2.10516900	-3.50754300
O	-1.29563800	-0.17944300	-2.38736800
C	1.03555400	-3.58969300	-0.49227600

H	4.07275400	1.49990100	0.11559200
H	4.08037500	-0.05604800	-2.50775700
H	4.19724500	1.69773200	-2.31208500
H	6.47152100	0.64432800	-2.65269700
H	6.34731400	1.46156700	-1.09644800
H	6.02941200	-1.54735400	-1.58061900
H	7.39861700	-0.77136000	-0.78854900
H	5.94396400	0.00984000	1.05650800
H	5.83819200	-1.74502200	0.87045400
H	3.72109600	-1.48876400	-0.43548700
H	-0.04243500	0.98580600	-1.18350800
H	1.82629900	0.03540900	-1.13705700
H	2.72787500	0.05177700	3.27829800
H	4.40398400	0.44840900	2.78099400
H	3.00318400	1.21630600	1.95973100
H	2.80871400	-2.30513500	2.87177100
H	3.67811400	-2.90628000	1.43439300
H	4.57923200	-2.01872000	2.69803600
H	-1.46149500	-3.22418900	-1.24896300
H	0.60079500	-3.69815600	0.50579400
H	0.77231600	-4.48618800	-1.06821800
H	2.12351700	-3.51769500	-0.43671000
H	-2.34323800	-1.42208100	-4.33478600
H	-1.52295200	-2.94100200	-3.84314800
H	-3.09123200	-2.52810300	-3.13849600
H	2.24086800	-0.90285900	1.22394200
H	-3.48407800	0.36062400	-0.48539200
H	-5.94686100	0.12602200	-0.66813800
H	-7.02171900	-2.07616700	-0.24038800
H	-5.61656600	-4.03234700	0.37163500
H	-3.16202400	-3.79002400	0.55162100
H	-0.18901600	3.70614700	-0.04686000
C	-1.48255000	3.24282600	-1.69333600
C	-1.66558100	2.33031100	0.66174700
C	-1.15908100	1.52823600	1.69215800
C	-3.02481400	2.68095900	0.66631200
C	-1.98453900	1.05340000	2.70598200
H	-0.10782000	1.24885600	1.67809700
C	-3.84075500	2.21268200	1.70278600
C	-3.33655800	1.39990600	2.71185300
H	-1.57101300	0.41187700	3.48011000
H	-4.89693400	2.47844700	1.69973300
H	-3.99461500	1.03417400	3.49513400
C	-1.11968500	-1.99596100	1.43101900

H	-1.71229600	-2.48119800	2.19405500
N	0.08914800	-1.63716300	1.77576600
O	0.80399500	-1.01362800	0.86357900
O	0.62462700	-1.86233400	2.90655900
H	-1.41022000	-0.47330100	0.01220900
H	-0.77558100	3.70408800	-2.39120300
H	-1.89531700	2.34956900	-2.18381700
C	-3.64462800	3.49289900	-0.45363300
H	-4.23273900	2.81351000	-1.09071100
H	-4.35890700	4.21100800	-0.03368600
C	-2.60783400	4.20532500	-1.32038900
H	-3.08495900	4.60981200	-2.21956600
H	-2.18646700	5.05747600	-0.76983900

PCM-B97-D/TZVP approximation

β-nitrostyrene

Zero-point correction= 0.132411 (Hartree/Particle)
Thermal correction to energy= 0.141769
Thermal correction to enthalpy= 0.142713
Thermal correction to Gibbs free energy= 0.096517
Sum of electronic and zero-point energies= -513.855790
Sum of electronic and thermal energies= -513.846432
Sum of electronic and thermal enthalpies= -513.845488
Sum of electronic and thermal free energies= -513.891684
Entropy= 97.227 cal mol^{-1} K^{-1}

XYZ coordinates

O	3.29191000	1.16760500	0.00020000
N	2.99832400	-0.03349400	-0.00002000
C	1.59808800	-0.44290300	-0.00005700
H	1.48778100	-1.52010700	-0.00021700
O	3.83030100	-0.95355600	-0.00021200
C	0.60467900	0.46522600	0.00007500
C	-0.82300200	0.18244600	0.00004700
H	0.89432400	1.51588400	0.00019500
C	-1.71915300	1.27365200	-0.00007200
C	-3.09878400	1.06493900	-0.00012800
C	-3.60729300	-0.23848100	-0.00004800
C	-2.72905700	-1.33322800	0.00008900
C	-1.35251500	-1.12832300	0.00013600
H	-1.31996200	2.28649500	-0.00012600
H	-3.77605100	1.91618900	-0.00022700

H	-4.68258500	-0.40436900	-0.00008200
H	-3.12405700	-2.34684100	0.00016700
H	-0.68318200	-1.98514700	0.00026000

2,4-pentanedione

Zero-point correction= 0.118141 (Hartree/Particle)
Thermal correction to energy= 0.126605
Thermal correction to enthalpy= 0.127549
Thermal correction to Gibbs free energy= 0.084425
Sum of electronic and zero-point energies= -345.578263
Sum of electronic and thermal energies= -345.569799
Sum of electronic and thermal enthalpies= -345.568855
Sum of electronic and thermal free energies= -345.611978
Entropy= 90.761 cal mol^{-1} K^{-1}

XYZ coordinates

O	-1.53586400	1.20854600	0.75516700
C	-1.21645000	0.31886500	-0.01174500
C	0.04242400	0.45096800	-0.88742900
O	2.20861800	0.86711300	0.07420800
C	1.31699200	0.06147600	-0.11133800
H	0.14706600	1.49116600	-1.20800700
C	-2.02015900	-0.95819000	-0.16757600
H	-2.75787700	-1.05084600	0.63502800
H	-2.53899200	-0.92275200	-1.13781900
H	-1.36125500	-1.83529500	-0.19285700
C	1.38184200	-1.36247900	0.40922900
H	0.65633600	-1.47740000	1.22831100
H	1.10073500	-2.07843900	-0.37431100
H	2.38492300	-1.58183800	0.78613600
H	-0.04086400	-0.21370700	-1.75833100

Catalyst 1b

Zero-point correction= 0.411722 (Hartree/Particle)
Thermal correction to energy= 0.433616
Thermal correction to enthalpy= 0.434560
Thermal correction to Gibbs free energy= 0.359290
Sum of electronic and zero-point energies= -1225.824017
Sum of electronic and thermal energies= -1225.802123
Sum of electronic and thermal enthalpies= -1225.801179

Sum of electronic and thermal free energies= -1225.876449
Entropy= 158.419 cal mol^{-1} K^{-1}

XYZ coordinates

C	2.58965300	-1.35285800	-0.06191400
N	1.29736300	-0.76479000	-0.44461900
C	0.07256500	-1.10994600	0.04756100
S	-0.14064900	-2.28318900	1.26306500
N	-0.95856500	-0.41865300	-0.52635800
C	-2.33352300	-0.42203200	-0.02008100
C	-3.01886700	0.89099200	-0.46401300
C	-4.42321900	0.96166800	0.17008300
C	-5.27420300	-0.24427000	-0.26710400
C	-4.57582800	-1.57154200	0.07477000
C	-3.15579600	-1.62352900	-0.51439100
N	-2.13891200	2.05543900	-0.24089700
C	-1.85448400	2.33613100	1.16815900
C	-2.60069300	3.25256300	-0.93967800
H	-2.30360300	-0.46515200	1.07852100
H	-3.20034400	-1.58957100	-1.61341000
H	-2.64332000	-2.54558400	-0.22081400
H	-5.16677300	-2.42013000	-0.29479400
H	-4.50998600	-1.67535000	1.16859600
H	-5.43223600	-0.19097000	-1.35567200
H	-6.26463400	-0.19864400	0.20605400
H	-4.32447100	0.96531200	1.26463600
H	-4.91301600	1.89988900	-0.12134500
H	-3.14771000	0.83140200	-1.55656100
H	1.33014500	-0.11745700	-1.22414100
H	-0.71822600	0.49570800	-0.91336900
H	-1.09554400	3.12697600	1.22317200
H	-2.74615300	2.67505700	1.72940900
H	-1.45407200	1.44033600	1.65558300
H	-1.82904100	4.03030300	-0.86920100
H	-2.76663300	3.01691100	-1.99893700
H	-3.54079700	3.66604400	-0.52297100
H	2.44371800	-1.74090600	0.95310100
C	2.94378700	-2.53150200	-0.97693200
C	3.62287500	-0.23285600	-0.00126300
C	3.48221200	0.75130500	0.99327700
C	4.69337300	-0.13295600	-0.89941300
C	4.38904100	1.80783200	1.08872300
H	2.65055600	0.67891700	1.69295200
C	5.60527100	0.92762600	-0.80760800

H	4.82680300	-0.88498900	-1.67328400
C	5.45645200	1.89983500	0.18464400
H	4.26887800	2.55735100	1.86905700
H	6.43242300	0.98941900	-1.51266900
H	6.16607400	2.72195000	0.25706100
H	2.15299800	-3.28542500	-0.90117600
H	3.02832700	-2.21022000	-2.02345800
H	3.89612300	-2.98288200	-0.67117100

Catalyst 1i

Zero-point correction= 0.446881 (hartree/particle)
Thermal correction to energy= 0.469775
Thermal correction to enthalpy= 0.470719
Thermal correction to Gibbs free energy= 0.393561
Sum of electronic and zero-point energies= -1303.179402
Sum of electronic and thermal energies= -1303.156508
Sum of electronic and thermal enthalpies= -1303.155563
Sum of electronic and thermal free energies= -1303.232722
Entropy= 162.393 cal mol^{-1} K^{-1}

XYZ coordinates

C	2.27930900	-0.84059400	0.11996400
N	0.95126300	-0.37882100	-0.28552700
C	-0.23976700	-0.83649600	0.19980000
S	-0.35236100	-1.95338400	1.47986600
N	-1.32657100	-0.30251600	-0.43511200
C	-2.71025500	-0.47618200	0.01394200
C	-3.55481600	0.70242600	-0.52070200
C	-4.98748200	0.58647600	0.04131200
C	-5.63011100	-0.74886700	-0.37459900
C	-4.76427900	-1.94082100	0.06700100
C	-3.32555200	-1.80561000	-0.45598300
N	-2.87159900	1.99371100	-0.30445900
C	-2.70955900	2.35867700	1.10475900
C	-3.47549600	3.08281800	-1.06949000
H	-2.72740800	-0.46814000	1.11343200
H	-3.31975100	-1.82349200	-1.55633600
H	-2.69896500	-2.62876600	-0.09704600
H	-5.20429100	-2.88386600	-0.28361700
H	-4.74053600	-1.98371700	1.16661400
H	-5.73566400	-0.76735800	-1.47064900
H	-6.64053900	-0.82892500	0.04915700

H	-4.95038200	0.64822500	1.13790800
H	-5.59264300	1.42942700	-0.31624900
H	-3.61469500	0.58514700	-1.61465600
H	0.92998400	0.17871000	-1.13214300
H	-1.18757600	0.61119000	-0.86869100
H	-2.09907400	3.26861100	1.16526400
H	-3.67299200	2.55635400	1.61308100
H	-2.18896500	1.55817800	1.64190900
H	-2.83292900	3.97044300	-1.00170000
H	-3.55788300	2.78736200	-2.12348700
H	-4.48399900	3.36400300	-0.70639800
H	2.16591600	-1.19741700	1.15243100
C	2.73730000	-2.03157200	-0.73936100
C	3.27289400	0.31973500	0.11538600
C	2.87216800	1.57993700	0.59181000
C	4.60767000	0.13217600	-0.30048100
C	3.76517200	2.65091100	0.64547600
H	1.84392800	1.71215100	0.92323700
C	5.49691900	1.21758900	-0.23724700
C	5.08857000	2.46896500	0.22653600
H	3.43394300	3.61833600	1.01873600
H	6.52853300	1.06834100	-0.55583300
H	5.79764400	3.29391500	0.26799400
H	2.06569600	-2.87466400	-0.53997800
H	2.64317100	-1.76556900	-1.80361900
C	5.10166100	-1.20434200	-0.82865200
H	5.14420800	-1.15311500	-1.92891300
H	6.13226500	-1.36975300	-0.48664000
C	4.19683200	-2.37748900	-0.42601000
H	4.50126100	-3.28806800	-0.95769000
H	4.30080600	-2.57644700	0.65094400

Product (*R*) obtained with catalyst 1b.

Complex C

Zero-point correction= 0.670747 (hartree/particle)
Thermal correction to energy= 0.712629
Thermal correction to enthalpy= 0.713573
Thermal correction to Gibbs free energy= 0.594270
Sum of electronic and zero-point energies= -2085.302646
Sum of electronic and thermal energies= -2085.260764

Sum of electronic and thermal enthalpies= -2085.259820
Sum of electronic and thermal free energies= -2085.379122
Entropy= 251.094 cal mol^{-1} K^{-1}

XYZ coordinates

C	-1.09049700	3.12657200	-0.85716000
N	-0.11805000	2.03328000	-0.90559200
C	1.18863400	2.10659600	-0.56553900
S	1.93878900	3.55341600	-0.02083400
N	1.85753700	0.91379300	-0.65691400
C	3.30848200	0.81943100	-0.71386900
C	3.83015400	-0.40739000	0.05176100
C	5.35914600	-0.39125500	0.10860800
C	5.91906500	-0.42201600	-1.32765500
C	5.37981900	0.74809300	-2.16574900
C	3.84303300	0.77078700	-2.15894400
N	3.17132600	-0.49666300	1.42628200
C	3.35186700	0.72168500	2.28104800
C	3.54381900	-1.74664300	2.16566700
O	0.55074900	-0.56994700	2.84868800
N	-0.21156600	-1.49364400	2.47656200
O	-0.10863500	-2.65537800	2.89138900
C	-1.24726400	-1.12410800	1.55532400
C	-2.08697100	-2.04315300	1.03144000
C	-0.37160900	-2.90826700	-1.42473800
C	0.65633900	-3.00577700	-0.45357400
O	1.32897700	-2.04030800	0.00042300
C	-3.21680500	-1.74714000	0.16649600
C	-3.59533500	-0.42946700	-0.17088300
C	-4.69926100	-0.20214300	-0.98850300
C	-5.44819500	-1.27775600	-1.48487100
C	-5.08529600	-2.59004500	-1.15551500
C	-3.98217800	-2.82135300	-0.33601200
C	-0.80131500	-1.72743000	-2.08599000
C	-1.94603600	-1.86094800	-3.08871500
O	-0.32166000	-0.57277600	-1.91369000
C	0.96828000	-4.39900200	0.10273000
H	3.70439600	1.72556000	-0.24278600
H	3.44296000	-0.12368100	-2.65851700
H	3.46151300	1.65147000	-2.68887700
H	5.75319600	0.67936400	-3.19564000
H	5.75089600	1.69513000	-1.74616000
H	5.62845000	-1.37235500	-1.79953800
H	7.01550500	-0.39812100	-1.29021300

H	5.70442200	0.51991100	0.61627400
H	5.73362700	-1.25579100	0.66902100
H	3.48360100	-1.31731000	-0.44651300
H	-0.44820900	1.14323800	-1.29776300
H	1.32221900	0.10014500	-0.99481000
H	2.81863200	0.54692500	3.21661800
H	4.42027300	0.85836600	2.46336400
H	2.93135000	1.58724400	1.76225600
H	2.86366700	-1.83110000	3.01561700
H	3.39628300	-2.58699500	1.48578800
H	4.58073700	-1.66705100	2.49919600
H	-0.87278800	-3.83187900	-1.70373300
H	0.85273800	-4.38046200	1.19377700
H	0.32529200	-5.18116900	-0.31888700
H	2.01704300	-4.64697500	-0.11706700
H	-2.25644400	-2.90004200	-3.24667800
H	-2.80558800	-1.28686800	-2.71994200
H	-1.63868300	-1.41982200	-4.04664400
H	2.16716800	-0.59852000	1.21243700
H	-1.25073200	-0.06595100	1.33490800
H	-1.93867600	-3.08387000	1.31138900
H	-3.03831400	0.41825800	0.21471100
H	-4.97798800	0.81999900	-1.23345500
H	-6.30918000	-1.09430000	-2.12462100
H	-5.66247300	-3.42898500	-1.53876400
H	-3.69141600	-3.83945900	-0.08331600
H	-0.51716700	4.02770500	-0.60463200
C	-1.70608800	3.30764300	-2.25149800
C	-2.09983300	2.88850000	0.26643500
C	-1.62672800	2.47723700	1.52513700
C	-3.47911400	3.08276300	0.10351000
C	-2.50805800	2.24329200	2.58214500
H	-0.55814500	2.33106500	1.66593700
C	-4.36560500	2.84930700	1.16205400
H	-3.87411200	3.40335200	-0.85676800
C	-3.88567500	2.42214500	2.40264000
H	-2.11924200	1.91261300	3.54350000
H	-5.43417700	2.99062000	1.00987000
H	-4.57582300	2.23072700	3.22195500
H	-0.90488800	3.47836600	-2.97865800
H	-2.26951800	2.41415300	-2.55158700
H	-2.38185000	4.17078000	-2.26922200

TS

Zero-point correction= 0.669881 (Hartree/Particle)
Thermal correction to energy= 0.710695
Thermal correction to enthalpy= 0.711639
Thermal correction to Gibbs free energy= 0.594955
Sum of electronic and zero-point energies= -2085.292884
Sum of electronic and thermal energies= -2085.252069
Sum of electronic and thermal enthalpies= -2085.251125
Sum of electronic and thermal free energies= -2085.367810
Entropy= 245.584 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.68366000	3.14896100	-0.94604800
N	0.17160400	1.96807900	-0.80706700
C	1.50685400	1.97092300	-0.59212200
S	2.41773300	3.40258700	-0.32561900
N	2.05906900	0.72356400	-0.57604000
C	3.48096800	0.42798700	-0.62504700
C	3.86022400	-0.62870000	0.43239400
C	5.35737100	-0.95604100	0.37082000
C	5.74181500	-1.45574700	-1.03308700
C	5.37792300	-0.41583300	-2.10158900
C	3.88433200	-0.07233200	-2.02816100
N	3.42453100	-0.19502700	1.83009100
C	3.97947300	1.11933200	2.28643600
C	3.66619500	-1.26003100	2.85501700
O	0.78439000	0.09289500	2.22629600
N	0.16341700	-0.97611200	1.83894700
O	0.67428400	-2.11399600	2.04055400
C	-1.04620000	-0.81351000	1.22839400
C	-1.79656100	-1.92467800	0.79265000
C	-1.14416900	-2.53426600	-1.09506900
C	0.28407800	-2.78908100	-0.89506900
O	1.17467600	-1.94088400	-1.04319800
C	-3.25230600	-1.78412400	0.55046000
C	-3.86093100	-0.54722900	0.26966600
C	-5.23103600	-0.47721800	0.01198900
C	-6.01795300	-1.63422100	0.02647900
C	-5.42360200	-2.87021900	0.30993800
C	-4.05363800	-2.94128000	0.56782500
C	-1.62156500	-1.45097700	-1.95959500
C	-2.86466500	-1.76515600	-2.77899800
O	-1.09567800	-0.33210600	-2.01584200

C	0.63981300	-4.21690800	-0.49912700
H	4.01932400	1.35916900	-0.42287900
H	3.28121500	-0.95841700	-2.26605000
H	3.62441600	0.71433400	-2.74664400
H	5.62768000	-0.79259500	-3.10208400
H	5.97280400	0.49584100	-1.93831000
H	5.20560800	-2.39392800	-1.24009400
H	6.81591100	-1.68034500	-1.05554100
H	5.93996600	-0.05309300	0.60116300
H	5.61145800	-1.71848500	1.11577200
H	3.26756600	-1.53116300	0.24242400
H	-0.26129400	1.08378500	-1.08848100
H	1.46277500	-0.07575800	-0.81831500
H	3.57418600	1.31467300	3.28275200
H	5.06975500	1.05560100	2.32948300
H	3.65498200	1.90500800	1.59772500
H	3.11122200	-0.97844400	3.75251900
H	3.27122900	-2.20139700	2.46984500
H	4.73536600	-1.32647400	3.06852500
H	-1.74189500	-3.44397200	-1.15577800
H	1.66323100	-4.25445600	-0.11472700
H	-0.05579300	-4.59367700	0.26171000
H	0.55753000	-4.87291600	-1.37863600
H	-3.64554100	-2.18100900	-2.12883900
H	-3.22972400	-0.86003700	-3.27414900
H	-2.62639400	-2.52924800	-3.53389400
H	2.36252600	-0.07478700	1.82788700
H	-1.33698600	0.21527000	1.08297300
H	-1.50599800	-2.87373400	1.23945000
H	-3.27595500	0.36687100	0.24776000
H	-5.68061300	0.49045500	-0.19794200
H	-7.08551500	-1.57410300	-0.17629900
H	-6.02702700	-3.77578500	0.33183600
H	-3.58995600	-3.90295900	0.78416700
H	-0.09867200	3.98863700	-0.55118900
C	-0.96912000	3.41400700	-2.43072900
C	-1.91964500	2.98874100	-0.06287300
C	-1.73764900	2.71872900	1.30519500
C	-3.22696700	3.13019300	-0.54837600
C	-2.83182700	2.59404700	2.16303000
H	-0.72805000	2.58213700	1.68705000
C	-4.32623700	3.01565500	0.31249700
H	-3.39636600	3.33169100	-1.60269500
C	-4.13407600	2.74606800	1.66944500

H	-2.66858400	2.37276800	3.21614000
H	-5.33352200	3.13099500	-0.08437400
H	-4.98857300	2.64412700	2.33556400
H	-0.01645700	3.54978100	-2.95447500
H	-1.50396500	2.56780300	-2.87986800
H	-1.57075500	4.32311400	-2.55562700

Complex D

Zero-point correction= 0.670820 (hartree/particle)
Thermal correction to energy= 0.711438
Thermal correction to enthalpy= 0.712382
Thermal correction to Gibbs free energy= 0.596999
Sum of electronic and zero-point energies= -2085.300291
Sum of electronic and thermal energies= -2085.259673
Sum of electronic and thermal enthalpies= -2085.258729
Sum of electronic and thermal free energies= -2085.374112
Entropy= 242.844 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.52137200	3.14199900	-0.99387500
N	0.30593500	1.94074700	-0.84832000
C	1.63759300	1.91011100	-0.61380100
S	2.58341200	3.32100300	-0.36627500
N	2.15884900	0.65057500	-0.57201400
C	3.56890800	0.30437700	-0.51940100
C	3.84115900	-0.73468200	0.58913800
C	5.32550000	-1.12782400	0.61371400
C	5.77256600	-1.67390100	-0.75295200
C	5.51838400	-0.64455700	-1.86178100
C	4.03818400	-0.24242700	-1.88438300
N	3.35205600	-0.24908300	1.94430700
C	3.92485900	1.05489000	2.39410700
C	3.50731400	-1.29000100	3.00579800
O	0.78291900	0.05681200	2.14740200
N	0.18544600	-0.95509600	1.54879300
O	0.81179500	-2.07553800	1.45855600
C	-1.03739800	-0.78440800	1.06005100
C	-1.77930700	-1.93727300	0.49801900
C	-1.40780400	-2.31819900	-1.02769000
C	0.08469100	-2.62516900	-1.19005300
O	0.89498400	-1.80738300	-1.60386700
C	-3.29037200	-1.77702200	0.57221000

C	-3.92597500	-0.54277300	0.36709200
C	-5.32109300	-0.45486500	0.37171000
C	-6.10309800	-1.59692400	0.57396600
C	-5.47807800	-2.83263300	0.77875700
C	-4.08260800	-2.91729400	0.77648700
C	-1.92645300	-1.25483300	-1.98261100
C	-3.04718100	-1.69222200	-2.90011600
O	-1.49236300	-0.11181600	-1.98790100
C	0.46369200	-4.05959800	-0.88815900
H	4.12426400	1.22269300	-0.30608200
H	3.41740900	-1.11101900	-2.14339700
H	3.85066300	0.53666600	-2.63309800
H	5.81181000	-1.05174900	-2.83829600
H	6.13879700	0.24619800	-1.67958500
H	5.21096900	-2.59409900	-0.97480500
H	6.83553100	-1.94375300	-0.70566600
H	5.93127400	-0.24472000	0.86134600
H	5.50404600	-1.88260700	1.38756800
H	3.22044200	-1.61817100	0.39568100
H	-0.17814400	1.06376300	-1.04854400
H	1.54886200	-0.11898000	-0.84824600
H	3.47363800	1.29203100	3.36165800
H	5.01000900	0.96585600	2.50168000
H	3.66430800	1.83455100	1.67286100
H	2.92884900	-0.95691100	3.87114100
H	3.08168600	-2.22184700	2.62930300
H	4.56138900	-1.40178800	3.27360000
H	-1.95108300	-3.25386000	-1.20957800
H	1.55027100	-4.15480000	-0.81059900
H	-0.01173100	-4.38590600	0.04445100
H	0.09374900	-4.70482700	-1.69985300
H	-3.88382000	-2.05605800	-2.28640500
H	-3.37406700	-0.86200000	-3.53298700
H	-2.71306200	-2.53639500	-3.52134800
H	2.25383700	-0.10759500	1.89782500
H	-1.45320000	0.20507600	1.16802700
H	-1.49168200	-2.83868800	1.05498200
H	-3.34394000	0.35826500	0.20041100
H	-5.79118000	0.51411200	0.21822200
H	-7.18916300	-1.52531100	0.57713900
H	-6.07525300	-3.72741000	0.94564100
H	-3.59627400	-3.87915400	0.93772300
H	0.08424500	3.96744500	-0.60010700
C	-0.79819600	3.41375900	-2.47887400

C	-1.76104800	3.01319200	-0.11102500
C	-1.58469500	2.74868400	1.25851000
C	-3.06474700	3.17307600	-0.59970900
C	-2.68187800	2.64964200	2.11581600
H	-0.57905600	2.58743500	1.64070300
C	-4.16721700	3.08236200	0.26031600
H	-3.22907000	3.36780900	-1.65610000
C	-3.98081800	2.82192700	1.61991000
H	-2.52352300	2.43154000	3.17034400
H	-5.17206600	3.20979100	-0.13920900
H	-4.83741100	2.73973800	2.28610300
H	0.15832000	3.52453100	-3.00160400
H	-1.35667200	2.58345700	-2.92781300
H	-1.37431700	4.33955300	-2.60259400

Product (*S*) obtained with catalyst 1b.

Complex C

Zero-point correction= 0.669989 (Hartree/Particle)
Thermal correction to energy= 0.711725
Thermal correction to enthalpy= 0.712670
Thermal correction to Gibbs free energy= 0.593217
Sum of electronic and zero-point energies= -2085.301352
Sum of electronic and thermal energies= -2085.259616
Sum of electronic and thermal enthalpies= -2085.258671
Sum of electronic and thermal free energies= -2085.378124
Entropy= 251.410 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.60963600	3.29755300	-0.22495700
N	0.28240500	2.16818800	-0.48212300
C	1.62025000	2.16100900	-0.29451400
S	2.49408100	3.44758200	0.43386000
N	2.22397800	1.01160200	-0.72451200
C	3.62573000	0.68720400	-0.52561400
C	3.82209000	-0.76743500	-0.04624900
C	5.30202100	-1.01463400	0.26981900
C	6.16121800	-0.76379700	-0.98489000
C	5.94954400	0.65268000	-1.53800400
C	4.46042800	0.91527700	-1.80169900
N	2.88654700	-1.11120300	1.11328400

C	2.88156600	-0.10824700	2.22498500
C	3.11528900	-2.48823300	1.65423300
C	-2.20826800	-1.44184400	0.92927300
C	-0.63119100	-2.05509000	-2.19783100
C	0.29427500	-2.22726900	-1.16483500
O	0.73208500	-1.29041500	-0.40435600
C	-3.37066100	-1.34946100	0.06830000
C	-3.78647100	-0.06226100	-0.33166400
C	-4.91773700	0.10023300	-1.12981500
C	-5.63979500	-1.01962100	-1.55577000
C	-5.22522000	-2.30797100	-1.18054500
C	-4.10268900	-2.47413700	-0.37605800
C	-1.25921900	-0.83446200	-2.60725100
C	-2.32813300	-0.95416100	-3.69676100
O	-1.03802500	0.30963200	-2.14622200
C	0.82623800	-3.63333600	-0.90589200
H	4.01368700	1.36449800	0.24486000
H	4.08910200	0.24973900	-2.59528500
H	4.29260500	1.94892500	-2.12435700
H	6.52899700	0.79127300	-2.45983200
H	6.31833900	1.38781700	-0.80719800
H	5.88470600	-1.49998900	-1.75492800
H	7.21708900	-0.93282600	-0.73829400
H	5.61928800	-0.33716300	1.07491400
H	5.45614100	-2.04301900	0.61434400
H	3.49779900	-1.45314500	-0.84013600
H	-0.14387600	1.37492200	-0.98790400
H	1.59799600	0.23577700	-0.97259300
H	2.16525900	-0.45242900	2.97285700
H	3.88746900	-0.05573100	2.65159800
H	2.58455700	0.86779900	1.83782400
H	2.26672800	-2.73493000	2.29681300
H	3.16386100	-3.18739400	0.81623000
H	4.04663900	-2.50866200	2.22448800
H	-0.92662900	-2.95203000	-2.73649300
H	0.37155200	-4.38097800	-1.56516800
H	1.91497500	-3.64536700	-1.06603200
H	0.64439700	-3.91818000	0.13850700
H	-2.31984400	-1.92905400	-4.19908700
H	-3.31186700	-0.80704800	-3.23028500
H	-2.18788700	-0.15375600	-4.43423900
H	1.92141400	-1.17016900	0.63728200
H	-3.21903000	0.80259600	-0.00393200
H	-5.22830400	1.09939100	-1.42698600

H	-6.51815700	-0.89549700	-2.18623900
H	-5.78000100	-3.17865100	-1.52381400
H	-3.78185000	-3.47549800	-0.09893900
H	0.00265700	4.05377000	0.28417600
C	-1.09377200	3.88159000	-1.56199300
C	-1.72199600	2.88235900	0.73821100
C	-1.42137000	2.03147900	1.81635200
C	-3.03644600	3.36012300	0.61733100
C	-2.40318500	1.66093700	2.73773500
H	-0.41061000	1.64465000	1.91863500
C	-4.02294600	2.99079900	1.53973800
H	-3.30358700	4.01490200	-0.20742100
C	-3.71239900	2.13736300	2.60191700
H	-2.14573200	0.98878000	3.55407700
H	-5.03837800	3.36413200	1.41856600
H	-4.48165800	1.84245900	3.31298200
C	-1.75964000	-2.55712400	1.54056900
H	-2.17064000	-3.55409900	1.44403900
N	-0.57166200	-2.52764100	2.35647800
O	-0.07974500	-1.44588400	2.71168600
O	-0.08403900	-3.63227100	2.66806800
H	-1.65692500	-0.52023300	1.09599400
H	-0.21973600	4.14464300	-2.16819600
H	-1.69661200	3.14609200	-2.10889300
H	-1.68755800	4.79012000	-1.40371800

TS

Zero-point correction= 0.670470 (hartree/particle)
Thermal correction to energy= 0.710988
Thermal correction to enthalpy= 0.711932
Thermal correction to Gibbs free energy= 0.596985
Sum of electronic and zero-point energies= -2085.289365
Sum of electronic and thermal energies= -2085.248847
Sum of electronic and thermal enthalpies= -2085.247902
Sum of electronic and thermal free energies= -2085.362850
Entropy= 241.927 cal mol^{-1} K^{-1}

XYZ coordinates

C	0.69817700	3.16691600	0.57130500
N	-0.23290500	2.04773500	0.72298200
C	-1.52069400	2.01883400	0.31148200
S	-2.29340100	3.32958800	-0.48459400

N	-2.15198400	0.83651500	0.56474500
C	-3.58702100	0.62249000	0.51736200
C	-3.91902700	-0.71788400	-0.16267100
C	-5.43552900	-0.93815000	-0.22913400
C	-6.03778900	-0.90875300	1.18805100
C	-5.71196900	0.41212300	1.89851400
C	-4.19516900	0.64376100	1.93506400
N	-3.25434100	-0.82296400	-1.53297100
C	-3.60417000	0.27557100	-2.49043300
C	-3.46001100	-2.16695400	-2.16248600
C	1.85956800	-1.28048800	-0.40111100
C	1.07288700	-2.11047100	1.38901500
C	-0.34607400	-2.39937400	1.17355300
O	-1.29377000	-1.69230800	1.55224700
C	3.30630200	-1.37188400	-0.10500100
C	3.97611700	-0.22623200	0.35421400
C	5.33748600	-0.27646300	0.66071500
C	6.04591700	-1.47483300	0.52401300
C	5.38464500	-2.62442200	0.06990700
C	4.02552100	-2.57290600	-0.24326200
C	1.50869300	-1.09795600	2.35582400
C	2.68886900	-1.48140300	3.23422700
O	0.99252700	0.02483300	2.44716400
C	-0.61445900	-3.71231100	0.44993600
H	-4.02467800	1.44463800	-0.05745700
H	-3.70776500	-0.13711200	2.53608900
H	-3.95325500	1.61384500	2.38504300
H	-6.11788000	0.40641200	2.91837100
H	-6.19291500	1.24238100	1.35974300
H	-5.62490800	-1.74641600	1.76956600
H	-7.12284100	-1.05953400	1.12261600
H	-5.89657800	-0.14459000	-0.83367400
H	-5.66226000	-1.89867000	-0.70607400
H	-3.44709300	-1.52057700	0.41569100
H	0.12337000	1.24907200	1.25973100
H	-1.63120800	0.09895800	1.05065000
H	-3.04214900	0.09385500	-3.40995500
H	-4.67857600	0.24935200	-2.68857800
H	-3.30473300	1.23448000	-2.05712500
H	-2.72930900	-2.26184300	-2.96908200
H	-3.27529500	-2.93373500	-1.40574000
H	-4.48222700	-2.24028800	-2.54006200
H	1.69272000	-3.00620900	1.36923100
H	-0.21733200	-4.55523300	1.03214300

H	-1.68934000	-3.85006200	0.29620400
H	-0.09082300	-3.71860200	-0.51712000
H	3.48041500	-1.93526400	2.62429200
H	3.07399600	-0.60146900	3.75900200
H	2.36636700	-2.23508900	3.96853300
H	-2.20312500	-0.75008100	-1.40150100
H	3.42550300	0.70447200	0.45653100
H	5.84372400	0.62280500	1.00615200
H	7.10546500	-1.51633500	0.76914600
H	5.92992700	-3.56033300	-0.03706800
H	3.51374500	-3.47109300	-0.58456400
H	0.12198800	3.96903400	0.09227500
C	1.13216700	3.64611200	1.96603400
C	1.84673600	2.79823900	-0.37010100
C	1.59613700	1.97455700	-1.48106000
C	3.14466100	3.30482500	-0.19549400
C	2.61471600	1.65732600	-2.38238000
H	0.60308500	1.55647400	-1.62195000
C	4.16498500	2.99213200	-1.10150800
H	3.37221000	3.94262200	0.65428800
C	3.90528300	2.16496400	-2.19726700
H	2.40040300	1.00152100	-3.22413800
H	5.16633300	3.38816700	-0.94078100
H	4.70172900	1.90926300	-2.89341300
C	1.36908300	-1.93273900	-1.55105700
H	1.90167900	-2.70719400	-2.08656600
N	0.14422800	-1.61506400	-2.07476700
O	-0.55847500	-0.70982600	-1.48478500
O	-0.28276100	-2.19327100	-3.11263700
H	1.40763000	-0.31711300	-0.18753400
H	0.23812300	3.87902500	2.55516100
H	1.70497000	2.86735700	2.48496600
H	1.74394200	4.55295500	1.89712700

Complex D

Zero-point correction= 0.671224 (hartree/particle)
Thermal correction to energy= 0.711786
Thermal correction to enthalpy= 0.712730
Thermal correction to Gibbs free energy= 0.597208
Sum of electronic and zero-point energies= -2085.299654
Sum of electronic and thermal energies= -2085.259092
Sum of electronic and thermal enthalpies= -2085.258148

Sum of electronic and thermal free energies= -2085.373670
Entropy= 243.136 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.67680200	3.00427200	-1.01476100
N	0.27745300	1.89809500	-1.10769800
C	1.57194800	1.92335900	-0.70915800
S	2.36410200	3.34679000	-0.17214300
N	2.19397200	0.71177000	-0.76635300
C	3.61400100	0.47225900	-0.58280300
C	3.86752700	-0.72588100	0.35676300
C	5.37500100	-0.93339400	0.55671100
C	6.07170600	-1.17545300	-0.79431200
C	5.81861700	-0.01029000	-1.76060500
C	4.31237300	0.22415400	-1.93684700
N	3.12102800	-0.59025000	1.67638400
C	3.36420900	0.68444300	2.41617600
C	3.33223100	-1.77066100	2.57296700
C	-1.86997500	-1.25652300	0.23637900
C	-1.26353600	-2.14950900	-0.94657400
C	0.24726600	-2.44834700	-0.86730100
O	1.08476000	-1.91250200	-1.58643600
C	-3.38371300	-1.26665000	0.10574400
C	-4.06568900	-0.08692700	-0.21577900
C	-5.45707300	-0.08842800	-0.36110300
C	-6.18206600	-1.27177900	-0.18648500
C	-5.50759100	-2.45537100	0.14006200
C	-4.11727600	-2.45034400	0.28254300
C	-1.62608300	-1.46662900	-2.26359400
C	-2.44682900	-2.27824100	-3.23608700
O	-1.28264800	-0.31590500	-2.49596900
C	0.60088300	-3.61865500	0.02567500
H	4.03898200	1.37747000	-0.13757500
H	3.84837700	-0.65005400	-2.41614200
H	4.11991600	1.09626500	-2.57279000
H	6.28468100	-0.21197700	-2.73381300
H	6.28321400	0.90276300	-1.35911300
H	5.68179200	-2.10536300	-1.23517600
H	7.14708500	-1.31840900	-0.62829500
H	5.80327800	-0.03901500	1.03016000
H	5.55649300	-1.78449800	1.22206200
H	3.42823800	-1.62188400	-0.10071100
H	-0.11835000	1.01732800	-1.44135100
H	1.65816800	-0.08758300	-1.10348100

H	2.73672800	0.66190800	3.31142300
H	4.41991100	0.74968900	2.69520000
H	3.07598600	1.52989200	1.78590700
H	2.52672000	-1.75573900	3.31112800
H	3.26030800	-2.68132300	1.97157400
H	4.31433200	-1.70623700	3.04822600
H	-1.76581200	-3.12332700	-0.88835400
H	0.30326700	-4.54431900	-0.49061900
H	1.67924400	-3.64334400	0.20732900
H	0.04207100	-3.57986200	0.96829600
H	-3.39667900	-2.54819400	-2.75104800
H	-2.63630900	-1.71348600	-4.15358700
H	-1.92632500	-3.21956800	-3.46570000
H	2.04891000	-0.62408800	1.45847200
H	-3.50421300	0.83551100	-0.33770000
H	-5.97281500	0.83850800	-0.60552700
H	-7.26474400	-1.27352500	-0.29881100
H	-6.06485300	-3.37938000	0.28482300
H	-3.59611300	-3.37237600	0.53793000
H	-0.07725200	3.89523700	-0.78905600
C	-1.34494600	3.19351700	-2.38739100
C	-1.65989900	2.79581100	0.14269100
C	-1.29483600	2.02391400	1.25776700
C	-2.92500400	3.40779200	0.14390400
C	-2.17463000	1.84653600	2.32931900
H	-0.32875200	1.52945700	1.27566100
C	-3.80477300	3.23635000	1.21817300
H	-3.23806100	4.01887700	-0.69848900
C	-3.43598700	2.44996800	2.31368300
H	-1.87163300	1.22719300	3.17104300
H	-4.78389900	3.71188500	1.19167300
H	-4.12640100	2.30365200	3.14216600
C	-1.45887900	-1.62296700	1.62141600
H	-2.13806800	-2.03018900	2.35865400
N	-0.24307600	-1.29992700	2.05157300
O	0.58362000	-0.79782900	1.14017000
O	0.16512600	-1.45708800	3.24626800
H	-1.50406100	-0.24600300	0.02872500
H	-0.56758900	3.32255700	-3.14896800
H	-1.95318900	2.31912400	-2.64790400
H	-1.98176500	4.08458200	-2.39461400

Product (*R*) obtained with catalyst 1i.

Complex C

Zero-point correction= 0.706550 (hartree/particle)
Thermal correction to energy= 0.749229
Thermal correction to enthalpy= 0.750173
Thermal correction to Gibbs free energy= 0.628983
Sum of electronic and zero-point energies= -2162.658869
Sum of electronic and thermal energies= -2162.616189
Sum of electronic and thermal enthalpies= -2162.615245
Sum of electronic and thermal free energies= -2162.736436
Entropy= 255.067 cal mol^{-1} K^{-1}

XYZ coordinates

C	-1.13066900	2.86105600	-0.32409800
N	-0.05468400	1.88763100	-0.48119500
C	1.25921900	2.10074800	-0.25132500
S	1.88542700	3.55691000	0.41146300
N	2.05131600	1.03128700	-0.56448400
C	3.50217900	1.07009300	-0.59990600
C	4.12032100	-0.22607400	-0.04845100
C	5.64227900	-0.09536200	0.04374100
C	6.21939000	0.17938500	-1.35968600
C	5.58742000	1.42926700	-1.99166500
C	4.05476000	1.32098900	-2.01734300
N	3.46116100	-0.61187400	1.27650700
C	3.48527200	0.46847500	2.31573800
C	3.97543900	-1.90845300	1.82292900
O	0.84895800	-1.09869800	2.78803400
N	0.18286100	-2.03426300	2.28924000
O	0.47204300	-3.22774700	2.45785100
C	-0.96721700	-1.65383100	1.52109400
C	-1.72551900	-2.57214100	0.88427800
C	-0.05320700	-2.78946700	-1.76930500
C	1.04979200	-2.78744600	-0.89049600
O	1.54826500	-1.75854700	-0.34064500
C	-2.94382200	-2.28476500	0.14654800
C	-3.47321700	-0.98163700	0.01773900
C	-4.65998700	-0.77266400	-0.67964700
C	-5.34121900	-1.84967800	-1.26310000
C	-4.82665600	-3.14672900	-1.14392300
C	-3.64037200	-3.36115300	-0.44481500

C	-0.76400200	-1.64977700	-2.25042100
C	-1.93935800	-1.91130900	-3.19390500
O	-0.51105800	-0.45119500	-1.97197700
C	1.70399100	-4.13151300	-0.56638600
H	3.81544500	1.90967200	0.03076100
H	3.73952500	0.49724600	-2.67471500
H	3.60270100	2.24519500	-2.39530200
H	5.97339800	1.57446500	-3.00891400
H	5.87293400	2.31595900	-1.40612100
H	6.02155800	-0.69311700	-2.00025500
H	7.30875400	0.28965900	-1.28752400
H	5.90124400	0.73473900	0.71521600
H	6.08390300	-1.01209300	0.45128300
H	3.85424200	-1.06104700	-0.70529600
H	-0.30980400	1.01381500	-0.95991400
H	1.59943900	0.16412300	-0.88187700
H	2.98364600	0.08196100	3.20346400
H	4.52806900	0.71045800	2.53514000
H	2.95686000	1.34551100	1.93402000
H	3.28873500	-2.21935300	2.61342800
H	3.97052700	-2.64010900	1.01279200
H	4.98322800	-1.75856100	2.21577300
H	-0.37841500	-3.75751900	-2.14245000
H	2.73580400	-4.12747800	-0.94910700
H	1.74927500	-4.25867200	0.52186100
H	1.17100700	-4.98069200	-1.01025000
H	-2.06840900	-2.97248000	-3.43649700
H	-2.85669000	-1.53984600	-2.72000100
H	-1.78979900	-1.33914900	-4.11969200
H	2.48202900	-0.81900100	1.00269100
H	-1.12418000	-0.58471100	1.50610000
H	-1.43074000	-3.61640500	0.96268400
H	-2.96739200	-0.13338800	0.46776200
H	-5.05626500	0.23581400	-0.76397900
H	-6.26725100	-1.67844300	-1.80848300
H	-5.34984400	-3.98630000	-1.59685900
H	-3.23230600	-4.36637000	-0.35470100
H	-0.66274300	3.78360400	0.04326500
C	-1.77336800	3.14366500	-1.69296800
C	-2.14070500	2.40023700	0.72671600
C	-1.66716800	1.85412600	1.93066600
C	-3.52902800	2.55170100	0.53616400
C	-2.54677400	1.43015000	2.92733000
H	-0.59318100	1.75035500	2.07083900

C	-4.40375200	2.12569000	1.54866900
C	-3.92712400	1.56104400	2.73251400
H	-2.15789200	0.99693000	3.84686600
H	-5.47711700	2.23678100	1.39570900
H	-4.62514000	1.23078200	3.49951800
C	-3.05807600	3.96233700	-1.52360200
C	-4.09318200	3.13788500	-0.74543000
H	-2.83499600	4.89047200	-0.97655400
H	-3.46402200	4.24751700	-2.50277900
H	-1.04060700	3.66735000	-2.31893700
H	-2.00823300	2.18776600	-2.18328000
H	-4.43751000	2.31432100	-1.39224700
H	-4.98072500	3.74059900	-0.50932700

TS

Zero-point correction= 0.705670 (hartree/particle)
Thermal correction to energy= 0.747267
Thermal correction to enthalpy= 0.748212
Thermal correction to Gibbs free energy= 0.630535
Sum of electronic and zero-point energies= -2162.648637
Sum of electronic and thermal energies= -2162.607039
Sum of electronic and thermal enthalpies= -2162.606095
Sum of electronic and thermal free energies= -2162.723771
Entropy= 247.671 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.96346100	2.86054700	-0.55794900
N	0.06407500	1.82158200	-0.55878000
C	1.38976200	1.98715800	-0.35481800
S	2.10695800	3.49284100	0.05169000
N	2.10370400	0.82970600	-0.47561500
C	3.54795200	0.73336300	-0.59690700
C	4.09781700	-0.38301000	0.31405800
C	5.61976600	-0.50975500	0.17105400
C	6.00047700	-0.79197300	-1.29327600
C	5.47134300	0.31313600	-2.21734500
C	3.95169300	0.45644300	-2.06156800
N	3.67350000	-0.17574300	1.76557400
C	4.07278100	1.14054200	2.35722300
C	4.09392500	-1.31044100	2.64779100
O	1.05118000	-0.26529100	2.28036800
N	0.52430900	-1.34185400	1.78584600

O	1.15088100	-2.43681500	1.83841700
C	-0.71682500	-1.23119200	1.23139600
C	-1.38678800	-2.35040100	0.69972900
C	-0.74463000	-2.71361300	-1.26000500
C	0.71156100	-2.80928400	-1.13693400
O	1.48719700	-1.84676800	-1.22477300
C	-2.85604900	-2.29969300	0.50786500
C	-3.56695900	-1.09097900	0.38325000
C	-4.94544900	-1.10270100	0.16370700
C	-5.63984300	-2.31350600	0.06287400
C	-4.94363900	-3.52195700	0.19155600
C	-3.56498300	-3.51159800	0.41041100
C	-1.38538800	-1.62726800	-2.00623900
C	-2.61501300	-2.01803400	-2.81291900
O	-1.00133500	-0.45105100	-1.97634900
C	1.25284400	-4.21529000	-0.90899000
H	3.97156300	1.69672100	-0.29634900
H	3.45103800	-0.46448100	-2.38915500
H	3.56718100	1.28338600	-2.67067100
H	5.72294100	0.09113200	-3.26264600
H	5.95814500	1.26592700	-1.95914800
H	5.56926700	-1.75761200	-1.59630200
H	7.09157000	-0.88028300	-1.37310400
H	6.09703000	0.42720900	0.49027100
H	5.99761200	-1.31427600	0.81197100
H	3.61226600	-1.32412900	0.03051500
H	-0.24950400	0.91548400	-0.91955600
H	1.60802000	-0.01245600	-0.78926800
H	3.69738600	1.16402300	3.38370100
H	5.16248500	1.22496700	2.35244100
H	3.61070000	1.94608500	1.77962100
H	3.54273500	-1.21400400	3.58570400
H	3.81205600	-2.24554100	2.16064800
H	5.17039000	-1.25790000	2.82638400
H	-1.23271600	-3.68087500	-1.38260600
H	1.16457600	-4.79972700	-1.83686400
H	2.30353400	-4.16716800	-0.60850000
H	0.67066000	-4.73121000	-0.13471800
H	-3.33404500	-2.53940800	-2.16701700
H	-3.07962400	-1.12778900	-3.24802100
H	-2.32938500	-2.71655000	-3.61317600
H	2.60427200	-0.19694100	1.81213100
H	-1.10771600	-0.22657600	1.21633000
H	-1.00785300	-3.31451400	1.03359200

H	-3.05758200	-0.13486500	0.45457000
H	-5.47375700	-0.15599200	0.07673500
H	-6.71448700	-2.31695700	-0.10903500
H	-5.47442600	-4.46961300	0.12206000
H	-3.02147800	-4.45101700	0.50318600
H	-0.47057400	3.78108100	-0.22050000
C	-1.48219200	3.07117000	-1.99311300
C	-2.06866600	2.52614900	0.44519400
C	-1.70691000	2.11082800	1.73718700
C	-3.43300600	2.67567500	0.12434300
C	-2.67489000	1.81890700	2.69871600
H	-0.65211400	1.98768000	1.97339500
C	-4.39689800	2.38889100	1.10458800
C	-4.03103600	1.95788400	2.38042100
H	-2.37205500	1.48133400	3.68798300
H	-5.45096000	2.50871200	0.85383000
H	-4.79627800	1.73238100	3.12096000
C	-2.77209300	3.89886000	-1.99548800
C	-3.87386700	3.12563500	-1.25622600
H	-2.59868000	4.86432600	-1.49688200
H	-3.08696900	4.11239300	-3.02538000
H	-0.68942500	3.55397000	-2.57785800
H	-1.68116900	2.08918200	-2.44421600
H	-4.13837000	2.23674900	-1.85231300
H	-4.78809900	3.72829900	-1.16778600

Complex D

Zero-point correction= 0.706236 (hartree/particle)
Thermal correction to energy= 0.747839
Thermal correction to enthalpy= 0.748783
Thermal correction to Gibbs free energy= 0.631611
Sum of electronic and zero-point energies= -2162.656059
Sum of electronic and thermal energies= -2162.614456
Sum of electronic and thermal enthalpies= -2162.613512
Sum of electronic and thermal free energies= -2162.730684
Entropy= 246.610 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.83149700	2.91786600	-0.51438000
N	0.15842700	1.84235100	-0.51625700
C	1.49256700	1.96466100	-0.33545000
S	2.26291800	3.45217400	0.03612000

N	2.16895300	0.78590700	-0.45819600
C	3.61150400	0.62349000	-0.50846900
C	4.06952800	-0.50280500	0.44300900
C	5.58937500	-0.70799700	0.35453500
C	6.01653200	-1.01892400	-1.09007300
C	5.58302500	0.10569800	-2.03929300
C	4.06657500	0.31914900	-1.95176100
N	3.60459000	-0.25216600	1.87000800
C	4.03199600	1.05563000	2.45026600
C	3.95485900	-1.38273400	2.78314100
O	1.03437200	-0.30308800	2.22173500
N	0.52612400	-1.30603900	1.53053100
O	1.25212500	-2.34769200	1.33080900
C	-0.71367600	-1.20314800	1.06616500
C	-1.35991000	-2.35842500	0.40293500
C	-0.97133500	-2.56833100	-1.15265600
C	0.54382800	-2.69285400	-1.35154100
O	1.25548400	-1.75045500	-1.67100800
C	-2.87944700	-2.33108200	0.48862100
C	-3.61753300	-1.13846700	0.42003000
C	-5.01542500	-1.17000500	0.41826900
C	-5.69779000	-2.38940700	0.47926100
C	-4.97062000	-3.58331700	0.55191900
C	-3.57309700	-3.54939100	0.55563500
C	-1.61670900	-1.48981800	-2.00664800
C	-2.69166300	-1.96435400	-2.95925700
O	-1.31557500	-0.30903500	-1.90518600
C	1.07933100	-4.10179800	-1.21215100
H	4.06007500	1.57204300	-0.19827700
H	3.54046600	-0.57992900	-2.29994100
H	3.74738100	1.15896500	-2.58084900
H	5.87064200	-0.13060100	-3.07220700
H	6.10120700	1.03575300	-1.76019000
H	5.54971500	-1.96347900	-1.40783800
H	7.10415400	-1.16332400	-1.12427200
H	6.10096200	0.20533700	0.68915600
H	5.90001800	-1.52521900	1.01471400
H	3.54961300	-1.42666200	0.16119500
H	-0.20959100	0.93410200	-0.80361700
H	1.64847900	-0.02224500	-0.80077500
H	3.62076000	1.11505400	3.46193500
H	5.12425900	1.10612200	2.48839400
H	3.62274700	1.86959000	1.84555300
H	3.38978700	-1.23890900	3.70734600

H	3.63167700	-2.31109900	2.30852200
H	5.02874600	-1.38385300	2.98877000
H	-1.41416700	-3.53781900	-1.41149200
H	0.76950500	-4.69071500	-2.08923500
H	2.17076000	-4.08639200	-1.14794500
H	0.65526600	-4.57825100	-0.32020600
H	-3.48128200	-2.46092800	-2.37691700
H	-3.10813900	-1.12284600	-3.52064800
H	-2.27844200	-2.71617200	-3.64751100
H	2.49616800	-0.25162000	1.89187300
H	-1.21837300	-0.27508600	1.27929500
H	-0.99343900	-3.27984100	0.87454100
H	-3.11501800	-0.17727200	0.36470100
H	-5.56575700	-0.23272500	0.37309800
H	-6.78603700	-2.41035000	0.47753500
H	-5.49003000	-4.53820100	0.61135000
H	-3.00759400	-4.47918700	0.61362600
H	-0.31735700	3.80433700	-0.12218500
C	-1.29027000	3.21225800	-1.95532500
C	-1.98132500	2.58057100	0.43566200
C	-1.67894600	2.10444300	1.72195400
C	-3.32761300	2.78579200	0.07345900
C	-2.68954800	1.80597500	2.63626600
H	-0.63823300	1.93166500	1.98786100
C	-4.33506600	2.48859500	1.00620800
C	-4.02866600	1.99843200	2.27622400
H	-2.43293200	1.41963600	3.62074000
H	-5.37523900	2.65018400	0.72260900
H	-4.82648000	1.76599300	2.97930400
C	-2.55168300	4.08317900	-1.96147300
C	-3.70369600	3.31319400	-1.29909200
H	-2.36439000	5.01672600	-1.40990200
H	-2.82223500	4.35729800	-2.98965500
H	-0.46090000	3.69485300	-2.48704900
H	-1.50704800	2.26087400	-2.45918300
H	-3.97531700	2.46294800	-1.94606900
H	-4.60061600	3.94178100	-1.21340000

Product (*S*) obtained with catalyst 1i.

Complex C

Zero-point correction= 0.705711 (hartree/particle)
Thermal correction to energy= 0.748457
Thermal correction to enthalpy= 0.749401
Thermal correction to Gibbs free energy= 0.628614
Sum of electronic and zero-point energies= -2162.660077
Sum of electronic and thermal energies= -2162.617330
Sum of electronic and thermal enthalpies= -2162.616386
Sum of electronic and thermal free energies= -2162.737174
Entropy= 254.219 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.99908700	2.64103000	1.00289200
N	0.16248400	2.07618600	0.32277500
C	1.41319400	1.96561200	0.82181900
S	1.88293800	2.54806600	2.36672800
N	2.27737400	1.32903600	-0.02363000
C	3.65682800	1.00111400	0.28111700
C	3.99273600	-0.45784800	-0.09455500
C	5.42487200	-0.79405700	0.34087600
C	6.42653500	0.16457200	-0.33082200
C	6.09439500	1.63054700	-0.02082500
C	4.64757800	1.95217100	-0.42011400
N	2.95431000	-1.43846700	0.45204600
C	2.63822700	-1.27169600	1.90636500
C	3.29891800	-2.86410000	0.15124200
C	-1.84498400	-2.18869800	0.08928800
C	0.16616100	-0.64477900	-3.41408400
C	0.65754900	-1.37294000	-2.32506200
O	0.97941000	-0.85980700	-1.19282600
C	-2.84401200	-1.38713200	-0.58811100
C	-2.40920100	-0.20611600	-1.22427700
C	-3.30782000	0.58974600	-1.93225000
C	-4.65766200	0.23331200	-1.99542700
C	-5.10908000	-0.92794600	-1.34643300
C	-4.21305000	-1.73227100	-0.65048100
C	-0.07479900	0.76478000	-3.46250200
C	-0.61874000	1.32140300	-4.78122100
O	0.09013800	1.57802600	-2.51975400
C	0.81068200	-2.88169600	-2.46988900

H	3.78980100	1.12602500	1.36212600
H	4.52206400	1.86027800	-1.50927200
H	4.37718000	2.97587300	-0.13758400
H	6.79047600	2.29798500	-0.54488400
H	6.21732500	1.81154600	1.05740600
H	6.39251300	0.00626100	-1.41939800
H	7.44190700	-0.08479100	0.00232400
H	5.50290100	-0.70058000	1.43291600
H	5.67634900	-1.82582500	0.07260400
H	3.90425600	-0.57759600	-1.18275800
H	0.01591100	1.75527300	-0.64230000
H	1.85609200	0.87571500	-0.83931700
H	1.86835100	-2.00312900	2.16047700
H	3.54532300	-1.45616400	2.48917000
H	2.27349300	-0.25883600	2.08866600
H	2.40562300	-3.46346000	0.33583000
H	3.59519700	-2.93661700	-0.89825800
H	4.11528400	-3.19007500	0.79941400
H	-0.06787500	-1.21011900	-4.31258000
H	0.31501800	-3.37778200	-1.62495300
H	0.39172600	-3.25616800	-3.41011600
H	1.87490100	-3.15419800	-2.42796700
H	-1.67410500	1.59639600	-4.63903300
H	-0.07382800	2.23819500	-5.03942000
H	-0.55373100	0.60444100	-5.60823900
H	2.06742500	-1.25122400	-0.13476600
H	-1.35990200	0.06371300	-1.17654900
H	-2.94934900	1.48968500	-2.42530600
H	-5.36255300	0.85635100	-2.54288300
H	-6.16214500	-1.19862900	-1.38649100
H	-4.57247300	-2.62544900	-0.14484100
H	-0.61155400	3.23730600	1.83927800
C	-1.74677600	3.57166400	0.03545800
C	-1.89829000	1.54837200	1.59308900
C	-1.30863900	0.46054700	2.25589000
C	-3.30287200	1.63727400	1.53058800
C	-2.08735000	-0.54182300	2.83289000
H	-0.22502300	0.41251600	2.32027300
C	-4.07610500	0.61753600	2.11015600
C	-3.48314600	-0.46556700	2.75615600
H	-1.60911000	-1.37848100	3.33854300
H	-5.16194400	0.68435000	2.04683900
H	-4.10156500	-1.24604100	3.19630900
C	-2.03350700	-3.41905300	0.61400400

H	-2.95994800	-3.97932300	0.61805800
N	-0.95864100	-4.13089500	1.25753000
O	0.17341500	-3.61539000	1.33684800
O	-1.22601000	-5.25639500	1.71065200
H	-0.84540800	-1.76140400	0.13951700
H	-1.10480600	4.43195000	-0.18907100
H	-1.92693500	3.04006800	-0.90914200
C	-3.99680400	2.78775800	0.82787200
H	-4.32816300	2.43707600	-0.16195100
H	-4.90485500	3.05917700	1.38365200
C	-3.08494800	4.00899200	0.64112800
H	-3.57437200	4.74818600	-0.00636600
H	-2.90561500	4.49171600	1.61334200

TS

Zero-point correction= 0.705537 (hartree/particle)
Thermal correction to energy= 0.747068
Thermal correction to enthalpy= 0.748012
Thermal correction to Gibbs free energy= 0.631313
Sum of electronic and zero-point energies= -2162.646197
Sum of electronic and thermal energies= -2162.604667
Sum of electronic and thermal enthalpies= -2162.603723
Sum of electronic and thermal free energies= -2162.720422
Entropy= 245.613 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.87310800	2.88975500	-0.22916300
N	0.17343400	1.91904900	-0.53668100
C	1.47270000	1.99854300	-0.16923300
S	2.13885700	3.33293600	0.68326200
N	2.21016800	0.90723100	-0.52180000
C	3.65918800	0.82081700	-0.51004500
C	4.12677000	-0.51041800	0.11308000
C	5.65771000	-0.58315000	0.14823100
C	6.22708700	-0.45908800	-1.27630800
C	5.76581000	0.84651100	-1.94007300
C	4.23339200	0.94100100	-1.93771800
N	3.50474500	-0.73952300	1.48669900
C	3.74808900	0.35532500	2.47937100
C	3.87312800	-2.07441900	2.06221200
C	-1.56750000	-1.67804500	0.34471800
C	-0.75485400	-2.25751100	-1.55037100

C	0.69289600	-2.39413300	-1.39312000
O	1.54209300	-1.55486800	-1.73656400
C	-3.00531900	-1.88501700	0.07160900
C	-3.80227100	-0.76883500	-0.22873900
C	-5.16167700	-0.92278600	-0.50763700
C	-5.74050700	-2.19629300	-0.50438400
C	-4.95105200	-3.31712800	-0.21090500
C	-3.59417100	-3.16257100	0.07670100
C	-1.34457500	-1.21757000	-2.39662300
C	-2.51544300	-1.64903400	-3.26528200
O	-0.96494600	-0.03769200	-2.39014400
C	1.13479700	-3.72126400	-0.79119900
H	4.03502200	1.65758200	0.08767400
H	3.80307800	0.13928000	-2.55414000
H	3.89654100	1.89908800	-2.35086400
H	6.14545500	0.90763300	-2.96818400
H	6.18250500	1.70137300	-1.38616700
H	5.88075600	-1.31467800	-1.87508800
H	7.32255700	-0.51008500	-1.23495500
H	6.04961200	0.23661100	0.76622200
H	5.98526800	-1.52789300	0.59616500
H	3.72392800	-1.32998400	-0.49415700
H	-0.12174800	1.12655400	-1.11764100
H	1.74669400	0.14997400	-1.03645900
H	3.23055500	0.07850500	3.40158500
H	4.82264700	0.44324400	2.65907600
H	3.33607900	1.29009600	2.08815900
H	3.15494400	-2.29471900	2.85506800
H	3.79090500	-2.82616100	1.27253200
H	4.89430300	-2.03680400	2.44781600
H	-1.26988200	-3.21691900	-1.58791200
H	0.58259600	-3.91855700	0.13878100
H	0.90057000	-4.54290300	-1.48280100
H	2.21156300	-3.70919000	-0.59527800
H	-2.99641300	-0.77497400	-3.71554000
H	-2.15728200	-2.32295000	-4.05786300
H	-3.24082500	-2.20903200	-2.66098600
H	2.44997400	-0.79028300	1.36626700
H	-3.35064500	0.21843700	-0.22617100
H	-5.76792300	-0.04616400	-0.72772800
H	-6.79823500	-2.31864300	-0.72948400
H	-5.39491500	-4.31095500	-0.21025300
H	-2.98109000	-4.03657300	0.28985200
H	-0.37265800	3.72557200	0.27690400

C	-1.49907600	3.41847100	-1.52942100
C	-1.91152500	2.32051200	0.74042500
C	-1.49539400	1.47865500	1.78422600
C	-3.27301100	2.67521900	0.64018900
C	-2.40669300	0.98076600	2.71600800
H	-0.44962300	1.19036600	1.84529100
C	-4.17627500	2.17969100	1.59431400
C	-3.75657000	1.33699300	2.62426300
H	-2.06410600	0.31440300	3.50526100
H	-5.22843000	2.45236000	1.51169600
H	-4.47752800	0.95489500	3.34472100
C	-0.97880700	-2.38453800	1.41092000
H	-1.42251100	-3.24537500	1.89306900
N	0.22853200	-1.99663800	1.92909200
O	0.82963700	-0.99353100	1.38715100
O	0.73479400	-2.60507400	2.91146100
H	-1.21192800	-0.66149700	0.20810500
H	-0.72562800	3.95387600	-2.09367900
H	-1.83527700	2.56994500	-2.14218200
C	-3.79174600	3.52693900	-0.50522500
H	-4.26270000	2.86014700	-1.24674900
H	-4.58631200	4.19060200	-0.13725100
C	-2.68717900	4.33201800	-1.20467800
H	-3.08111200	4.79131100	-2.12063400
H	-2.35016400	5.14751600	-0.54754600

Complex D

Zero-point correction= 0.706702 (hartree/particle)
Thermal correction to energy= 0.748089
Thermal correction to enthalpy= 0.749033
Thermal correction to Gibbs free energy= 0.632375
Sum of electronic and zero-point energies= -2162.656113
Sum of electronic and thermal energies= -2162.614727
Sum of electronic and thermal enthalpies= -2162.613783
Sum of electronic and thermal free energies= -2162.730441
Entropy= 245.528 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.84638300	2.86637000	-0.40392900
N	0.20010000	1.89383100	-0.70748900
C	1.50350300	1.98783400	-0.35079800
S	2.18113100	3.37927500	0.39035600

N	2.23619800	0.87320700	-0.62912700
C	3.67838100	0.74936700	-0.52624900
C	4.08077100	-0.55348700	0.19591900
C	5.60881700	-0.65015700	0.31092800
C	6.26092300	-0.59839200	-1.08223200
C	5.86111000	0.68048400	-1.83013500
C	4.33345900	0.79224600	-1.92240200
N	3.38744800	-0.69888900	1.54358200
C	3.56067000	0.45798900	2.47327100
C	3.73604800	-1.98410000	2.22712600
C	-1.55365300	-1.63709900	0.14476700
C	-0.87391100	-2.28186300	-1.15567100
C	0.65852000	-2.44282000	-1.12432600
O	1.42941000	-1.73888100	-1.76947400
C	-3.05648000	-1.81157300	0.00845000
C	-3.86864900	-0.69657000	-0.22705600
C	-5.24957000	-0.84377800	-0.39192400
C	-5.83443000	-2.11249800	-0.32586100
C	-5.02927900	-3.23422500	-0.08841300
C	-3.64955900	-3.08247400	0.07469000
C	-1.31609100	-1.45612600	-2.36218000
C	-2.04191400	-2.20339400	-3.45405200
O	-1.10613600	-0.25225100	-2.41914900
C	1.13534100	-3.68368500	-0.40017600
H	4.03855900	1.60875700	0.04778300
H	3.93088000	-0.03444900	-2.52549000
H	4.03306500	1.73246100	-2.39958600
H	6.30238000	0.68992700	-2.83524800
H	6.25591800	1.55498100	-1.29131000
H	5.93559800	-1.47542300	-1.66194200
H	7.35124400	-0.66370600	-0.97528900
H	5.97928200	0.18899800	0.91635400
H	5.89363300	-1.57932200	0.81691200
H	3.69874600	-1.40115000	-0.38755400
H	-0.12302100	1.04140700	-1.16852300
H	1.76680400	0.08756400	-1.07807200
H	2.98327500	0.23660700	3.37495300
H	4.62032800	0.57337800	2.71959900
H	3.17097300	1.36347800	2.00003900
H	2.96687200	-2.15915700	2.98373800
H	3.71258600	-2.78881000	1.48689800
H	4.73040400	-1.91146500	2.67515000
H	-1.27893800	-3.29822200	-1.24059600
H	0.60401900	-3.81514200	0.55002100

H	0.89761100	-4.55701200	-1.02671000
H	2.21750000	-3.64222100	-0.24591900
H	-2.28797600	-1.53831700	-4.28702000
H	-1.42411100	-3.04387300	-3.80282500
H	-2.95917800	-2.63640800	-3.02783200
H	2.30991700	-0.79001900	1.36234200
H	-3.41496500	0.28915200	-0.26389400
H	-5.86750800	0.03538800	-0.56607300
H	-6.90911200	-2.22885300	-0.45374200
H	-5.47705100	-4.22477200	-0.02873400
H	-3.02737900	-3.95757700	0.25925400
H	-0.33231800	3.73548200	0.02634300
C	-1.54745000	3.31746600	-1.69443600
C	-1.82701800	2.33977600	0.64581500
C	-1.36005200	1.52111300	1.68646300
C	-3.18770500	2.71032500	0.61436500
C	-2.22067100	1.06169800	2.68394200
H	-0.31791400	1.21441700	1.69204600
C	-4.03820900	2.25603800	1.63485500
C	-3.56842500	1.43694500	2.66225300
H	-1.83917200	0.41095700	3.46787200
H	-5.09029000	2.53995000	1.60579800
H	-4.25031600	1.08545700	3.43453000
C	-1.07181400	-2.13708900	1.46329500
H	-1.68120500	-2.71730400	2.14338200
N	0.11121500	-1.73854400	1.92140300
O	0.84881200	-1.01832500	1.08302200
O	0.56942900	-2.01476000	3.07573600
H	-1.31202600	-0.57114500	0.07696900
H	-0.80813200	3.80676600	-2.34030500
H	-1.93266900	2.43752900	-2.22967100
C	-3.76772600	3.52509300	-0.52927500
H	-4.31054300	2.83852800	-1.20016600
H	-4.51563800	4.22761700	-0.13654300
C	-2.70131000	4.26686800	-1.34795100
H	-3.14955500	4.67857600	-2.26157200
H	-2.30899000	5.11337500	-0.76515400

PCM-B98/TZVP approximation

β-nitrostyrene

Zero-point correction= 0.135694 (Hartree/Particle)
Thermal correction to Energy= 0.144901
Thermal correction to Enthalpy= 0.145845
Thermal correction to Gibbs Free Energy= 0.099880
Sum of electronic and zero-point Energies= -513.990530
Sum of electronic and thermal Energies= -513.981324
Sum of electronic and thermal Enthalpies= -513.980380
Sum of electronic and thermal Free Energies= -514.026344
Entropy= 96.741 cal mol^{-1} K^{-1}

XYZ coordinates

O	3.26257100	1.16511400	-0.00022700
N	2.98699300	-0.03206800	-0.00002100
C	1.60020700	-0.45605100	-0.00013300
H	1.51033400	-1.53118400	-0.00021000
O	3.82597900	-0.93316200	0.00028300
C	0.61220700	0.44655400	0.00002500
C	-0.82066600	0.17272600	0.00002100
H	0.90688400	1.49210100	0.00014700
C	-1.70450000	1.26550700	0.00009300
C	-3.08143500	1.06786500	0.00007700
C	-3.59771900	-0.22616800	-0.00000500
C	-2.73098900	-1.32260400	-0.00007000
C	-1.35713900	-1.12838400	-0.00005500
H	-1.30304900	2.27340700	0.00015700
H	-3.74937700	1.92151500	0.00013000
H	-4.67036300	-0.38359400	-0.00001500
H	-3.13159600	-2.32984600	-0.00012700
H	-0.69998600	-1.99021100	-0.00009900

2,4-pentanedione

Zero-point correction= 0.121448 (Hartree/Particle)
Thermal correction to Energy= 0.129801
Thermal correction to Enthalpy= 0.130745
Thermal correction to Gibbs Free Energy= 0.087878
Sum of electronic and zero-point Energies= -345.668453
Sum of electronic and thermal Energies= -345.660100

Sum of electronic and thermal Enthalpies= -345.659156
Sum of electronic and thermal Free Energies= -345.702024
Entropy= 90.222 cal mol^{-1} K^{-1}

XYZ coordinates

O	-1.45321000	1.42023400	-0.27186900
C	-1.21349800	0.29214900	0.09640600
C	0.00014400	0.00012500	0.99350500
O	1.45287100	-1.42021200	-0.27183400
C	1.21345000	-0.29206000	0.09656600
H	-0.18431100	-0.87884900	1.61244300
C	-2.04692400	-0.90074700	-0.30575500
H	-1.40275000	-1.70185100	-0.68048500
H	-2.56191900	-1.29392400	0.57734200
H	-2.78024000	-0.61506000	-1.05879900
C	2.04711700	0.90057500	-0.30589200
H	1.40322300	1.70212200	-0.68009900
H	2.56271500	1.29323600	0.57712800
H	2.78003200	0.61471400	-1.05926100
H	0.18421700	0.87917400	1.61238400

Catalyst 1b

Zero-point correction= 0.421143 (Hartree/Particle)
Thermal correction to Energy= 0.442851
Thermal correction to Enthalpy= 0.443795
Thermal correction to Gibbs Free Energy= 0.368335
Sum of electronic and zero-point Energies= -1226.017663
Sum of electronic and thermal Energies= -1225.995955
Sum of electronic and thermal Enthalpies= -1225.995011
Sum of electronic and thermal Free Energies= -1226.070471
Entropy= 158.818 cal mol^{-1} K^{-1}

XYZ coordinates

C	2.57968300	-1.33493200	-0.09731900
N	1.29056800	-0.73183900	-0.45093700
C	0.08144700	-1.07451100	0.06005000
S	-0.10436500	-2.26241100	1.26650400
N	-0.95789700	-0.37892200	-0.47152700
C	-2.33113100	-0.41632600	0.02734500
C	-3.03870400	0.87805600	-0.43959100
C	-4.46018500	0.92356400	0.15752900
C	-5.27636700	-0.30273400	-0.28275500

C	-4.55907400	-1.61193700	0.07447700
C	-3.12302600	-1.63767900	-0.46929500
N	-2.18944000	2.06256300	-0.22568700
C	-1.96523100	2.42509000	1.17185800
C	-2.60136600	3.21689800	-1.01662200
H	-2.30524500	-0.45285100	1.12362900
H	-3.13385500	-1.62752400	-1.56628800
H	-2.60772300	-2.54639500	-0.15274200
H	-5.11784400	-2.46867600	-0.31482200
H	-4.53193000	-1.72670900	1.16535900
H	-5.43208800	-0.25897400	-1.36840300
H	-6.26954200	-0.27472300	0.17695600
H	-4.40007200	0.94786000	1.25167200
H	-4.96589100	1.84211000	-0.15640900
H	-3.14323300	0.80103700	-1.53063800
H	1.30595600	-0.07655100	-1.22109600
H	-0.73678400	0.53862800	-0.85379700
H	-1.19449900	3.19902400	1.21725900
H	-2.86522200	2.81684000	1.67248300
H	-1.60531400	1.56324000	1.73681200
H	-1.83097800	3.99029800	-0.95401500
H	-2.70860000	2.92855400	-2.06542900
H	-3.55248400	3.66449300	-0.68292100
H	2.43784800	-1.74472900	0.90582600
C	2.92026900	-2.49623100	-1.03734200
C	3.62969400	-0.22901600	-0.01637000
C	3.53371500	0.71281900	1.01820700
C	4.67856200	-0.10816400	-0.93085900
C	4.45795900	1.74579000	1.13371200
H	2.72539700	0.62849400	1.73810400
C	5.60770800	0.92922100	-0.81837700
H	4.78626600	-0.82427600	-1.73708500
C	5.50088800	1.85826800	0.21194000
H	4.37020100	2.46021700	1.94514300
H	6.41603000	1.00514800	-1.53767600
H	6.22386800	2.66164800	0.30082600
H	2.13695400	-3.25282000	-0.96406000
H	2.98612700	-2.16974500	-2.07914900
H	3.87083400	-2.95670500	-0.75608400

Catalyst 1i

Zero-point correction= 0.457700 (Hartree/Particle)

Thermal correction to Energy= 0.480216
Thermal correction to Enthalpy= 0.481160
Thermal correction to Gibbs Free Energy= 0.404768
Sum of electronic and zero-point Energies= -1303.400979
Sum of electronic and thermal Energies= -1303.378464
Sum of electronic and thermal Enthalpies= -1303.377519
Sum of electronic and thermal Free Energies= -1303.453912
Entropy= 160.781 cal mol^{-1} K^{-1}

XYZ coordinates

C	2.27131400	-0.86160900	0.08139500
N	0.94374500	-0.39549900	-0.30797600
C	-0.23338500	-0.83391600	0.20786600
S	-0.31941500	-1.93964700	1.49982900
N	-1.32873800	-0.30011300	-0.39348800
C	-2.70484500	-0.47521000	0.06656400
C	-3.54914300	0.68663200	-0.50877400
C	-4.99104800	0.58561500	0.03025600
C	-5.62630600	-0.76209900	-0.34904300
C	-4.76555300	-1.94013700	0.12721700
C	-3.31829900	-1.81740900	-0.36834600
N	-2.86732600	1.98178100	-0.33923700
C	-2.76018300	2.45218100	1.03976400
C	-3.38541600	3.02449000	-1.21797700
H	-2.71617600	-0.43776200	1.16271500
H	-3.28727500	-1.87928600	-1.46333100
H	-2.70592500	-2.63067100	0.02552200
H	-5.19537500	-2.88668800	-0.21498600
H	-4.76866300	-1.97419200	1.22389200
H	-5.73846000	-0.81247000	-1.43976300
H	-6.63436700	-0.83057500	0.07247900
H	-4.98667800	0.68986500	1.12143200
H	-5.59349700	1.40843100	-0.36715400
H	-3.59391000	0.53176600	-1.59566700
H	0.90123900	0.15738700	-1.15410500
H	-1.20306200	0.60706700	-0.83800800
H	-2.09586700	3.31997500	1.06781300
H	-3.72646900	2.75457200	1.47459700
H	-2.32450700	1.67872900	1.67479300
H	-2.72294700	3.89345900	-1.17639400
H	-3.40770800	2.66347100	-2.24933600
H	-4.39950200	3.36511400	-0.94958200
H	2.15015400	-1.25291400	1.09699300
C	2.74511600	-2.01429800	-0.81753000

C	3.25973000	0.30350700	0.12367100
C	2.84944600	1.53896200	0.64380300
C	4.59201600	0.14542400	-0.29623400
C	3.72826100	2.61204800	0.73790800
H	1.82453100	1.65270500	0.98024600
C	5.46687500	1.23523700	-0.19342100
C	5.04806900	2.45989100	0.31350300
H	3.38848900	3.55800400	1.14532400
H	6.49675700	1.11236600	-0.51604500
H	5.74619700	3.28694500	0.38411700
H	2.09072900	-2.87387900	-0.65130500
H	2.64222900	-1.72163500	-1.87039400
C	5.10288500	-1.16487600	-0.86889500
H	5.16538200	-1.07046300	-1.96144300
H	6.12589600	-1.33610100	-0.51964300
C	4.20621500	-2.35672900	-0.52199900
H	4.51563400	-3.23723500	-1.09242100
H	4.31552800	-2.61104300	0.53891700

Product (*R*) obtained with catalyst 1b.

Complex C

Zero-point correction= 0.684929 (Hartree/Particle)
Thermal correction to Energy= 0.727069
Thermal correction to Enthalpy= 0.728013
Thermal correction to Gibbs Free Energy= 0.604069
Sum of electronic and zero-point Energies= -2085.690112
Sum of electronic and thermal Energies= -2085.647972
Sum of electronic and thermal Enthalpies= -2085.647028
Sum of electronic and thermal Free Energies= -2085.770972
Entropy= 260.862 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.49894400	3.43394300	-0.63038900
N	0.30439100	2.21702000	-0.71499700
C	1.58742600	2.09553400	-0.32757300
S	2.46336700	3.37136600	0.42471600
N	2.12702000	0.86410300	-0.54579600
C	3.55575400	0.60471500	-0.47868700
C	3.87049600	-0.77223700	0.13749000
C	5.38188900	-0.93851200	0.32630500

C	6.09247300	-0.81692100	-1.03488300
C	5.75639800	0.50469300	-1.73569800
C	4.23985200	0.70185100	-1.85680100
N	3.06296400	-0.99733000	1.41215800
C	3.20209200	0.06814500	2.45026500
C	3.28808000	-2.35031000	2.00750000
O	0.19245200	-0.96740600	2.75614900
N	-0.64991800	-1.79806600	2.39295300
O	-0.58950500	-2.98997200	2.68470300
C	-1.73776400	-1.29147500	1.59608400
C	-2.66368200	-2.12708500	1.10596600
C	-0.39692700	-2.55256500	-1.97656000
C	0.48583600	-2.89359900	-0.92728400
O	1.19832500	-2.09202300	-0.27083100
C	-3.80638100	-1.76933600	0.27650700
C	-4.09596200	-0.44666900	-0.10791100
C	-5.20017900	-0.17462300	-0.90334300
C	-6.03478700	-1.21021000	-1.33196600
C	-5.76067300	-2.52455900	-0.95779500
C	-4.65622600	-2.80115200	-0.15961300
C	-0.64233100	-1.25106500	-2.47323600
C	-1.70558000	-1.10197500	-3.55856300
O	-0.06622300	-0.19848900	-2.09934700
C	0.58287600	-4.37177000	-0.54799200
H	3.97894900	1.38805800	0.15516500
H	3.80856400	-0.04967500	-2.52881300
H	4.01104900	1.68427400	-2.27761400
H	6.21824000	0.53179300	-2.72710800
H	6.18326700	1.33911600	-1.16610500
H	5.78838800	-1.65679500	-1.67137300
H	7.17208500	-0.90935600	-0.88571300
H	5.76566700	-0.16981200	1.00655700
H	5.61251800	-1.91201100	0.76600900
H	3.49088600	-1.55412300	-0.52475200
H	-0.08985700	1.42875900	-1.23626200
H	1.52918700	0.17866800	-1.02778000
H	2.52593600	-0.17488700	3.26692700
H	4.23079100	0.08259400	2.80748900
H	2.93551700	1.03552000	2.02806100
H	2.49893500	-2.52673200	2.73641200
H	3.22150900	-3.09181600	1.21525100
H	4.26175100	-2.37784600	2.49254000
H	-0.95503900	-3.36255000	-2.43025900
H	0.35369500	-4.48491200	0.51570600

H	-0.08648900	-5.00749200	-1.13015800
H	1.61159000	-4.71502000	-0.69949000
H	-2.11522400	-2.05750700	-3.89020700
H	-2.52237200	-0.48390400	-3.17188100
H	-1.27521200	-0.57528200	-4.41499600
H	2.08851000	-1.02077100	1.06946500
H	-1.66660600	-0.22583300	1.44322500
H	-2.55245000	-3.17965300	1.34898800
H	-3.46354300	0.37171600	0.21535300
H	-5.41206300	0.84881500	-1.19123600
H	-6.89487100	-0.99083800	-1.95473700
H	-6.40520800	-3.33130700	-1.28758600
H	-4.44120100	-3.82408100	0.13105100
H	0.14618600	4.17230300	-0.14566900
C	-0.83060800	3.93712900	-2.03986500
C	-1.70848500	3.21824600	0.28264900
C	-1.49616700	2.72817200	1.58015300
C	-3.01535600	3.53406700	-0.09913900
C	-2.55606300	2.56351600	2.46690400
H	-0.48704100	2.48401100	1.89562700
C	-4.08147800	3.36900700	0.78904200
H	-3.21524900	3.91738700	-1.09249000
C	-3.85746400	2.88349200	2.07383200
H	-2.36675700	2.18922900	3.46741800
H	-5.08733400	3.62346400	0.47183500
H	-4.68442700	2.75728100	2.76382900
H	0.09854600	4.09433900	-2.59093900
H	-1.43903000	3.21666500	-2.59445700
H	-1.36595900	4.88872300	-2.00074100

TS

Zero-point correction= 0.684739 (Hartree/Particle)
Thermal correction to Energy= 0.725476
Thermal correction to Enthalpy= 0.726420
Thermal correction to Gibbs Free Energy= 0.608495
Sum of electronic and zero-point Energies= -2085.674521
Sum of electronic and thermal Energies= -2085.633784
Sum of electronic and thermal Enthalpies= -2085.632840
Sum of electronic and thermal Free Energies= -2085.750765
Entropy= 248.193 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.37310500	3.34419700	-0.91089700
N	0.36243500	2.08199900	-0.82648300
C	1.67424000	1.95959000	-0.56153100
S	2.69255300	3.30605500	-0.23032400
N	2.12861400	0.67793500	-0.54839600
C	3.53329700	0.30363000	-0.56243000
C	3.83139900	-0.81338300	0.46139900
C	5.31918300	-1.19006500	0.44165800
C	5.74749600	-1.63983300	-0.96511900
C	5.44884600	-0.55911000	-2.00888700
C	3.97032500	-0.15823400	-1.96862100
N	3.34316500	-0.44477200	1.85990600
C	3.88233000	0.83569100	2.41041600
C	3.52741400	-1.55813300	2.84064300
O	0.64889500	-0.22531900	2.25830700
N	-0.02642700	-1.23101700	1.84646900
O	0.41718800	-2.39315100	1.99034200
C	-1.24224800	-0.98256200	1.27174100
C	-2.00356400	-2.02477800	0.74424200
C	-1.29581000	-2.43048300	-1.32951100
C	0.10602700	-2.73695400	-1.10310800
O	1.01397500	-1.89985200	-1.07667600
C	-3.45549600	-1.88055600	0.50528800
C	-4.08881500	-0.63246100	0.39645800
C	-5.46382200	-0.55332300	0.19685100
C	-6.23339400	-1.71267300	0.10291100
C	-5.61686900	-2.95913000	0.21335100
C	-4.24255200	-3.03991300	0.41226600
C	-1.72568900	-1.22181500	-2.01733600
C	-2.96081300	-1.34739100	-2.89779600
O	-1.15351400	-0.13349700	-1.92874700
C	0.44814200	-4.21094100	-0.92247800
H	4.09913100	1.20192200	-0.30568300
H	3.34199200	-1.00273000	-2.27252600
H	3.77163200	0.66226400	-2.66329000
H	5.71024100	-0.91630300	-3.00944400
H	6.07457100	0.32070900	-1.81432200
H	5.21379500	-2.56108400	-1.22787200
H	6.81370800	-1.88394300	-0.95359500
H	5.92692700	-0.32845000	0.74048300
H	5.51950200	-1.99457500	1.15342200
H	3.22466400	-1.68563000	0.19874800
H	-0.14823700	1.24389300	-1.11141000

H	1.48000200	-0.06647200	-0.82095900
H	3.41614400	0.99969900	3.38136400
H	4.96162500	0.75677200	2.53166200
H	3.62838600	1.66045100	1.74407900
H	2.90788100	-1.34044000	3.70847400
H	3.18511800	-2.48700000	2.38979100
H	4.57340500	-1.62554500	3.13250400
H	-1.91896800	-3.30142400	-1.50937700
H	1.37698600	-4.30706200	-0.36066500
H	-0.34795300	-4.75776300	-0.41197600
H	0.58649800	-4.66839400	-1.90849000
H	-3.71846900	-1.99155000	-2.44601200
H	-3.37769700	-0.35915200	-3.09321700
H	-2.66941500	-1.80048900	-3.85233000
H	2.29893300	-0.32248700	1.80982900
H	-1.49162300	0.06377700	1.21741500
H	-1.68541500	-3.02025400	1.02834300
H	-3.51485900	0.28369400	0.46568900
H	-5.93465300	0.42027200	0.11666600
H	-7.30468300	-1.64572900	-0.05063100
H	-6.20696400	-3.86667200	0.14922400
H	-3.76801300	-4.01221600	0.50146400
H	0.29346100	4.09568400	-0.47909600
C	-0.62161200	3.71604000	-2.37719100
C	-1.62383800	3.27516600	-0.03371500
C	-1.47621200	2.96772800	1.32698900
C	-2.90753000	3.53710500	-0.51832800
C	-2.57772600	2.92735200	2.17607700
H	-0.48770300	2.75084900	1.71830800
C	-4.01550900	3.49813800	0.33211100
H	-3.05674300	3.77532800	-1.56442200
C	-3.85591100	3.19460400	1.68090600
H	-2.43960200	2.68740600	3.22485700
H	-5.00294000	3.70795200	-0.06555300
H	-4.71534000	3.16516500	2.34179300
H	0.33847900	3.77975800	-2.89309900
H	-1.23532800	2.96548800	-2.88242700
H	-1.11530000	4.68790700	-2.45696800

Complex D

Zero-point correction= 0.685431 (Hartree/Particle)
Thermal correction to Energy= 0.726099

Thermal correction to Enthalpy= 0.727044
Thermal correction to Gibbs Free Energy= 0.609491
Sum of electronic and zero-point Energies= -2085.693184
Sum of electronic and thermal Energies= -2085.652516
Sum of electronic and thermal Enthalpies= -2085.651571
Sum of electronic and thermal Free Energies= -2085.769124
Entropy= 247.411 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.20754600	3.37092900	-0.90777700
N	0.47873100	2.08084300	-0.81841600
C	1.78738300	1.90802000	-0.55493100
S	2.85385000	3.21824600	-0.24407400
N	2.19591400	0.61267300	-0.53660500
C	3.57762000	0.17165800	-0.43212300
C	3.75337500	-0.93065400	0.63884700
C	5.22330700	-1.37710700	0.70822500
C	5.71942100	-1.87703500	-0.65719100
C	5.54442900	-0.80513600	-1.73612200
C	4.08806200	-0.33415300	-1.79816500
N	3.20908700	-0.51429800	1.99421100
C	3.75666700	0.75817000	2.54044400
C	3.31685800	-1.60596000	3.00513100
O	0.63750900	-0.22554200	2.14432000
N	0.01173400	-1.17143800	1.47727000
O	0.62632700	-2.28527000	1.28279400
C	-1.20229400	-0.95340500	1.02817900
C	-1.93944100	-2.04271000	0.32752000
C	-1.57530500	-2.21629400	-1.21732000
C	-0.08851000	-2.55817000	-1.42752200
O	0.73024100	-1.72497900	-1.75953600
C	-3.45309000	-1.92825100	0.47866500
C	-4.13059800	-0.70692100	0.37261700
C	-5.51861900	-0.65158700	0.49122900
C	-6.25509700	-1.81315900	0.71682800
C	-5.59187700	-3.03413200	0.82630400
C	-4.20421700	-3.08713300	0.70826800
C	-1.99421400	-1.01332600	-2.05904400
C	-2.96804800	-1.29029300	-3.18152100
O	-1.56799100	0.10294400	-1.84622400
C	0.26491800	-4.02272800	-1.30785600
H	4.16004800	1.05239800	-0.15361300
H	3.44257500	-1.15304700	-2.13628300
H	3.97472300	0.48319900	-2.51560600

H	5.85198500	-1.19230100	-2.71225700
H	6.19788000	0.04767000	-1.51454000
H	5.15812600	-2.77644300	-0.93884800
H	6.76895300	-2.17394000	-0.57204900
H	5.85056600	-0.53765100	1.02987200
H	5.34283700	-2.17319600	1.44632300
H	3.12345000	-1.78366900	0.36620800
H	-0.09233300	1.26235100	-1.01968100
H	1.53610500	-0.08882600	-0.86513000
H	3.24188600	0.96358700	3.47892700
H	4.82607400	0.65956600	2.72918300
H	3.56716600	1.57641900	1.84604800
H	2.67935200	-1.33830800	3.84664700
H	2.94052300	-2.52670100	2.56404400
H	4.34675500	-1.71877800	3.34152500
H	-2.14570300	-3.08974400	-1.54912500
H	1.34568800	-4.13709400	-1.24030200
H	-0.21197000	-4.47307100	-0.43544100
H	-0.09831200	-4.54655700	-2.19982500
H	-3.89354700	-1.70665500	-2.77003500
H	-3.18422800	-0.37432300	-3.72995900
H	-2.55214600	-2.04234500	-3.86073000
H	2.11973800	-0.37637100	1.91148400
H	-1.61207800	0.02169000	1.23122900
H	-1.62821400	-2.98807700	0.78215300
H	-3.58208800	0.21213800	0.20055100
H	-6.02232400	0.30567300	0.41114200
H	-7.33430100	-1.76668200	0.81200500
H	-6.15206000	-3.94438700	1.01097600
H	-3.69501300	-4.04143200	0.80561600
H	0.48631700	4.09384700	-0.46900300
C	-0.42676000	3.75669600	-2.37559800
C	-1.46798000	3.34688700	-0.04206000
C	-1.37230300	2.90076400	1.28422800
C	-2.71132700	3.78397300	-0.50633200
C	-2.48578700	2.89499600	2.11889500
H	-0.42145500	2.53617300	1.65823300
C	-3.83019200	3.77960300	0.33009700
H	-2.82194500	4.12986700	-1.52677900
C	-3.72258000	3.33635500	1.64499800
H	-2.38839500	2.54192600	3.13993300
H	-4.78546000	4.12361000	-0.05238300
H	-4.59079600	3.33179400	2.29505000
H	0.53713500	3.75426300	-2.88833300

H	-1.09131500	3.04984700	-2.87985000
H	-0.85030200	4.76057700	-2.45972400

Product (*S*) obtained with catalyst 1b.

Complex C

Zero-point correction= 0.684665 (Hartree/Particle)
Thermal correction to Energy= 0.726888
Thermal correction to Enthalpy= 0.727832
Thermal correction to Gibbs Free Energy= 0.603604
Sum of electronic and zero-point Energies= -2085.689746
Sum of electronic and thermal Energies= -2085.647523
Sum of electronic and thermal Enthalpies= -2085.646579
Sum of electronic and thermal Free Energies= -2085.770806
Entropy= 261.459 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.51520800	3.50651900	-0.41854400
N	0.30137400	2.31070300	-0.60589200
C	1.57084100	2.15363300	-0.18688100
S	2.40918000	3.34816600	0.72544600
N	2.12678800	0.95428000	-0.51239300
C	3.54739200	0.67723700	-0.38492100
C	3.82376200	-0.75354600	0.11923300
C	5.32141300	-0.93926400	0.38629900
C	6.11563900	-0.69936100	-0.91092600
C	5.82130700	0.68055100	-1.51120500
C	4.31462700	0.89498600	-1.70471400
N	2.93683600	-1.10166300	1.31006600
C	2.97716200	-0.13051300	2.44506800
C	3.15480100	-2.49703600	1.80271700
C	-2.41023100	-1.47396000	0.98237600
C	-0.40483900	-2.29551000	-2.30637300
C	0.43972100	-2.75141000	-1.26948700
O	1.17431500	-2.03568300	-0.54239000
C	-3.63639200	-1.48862900	0.19692700
C	-4.06981300	-0.27797600	-0.37100400
C	-5.23799300	-0.22609600	-1.12442200
C	-5.98790200	-1.38265300	-1.32660300
C	-5.56605500	-2.59442000	-0.77119400
C	-4.40306100	-2.64984000	-0.01732600

C	-0.58652100	-0.95303600	-2.71236200
C	-1.60675100	-0.68536300	-3.81608900
O	0.01334900	0.04811200	-2.24553000
C	0.47083300	-4.25795400	-1.00697100
H	3.93313800	1.39564300	0.34292100
H	3.92499500	0.20997500	-2.46726500
H	4.11160300	1.91253100	-2.04832000
H	6.34147700	0.79346100	-2.46705300
H	6.21266000	1.45921700	-0.84531200
H	5.85429400	-1.47830100	-1.63744100
H	7.18396000	-0.80819700	-0.70301700
H	5.65941500	-0.23569500	1.15551700
H	5.52851800	-1.94849100	0.74977200
H	3.49318200	-1.46821100	-0.63868300
H	-0.06887200	1.57651200	-1.21620000
H	1.55257500	0.32041900	-1.08494800
H	2.24855000	-0.45743000	3.18411800
H	3.97712100	-0.13057300	2.87675400
H	2.72121100	0.86674700	2.09179200
H	2.33036900	-2.74958500	2.46782000
H	3.14970400	-3.16995500	0.94858800
H	4.09967900	-2.55059400	2.33990500
H	-0.98451900	-3.04584700	-2.83016400
H	-0.23554800	-4.81510700	-1.62450500
H	1.48011000	-4.63449600	-1.20366500
H	0.25505400	-4.44853700	0.04873800
H	-2.04181400	-1.59744200	-4.22789700
H	-2.41148400	-0.06236000	-3.41248400
H	-1.12771000	-0.11786900	-4.61902400
H	1.98857600	-1.11652400	0.89612200
H	-3.48872300	0.62355300	-0.20985900
H	-5.56102100	0.71595900	-1.55248600
H	-6.89736100	-1.34519800	-1.91582300
H	-6.14727200	-3.49528400	-0.93179600
H	-4.08715600	-3.59900300	0.39960600
H	0.11785100	4.20287300	0.13970500
C	-0.83530900	4.13368500	-1.78065400
C	-1.73428600	3.20098700	0.45611000
C	-1.55298900	2.49148900	1.65253300
C	-3.02146000	3.64990200	0.14406000
C	-2.62102200	2.24447300	2.50995800
H	-0.56190700	2.13715100	1.91378200
C	-4.09581500	3.40106200	1.00214400
H	-3.19986400	4.20230600	-0.77052800

C	-3.90107100	2.69877800	2.18771400
H	-2.45362100	1.69669900	3.43124600
H	-5.08527000	3.75960600	0.73867100
H	-4.73473200	2.50648500	2.85397700
C	-1.88185800	-2.50866200	1.65199100
H	-2.25973900	-3.51759700	1.70406200
N	-0.64469900	-2.36392700	2.37215000
O	-0.11290900	-1.25753700	2.48078200
O	-0.16877300	-3.39425000	2.85806600
H	-1.87625900	-0.52949600	1.02881300
H	0.09793200	4.32654800	-2.31300100
H	-1.45077300	3.47096600	-2.39632400
H	-1.35868800	5.08515400	-1.66290200

TS

Zero-point correction= 0.684780 (Hartree/Particle)
Thermal correction to Energy= 0.725505
Thermal correction to Enthalpy= 0.726450
Thermal correction to Gibbs Free Energy= 0.608347
Sum of electronic and zero-point Energies= -2085.670034
Sum of electronic and thermal Energies= -2085.629308
Sum of electronic and thermal Enthalpies= -2085.628364
Sum of electronic and thermal Free Energies= -2085.746466
Entropy= 248.567 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.39547200	3.45677900	-0.41960300
N	0.36960400	2.21739600	-0.54882000
C	1.66092500	2.06119700	-0.21113100
S	2.59609200	3.30265300	0.52376100
N	2.16754000	0.82445400	-0.46909500
C	3.58768300	0.51566600	-0.46257200
C	3.86356500	-0.85311400	0.18725700
C	5.37060800	-1.13932600	0.23329800
C	5.96304900	-1.10728600	-1.18644900
C	5.67958300	0.22773600	-1.88214700
C	4.17775300	0.53411300	-1.88765100
N	3.19563000	-0.97018300	1.55396900
C	3.56895000	0.08653400	2.54406600
C	3.36023500	-2.33294700	2.14978500
C	-1.97522800	-1.49251700	0.42229700
C	-1.16379800	-2.07556200	-1.56188000

C	0.20778600	-2.49131600	-1.30243500
O	1.20702300	-1.77213900	-1.39149200
C	-3.42043900	-1.61850300	0.12311300
C	-4.15625500	-0.46215800	-0.17258100
C	-5.52493400	-0.53588400	-0.42147200
C	-6.17831800	-1.76606400	-0.39142700
C	-5.45417200	-2.92491500	-0.10488300
C	-4.08948900	-2.85236300	0.15234200
C	-1.46833900	-0.88030500	-2.33818300
C	-2.62227700	-0.98379600	-3.32267000
O	-0.85484300	0.18482500	-2.22958100
C	0.36535600	-3.94586100	-0.88279800
H	4.07344100	1.30526500	0.11511100
H	3.64376700	-0.19878900	-2.50378100
H	3.98481100	1.52135000	-2.31553900
H	6.06052100	0.20782100	-2.90745900
H	6.21410700	1.03196300	-1.36200400
H	5.53222100	-1.92624400	-1.77485000
H	7.03956700	-1.29213200	-1.12873600
H	5.87788200	-0.38907800	0.85032700
H	5.56346100	-2.11705500	0.68167700
H	3.35882300	-1.62068500	-0.40615800
H	-0.07670900	1.45873000	-1.06774200
H	1.56879800	0.14246900	-0.94126200
H	2.98656700	-0.08899200	3.44742800
H	4.63187700	0.01438400	2.76901100
H	3.32736900	1.06974900	2.14072400
H	2.60689100	-2.45015100	2.92731300
H	3.19296100	-3.07878600	1.37359100
H	4.36249100	-2.43559600	2.56080700
H	-1.84017600	-2.90759100	-1.73036300
H	-0.08560500	-4.61752000	-1.61839600
H	1.42083300	-4.19113100	-0.76438000
H	-0.15525700	-4.11053300	0.06805700
H	-3.45511000	-1.55301600	-2.90323500
H	-2.95754200	0.01265700	-3.61150200
H	-2.27883000	-1.51424100	-4.21810600
H	2.16483300	-0.86745700	1.41040400
H	-3.65603500	0.50007500	-0.19173100
H	-6.07881600	0.37071800	-0.63885300
H	-7.24276900	-1.82432700	-0.58957100
H	-5.95526800	-3.88642400	-0.08254100
H	-3.53858800	-3.76259900	0.36410500
H	0.22923700	4.11581600	0.19029800

C	-0.57223500	4.10979700	-1.79601000
C	-1.69077900	3.20582200	0.35427500
C	-1.63351200	2.51156800	1.57184000
C	-2.92972500	3.69280500	-0.07222600
C	-2.77639200	2.32190500	2.34254700
H	-0.68364200	2.11483100	1.91372700
C	-4.07866800	3.50251900	0.69948600
H	-3.01171300	4.23012500	-1.00914200
C	-4.00673300	2.81992900	1.91019000
H	-2.70760600	1.78298300	3.28132500
H	-5.02888800	3.89204700	0.34946300
H	-4.89799600	2.67210600	2.51000100
C	-1.43562200	-2.24590400	1.46994700
H	-1.90373500	-3.11263600	1.90826500
N	-0.23885700	-1.91469200	2.04996500
O	0.40769700	-0.90070000	1.63489600
O	0.19978800	-2.61080900	2.99780700
H	-1.54671900	-0.50768200	0.28306600
H	0.41150800	4.26786600	-2.24248800
H	-1.15935100	3.47723100	-2.46772200
H	-1.06245100	5.08249600	-1.71043100

Complex D

Zero-point correction= 0.686200 (Hartree/Particle)
Thermal correction to Energy= 0.726622
Thermal correction to Enthalpy= 0.727566
Thermal correction to Gibbs Free Energy= 0.610455
Sum of electronic and zero-point Energies= -2085.689705
Sum of electronic and thermal Energies= -2085.649284
Sum of electronic and thermal Enthalpies= -2085.648340
Sum of electronic and thermal Free Energies= -2085.765451
Entropy= 246.481 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.49256500	3.25289000	-0.81163400
N	0.33452800	2.04600400	-0.82155400
C	1.63005500	1.98305600	-0.45887700
S	2.49471600	3.33566800	0.15125400
N	2.20204400	0.75753800	-0.58843800
C	3.62290600	0.49430600	-0.43312900
C	3.89830500	-0.80382100	0.35569200
C	5.41253600	-0.99505600	0.53630400

C	6.12686900	-1.05085800	-0.82398600
C	5.83908000	0.20081700	-1.65862800
C	4.32999700	0.42492600	-1.80332900
N	3.13688600	-0.87159200	1.66992700
C	3.29367600	0.30884300	2.56697700
C	3.41138500	-2.13580400	2.41874400
C	-1.90644600	-1.49398100	0.18261600
C	-1.36065200	-2.11167800	-1.17542100
C	0.15226400	-2.41468800	-1.23634600
O	0.93525200	-1.71390500	-1.85079600
C	-3.43158100	-1.52102200	0.14816500
C	-4.15454100	-0.32801700	0.06028300
C	-5.54910600	-0.34100500	0.02290300
C	-6.24202500	-1.54823300	0.07347800
C	-5.53097700	-2.74509100	0.16399200
C	-4.13856400	-2.72972200	0.19907700
C	-1.72580200	-1.17047900	-2.32828300
C	-2.40404500	-1.78724000	-3.52637800
O	-1.47092400	0.01500700	-2.27214900
C	0.56914900	-3.74239000	-0.64733700
H	4.03200000	1.34650600	0.11417200
H	3.88218800	-0.38186500	-2.39649100
H	4.12678100	1.36243700	-2.32756700
H	6.30005600	0.11342900	-2.64696800
H	6.29147400	1.07537100	-1.17551300
H	5.79190200	-1.94121500	-1.37030900
H	7.20206000	-1.16796800	-0.66045600
H	5.82099900	-0.16568500	1.12483500
H	5.61590200	-1.91556800	1.08759100
H	3.49832300	-1.64900800	-0.21595600
H	-0.11360800	1.21147900	-1.19506700
H	1.64918000	0.01954200	-1.01786900
H	2.65849800	0.14410200	3.43677500
H	4.33224600	0.40349600	2.88407600
H	2.97407700	1.21396500	2.05252700
H	2.58229900	-2.28806200	3.10906400
H	3.44026800	-2.96628300	1.71359000
H	4.35991800	-2.06328200	2.94861200
H	-1.86250400	-3.07311900	-1.32294900
H	0.20344900	-4.54077500	-1.30354700
H	1.65533600	-3.80264200	-0.59075100
H	0.11986600	-3.90006300	0.33577200
H	-3.37105000	-2.20027000	-3.21886600
H	-2.55154800	-1.04234000	-4.30735200

H	-1.80601800	-2.62037800	-3.91003900
H	2.07962700	-0.94277100	1.43358500
H	-3.62459000	0.61774800	0.02617100
H	-6.09101300	0.59630600	-0.04260900
H	-7.32611200	-1.55856900	0.04646900
H	-6.06099800	-3.69037000	0.21105600
H	-3.60004900	-3.66954000	0.27825700
H	0.16903000	4.04459200	-0.44796600
C	-0.91764300	3.59869800	-2.24437800
C	-1.64100800	3.12260400	0.19249500
C	-1.40256900	2.53618200	1.44353600
C	-2.91772500	3.63322200	-0.06493100
C	-2.40527000	2.46813300	2.40680800
H	-0.42305400	2.12650700	1.66195300
C	-3.92455400	3.56651200	0.90027600
H	-3.14107600	4.08976800	-1.02132100
C	-3.67315400	2.98535400	2.13993100
H	-2.19642600	2.00678200	3.36592200
H	-4.90667500	3.96991100	0.67703300
H	-4.45550300	2.93082600	2.88887500
C	-1.40453200	-2.11279900	1.45189500
H	-2.03365500	-2.66835400	2.12981400
N	-0.18729700	-1.85074400	1.87882700
O	0.59853100	-1.16399300	1.07160300
O	0.27367100	-2.24229800	3.00135900
H	-1.57901000	-0.45147500	0.16598000
H	-0.02754700	3.67339500	-2.87248800
H	-1.57514400	2.83224200	-2.66302000
H	-1.43151200	4.56160400	-2.27964700

Product (*R*) obtained with catalyst 1i.

Complex C

Zero-point correction= 0.721665 (Hartree/Particle)
Thermal correction to Energy= 0.764639
Thermal correction to Enthalpy= 0.765583
Thermal correction to Gibbs Free Energy= 0.640778
Sum of electronic and zero-point Energies= -2163.073793
Sum of electronic and thermal Energies= -2163.030819
Sum of electronic and thermal Enthalpies= -2163.029875
Sum of electronic and thermal Free Energies= -2163.154680

Entropy= 262.674 cal mol^{-1} K^{-1}

XYZ coordinates

C	-1.08075300	3.00683400	-0.33246800
N	-0.04540000	1.99186600	-0.47851400
C	1.25028700	2.13427700	-0.14399900
S	1.86378600	3.52854600	0.65413500
N	2.03166700	1.06204500	-0.45507200
C	3.48427600	1.11799000	-0.44937800
C	4.11586000	-0.19623800	0.04695600
C	5.63560500	-0.04552500	0.17202200
C	6.23767800	0.32335700	-1.19696200
C	5.59512300	1.58895300	-1.77601400
C	4.06758200	1.46162000	-1.83483700
N	3.43871200	-0.67794800	1.32727200
C	3.38832800	0.32216400	2.43626400
C	3.98345600	-1.98230600	1.81507600
O	0.71710700	-1.41877000	2.73457600
N	0.00457000	-2.32433600	2.28117300
O	0.25916700	-3.51695300	2.42435800
C	-1.17443400	-1.90602200	1.56825100
C	-1.96465400	-2.80961200	0.97259200
C	0.26039100	-2.74220200	-2.06567200
C	1.24756100	-2.94731100	-1.07520100
O	1.78129400	-2.05480500	-0.36876000
C	-3.17919200	-2.53274200	0.21660400
C	-3.73711600	-1.24566000	0.10050000
C	-4.89428700	-1.04867200	-0.64043000
C	-5.51674100	-2.12434300	-1.27900800
C	-4.97730800	-3.40492900	-1.16883300
C	-3.82018300	-3.60728800	-0.42485100
C	-0.30433100	-1.49928500	-2.43717500
C	-1.42607600	-1.51814000	-3.47228500
O	0.03096300	-0.37472500	-1.98785100
C	1.70678100	-4.38530100	-0.83196500
H	3.75551400	1.92958900	0.23060200
H	3.77521800	0.68633300	-2.55317400
H	3.61585700	2.40001900	-2.16655700
H	5.99304200	1.78929800	-2.77522200
H	5.86055200	2.45116000	-1.15212800
H	6.08860500	-0.51393300	-1.88945800
H	7.31822700	0.45480400	-1.08971700
H	5.88037800	0.73755100	0.89848000
H	6.08811200	-0.97554000	0.52474700

H	3.88018400	-0.99500500	-0.66051700
H	-0.28348800	1.15926900	-1.02510000
H	1.57566800	0.29447500	-0.96622200
H	2.83690400	-0.12449800	3.26073900
H	4.40498300	0.55597300	2.74910900
H	2.88011300	1.22461400	2.10172500
H	3.28631600	-2.37500900	2.55321000
H	4.04325500	-2.66753500	0.97330200
H	4.96060900	-1.82397300	2.26694500
H	-0.11387400	-3.62179600	-2.57536800
H	2.77942800	-4.45995400	-1.03947600
H	1.55872700	-4.63498100	0.22275400
H	1.18020300	-5.11325400	-1.45149800
H	-1.61527000	-2.51266200	-3.87966600
H	-2.34499200	-1.14796700	-3.00603500
H	-1.17577600	-0.83396300	-4.28797600
H	2.47805400	-0.89637100	1.01620800
H	-1.28605500	-0.83311100	1.56048500
H	-1.67181100	-3.85188400	1.05599700
H	-3.27462900	-0.39845600	0.59335200
H	-5.31552100	-0.05267800	-0.71710800
H	-6.41980400	-1.96324000	-1.85714000
H	-5.45742400	-4.24324300	-1.66057900
H	-3.39883000	-4.60343600	-0.34013800
H	-0.57733500	3.88496300	0.08439200
C	-1.64937600	3.37293100	-1.71191900
C	-2.16244300	2.58191300	0.66407500
C	-1.77891700	1.98209900	1.87152700
C	-3.52378700	2.84337400	0.43175100
C	-2.71871100	1.62869800	2.83409600
H	-0.72504000	1.80223300	2.05601400
C	-4.46052200	2.48044300	1.40951500
C	-4.07204800	1.87561600	2.59965000
H	-2.39758900	1.16996300	3.76308700
H	-5.51225900	2.68563600	1.23049200
H	-4.81557600	1.60799500	3.34250200
C	-2.88468100	4.26381400	-1.57117000
C	-4.00015700	3.50100500	-0.85111500
H	-2.62589900	5.16646200	-1.00490200
H	-3.23080200	4.59339000	-2.55519600
H	-0.86539400	3.86859600	-2.29111800
H	-1.91830900	2.45637100	-2.25184200
H	-4.39214900	2.72611700	-1.52417900
H	-4.84105300	4.16451300	-0.62616100

TS

Zero-point correction= 0.721655 (Hartree/Particle)
Thermal correction to Energy= 0.763085
Thermal correction to Enthalpy= 0.764029
Thermal correction to Gibbs Free Energy= 0.644796
Sum of electronic and zero-point Energies= -2163.057781
Sum of electronic and thermal Energies= -2163.016351
Sum of electronic and thermal Enthalpies= -2163.015407
Sum of electronic and thermal Free Energies= -2163.134640
Entropy= 250.948 cal mol^{-1} K^{-1}

XYZ coordiantes

C	-0.65240600	3.14609500	-0.44500000
N	0.23065000	1.98640800	-0.50723000
C	1.55501500	1.99480700	-0.27931300
S	2.42016600	3.40541800	0.18878800
N	2.15518400	0.78234000	-0.42206700
C	3.59234900	0.58217700	-0.50470600
C	4.04548800	-0.61039600	0.36458700
C	5.56443700	-0.80952300	0.27232800
C	5.99615900	-1.02657400	-1.18747000
C	5.55024100	0.13752100	-2.07718500
C	4.03821900	0.35805200	-1.96552800
N	3.56316600	-0.47322800	1.80625900
C	3.97106200	0.78652200	2.50021400
C	3.90432200	-1.66766800	2.63864500
O	0.87399300	-0.65735600	2.26896900
N	0.32101700	-1.68268400	1.73946100
O	0.92075200	-2.78129500	1.71054500
C	-0.94086900	-1.52891100	1.23542300
C	-1.58335300	-2.58349700	0.58934300
C	-0.91668000	-2.60713600	-1.54299100
C	0.52053700	-2.75397300	-1.39481700
O	1.31545400	-1.81627600	-1.27387000
C	-3.05054300	-2.59780800	0.40893200
C	-3.83708100	-1.43685200	0.48054300
C	-5.21885800	-1.50933300	0.33264000
C	-5.84330800	-2.73701900	0.11283800
C	-5.07372500	-3.89830500	0.04276600
C	-3.69212800	-3.82735500	0.18884300
C	-1.52756500	-1.38324400	-2.03984200
C	-2.77687100	-1.54990800	-2.89331400

O	-1.09608300	-0.25071500	-1.81346900
C	1.05522100	-4.18073900	-1.43023900
H	4.05774300	1.50179200	-0.14326800
H	3.49904900	-0.50572000	-2.36990000
H	3.72980600	1.23389500	-2.54287200
H	5.82278200	-0.05527500	-3.11909600
H	6.07829000	1.05073500	-1.77623300
H	5.55825000	-1.96089700	-1.55884900
H	7.08249600	-1.14918000	-1.22459400
H	6.08223300	0.07108300	0.66906900
H	5.87572000	-1.66900300	0.87041100
H	3.53226200	-1.50804600	0.00544100
H	-0.18393000	1.12831600	-0.87646300
H	1.58980000	0.00533500	-0.77627400
H	3.52653800	0.77412000	3.49462200
H	5.05628200	0.82250500	2.58470800
H	3.59873200	1.65037200	1.94865000
H	3.31601100	-1.61291800	3.55272100
H	3.62358200	-2.56760900	2.09578100
H	4.96644000	-1.66487500	2.87471500
H	-1.43148300	-3.52004500	-1.82736400
H	1.22210000	-4.47287900	-2.47304800
H	2.00574200	-4.23042600	-0.89940900
H	0.35266800	-4.89477100	-0.99434400
H	-3.42295600	-2.34619700	-2.51688900
H	-3.32665300	-0.60914800	-2.93174600
H	-2.47559700	-1.82249500	-3.91128600
H	2.51093700	-0.47132700	1.79034300
H	-1.32857900	-0.52882000	1.33038400
H	-1.12870900	-3.55742500	0.72233400
H	-3.37662200	-0.47095600	0.65073800
H	-5.80914100	-0.60166600	0.39316500
H	-6.92060800	-2.78902100	0.00136300
H	-5.55013900	-4.85866800	-0.12079100
H	-3.09827700	-4.73473100	0.13814100
H	-0.05325000	3.94714300	-0.00093000
C	-1.06938100	3.57841600	-1.85941300
C	-1.84645200	2.88236100	0.47517700
C	-1.63774900	2.22811100	1.69712100
C	-3.13779700	3.33159100	0.15085400
C	-2.68479800	2.00266800	2.58435500
H	-0.64012900	1.88373000	1.94791400
C	-4.18329900	3.09922300	1.05520100
C	-3.96976800	2.43939600	2.26016100

H	-2.49851700	1.49145100	3.52269500
H	-5.18058100	3.44964700	0.80421000
H	-4.79504100	2.27391400	2.94446700
C	-2.17052800	4.63842400	-1.79824400
C	-3.42874700	4.04694000	-1.15586500
H	-1.82321500	5.49920400	-1.21409000
H	-2.40082900	5.00768300	-2.80205900
H	-0.18444000	3.95380800	-2.38100100
H	-1.42962200	2.70307700	-2.41249200
H	-3.88336700	3.33274700	-1.85549500
H	-4.17835000	4.82576600	-0.98261900

Complex D

Zero-point correction= 0.722295 (Hartree/Particle)
Thermal correction to Energy= 0.763655
Thermal correction to Enthalpy= 0.764599
Thermal correction to Gibbs Free Energy= 0.646065
Sum of electronic and zero-point Energies= -2163.076511
Sum of electronic and thermal Energies= -2163.035152
Sum of electronic and thermal Enthalpies= -2163.034208
Sum of electronic and thermal Free Energies= -2163.152741
Entropy= 249.475 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.49342800	3.20427400	-0.40259100
N	0.33377100	2.00344100	-0.46478800
C	1.66127400	1.95333400	-0.24721000
S	2.58536100	3.32880700	0.20274800
N	2.21078500	0.71931600	-0.39469500
C	3.63600300	0.43094000	-0.38307900
C	3.96889900	-0.78212100	0.51617800
C	5.47987400	-1.06773400	0.49255200
C	5.97747300	-1.31142300	-0.94047300
C	5.65021000	-0.12331500	-1.84915500
C	4.14975200	0.18350800	-1.81685000
N	3.42867400	-0.61965900	1.92657900
C	3.84235000	0.62584700	2.63192400
C	3.70009100	-1.81660500	2.77482800
O	0.84267200	-0.68217000	2.17373900
N	0.31690200	-1.60282300	1.39487900
O	1.06168500	-2.58739900	1.02961800
C	-0.93251100	-1.49062700	1.00923900

C	-1.54718300	-2.55563700	0.16789900
C	-1.20934700	-2.45676300	-1.39031600
C	0.30110800	-2.57898900	-1.66629000
O	1.00272000	-1.61400600	-1.89251100
C	-3.05796600	-2.65947600	0.35103300
C	-3.88621200	-1.53222700	0.42631400
C	-5.26616500	-1.67224500	0.56837700
C	-5.84357000	-2.93898500	0.63691200
C	-5.02946200	-4.06801900	0.56510200
C	-3.65021500	-3.92588600	0.42406000
C	-1.79626500	-1.20628400	-2.03907200
C	-2.76827000	-1.43621000	-3.17366300
O	-1.49724500	-0.08862300	-1.67205500
C	0.82935700	-3.99217500	-1.76013300
H	4.12888100	1.32437200	0.00569900
H	3.58612700	-0.64706600	-2.25708800
H	3.92340600	1.07597800	-2.40679800
H	5.96666500	-0.32934600	-2.87611400
H	6.21245600	0.75755800	-1.51563700
H	5.50558100	-2.21840000	-1.33816400
H	7.05507900	-1.49905700	-0.92006300
H	6.02560300	-0.21833400	0.91939100
H	5.70863700	-1.94144600	1.10654500
H	3.42706200	-1.65527800	0.13797400
H	-0.14422400	1.15342600	-0.75684800
H	1.62394400	-0.00529400	-0.80209900
H	3.35034000	0.63339100	3.60423200
H	4.92346400	0.63894300	2.77352600
H	3.52309300	1.50094200	2.06636400
H	3.08791400	-1.72905400	3.67119400
H	3.39022400	-2.70517100	2.22840500
H	4.75331400	-1.86358300	3.04810900
H	-1.67875200	-3.33713300	-1.84061800
H	0.51841500	-4.41899600	-2.72106200
H	1.91694100	-3.98558200	-1.70729500
H	0.42206700	-4.62031000	-0.96604100
H	-3.62318300	-2.01763500	-2.81272400
H	-3.11029400	-0.48450600	-3.57844500
H	-2.28872200	-2.02638600	-3.96201900
H	2.33100300	-0.60501000	1.88473800
H	-1.45746200	-0.61621700	1.35514000
H	-1.10573200	-3.50791100	0.47675800
H	-3.46104200	-0.53597600	0.37853700
H	-5.88838400	-0.78604300	0.63041000

H	-6.91670600	-3.04519400	0.75096400
H	-5.46544100	-5.05931000	0.62653400
H	-3.02319200	-4.81147900	0.37935100
H	0.13318700	3.96282900	0.07708700
C	-0.84769700	3.69743200	-1.81368200
C	-1.72488300	2.97916600	0.47634500
C	-1.59672400	2.25133600	1.66734900
C	-2.97174600	3.53517700	0.14242900
C	-2.68186300	2.06119300	2.51630200
H	-0.63570500	1.81686900	1.92216200
C	-4.05492700	3.33829900	1.00949300
C	-3.92182100	2.60840000	2.18539200
H	-2.55900100	1.49066500	3.43053400
H	-5.01762000	3.77108500	0.75193700
H	-4.77508600	2.47203600	2.84125900
C	-1.86791300	4.83513100	-1.74140800
C	-3.17923900	4.32303100	-1.13898700
H	-1.46729600	5.64978700	-1.12631500
H	-2.05002900	5.24946600	-2.73754600
H	0.07264700	4.01909200	-2.30923000
H	-1.26222900	2.86554000	-2.39522200
H	-3.67866300	3.67525800	-1.87206200
H	-3.86654500	5.15314200	-0.94647700

Product (*S*) obtained with catalyst 1i.

Complex C

Zero-point correction= 0.721430 (Hartree/Particle)
Thermal correction to Energy= 0.764528
Thermal correction to Enthalpy= 0.765472
Thermal correction to Gibbs Free Energy= 0.639439
Sum of electronic and zero-point Energies= -2163.073480
Sum of electronic and thermal Energies= -2163.030381
Sum of electronic and thermal Enthalpies= -2163.029437
Sum of electronic and thermal Free Energies= -2163.155470
Entropy= 265.258 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.86553700	3.20110000	-0.01058300
N	0.10952300	2.16024400	-0.30610800
C	1.39393300	2.14635500	0.09550300

S	2.06413100	3.33950300	1.13720500
N	2.11246100	1.08380200	-0.36269100
C	3.56178700	1.01752500	-0.28705900
C	4.06515400	-0.40464200	0.02645500
C	5.58264100	-0.39389900	0.24177600
C	6.28595800	0.12589800	-1.02582700
C	5.77115800	1.51126900	-1.43364500
C	4.24387500	1.51775700	-1.57641000
N	3.28360900	-1.02206200	1.18174900
C	3.22481800	-0.19782300	2.42687700
C	3.72167400	-2.41771200	1.49251100
C	-1.97312300	-2.15313400	0.91179100
C	0.01402800	-2.28525300	-2.47942100
C	0.94052000	-2.72094400	-1.50521400
O	1.58469600	-1.98716000	-0.71387000
C	-3.21986300	-2.28522200	0.17093600
C	-3.80473900	-1.11717300	-0.34866200
C	-4.99511500	-1.17847300	-1.06549000
C	-5.61858800	-2.40648900	-1.27571500
C	-5.04832900	-3.57598600	-0.76419400
C	-3.86171600	-3.51905200	-0.04815900
C	-0.35130600	-0.94672200	-2.75249000
C	-1.41649400	-0.71424000	-3.82154400
O	0.12077600	0.07692000	-2.19614100
C	1.19387000	-4.22652200	-1.40964900
H	3.85561300	1.68981400	0.52314100
H	3.93475800	0.88616500	-2.41788100
H	3.88023400	2.52861300	-1.77798300
H	6.23678800	1.82391900	-2.37298000
H	6.06460800	2.24776600	-0.67575900
H	6.11483400	-0.58388200	-1.84420500
H	7.36549100	0.15235700	-0.85184900
H	5.83933100	0.25086700	1.08984400
H	5.94936000	-1.39772900	0.46866100
H	3.81583000	-1.06415000	-0.80893500
H	-0.15396200	1.45523700	-1.00038100
H	1.62700200	0.44488000	-1.00674900
H	2.58481900	-0.71771200	3.13656100
H	4.23028800	-0.09451900	2.83269500
H	2.80574300	0.78201300	2.20504400
H	2.96433400	-2.87257000	2.12927400
H	3.79296500	-2.97439700	0.56116100
H	4.67970000	-2.39323900	2.00815500
H	-0.47044400	-3.05304400	-3.07032100

H	1.06185500	-4.55591500	-0.37473600
H	0.54216000	-4.81252900	-2.05975600
H	2.23436900	-4.43068400	-1.68384200
H	-1.01783100	-0.04009300	-4.58523900
H	-1.75553500	-1.63631600	-4.29642300
H	-2.27696400	-0.21538900	-3.36432500
H	2.33196700	-1.12833300	0.78865200
H	-3.32197200	-0.16077400	-0.17873000
H	-5.43517200	-0.26882100	-1.45771500
H	-6.54560500	-2.45708000	-1.83586800
H	-5.53265500	-4.53175400	-0.92897200
H	-3.43129500	-4.43630900	0.33682200
H	-0.34238600	3.92275200	0.62491200
C	-1.29013200	3.90961400	-1.30594900
C	-2.05308200	2.65929500	0.78914400
C	-1.81583100	1.77170200	1.84802800
C	-3.36808300	3.08723900	0.53636700
C	-2.85466300	1.30297000	2.64481200
H	-0.79898000	1.45143000	2.04770200
C	-4.40602900	2.60322500	1.34480100
C	-4.16155500	1.71963300	2.38996500
H	-2.64550300	0.62002600	3.46113900
H	-5.42146000	2.93681800	1.15034000
H	-4.98110500	1.36380000	3.00491000
C	-1.29311900	-3.14214200	1.50986900
H	-1.53856700	-4.19238700	1.52252400
N	-0.05347000	-2.87382400	2.18965300
O	0.32822700	-1.71389800	2.35313900
O	0.58028900	-3.85719700	2.58456600
H	-1.55533000	-1.15336900	0.98198700
H	-0.42729300	4.44974100	-1.70534600
H	-1.57800500	3.16199100	-2.05570900
C	-3.68876700	4.05333900	-0.59043600
H	-4.08212900	3.48565800	-1.44473600
H	-4.49384000	4.72361000	-0.27312800
C	-2.46572900	4.85366200	-1.04686600
H	-2.70516500	5.42182100	-1.95059000
H	-2.18940000	5.58226900	-0.27554500

TS

Zero-point correction= 0.721241 (Hartree/Particle)
Thermal correction to Energy= 0.762925

Thermal correction to Enthalpy= 0.763869
Thermal correction to Gibbs Free Energy= 0.644203
Sum of electronic and zero-point Energies= -2163.053937
Sum of electronic and thermal Energies= -2163.012253
Sum of electronic and thermal Enthalpies= -2163.011309
Sum of electronic and thermal Free Energies= -2163.130975
Entropy= 251.858 cal mol^{-1} K^{-1}

XYZ coordinates

C	-0.68711600	3.14495400	-0.16362200
N	0.23744200	2.04605200	-0.41702700
C	1.54782500	2.03933700	-0.11989100
S	2.34322100	3.35140500	0.65671900
N	2.19571300	0.89174900	-0.45835000
C	3.64058400	0.73991800	-0.47055900
C	4.07286100	-0.59661800	0.16757300
C	5.60196700	-0.71277500	0.19765200
C	6.17174400	-0.61574800	-1.22767600
C	5.73601300	0.68240700	-1.91592500
C	4.20959200	0.82572800	-1.90210600
N	3.43895100	-0.80227500	1.53905200
C	3.69347200	0.28461900	2.53376400
C	3.77241900	-2.13981500	2.12316100
C	-1.64833200	-1.96281700	0.37190600
C	-0.81800600	-2.31115700	-1.66770700
C	0.60608900	-2.54126000	-1.47106800
O	1.49307800	-1.68511800	-1.54472200
C	-3.07781000	-2.22307500	0.08669500
C	-3.93881200	-1.13263500	-0.10393500
C	-5.29730000	-1.33385100	-0.33702200
C	-5.81535900	-2.62596400	-0.39587800
C	-4.96602100	-3.71903200	-0.21371600
C	-3.61093600	-3.52032300	0.02779900
C	-1.31789300	-1.12597700	-2.35224600
C	-2.46817300	-1.33263100	-3.32499000
O	-0.86689100	0.00938500	-2.17866500
C	0.98322300	-3.98033400	-1.14822400
H	4.04528700	1.57392500	0.10729100
H	3.74944800	0.04245700	-2.51534600
H	3.90702300	1.78806500	-2.32320200
H	6.10348900	0.70648000	-2.94603100
H	6.18695800	1.53831500	-1.39906100
H	5.82522400	-1.47579400	-1.81317000
H	7.26260200	-0.68199000	-1.18321700

H	6.02873700	0.09001100	0.80946400
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H	3.65196200	-1.41047700	-0.43038300
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H	1.67225000	0.16285800	-0.95096200
H	3.14757600	0.03412900	3.44241900
H	4.75987100	0.33782400	2.74743400
H	3.33280100	1.23572400	2.14158900
H	3.03754400	-2.35946600	2.89558400
H	3.70032100	-2.89433300	1.34061900
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H	-1.37599700	-3.21965700	-1.87105000
H	0.52683700	-4.27446600	-0.19571500
H	0.60604800	-4.66613200	-1.91185100
H	2.06684200	-4.07601200	-1.07590200
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H	-3.18668900	-2.06503200	-2.95009500
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H	2.40379700	-0.83246400	1.40129700
H	-3.54293400	-0.12400000	-0.05294200
H	-5.94979400	-0.47833800	-0.47196300
H	-6.87205000	-2.78290900	-0.58166600
H	-5.36172200	-4.72770100	-0.26016200
H	-2.96136800	-4.37939200	0.15827200
H	-0.11441000	3.88039600	0.40995300
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C	-1.86940200	2.69865100	0.69928000
C	-1.64398100	1.83713900	1.78177900
C	-3.16662600	3.19145200	0.47414400
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H	-2.47967900	0.78969300	3.46099600
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Complex D

Zero-point correction= 0.722750 (Hartree/Particle)
Thermal correction to Energy= 0.764060
Thermal correction to Enthalpy= 0.765005
Thermal correction to Gibbs Free Energy= 0.647167
Sum of electronic and zero-point Energies= -2163.073669
Sum of electronic and thermal Energies= -2163.032358
Sum of electronic and thermal Enthalpies= -2163.031414
Sum of electronic and thermal Free Energies= -2163.149251
Entropy= 248.009 cal mol^{-1} K^{-1}

XYZ coordiantes

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N	2.21769100	0.87613400	-0.48746500
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H	7.36033100	-0.56505300	-0.89914000
H	5.97881500	0.16780200	1.01381500
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H	3.87685400	-2.88393000	1.47085600
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H	-1.35534300	-3.31589500	-1.55179000
H	0.69395600	-4.07650900	0.07014300
H	0.86556200	-4.56330100	-1.61435600
H	2.21892900	-3.73451800	-0.81468500
H	-1.25719300	-2.57936600	-4.09359200
H	-2.88009400	-2.45656400	-3.41904500
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H	2.33979200	-0.98207200	1.38537000
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H	-6.93491500	-2.69873200	-0.07081100
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C	-1.86330600	2.66557500	0.63829900
C	-1.57737200	1.87978900	1.76306400
C	-3.17405900	3.13634000	0.44632800
C	-2.56347500	1.55881600	2.68960800
H	-0.56786700	1.51111300	1.90709400

C	-4.15657900	2.80811100	1.39026800
C	-3.86344000	2.02833900	2.50361900
H	-2.31867000	0.94478500	3.54923900
H	-5.16803200	3.17663100	1.24350400
H	-4.64137100	1.78764200	3.22008800
C	-0.98745000	-2.56254500	1.31845000
H	-1.53600400	-3.24829000	1.94536000
N	0.19189700	-2.18623300	1.76662800
O	0.87717900	-1.34006200	1.02106900
O	0.71090800	-2.61156300	2.85074500
H	-1.38910100	-0.83614100	0.17914000
H	-0.40041900	4.01520600	-2.21092100
H	-1.62972100	2.74897800	-2.25876200
C	-3.55608000	3.96802700	-0.76524600
H	-4.06498300	3.31785500	-1.48951300
H	-4.28790800	4.72595700	-0.46827200
C	-2.34939600	4.62022800	-1.44699800
H	-2.65210200	5.05967800	-2.40207900
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2. Experimental Part

2.1 Kinetic studies

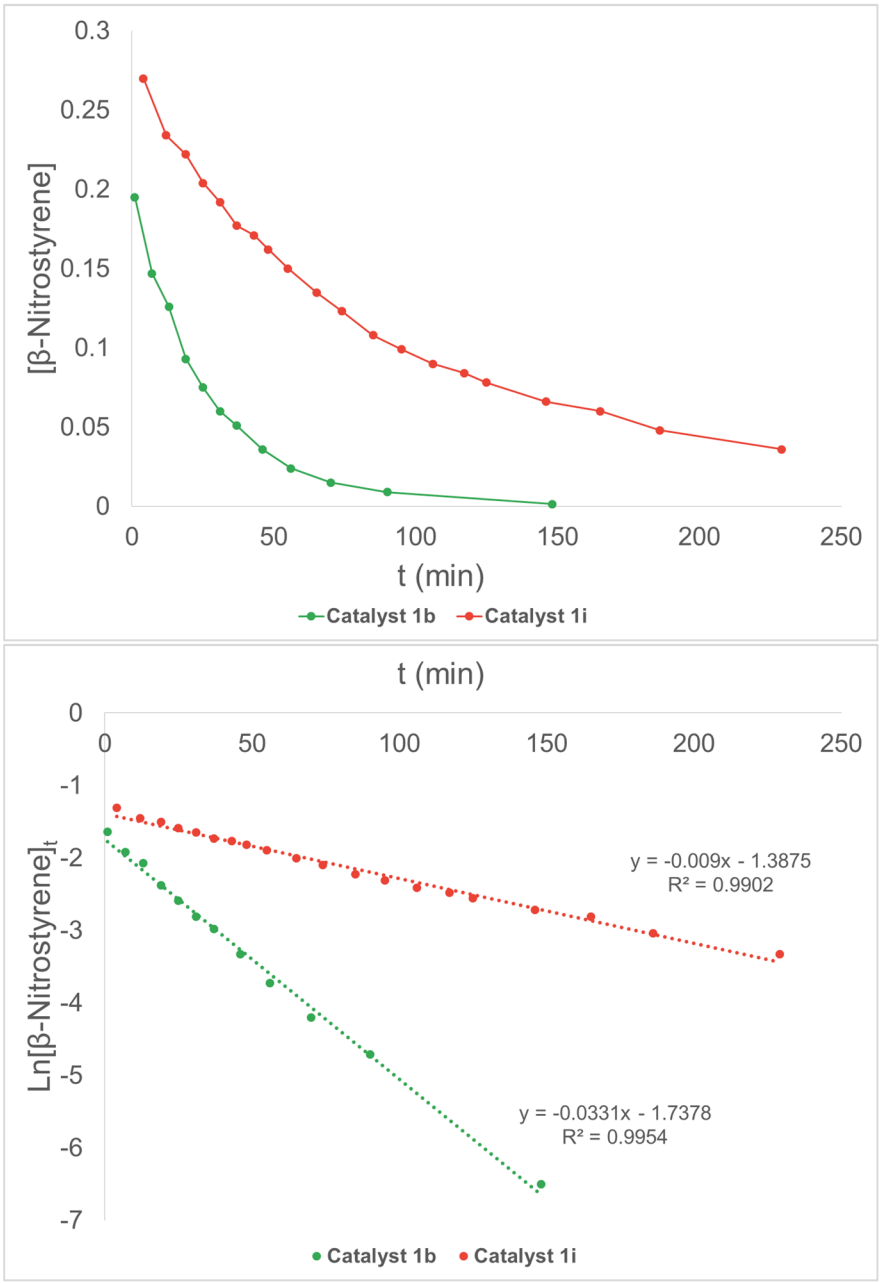
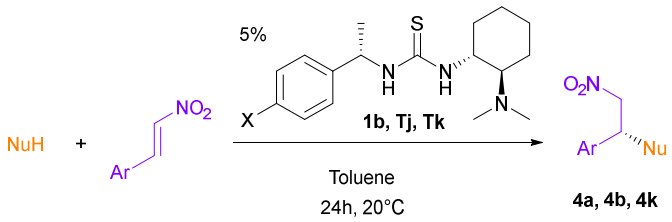
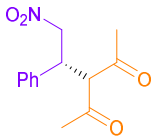
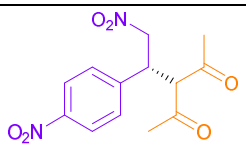
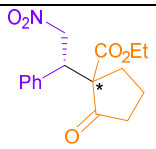


Fig. S8. Kinetics of the Michael addition under pseudo-first order conditions. (Top) Concentration of β-nitrostyrene as a function of time with catalysts **1i** and **1b**.[8] (Bottom) Plot on a logarithmic scale of the concentration of β-nitrostyrene as the reaction proceeds.

2.2 Evaluation of organocatalysts

Table S7. Evaluation of *p*-substituted catalysts with -OCH_3 or -NO_2 in the Michael reaction under consideration.



Entry	Product	X	Cat	Yield (%)[a]	*ee* (%)
1		-H	**1b**	87[b]	86
2		-OCH_3	**Tj**	88	86
3	**4a**	-NO_2	**Tk**	88	85
4		-H	**1b**	88	90
5		-OCH_3	**Tj**	85	90
6	**4b**	-NO_2	**Tk**	91	75
7		-H	**1b**	91	80
8		-OCH_3	**Tj**	88	76
9	**4k**	-NO_2	**Tk**	78	60

[a]Isolated yields, *ee* obtained by CSP-HPLC. [b]Ref. 8.

2.3 Synthesis of organocatalysts

The synthesis and characterization of compounds **4a**–**4l** and **1b** can be found in Ref. 8. All starting materials were used directly as obtained commercially. Flash column chromatography was carried out with silica gel 60 (0.4/0.63 mm, 230-400 mesh) and TLC was performed with silica gel F254 plates. Melting points are uncorrected. ^{1}H and ^{13}C NMR were recorded at 300 MHz and 75 MHz respectively. Chemical shifts (δ) are reported in ppm downfield from TMS and coupling constants are given in Hertz. Mass spectra were obtained by EI. HRMS (DART) were measured with a TOF mass spectrometer and the CSP-HPLC analysis was performed using the indicated chiral column and UV detector.

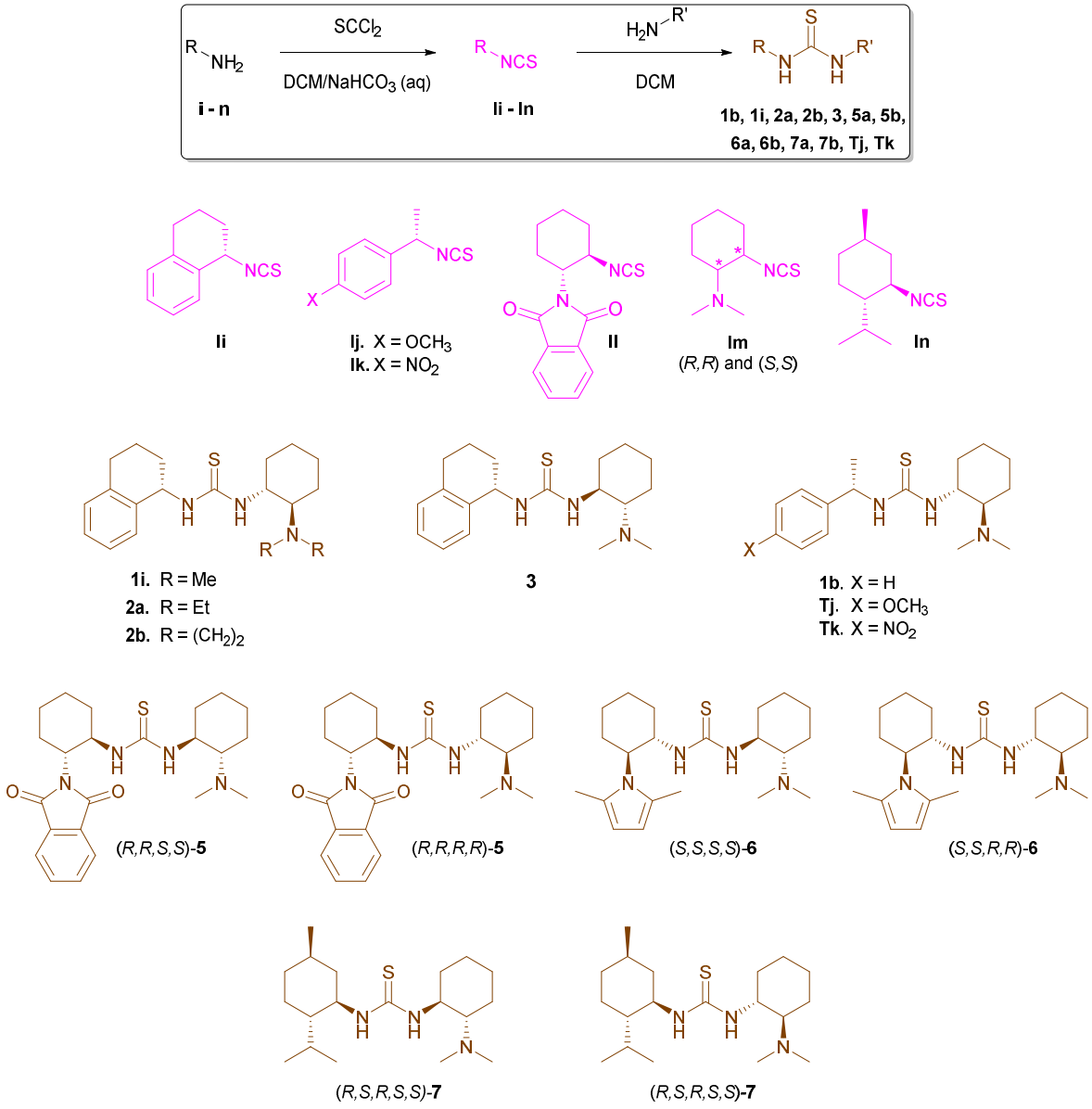


Fig. S9. Intermediaries and thioureas used in this work.

General procedure for the intermediaries (isothiocyanate synthesis)

The corresponding chiral amine (2 mmol, 1 eq) was dissolved in 20 mL of DCM and 20 mL of 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 DCM (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 (the proportion of solvents is reported in the R_f section for each compound).

(*S*)-1,2,3,4-Tetrahydro-1-naphthylisothiocyanate, **Ii**.
Yellow liquid (348 mg, 92%). R_f = 0.52 (hexane/ethyl acetate, 9:1). $[\alpha]_D^{25}$ +57.7 (*c* 1, $CHCl_3$). IR (film): $\tilde{\nu}$ cm^{-1} = 3062, 3021, 2945, 2933, 2865, 2837, 2108, 2078, 1491, 1452, 1342, 1307, 1201, 1157, 1078, 987, 927, 881, 738, 683, 604. ^1H NMR (300 MHz, $CDCl_3$): δ = 7.40 – 7.28 (1H, m), 7.28 – 7.18 (2H, m), 7.18 – 7.04 (1H, m), 4.92 (1H, t, *J* = 5.3 Hz), 2.93 – 2.67 (2H, m), 2.18 – 2.03 (2H, m), 2.03 – 1.92 (1H, m), 1.91 – 1.75 (1H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 136.5, 133.4, 129.6, 128.7, 128.5, 126.6, 55.9, 31.0, 28.7, 19.5. MS-EI (IE, 70 eV): *m/z* (%) = 189 (1) $[M]^+$, 131 (100), 116 (17), 91 (25), 77 (5). HRMS (DART/TOF): $[M-NCS]^+$ calcd. for $C_{10}H_{11}$ 131.0861; found 131.0860.

(*S*)-1-(*p*-Methoxyphenyl)ethylisothiocyanate, **Ij**.
Colorless oil (340 mg, 88%), R_f = 0.40 (hexane/ethyl acetate, 9:1). $[\alpha]_D^{25}$ +5.1 (*c* 2.11, $CHCl_3$). ^1H NMR (300 MHz, $CDCl_3$): δ = 7.22 (2H, d, *J* = 8.2 Hz), 6.88 (2H, d, *J* = 8.6 Hz), 4.83 (1H, q, *J* = 6.7 Hz), 3.77 (3H, s), 1.61 (3H, d, *J* = 6.8 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 159.4, 132.2, 131.9, 126.7, 114.2, 56.5, 55.3, 24.8. MS-DART (positive): *m/z* (%) = 135 (100) $[M-NCS]^+$.

(*S*)-1-(*p*-Nitrophenyl)ethylisothiocyanate, **Ik**.
Yellow oil (395 mg, 95%). R_f = 0.38 (hexane/ethyl acetate, 8:2). $[\alpha]_D^{25}$ +5.9 (*c* 1.4, $CHCl_3$). ^1H NMR (300 MHz, $CDCl_3$): δ = 8.24 (2H, d, *J* = 8.7 Hz), 7.54 (2H, d, *J* = 8.7 Hz), 5.11 (1H, q, *J* = 6.7 Hz), 1.74 (3H, d, *J* = 6.8 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 147.6, 147.2, 134.7, 126.5, 124.2, 56.4, 24.9. MS-DART (positive): *m/z* (%) = 209 (50) $[M+H]^+$, 150 (100). HRMS (DART/TOF): $[M+H]^+$ calcd for $C_9H_9N_2O_2S$ 209.0385; found 209.0377.

(*R,R*)-2-*N*-Phthaloylaminocyclohexylisothiocyanate, **Il**.
The required chiral amine was prepared according to the literature procedure.[9] Beige solid (447 mg, 78%), mp 97 – 99 °C. R_f = 0.54 (hexane/ethyl acetate, 7:3). $[\alpha]_D^{25}$ -8.0 (*c* 1.01, $CHCl_3$). ^1H NMR (300 MHz, $CDCl_3$): δ = 7.94 – 7.81 (2H, m), 7.80 – 7.67 (2H, m), 4.65 – 4.42 (1H, m), 4.31 – 4.03 (1H, m), 2.39 – 2.24 (1H, m), 2.23 – 2.05 (1H, m), 1.94 – 1.75 (3H, m), 1.70 – 1.55 (1H, m), 1.50 – 1.31 (2H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 167.9, 134.1, 133.8, 131.5, 123.3, 56.8, 54.7, 33.5, 28.8, 24.8, 23.9. MS-DART (positive): *m/z* (%) = 287 (100) $[M+H]^+$, 228 (72). HRMS (DART/TOF): $[M+H]^+$ calcd for $C_{15}H_{15}N_2O_2S$ 287.0854; found 287.0863.

(*R,R*)-2-Dimethylaminocyclohexylisothiocyanate, **Im**.
Orange oil (339 mg, 92%). R_f = 0.66 (hexane/ethyl acetate, 4:6, TLC Stain: $KMnO_4$). $[\alpha]_D^{25}$ -100.5 (*c* 0.34, $CHCl_3$) (lit.[10] $[\alpha]_D^{25}$ -99 (*c* 0.36, $CHCl_3$)). ^1H NMR (300 MHz, $CDCl_3$): δ = 3.56 (1H, td, *J* = 10.5, 4.1 Hz), 2.50 – 2.41 (1H, m), 2.34 (6H, s), 2.22 – 2.15 (1H, m), 1.89 – 1.67 (3H, m), 1.62 – 1.48 (1H, m), 1.29 – 1.13 (3H,

m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 132.7, 67.4, 58.4, 40.5, 33.7, 24.6, 24.5, 23.8. MS-DART (positive): *m/z* (%) = 185 (100) $[M+H]^+$, 171 (21). HRMS (DART/TOF): $[M+H]^+$ calcd for $C_9H_{17}N_2S$ 185.1112; found 185.1100.

(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexylisothiocyanate, **In**.
Yellow oil (374 mg, 95%). R_f = 0.75 (hexane/ethyl acetate, 9:1). $[\alpha]_D^{25}$ -51.0 (*c* 1.15, $CHCl_3$) (lit.[11] $[\alpha]_D^{25}$ -74.2 (*c* 0.52, $CHCl_3$)). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.44 (1H, td, *J* = 11.0, 3.9 Hz), 2.23 – 2.02 (2H, m), 1.79 – 1.61 (2H, m), 1.48 – 1.33 (2H, m), 1.32 – 1.21 (1H, m), 1.02 – 0.87 (8H, m), 0.82 (3H, d, *J* = 7.0 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 162.8, 58.9, 48.6, 43.0, 34.0, 31.7, 27.6, 23.3, 21.8, 20.8, 15.8. MS-DART (positive): *m/z* (%) = 198 (34) $[M+H]^+$, 155 (64), 139 (100), 83 (51). HRMS (DART/TOF): $[M+H]^+$ calcd for $C_{11}H_{20}NS$ 198.1316; found 198.1312.

General procedure for the preparation of bifunctional catalysts

The corresponding isothiocyanate (2 mmol, 1 equiv) was dissolved in 7 mL of DCM. The (*R,R*)- or (*S,S*)-*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. Note: Catalysts **6** were prepared with isothiocyanate **Im** and (1*S*,2*S*)-2-(2,5-dimethyl-1*H*-pyrrol-1-yl)cyclohexan-1-amine.

1-[(1*R*,2*R*)-2-(Dimethylamino)cyclohexyl]-3-[(*S*)-1,2,3,4-tetrahydro-1-naphthyl]-thiourea, **1i**.
White solid (504 mg, 76%), mp 55 – 58 °C. R_f = 0.37 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ +16.4 (*c* 1, $CHCl_3$). IR (KBr): $\tilde{\nu}$ cm^{-1} = 3244, 3020, 2927, 2856, 2781, 1526, 1448, 1357, 1319, 1265, 1235, 1206, 1150, 1078, 1038, 948, 872, 850, 775, 742, 705, 651, 597, 558, 480, 439. ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ = 7.88 (d, *J* = 8.7 Hz, 1H), 7.31 – 7.23 (m, 1H), 7.18 – 7.03 (m, 4H), 5.60 (br, 1H), 4.02 (br, 1H), 2.85 – 2.61 (m, 2H), 2.48 – 2.34 (m, 1H), 2.21 (s, 7H), 2.01 – 1.87 (m, 1H), 1.87 – 1.68 (m, 5H), 1.64 – 1.55 (m, 1H), 1.26 – 1.11 (m, 3H), 1.11 – 0.99 (m, 1H). ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ = 181.3, 137.943, 136.9, 128.7, 128.2, 126.7, 125.7, 65.4, 54.3, 50.9, 39.9, 32.9, 29.7, 28.8, 24.6, 24.4, 22.1, 20.1. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.94 (1H, br), 7.54 – 7.26 (1H, m), 7.26 – 6.96 (3H, m), 6.29 (1H, br), 5.33 (1H, br), 3.50 (1H, br), 2.79 (2H, br), 2.49 – 2.19 (2H, m), 2.06 (8H, s), 1.87 – 1.55 (5H, m), 1.36 – 1.04 (4H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 182.4, 137.4, 136.8, 129.1, 127.2, 126.2, 67.6, 56.2, 52.8, 40.1, 33.4, 29.5, 29.3, 24.8, 24.6, 22.2, 20.2. MS-EI (IE, 70 eV): *m/z* (%) = 331 (6) $[M]^+$, 155 (8), 146 (8), 125 (100), 98 (8), 84 (27), 71 (9), 58 (9). HRMS (DART/TOF): $[M+H]^+$ Calcd. for $C_{19}H_{30}N_3S$ 332.2160; found 332.2152.

1-[(1*R*,2*R*)-2-(Diethylamino)cyclohexyl]-3-[(*S*)-1,2,3,4-tetrahydro-1-naphthyl]-thiourea, **2a**.
Hygroscopic yellow solid (597 mg, 83%). R_f = 0.51 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ -11.7 (*c* 1.15, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.40 – 7.29 (1H, m), 7.24 – 7.02 (3H, m), 6.81 (1H, br), 6.43 (1H, br), 5.27 (1H, br), 3.80 – 3.48 (1H, br), 2.85 – 2.73 (2H, m), 2.70 – 2.47 (3H, m), 2.45 – 2.27 (2H, m), 2.26 – 2.10 (1H, m), 1.98 – 1.78 (5H, m), 1.77 – 1.68 (1H, m), 1.38 – 1.09 (6H, m), 0.97 (5H, t, *J* = 6.9 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 181.9, 137.4, 136.7, 129.2, 128.6, 127.4, 126.3, 63.8, 55.9, 52.5, 43.2, 33.4, 30.0, 29.2, 25.6, 24.6, 24.0, 20.3, 14.1. MS-DART (positive): *m/z* (%) = 360 (100) $[M+H]^+$, 131 (13). HRMS (DART/TOF): $[M+H]^+$ Calcd. for $C_{21}H_{34}N_3S$ 360.2473; found 360.2483.

1-[(1*R*,2*R*)-2-(Pyrrolidin-1-yl)cyclohexyl]-3-[(*S*)-1,2,3,4-tetrahydro-1-naphthyl]-thiourea, **2b**.
Yellow solid (607 mg, 85%), mp 65 – 67 °C. R_f = 0.45 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ +30.5 (*c* 1.02, $CHCl_3$). ^{1}H NMR (300 MHz, CDCl3): δ = 8.58 (1H, br), 7.50 – 7.30 (1H, m), 7.20 – 7.00 (3H, m), 6.36 (1H, br), 5.41 (1H, br), 3.65 (1H, br), 2.81 – 2.74 (2H, m), 2.72 – 2.52 (4H, m), 2.48 – 2.19 (2H, m), 2.06 – 1.38 (11H, m), 1.33 – 1.14 (4H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 182.6, 137.4, 136.8, 129.1, 128.2, 127.2, 126.2, 64.3, 57.9, 53.5, 53.2, 48.3, 33.1, 29.8, 29.4, 24.7, 24.5, 23.4, 20.7. MS-DART (positive): *m/z* (%) = 358 (100) $[M+H]^+$, 324 (11). HRMS (DART/TOF): $[M+H]^+$ Calcd for $C_{21}H_{32}N_3S$ 358.2317; found 358.2317.

1-[(1*S*,2*S*)-2-(Dimethylamino)cyclohexyl]-3-[(*S*)-1,2,3,4-tetrahydro-1-naphthyl]-thiourea, **3**.
White solid (524 mg, 79%), mp 68 – 69 °C. R_f = 0.28 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$-114.8 (*c* 1, $CHCl_3$). IR (KBr): $\tilde{\nu}$ cm^{-1} = 3252, 3019, 2927, 2856, 2785, 1530, 1448, 1357, 1318, 1265, 1237, 1208, 1077, 1035, 948, 872, 851, 773, 742, 705, 653, 559, 479, 438. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.07 (1H, br), 7.65 – 6.84 (4H, m), 6.42 (1H, br), 5.51 (1H, br), 3.64 (1H, br), 2.78 (2H, br), 2.56 – 2.19 (2H, m), 2.17 – 1.65 (13H, m), 1.20 (4H, br). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 182.1, 137.3, 136.6, 129.2, 128.9, 127.1, 126.0, 67.6, 56.0, 52.5, 40.0, 33.3, 29.7, 29.2, 24.6, 24.5, 22.6, 19.8. MS-DART (positive): m/z (%) = 332 (100) $[M+H]^+$. HRMS (DART/TOF): $[M+H]^+$ Calcd for $C_{19}H_{30}N_3S$ 332.2160; found 332.2156.

1-[(1*R*,2*R*)-2-(Dimethylamino)cyclohexyl]-3-[(*S*)-1-(*p*-methoxyphenyl)ethy]-thiourea, **Tj**.
Hygroscopic white solid (604 mg, 90%). R_f = 0.49 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ +3.8 (*c* 0.91, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.25 (3H, d, *J* = 8.7 Hz), 6.87 (2H, d, *J* = 8.7 Hz), 6.13 (1H, br), 4.98 (1H, br), 3.80 (3H, s), 3.57 (1H, br), 2.46 (1H, br), 2.23 (6H, s), 2.13 – 2.03 (1H, m), 1.85 – 1.72 (2H, m), 1.66 – 1.57 (1H, m), 1.49 (3H, d, *J* = 6.8 Hz), 1.27 – 1.06 (4H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 182.0, 159.0, 152.2, 127.3, 114.2, 67.4, 56.3, 55.4, 53.3, 40.2, 32.9, 24.9, 24.5, 22.1, 15.7. MS-DART (positive): *m/z* (%) = 336 (100) $[M+H]^+$, 143 (18), 135 (11). HRMS (DART/TOF): $[M+H]^+$ Calcd. for $C_{18}H_{30}N_3OS$ 336.2110; found 336.2111.

1-[(1*R*,2*R*)-2-(Dimethylamino)cyclohexyl]-3-[(*S*)-1-(*p*-nitrophenyl)ethy]-thiourea, **Tk**.
Yellow solid (686 mg, 98%), mp 59 – 60 °C. R_f = 0.49 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ +90.4 (*c* 1, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.07 (1H, br), 8.18 (2H, d, *J* = 8.2 Hz), 7.49 (2H, d, *J* = 8.3 Hz), 6.19 (1H, s), 5.42 (1H, s), 3.53 (1H, s), 2.28 (8H, s), 1.92 – 1.77 (2H, m), 1.74 – 1.64 (1H, m), 1.52 (3H, d, *J* = 6.7 Hz), 1.22 – 1.13 (4H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 183.1, 151.6, 147.0, 127.1, 124.0, 67.9, 56.5, 53.5, 40.5, 33.3, 24.7, 24.5, 22.6, 22.4. MS-DART (positive): *m/z* (%) = 351 (17) $[M+H]^+$, 143 (100). HRMS (DART/TOF): $[M+H]^+$ Calcd for $C_{17}H_{27}N_4O_2S$ 351.1855; found 355.1850.

1-[(1*S*,2*S*)-2-(Dimethylamino)cyclohexyl]-3-[(*R,R*)-2-*N*-phthaloylaminocyclohexyl]-thiourea, (*R,R,S,S*)-**5**.
Yellow solid (660 mg, 77%), mp 158 – 160 °C. R_f = 0.44 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ -80.0 (*c* 1, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.86 – 7.74 (2H, m), 7.72 – 7.62 (2H, m), 6.27 (1H, br), 4.75 (1H, br), 4.05 – 3.86 (1H, m), 3.51 (2H, br), 2.64 – 2.40 (2H, m), 2.28 (7H, s), 2.13 – 1.95 (1H, m), 1.94 – 1.69 (5H, m), 1.66 – 1.45 (2H, m), 1.41 – 1.02 (6H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 182.5, 168.9, 134.0, 132.1, 123.0, 67.5, 56.0, 55.2, 53.6, 40.3, 33.3, 33.0, 28.9, 25.5, 24.9, 24.7, 24.5, 22.9. MS-DART (positive): *m/z* (%) = 429 (100) $[M+H]^+$, 287 (19), 143 (69). HRMS (DART/TOF): $[M+H]^+$ Calcd. for $C_{23}H_{33}N_4O_2S$ 429.2324; found 429.2335.

1-[(1*R*,2*R*)-2-(Dimethylamino)cyclohexyl]-3-[(*R,R*)-2-*N*-phthaloylaminocyclohexyl]-thiourea, (*R,R,R,R*)-**5**. Yellow solid (831 mg, 97%). mp 152 – 154 °C. R_f = 0.37 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ -60.6 (*c* 1, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.87 – 7.74 (2H, m), 7.73 – 7.61 (2H, m), 7.20 – 7.09 (1H, m), 6.79 – 6.59 (1H, br), 5.09 – 4.90 (1H, m), 4.29 – 4.14 (1H, m), 4.08 – 3.91 (1H, m), 3.20 – 3.06 (1H, m), 2.63 (6H, s), 2.30 – 2.16 (1H, m), 2.05 – 1.75 (5H, m), 1.72 – 1.12 (10H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 181.8, 168.9, 133.7, 132.2, 123.2, 66.6, 55.2, 54.8, 54.1, 39.5, 32.8, 32.5, 28.7, 25.6, 24.7, 24.6, 24.2, 22.5. MS-DART (positive): *m/z* (%) = 429 (100) $[M+H]^+$, 143 (23). HRMS (DART/TOF): $[M+H]^+$ Calcd. for $C_{23}H_{33}N_4O_2S$ 429.2324; found 429.2334.

1-[(1*S*,2*S*)-2-(Dimethylamino)cyclohexyl]-3-[(1*S,*1*S*)-2-(2,5-dimethyl-1*H*-pyrrol-1-yl)cyclohexyl]-thiourea, (*S,S,S,S*)-**6**.
The required cyclohexanediamine with pyrrole was obtained by a previously reported procedure.[12] Slightly brown solid (670 mg, 89%), mp 83 – 85 °C. R_f = 0.29 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ +8.7 (*c* 0.55, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.64 (1H, s), 6.10 (1H, s), 5.66 (2H, s), 4.63 (2H, br), 3.98 – 3.73 (1H, m), 3.34 (1H, s), 2.70 – 2.48 (1H, m), 2.42 – 2.13 (12H, m), 1.98 – 1.59 (8H, m), 1.52 – 1.31 (3H, m), 1.24 – 1.10 (4H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 182.0, 128.3, 107.8, 105.9, 66.5, 59.4, 56.3, 54.9, 39.6, 33.7, 32.9, 32.4, 26.0, 24.8, 24.6, 24.3, 22.0, 15.0, 13.6. MS-DART (positive): *m/z* (%) = 377 (100) $[M+H]^+$. HRMS (DART/TOF): $[M+H]^+$ Calcd. for $C_{21}H_{37}N_4S$ 377.2739; found 377.2743.

1-[(1*R*,2*R*)-2-(Dimethylamino)cyclohexyl]-3-[(1*S,*1*S*)-2-(2,5-dimethyl-1H-pyrrol-1-yl)cyclohexyl]-thiourea, (*S,S,R,R*)-**6**.
The required cyclohexanediamine with pyrrole was obtained by a previously reported procedure.[12] Slightly brown solid (685 mg, 91%), mp 72 – 74 °C. R_f = 0.31 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ -8.4 (*c* 0.51, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.63 (1H, br), 5.67 (2H, s), 4.61 (1H, s), 4.40 – 3.94 (1H, br), 3.93 – 3.73 (1H, m), 3.72 – 3.36 (1H, br), 2.61 – 2.14 (12H, m), 2.07 – 1.57 (8H, m), 1.52 – 0.92 (8H, m). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 181.5, 129.0, 128.0, 108.0, 105.6, 67.3, 59.9, 56.1, 55.9, 40.5, 34.1, 32.5, 32.3, 26.0, 25.0, 24.9, 24.6, 22.8, 15.3, 13.8. MS-DART (positive): *m/z* (%) = 377 (100) $[M+H]^+$. HRMS (DART/TOF): $[M+H]^+$ Calcd. for $C_{21}H_{37}N_4S$ 377.2739; found 377.2731.

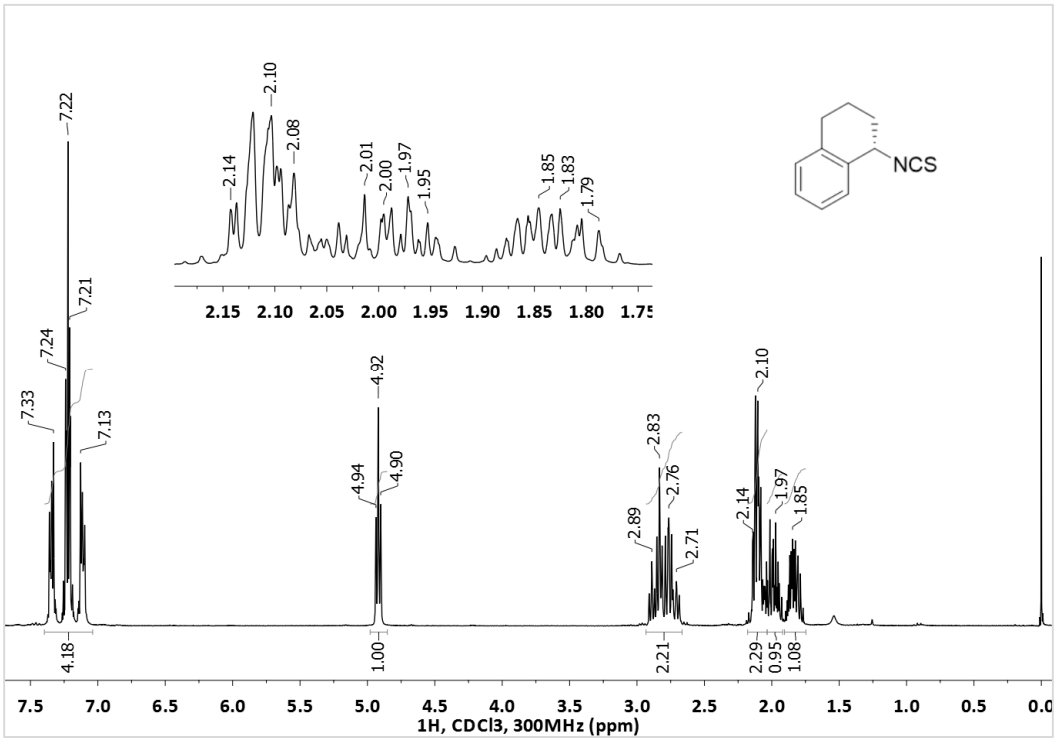
1-[(1*S*,2*S*)-2-(Dimethylamino)cyclohexyl]-3-[(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl]-thiourea, (*R,S,R,S,S*)-**7**.
White solid (584 mg, 86%), mp 62 – 65 °C. R_f = 0.39 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ = -73.5 (*c* 0.52, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.36 (1H, s), 3.99 (1H, br), 3.71 (1H, br), 2.85 – 2.52 (3H, m), 2.38 (7H, s), 2.18 (1H, d, *J* = 12.2 Hz), 2.07 – 1.98 (1H, m), 1.94 – 1.85 (2H, m), 1.76 – 1.67 (3H, m), 1.55 – 1.47 (1H, m), 1.31 – 1.12 (7H, m), 0.93 – 0.90 (6H, m), 0.83 (3H, d, *J* = 7.0 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 181.8, 67.7, 56.0, 55.2, 48.3, 42.3, 40.1, 34.6, 33.3, 31.8, 26.8, 24.8, 24.5, 23.8, 22.2, 21.2, 16.5. MS-DART (positive): *m/z* (%) = 340 (100) $[M+H]^+$. HRMS (DART/TOF): $[M+H]^+$ Calcd for $C_{19}H_{38}N_3S$ 340.2786; found 340.2784.

1-[(1*R*,2*R*)-2-(Dimethylamino)cyclohexyl]-3-[(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl]-thiourea, (*R,S,R,R,R*)-**7**.
White solid (563 mg, 83%), mp 91 – 93 °C. R_f = 0.31 (CH_2Cl_2/CH_3OH/NH_4OH, 90:10:1). $[\alpha]_D^{25}$ -40.2 (*c* 0.49, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.50 (d, *J* = 7.8 Hz, 1H), 6.75 (d, *J* = 7.2 Hz, 1H), 4.64 (q, *J* = 9.6, 8.2 Hz, 1H), 4.21 (q, *J* = 14.6, 12.8 Hz, 1H), 3.31 (t, *J* = 9.5 Hz, 1H), 2.79 (s, 6H), 2.33 (d, *J* = 11.0 Hz, 1H), 2.12

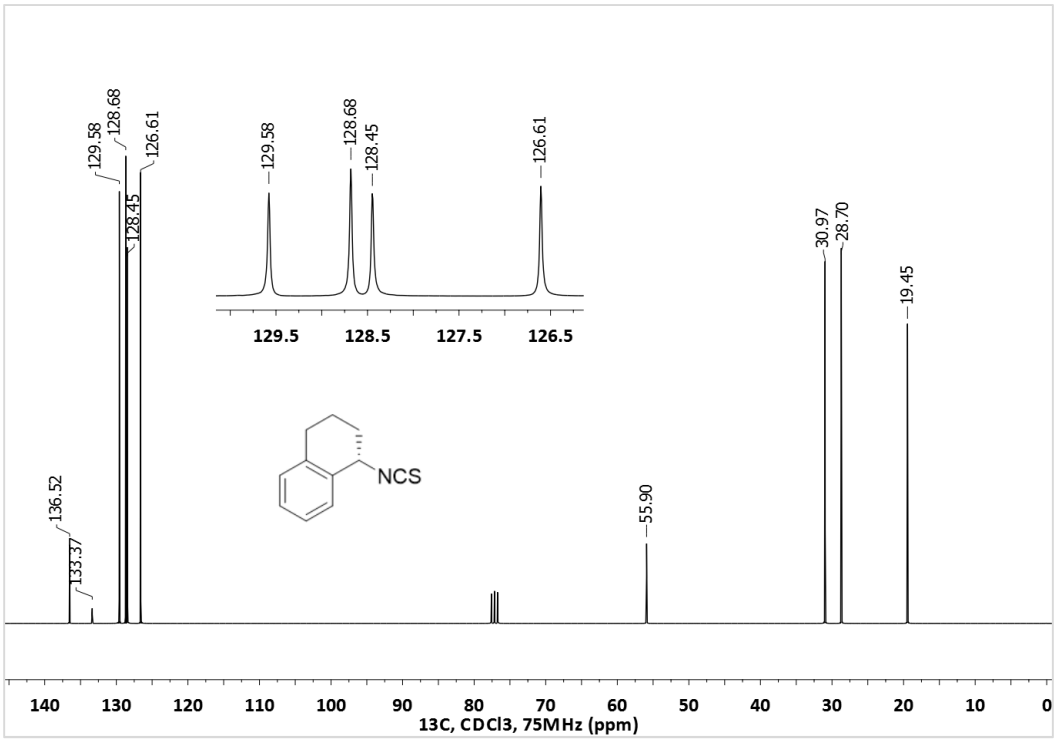
– 1.76 (m, 5H), 1.76 – 1.63 (m, 2H), 1.52 – 1.21 (m, 7H), 0.94 – 0.81 (m, 10H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 181.3, 67.3, 55.5, 53.9, 48.0, 42.2, 34.6, 33.2, 32.0, 27.1, 24.6, 24.2, 24.1, 23.0, 223, 21.2, 17.0. MS-DART (positive): *m/z* (%) = 340 (100) $[M+H]^+$. HRMS (DART/TOF): $[M+H]^+$ Calcd for $C_{19}H_{38}N_3S$ 340.2786; found 340.2789.

2.4 Characterization of all compounds

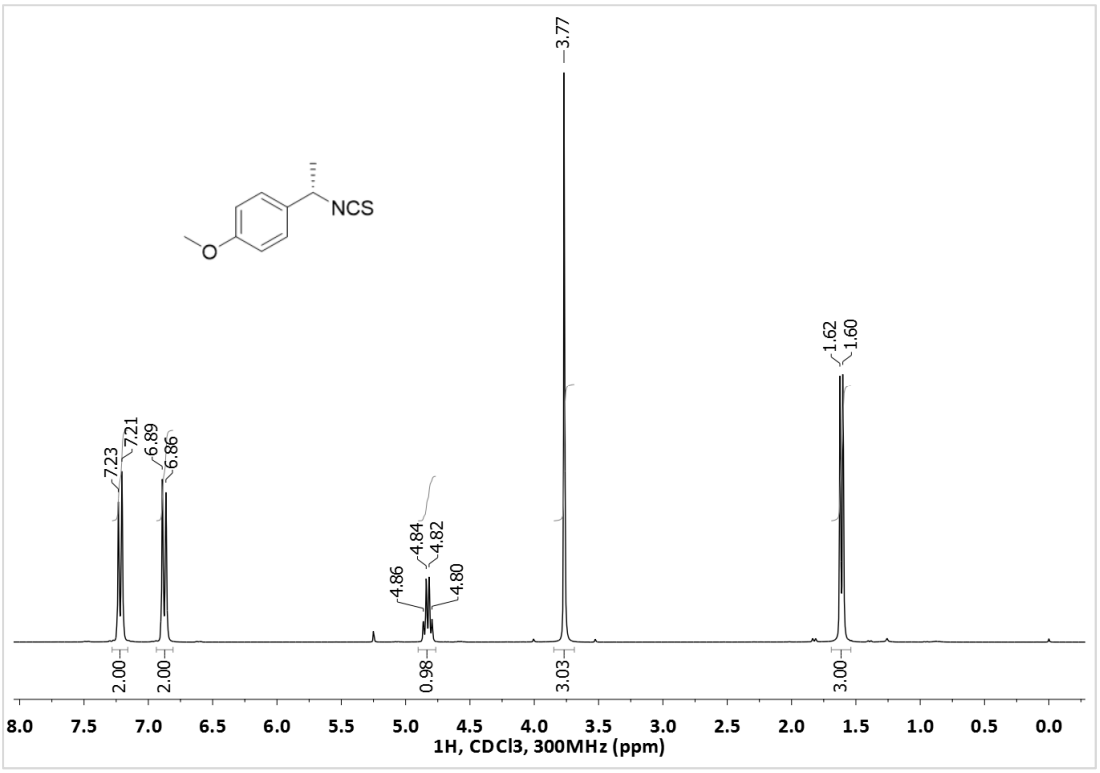
Spectra of intermediaries and catalysts



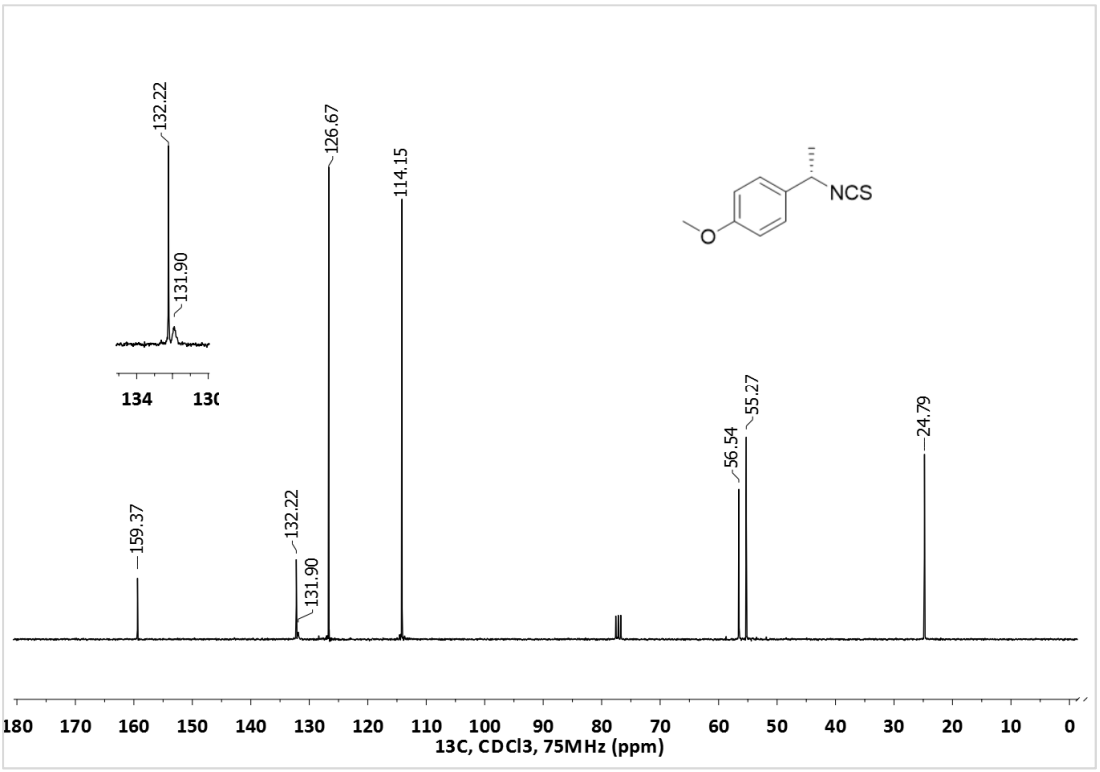
^{1}H NMR Spectrum (300 MHz) of **Ii**.



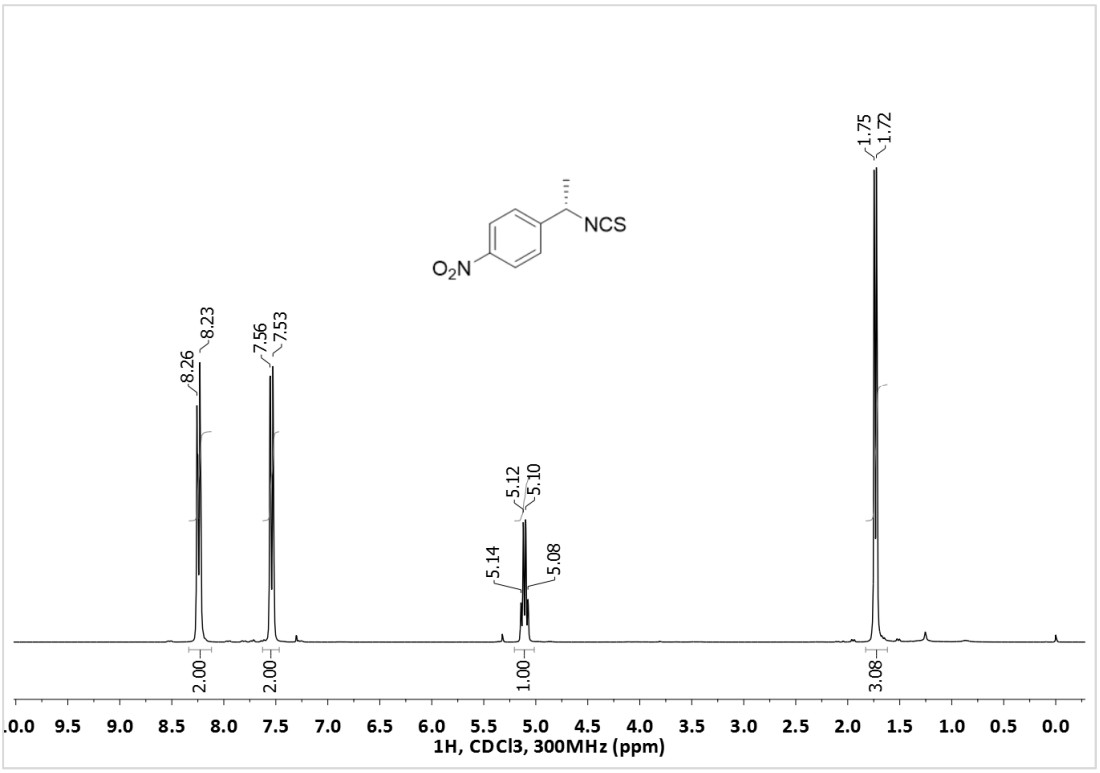
^{13}C NMR Spectrum (75 MHz) of **Ii**.



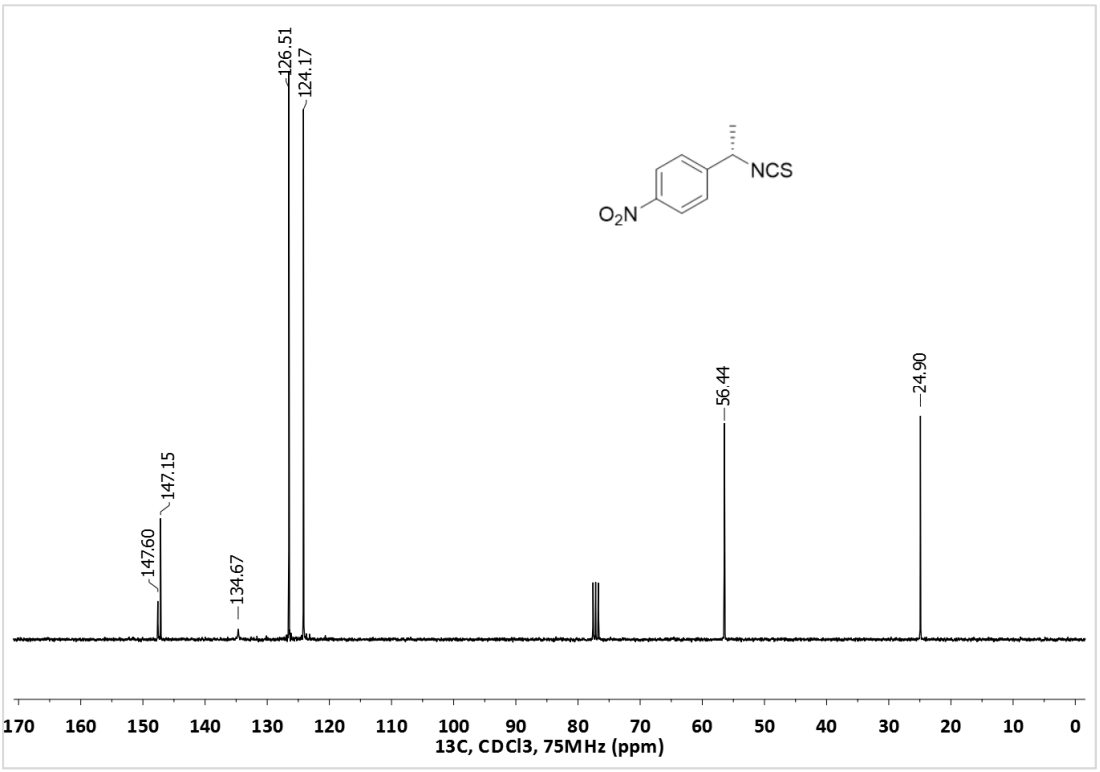
^{1}H NMR Spectrum (300 MHz) of **Ij**.



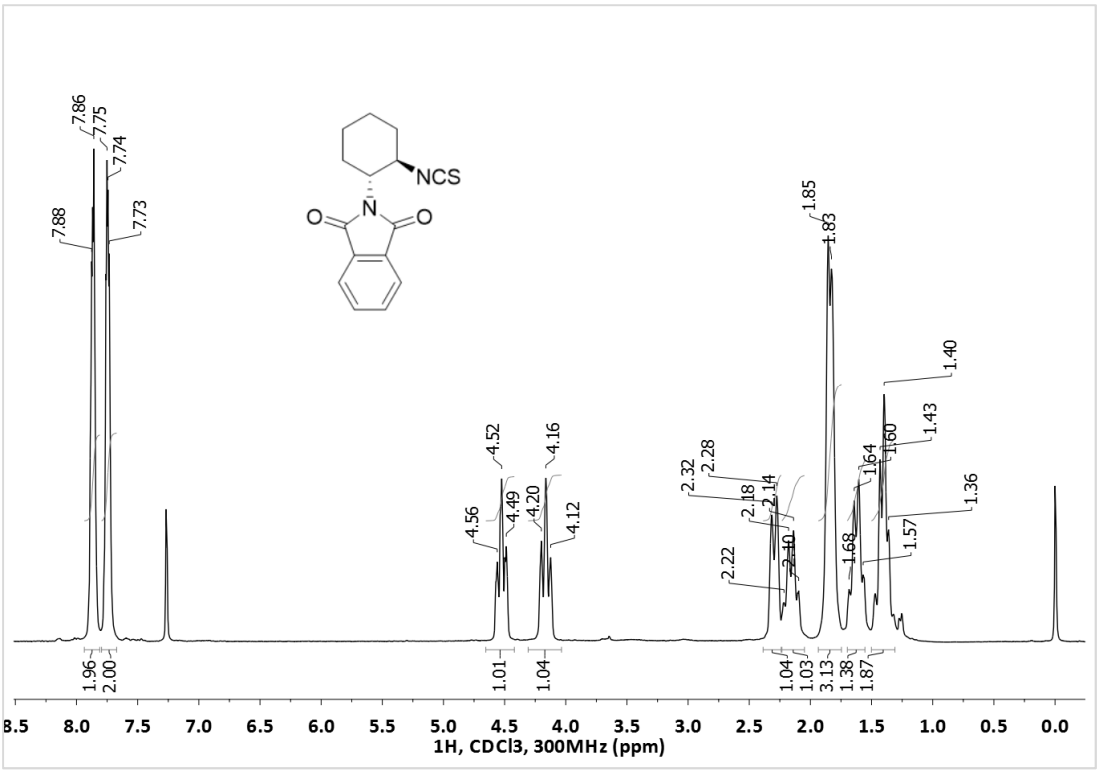
^{13}C NMR Spectrum (75 MHz) of **Ii**.



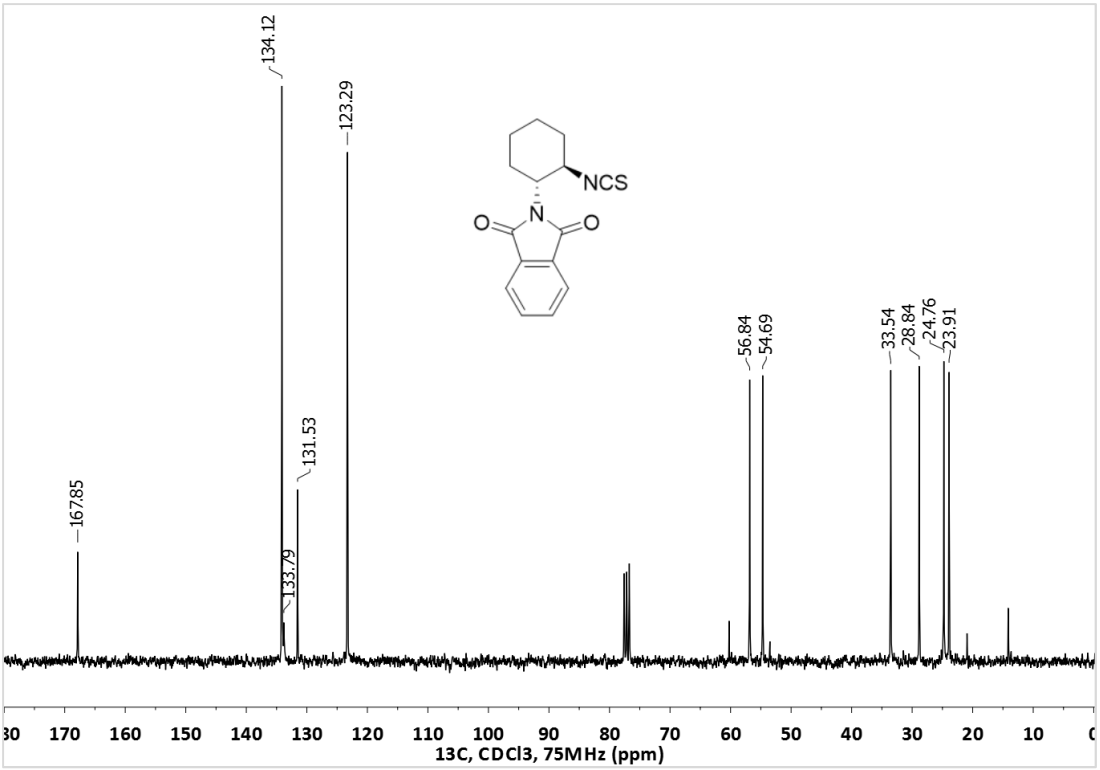
^{1}H NMR Spectrum (300 MHz) of **Ik**.



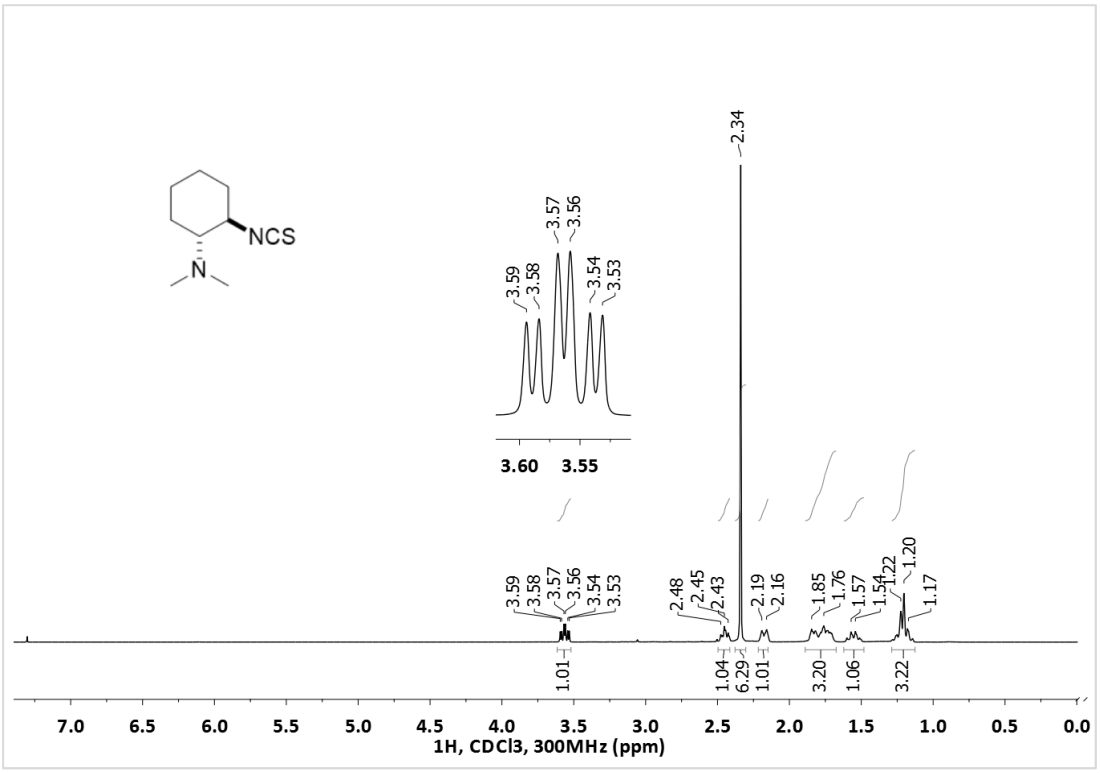
^{13}C NMR Spectrum (75 MHz) of **Ik**.



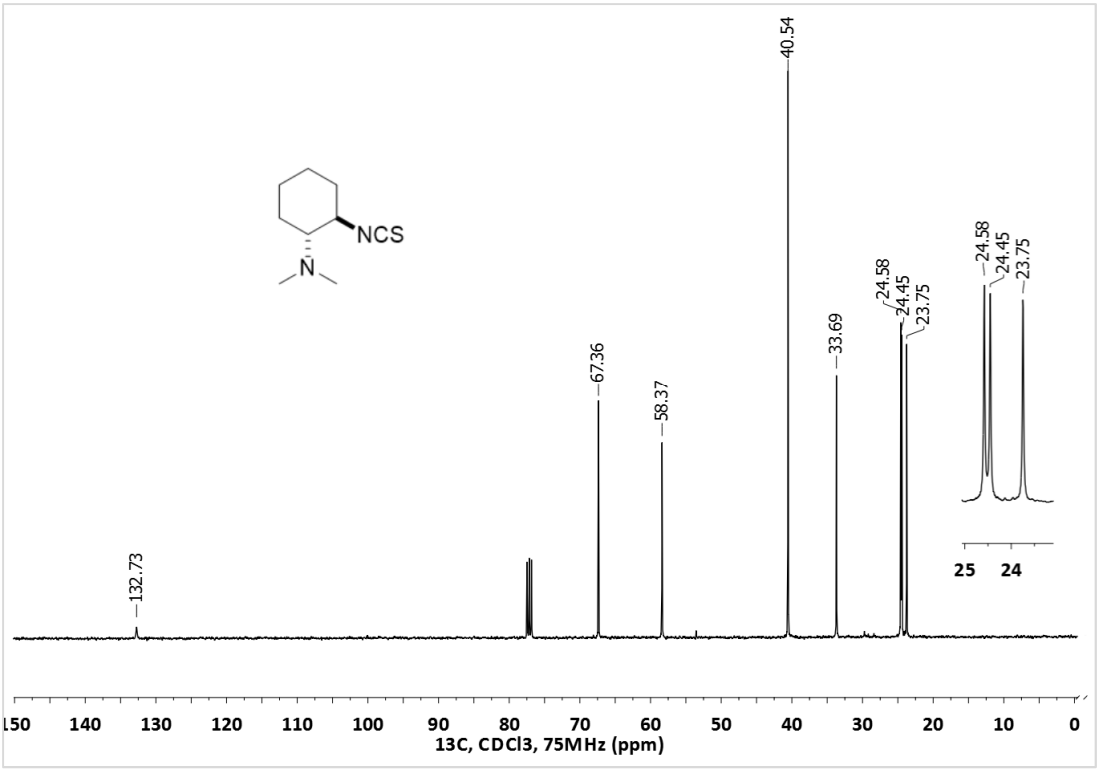
^{1}H NMR Spectrum (300 MHz) of **II**.



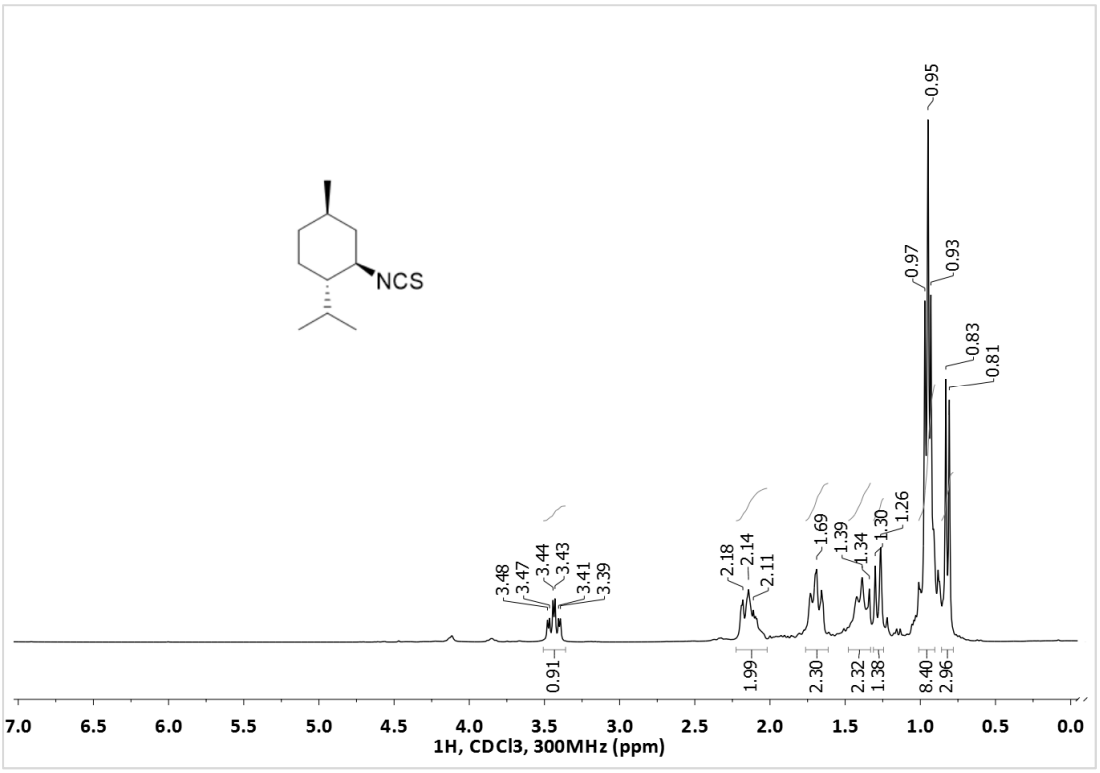
^{13}C NMR Spectrum (75 MHz) of **II**.



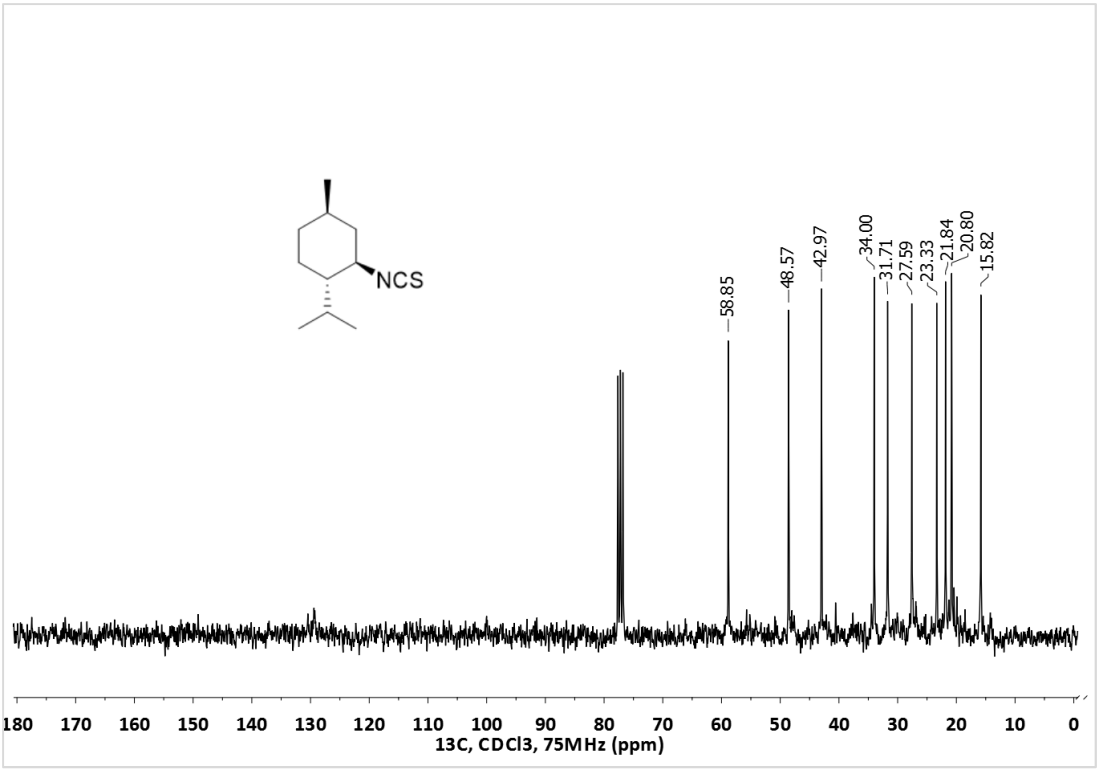
^{1}H NMR Spectrum (300 MHz) of **Im**.



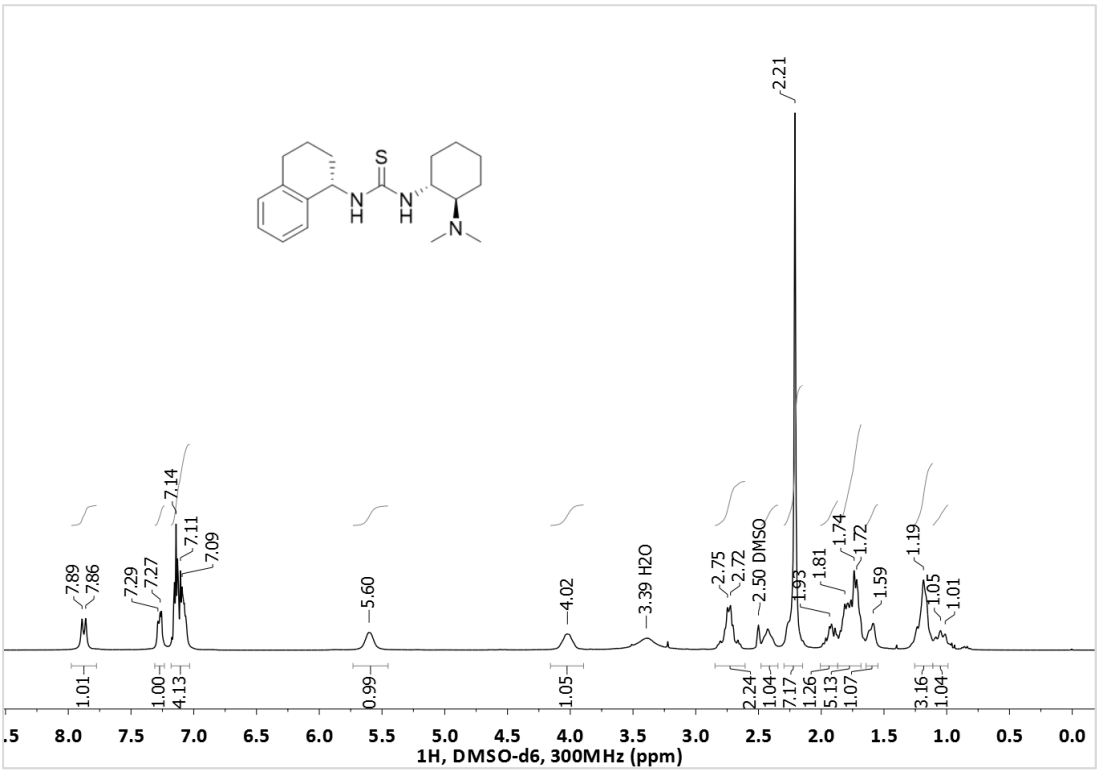
^{13}C NMR Spectrum (75 MHz) of **Im**.



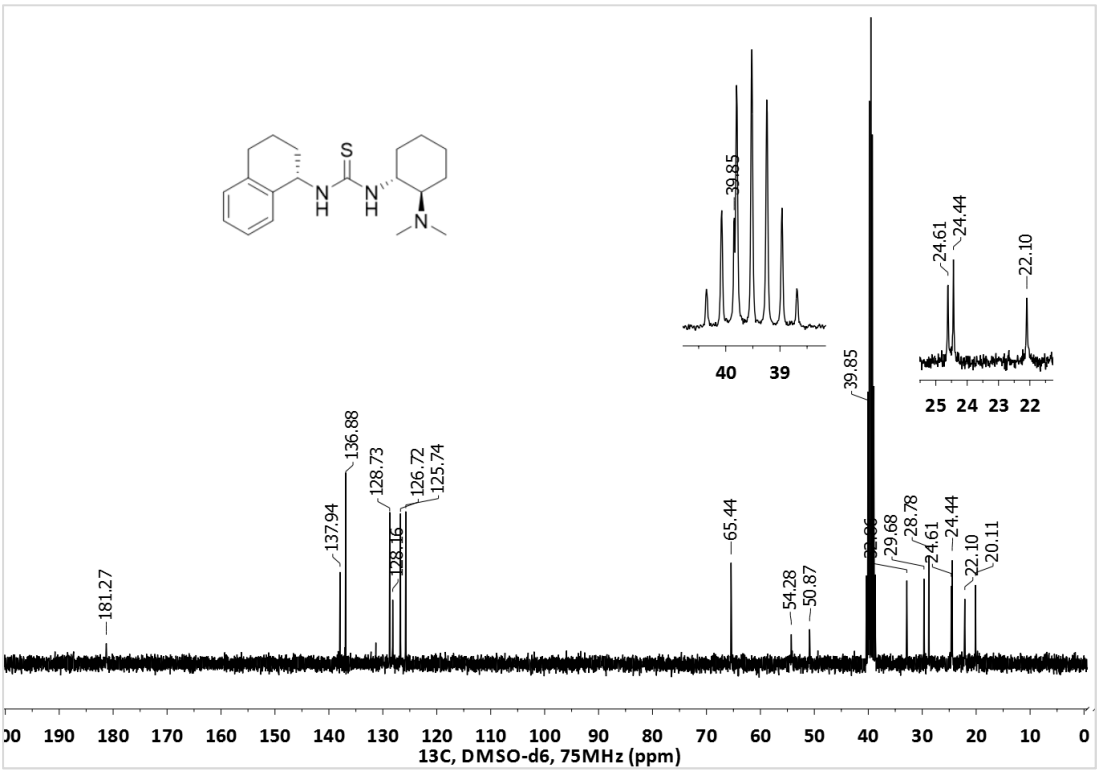
^{1}H NMR Spectrum (300 MHz) of **In**.



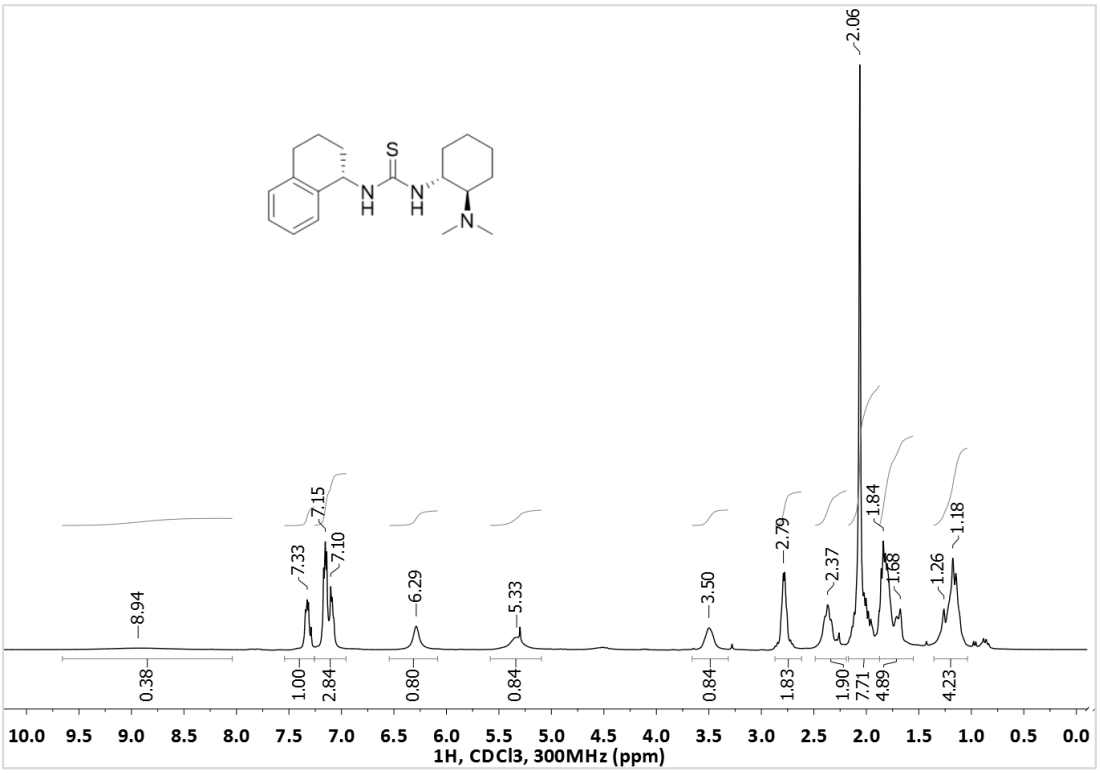
^{13}C NMR Spectrum (75 MHz) of **In**.



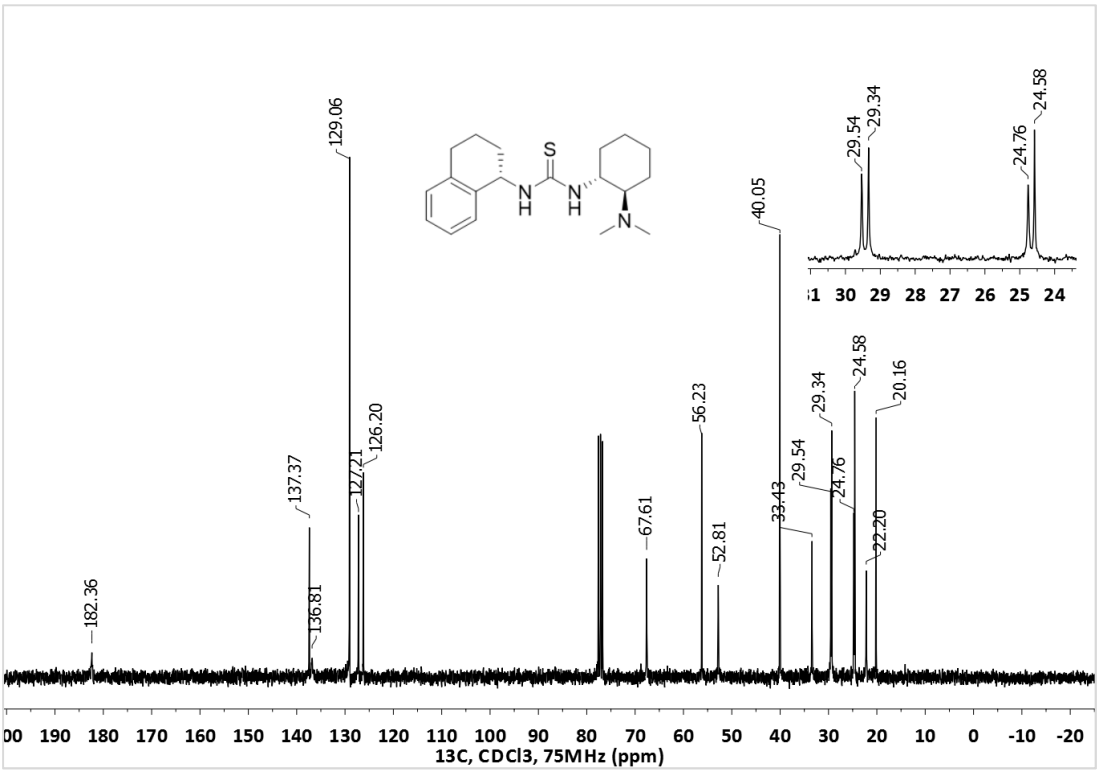
^{1}H NMR Spectrum (300 MHz) in DMSO-d_6 of **1i**.[13]



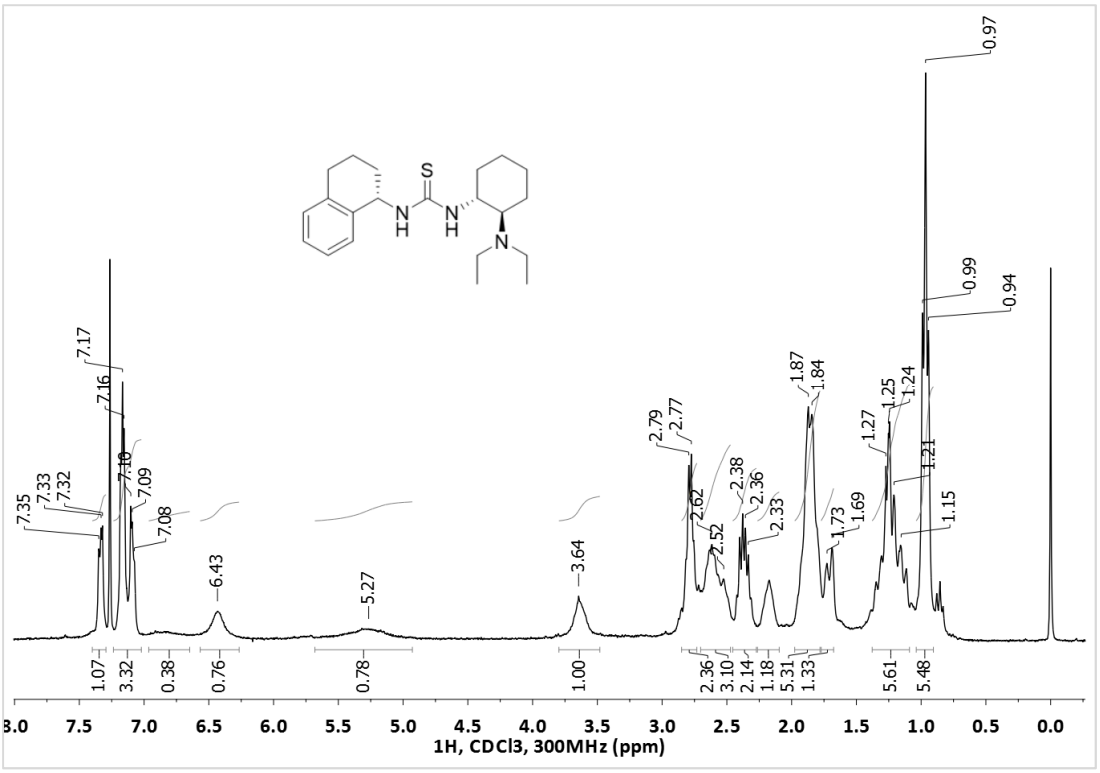
^{13}C NMR Spectrum (75 MHz) in DMSO-d_6 of **1i**.



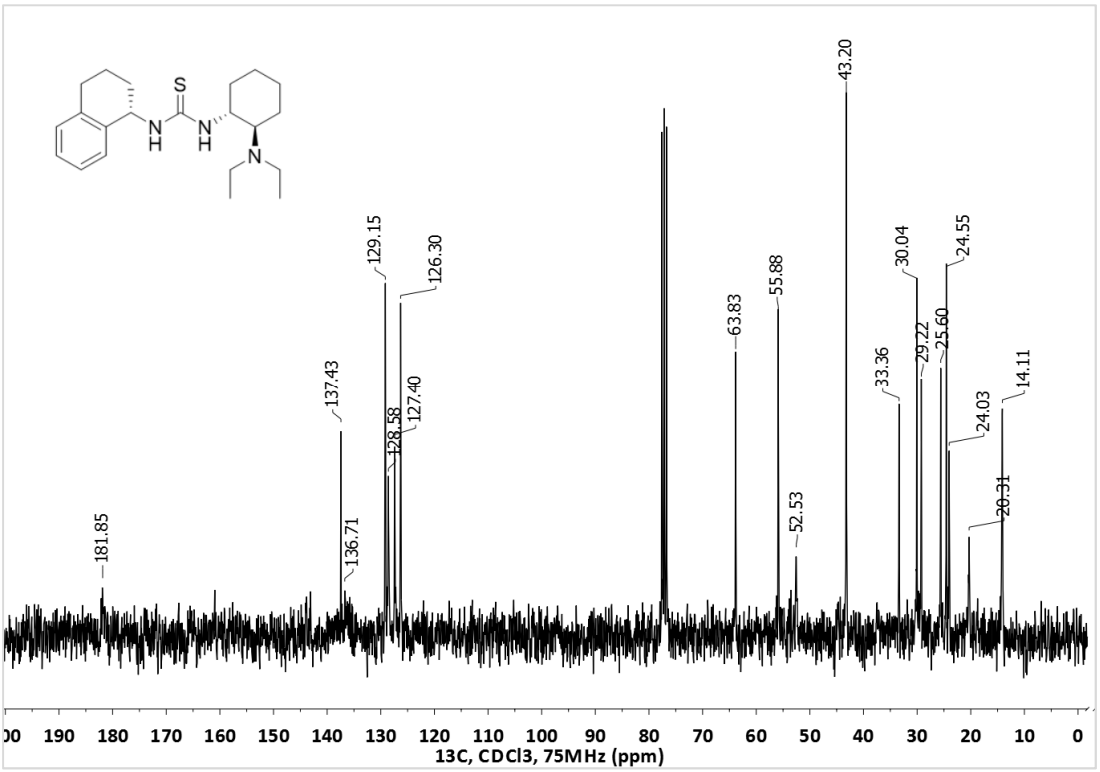
^{1}H NMR Spectrum (300 MHz) in $CDCl_3$ of **1i**.



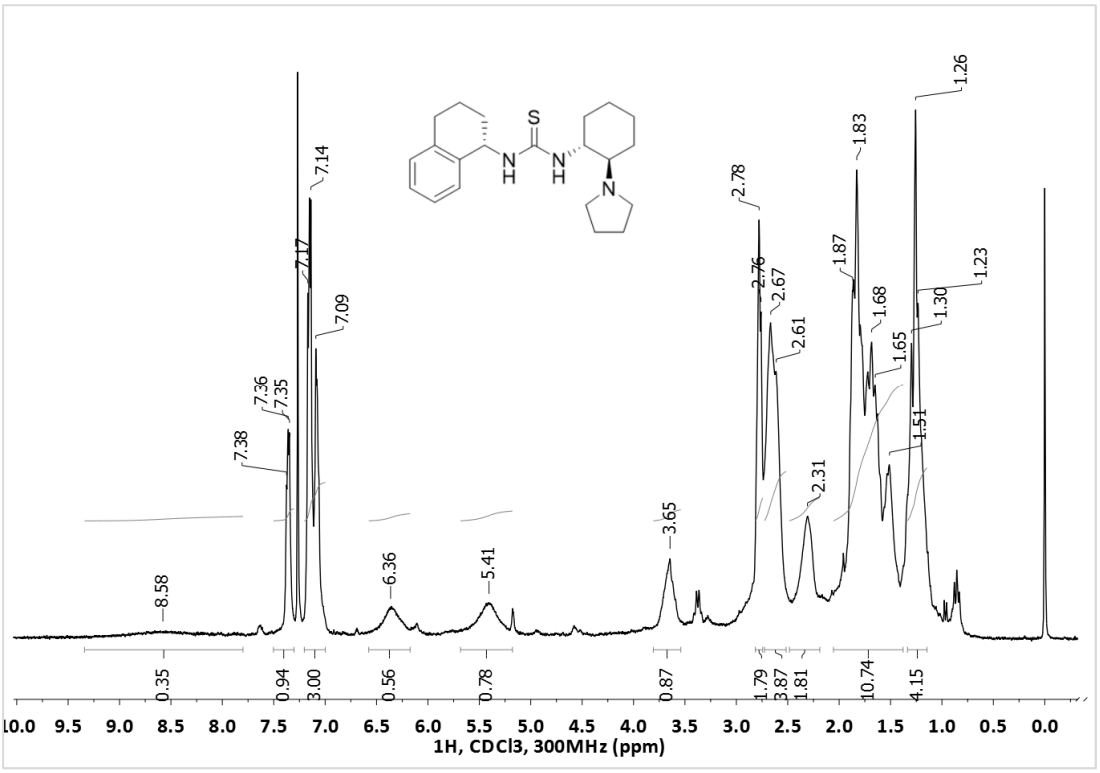
^{13}C NMR Spectrum (75 MHz) in $CDCl_3$ of **1i**.



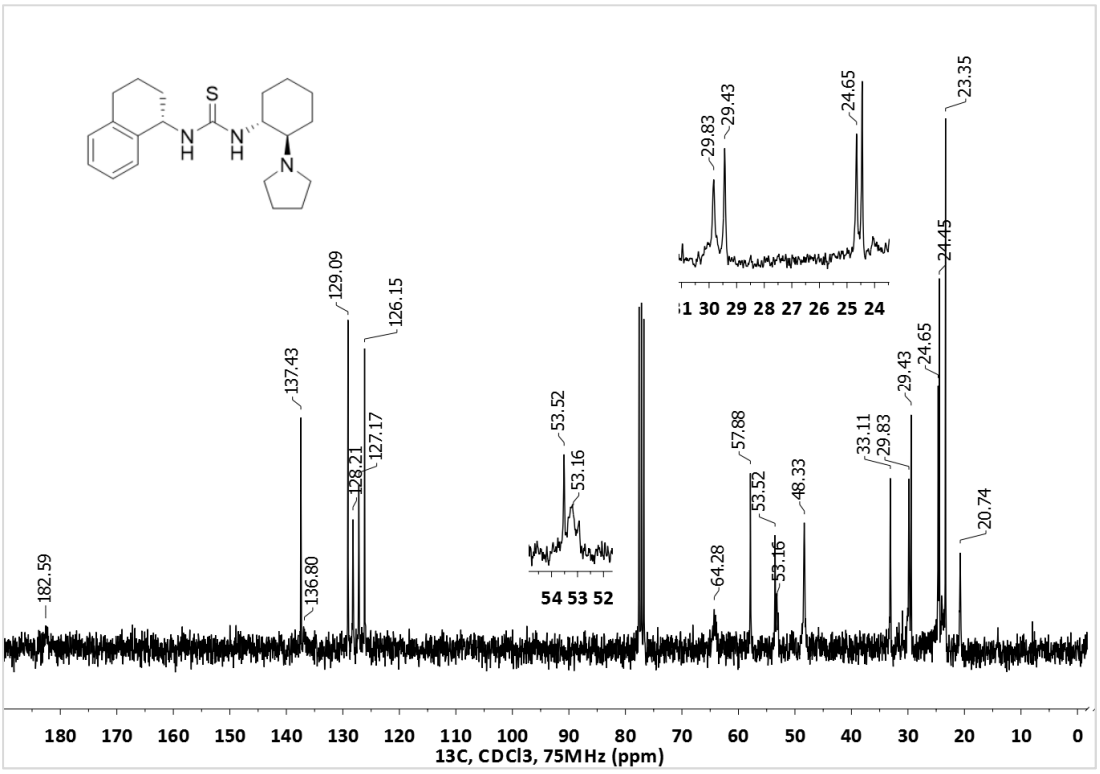
^{1}H NMR Spectrum (300 MHz) of **2a**.



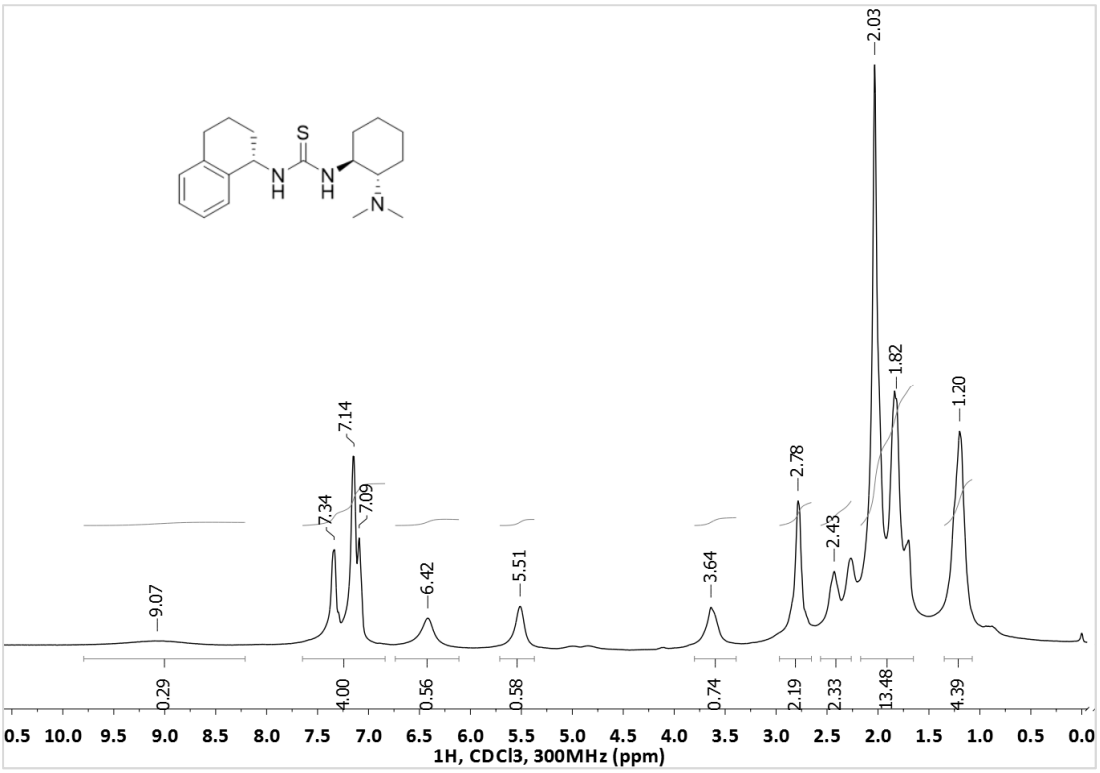
^{13}C NMR Spectrum (75 MHz) of **2a**.



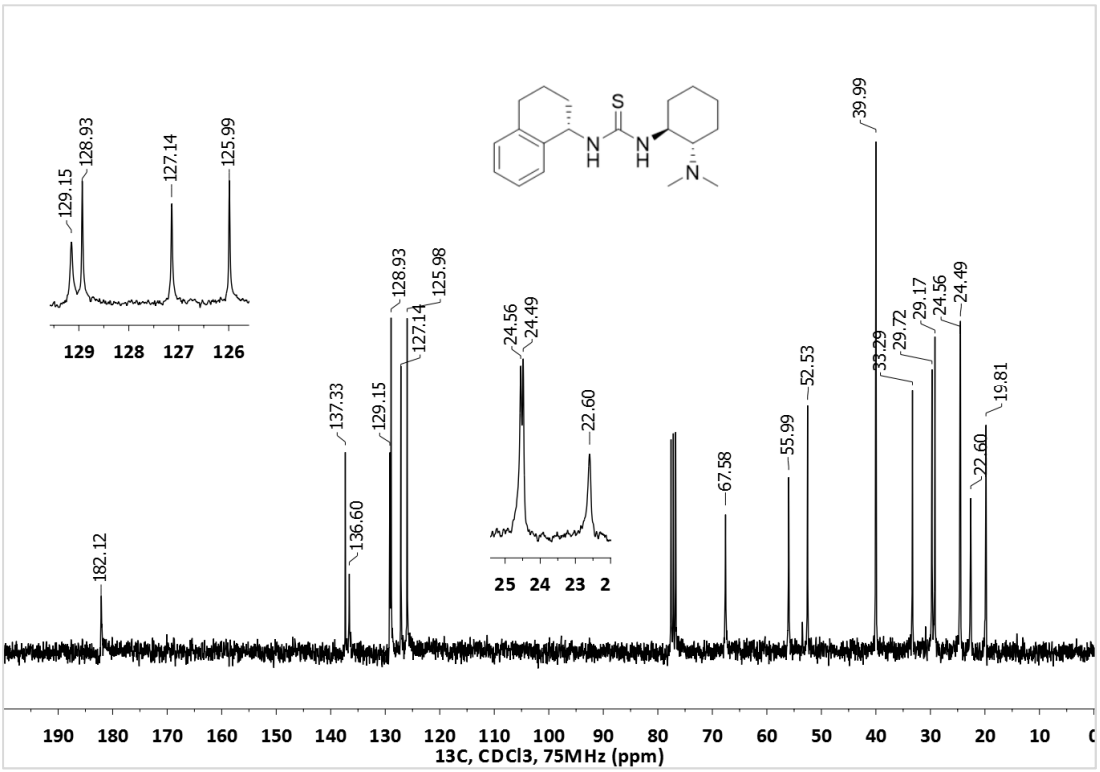
^{1}H NMR Spectrum (300 MHz) of **2b**.



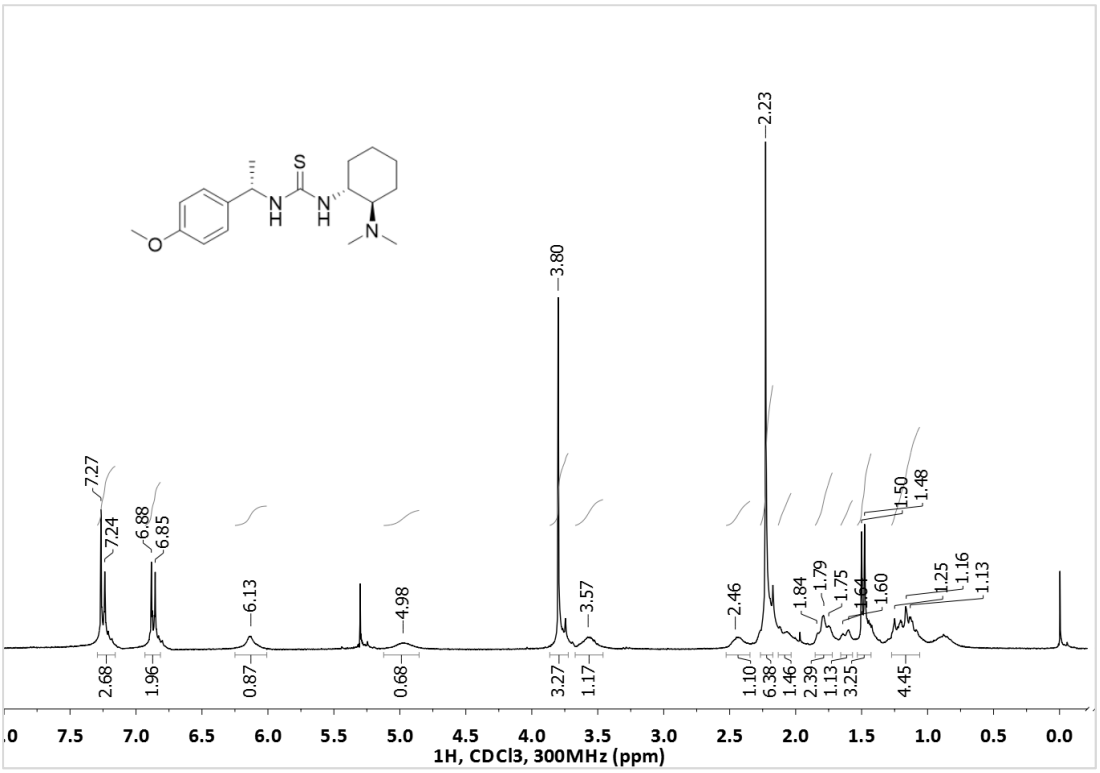
^{13}C NMR Spectrum (75 MHz) of **2b**.



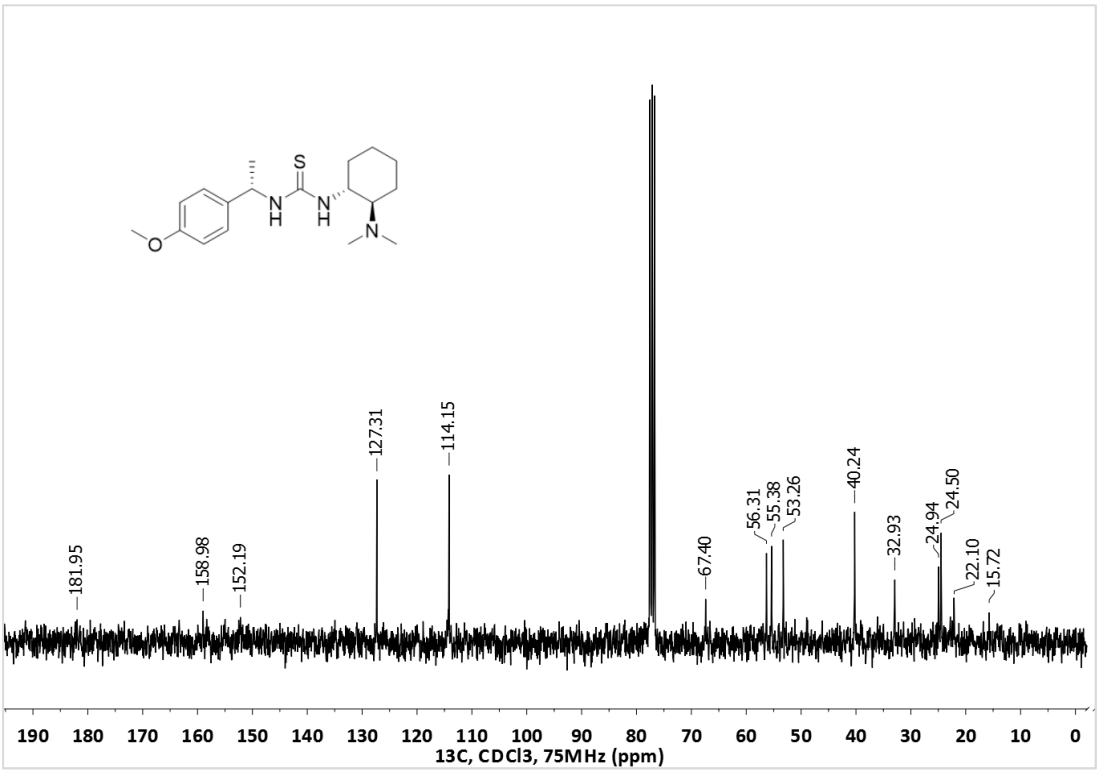
^{1}H NMR Spectrum (300 MHz) of **3**.



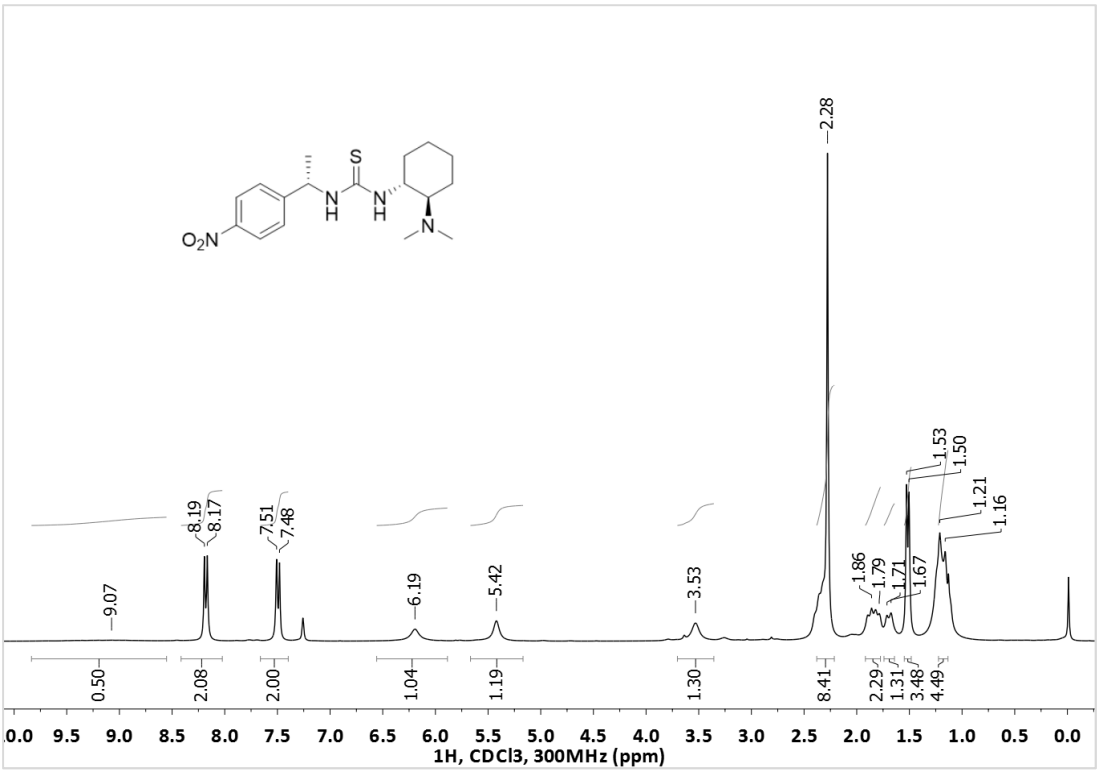
^{13}C NMR Spectrum (75 MHz) of **3**.



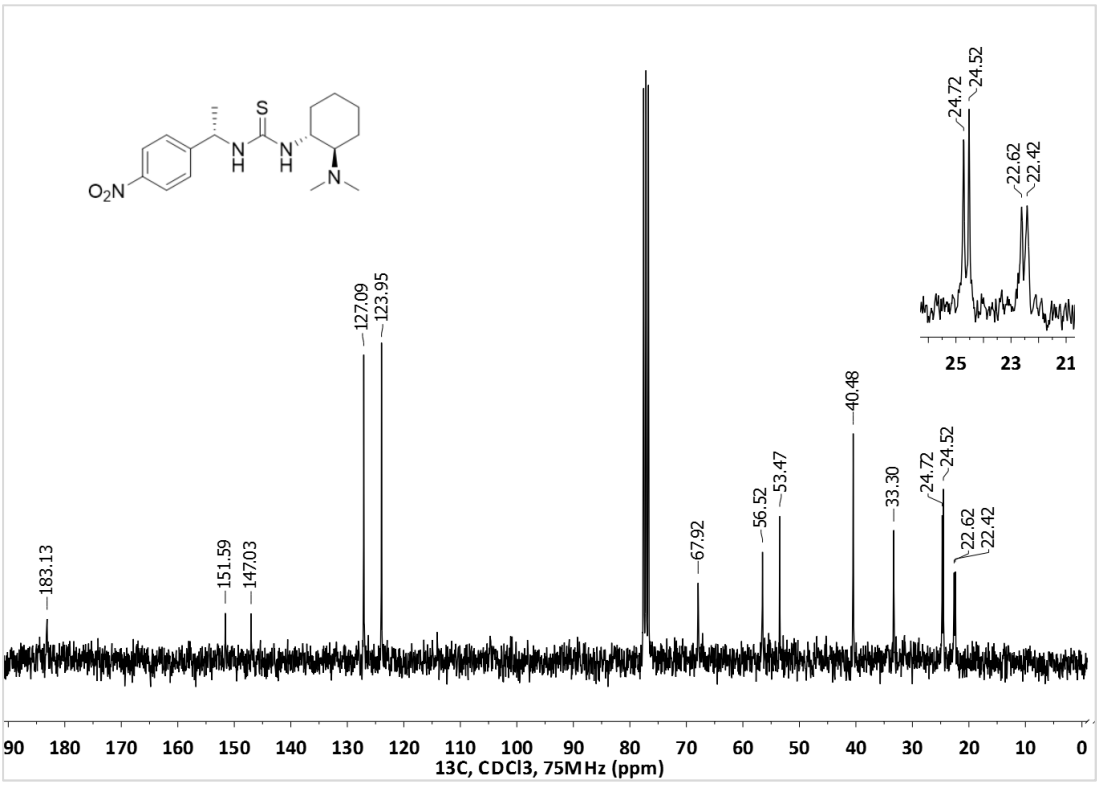
^{1}H NMR Spectrum (300 MHz) of **Tj**.



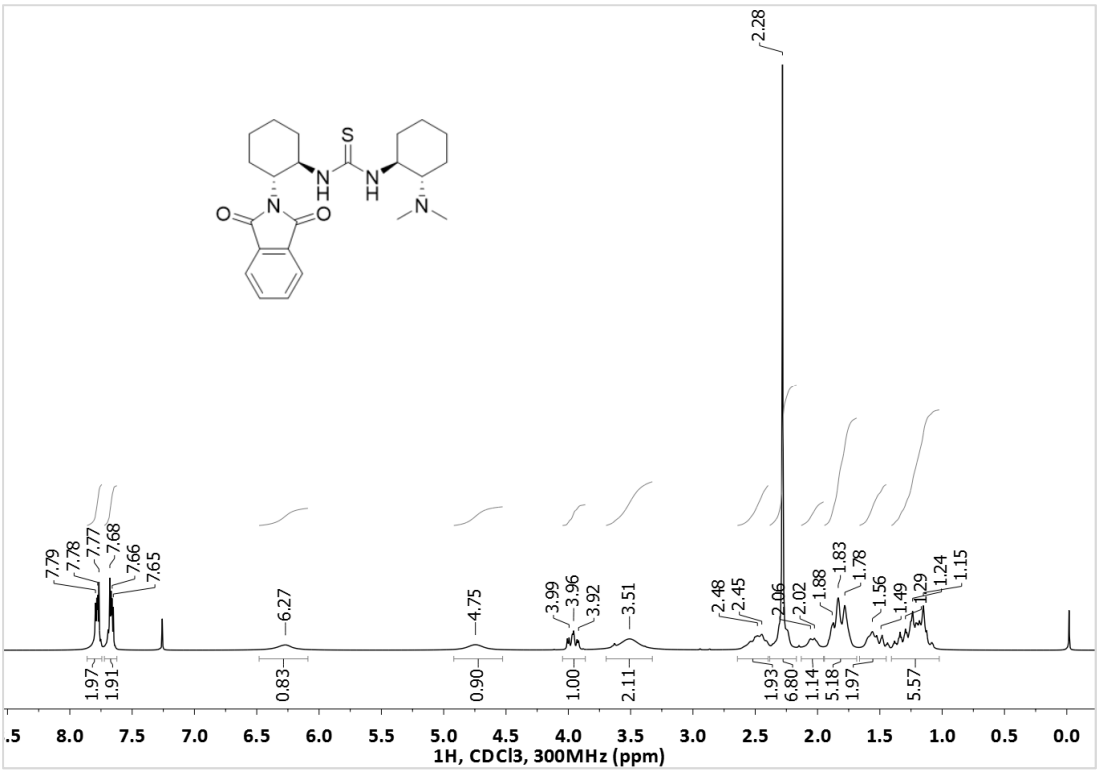
^{13}C NMR Spectrum (75 MHz) of **Tj**.



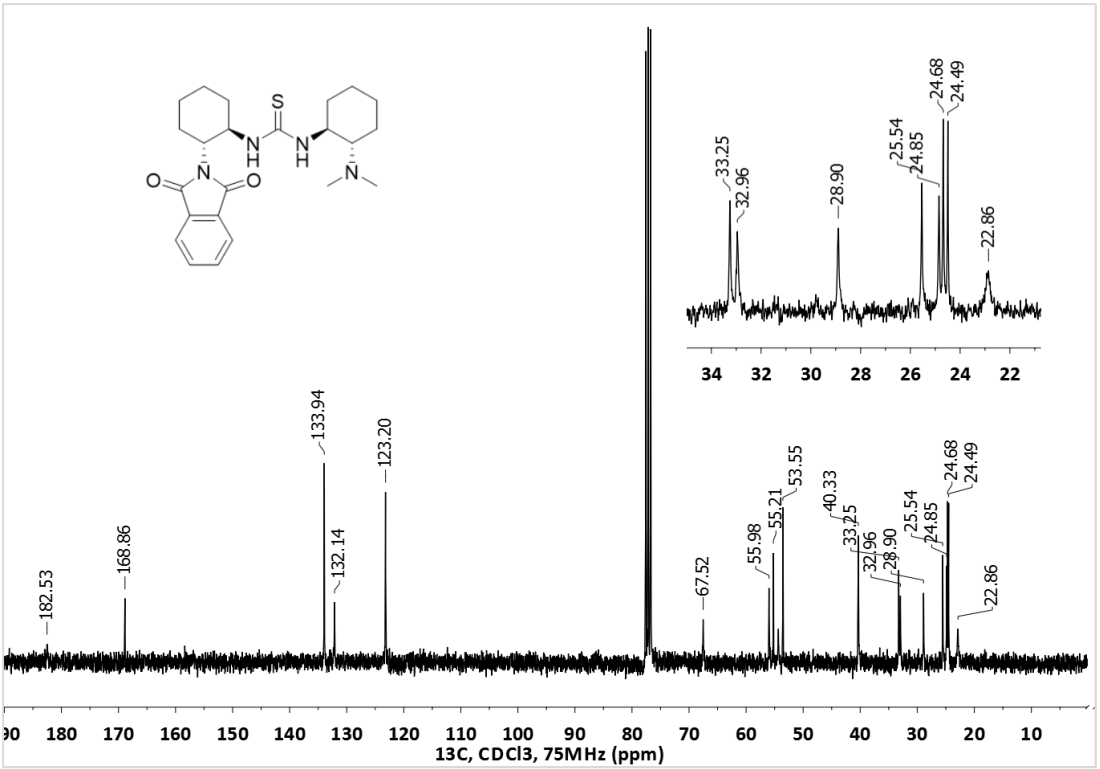
^{1}H NMR Spectrum (300 MHz) of **Tk**.



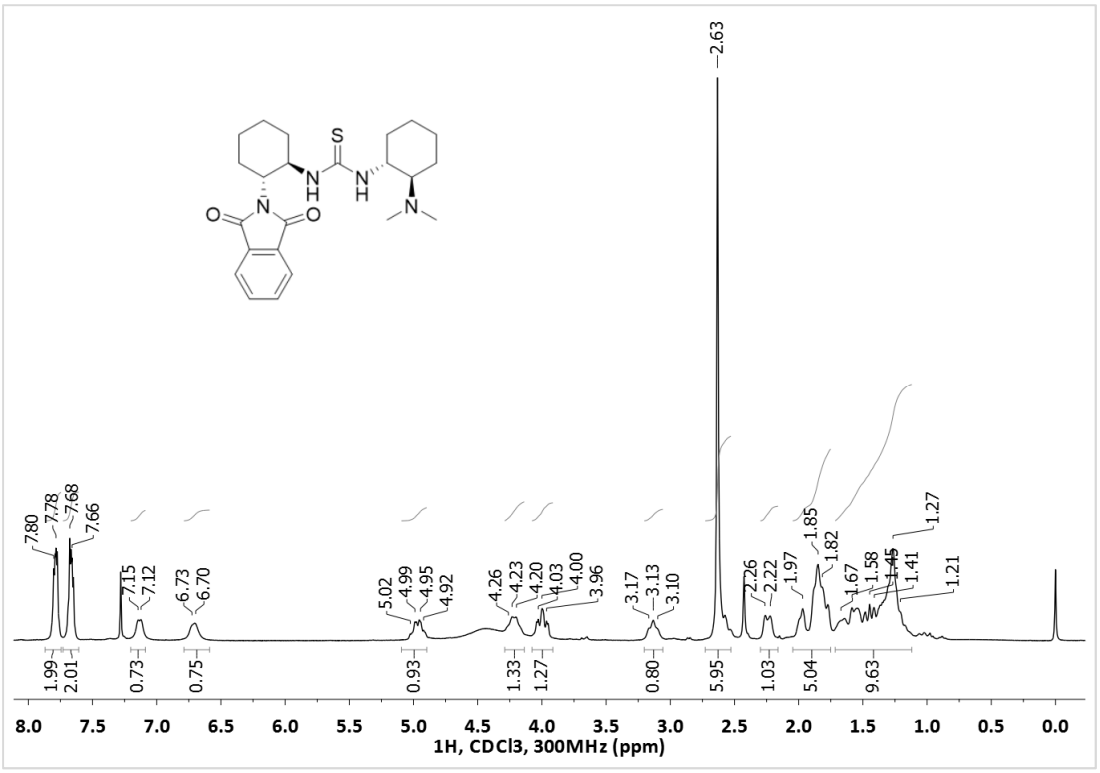
^{13}C NMR Spectrum (75 MHz) of **Tk**.



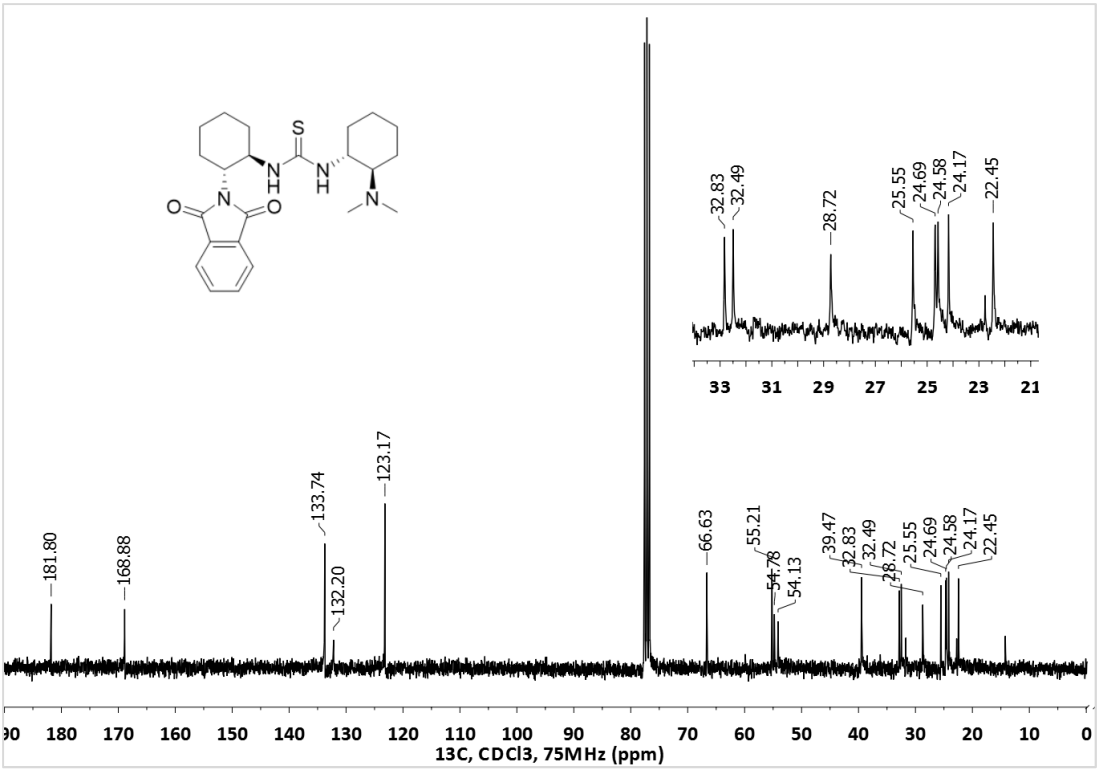
^{1}H NMR Spectrum (300 MHz) of (*R,R,S,S*)-**5**.



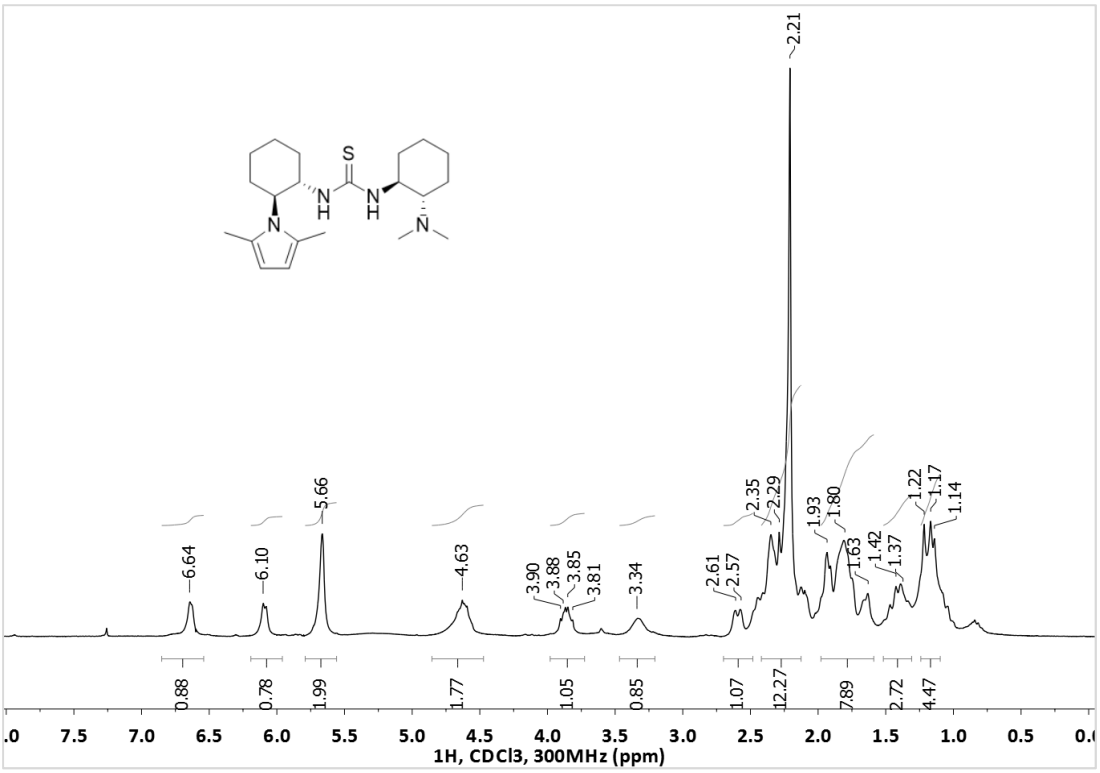
^{13}C NMR Spectrum (75 MHz) of (*R,R,S,S*)-**5**.



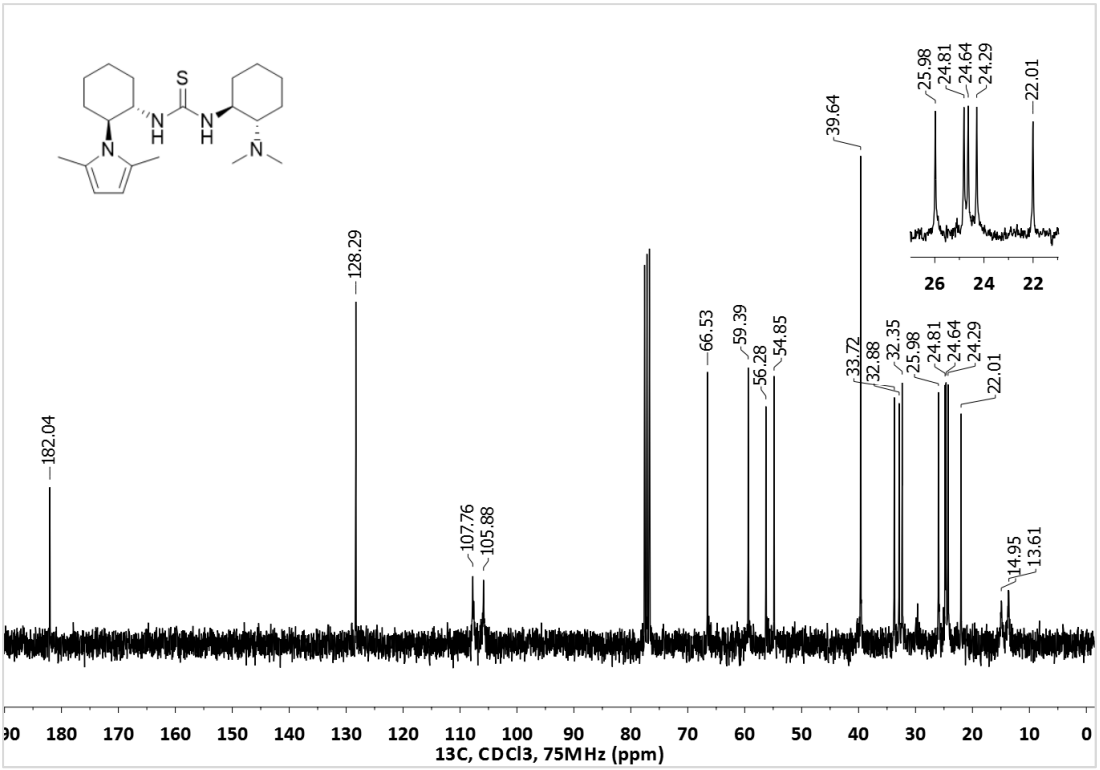
^{1}H NMR Spectrum (300 MHz) of (*R,R,R,R*)-**5**.



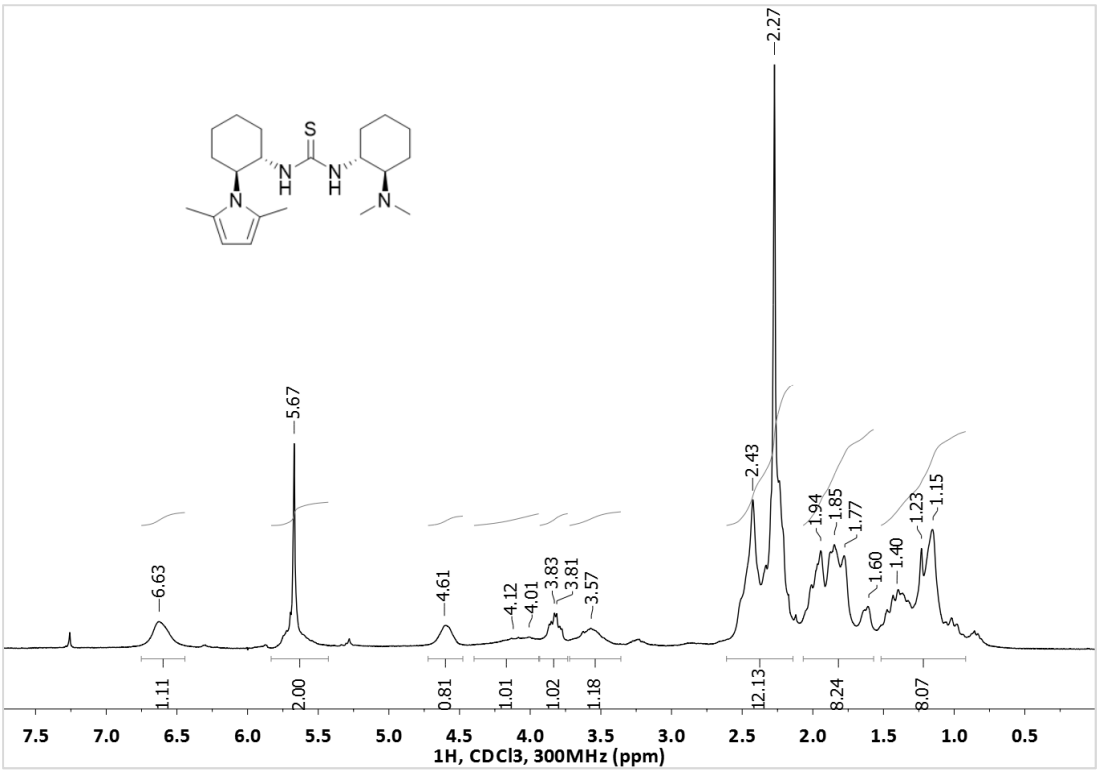
^{13}C NMR Spectrum (75 MHz) of (*R,R,R,R*)-**5**.



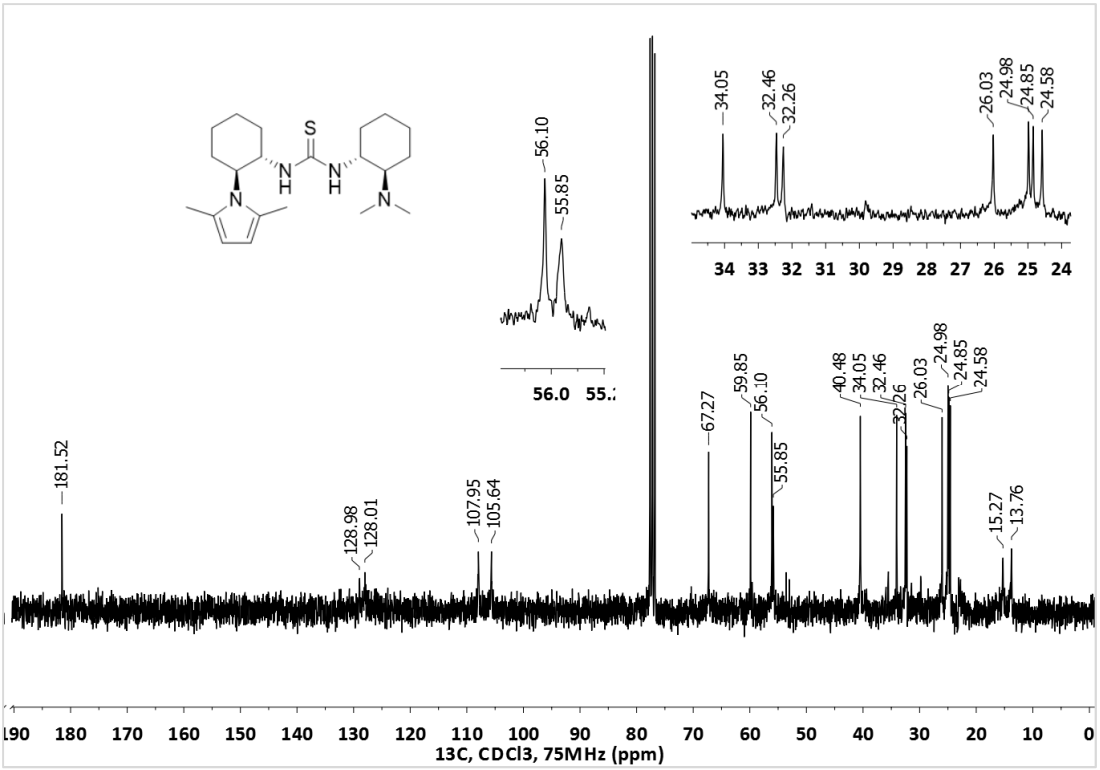
^{1}H NMR Spectrum (300 MHz) of (*S,S,S,S*)-**6**.



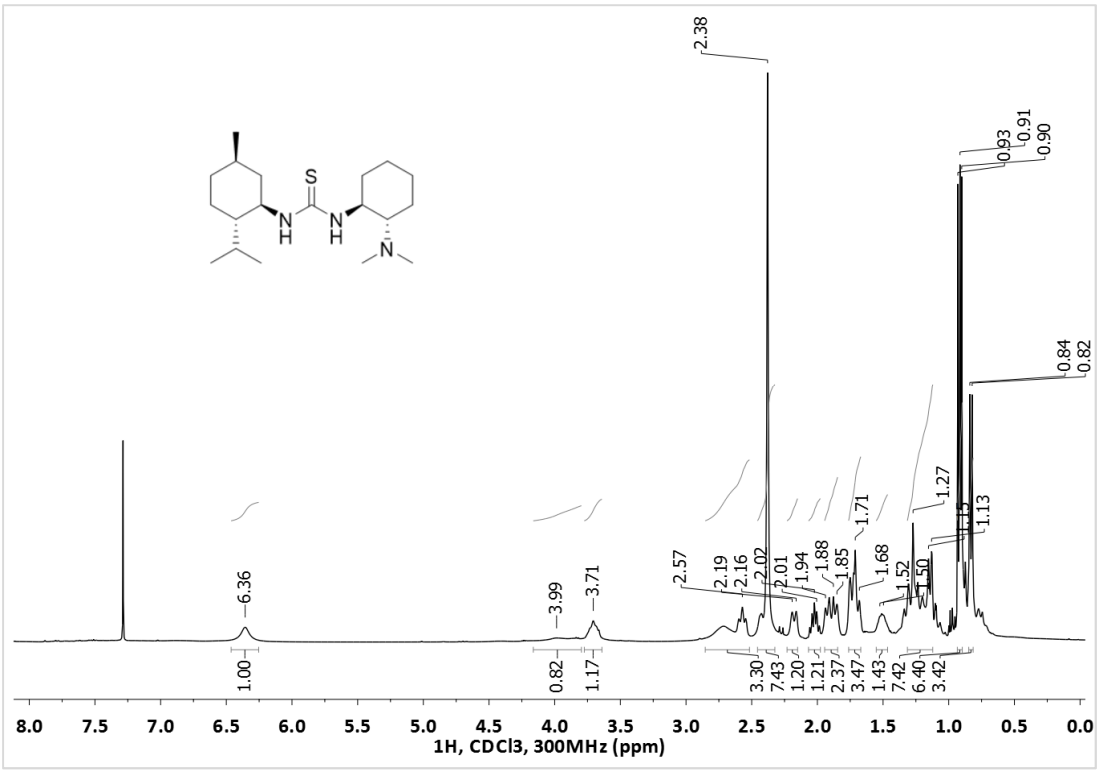
^{13}C NMR Spectrum (75 MHz) of (*S,S,S,S*)-**6**.



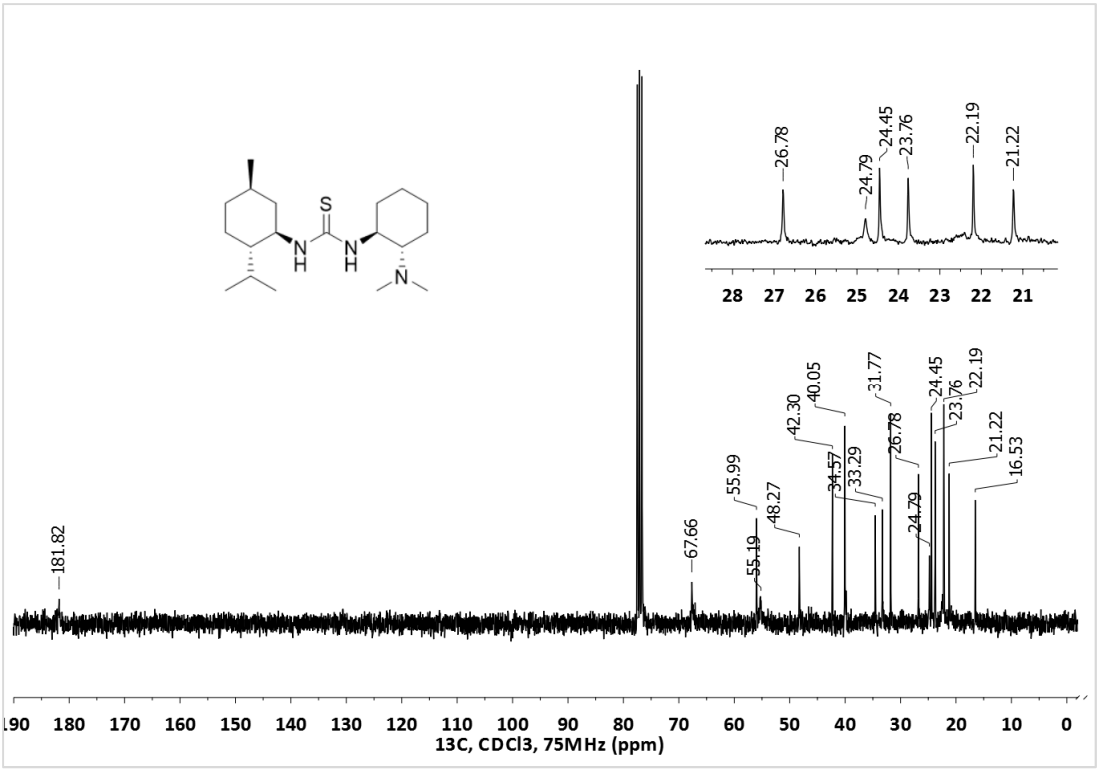
^{1}H NMR Spectrum (300 MHz) of (*S,S,R,R*)-**6**.



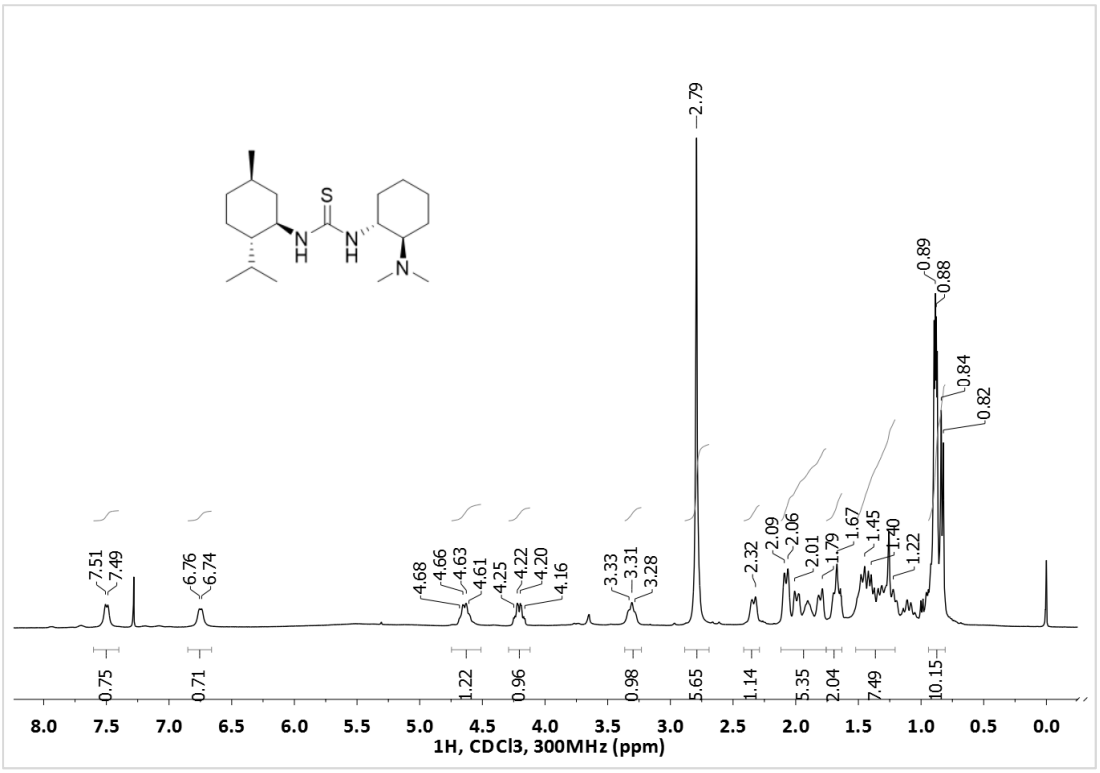
^{13}C NMR Spectrum (75 MHz) of (*S,S,R,R*)-**6**.



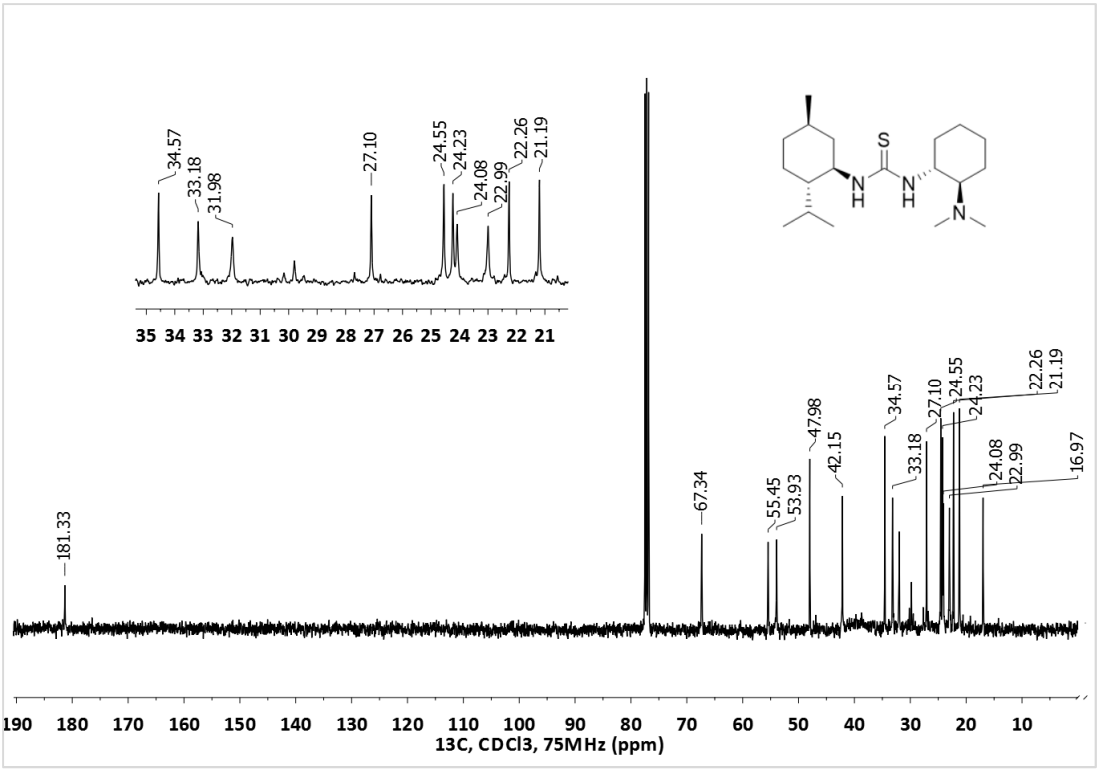
^{1}H NMR Spectrum (300 MHz) of (*R,S,R,S,S*)-**7**.



^{13}C NMR Spectrum (75 MHz) of (*R,S,R,S,S*)-**7**.



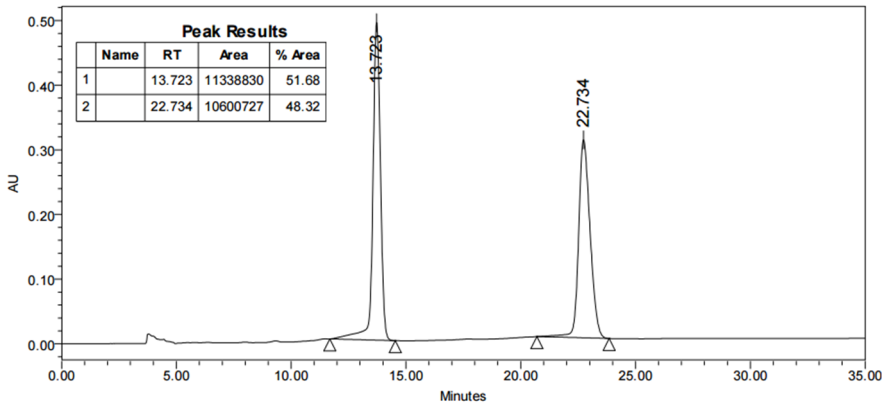
^{1}H NMR Spectrum (300 MHz) of (*R,S,R,R,R*)-**7**.



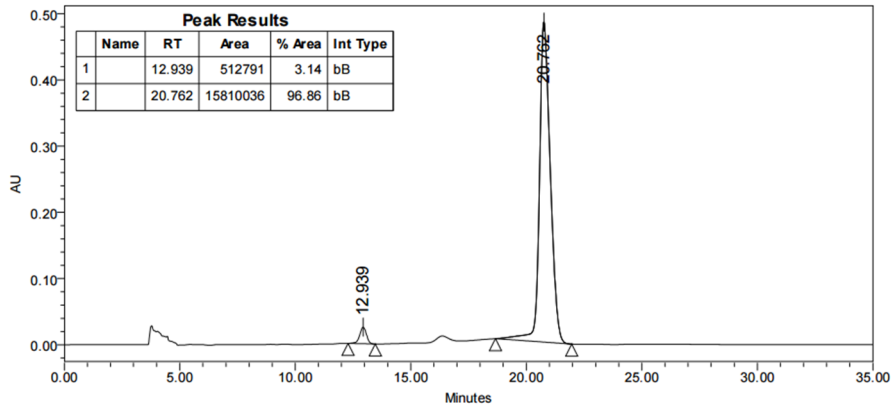
^{13}C NMR Spectrum (75 MHz) of (*R,S,R,R,R*)-**7**.

Selected CSP-HPLC traces

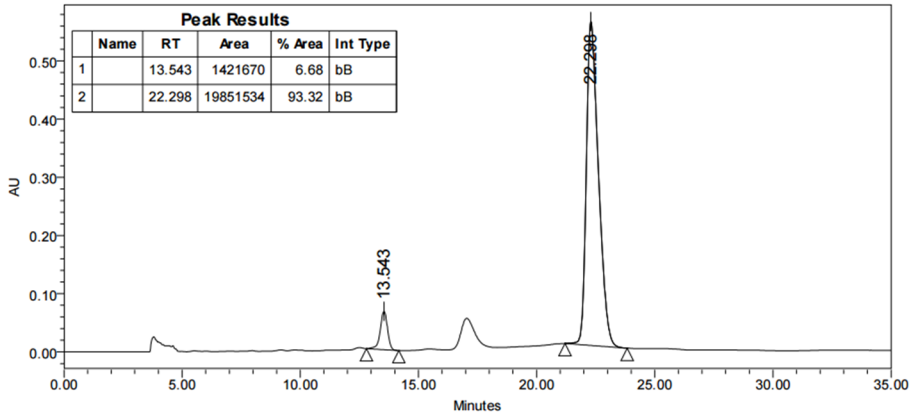
Compound **4a**. HPLC: Chiralpak IA, hexane/ethanol 85/15, 0.8 mL/min, λ = 220 nm, retention times 13.7 min (S), 22.7 min (R).



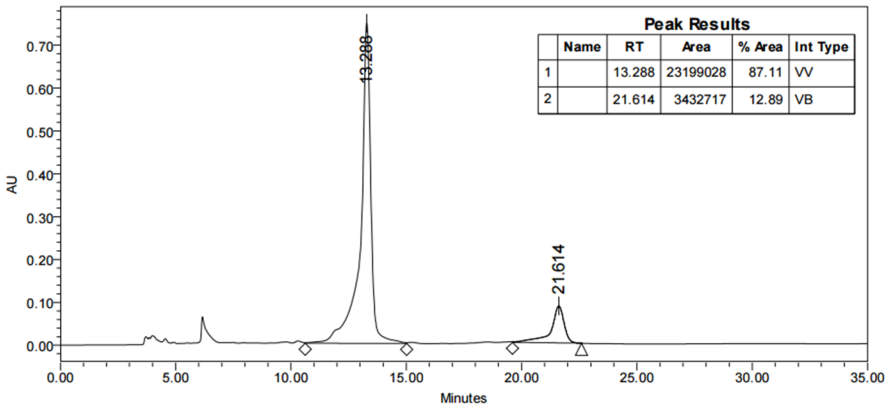
Racemic (**Table 3** of the body of the article).



With catalyst **1i** (**Table 3, entry 1** of the body of the article).

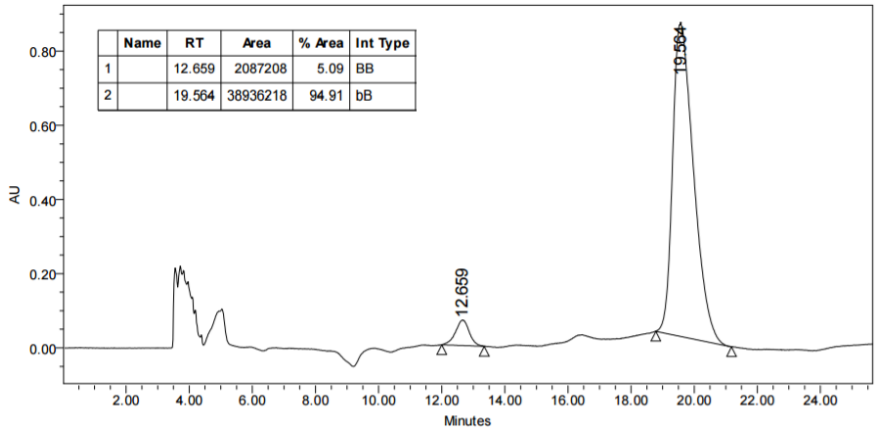


With catalyst **2b** (**Table 3, entry 3** of the body of the article).

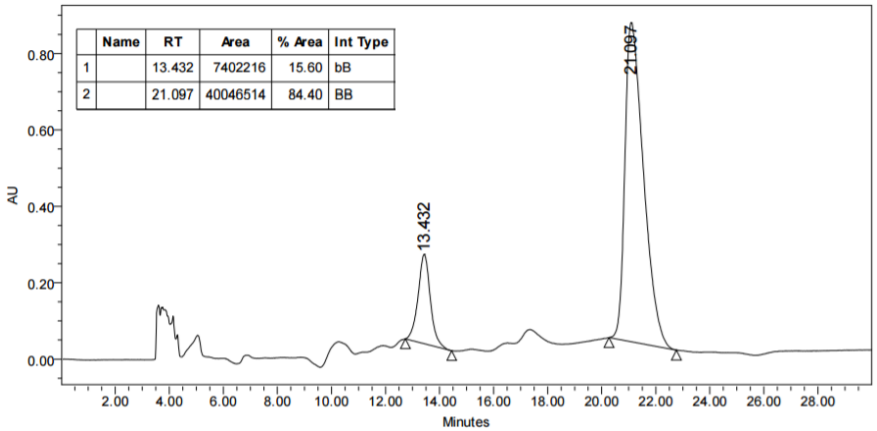


With catalyst **3** (**Table 3, entry 4** of the body of the article).

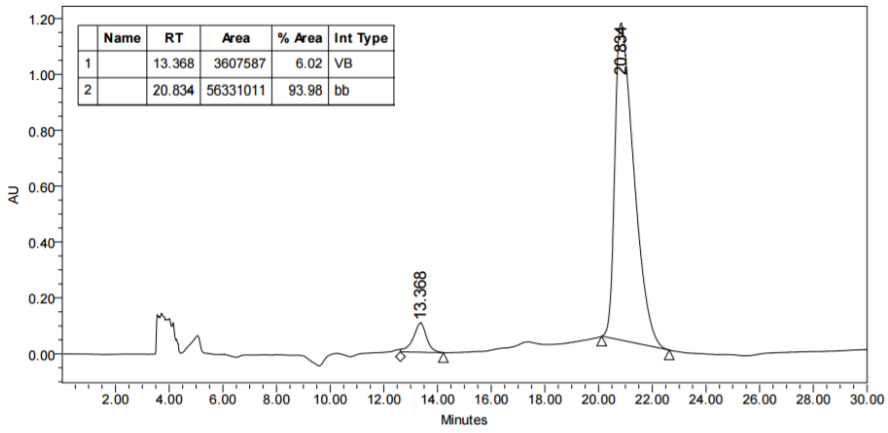
Compound **4a**. HPLC: Chiralpak IA, hexane/ethanol 85/15, 0.8 mL/min, λ = 220 nm, retention times 12.6 min (S), 19.5 min (R).



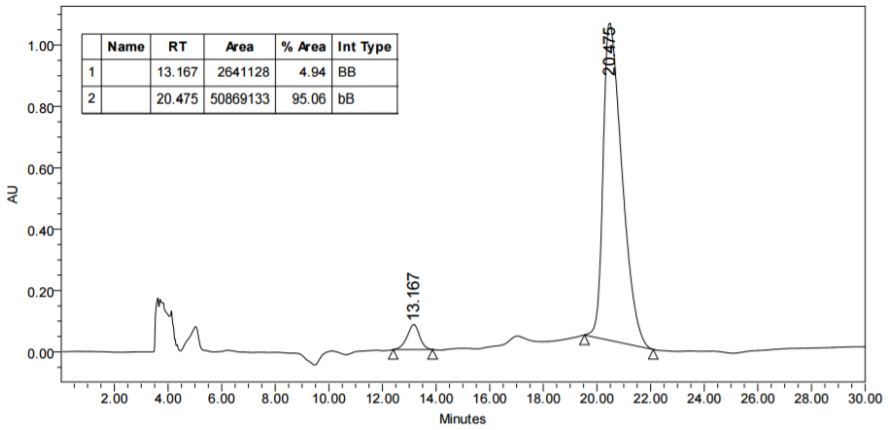
With catalyst **1i** (**Table 4, entry 4** of the body of the article).



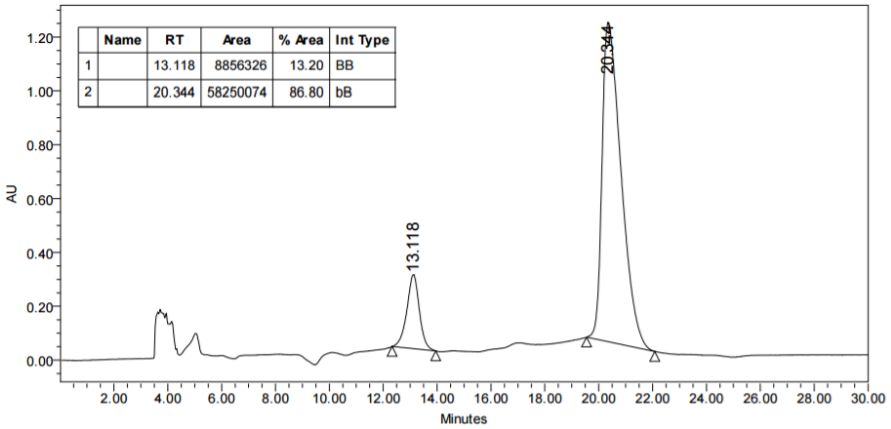
With catalyst **1i** (**Table 4, entry 6** of the body of the article).



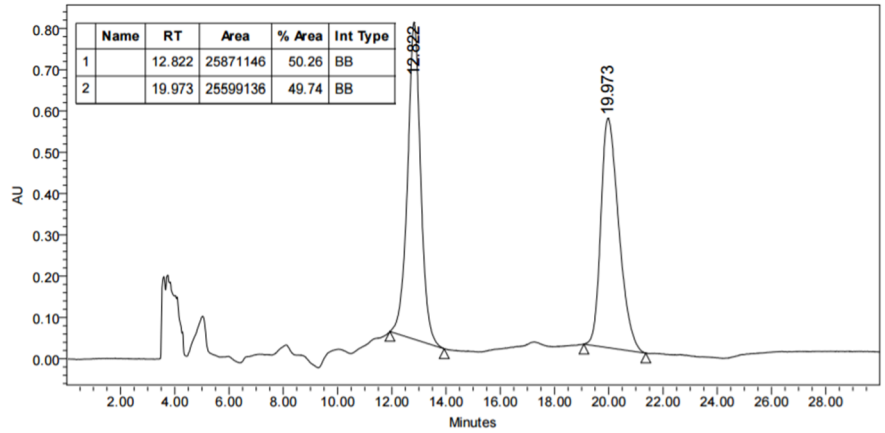
With catalyst **1i** (**Table 4, entry 7** of the body of the article).



With catalyst **1i** (**Table 4, entry 10** of the body of the article).

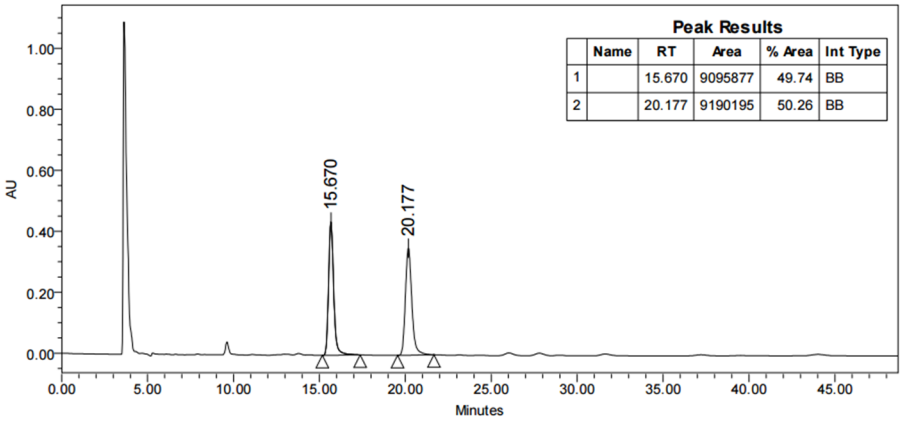


With catalyst **1i** (**Table 4, entry 12** of the body of the article).

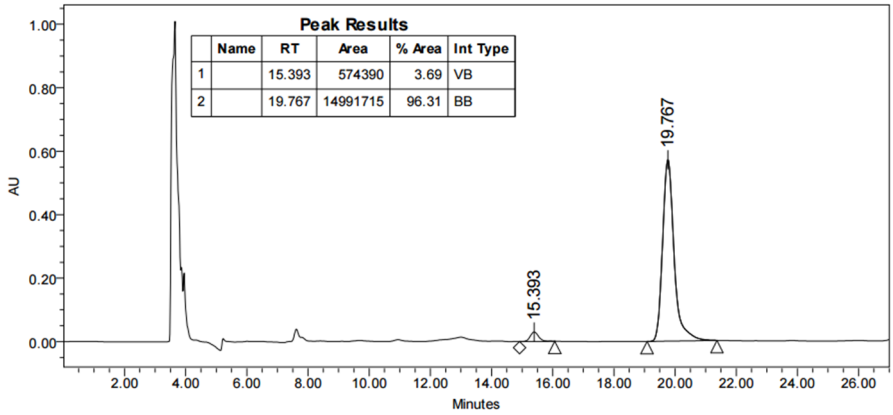


With catalyst **1i** (**Table 4, entry 15** of the body of the article).

Compound **4b**. HPLC: Chiralpak IC3, hexane/ethanol 85/15, 0.6 mL/min, λ = 250 nm, retention times 15.6 min (S), 20.1 (R).

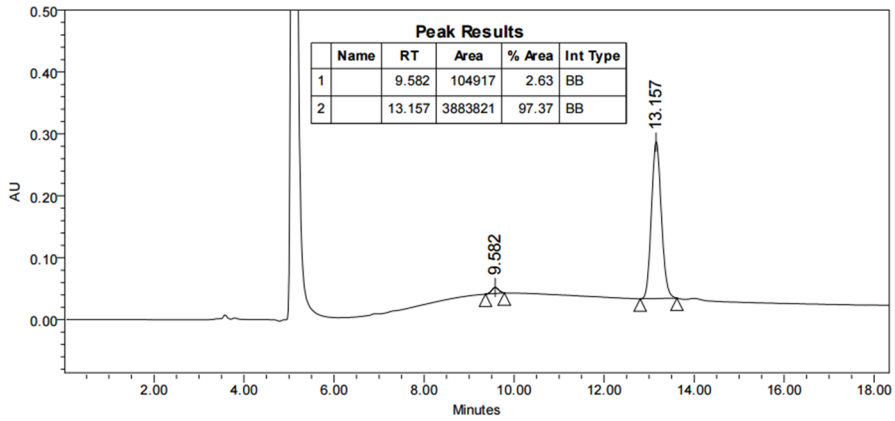


Racemic (**Table 5**).



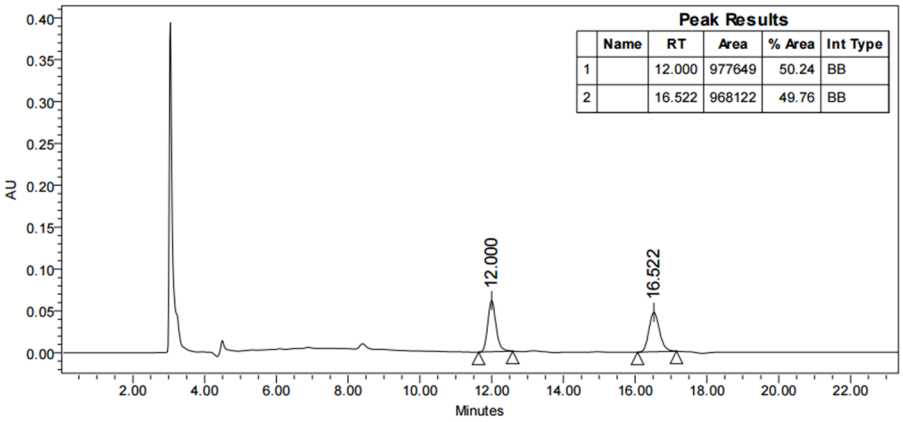
With catalyst **1i** (**Table 5, entry 1** of the body of the article).

Compound **4c**. HPLC: Chiralpak IC3, hexane/ethanol 85/15, 0.6 mL/min, λ = 220 nm, retention times 9.5 min (S), 13.1 (R).

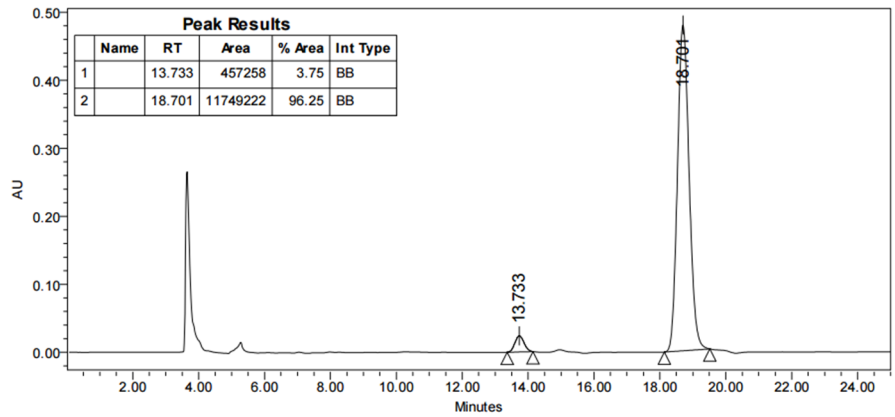


With catalyst **Ia** (**Table 5, entry 2** of the body of the article).

Compound **4d**. HPLC: Chiralpak IC3, hexane/ethanol 85/15, 0.6 mL/min, λ = 254 nm, retention times 12.0 min (S), 16.5 min (R).

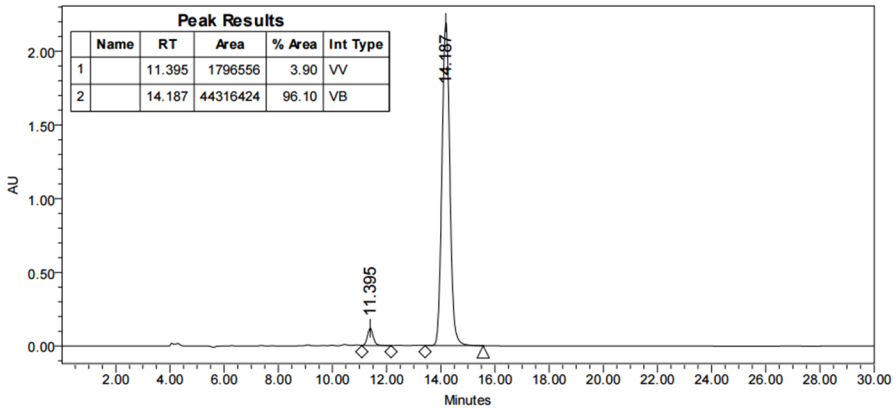


Racemic (**Table 5** of the body of the article).



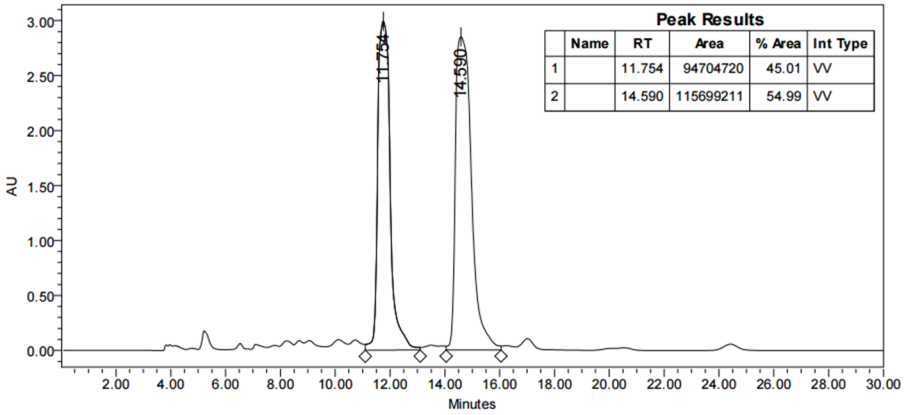
With catalyst **1i** (**Table 5, entry 3** of the body of the article).

Compound **4f**. HPLC: Chiralpak IA, hexane/ethanol 85/15, 0.8 mL/min, λ = 220 nm, retention times 11.3 min (S), 14.1 (R).

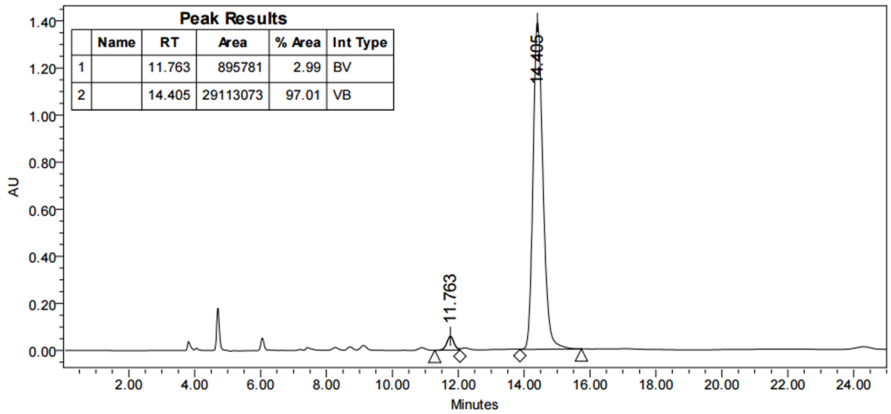


With catalyst **1i** (**Table 5, entry 5** of the body of the article).

Compound **4g**. HPLC: Chiralpak IA, hexane/ethanol 85/15, 0.8 mL/min, λ = 220 nm, retention times 11.7 min (S), 14.5 min (R).

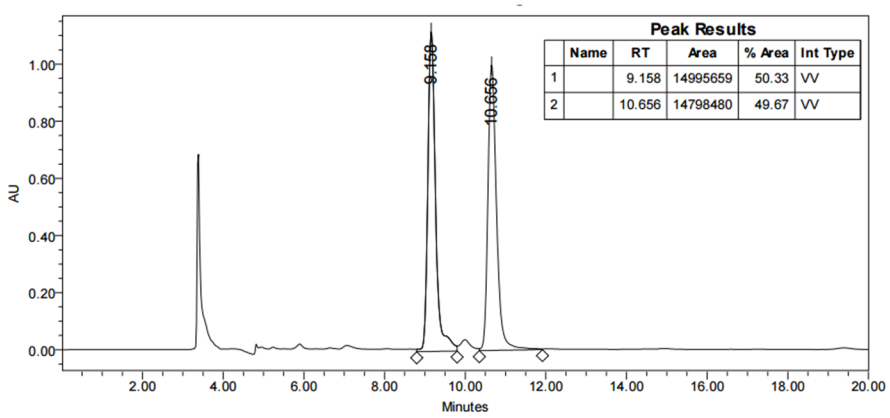


Racemic (**Table 5** of the body of the article).

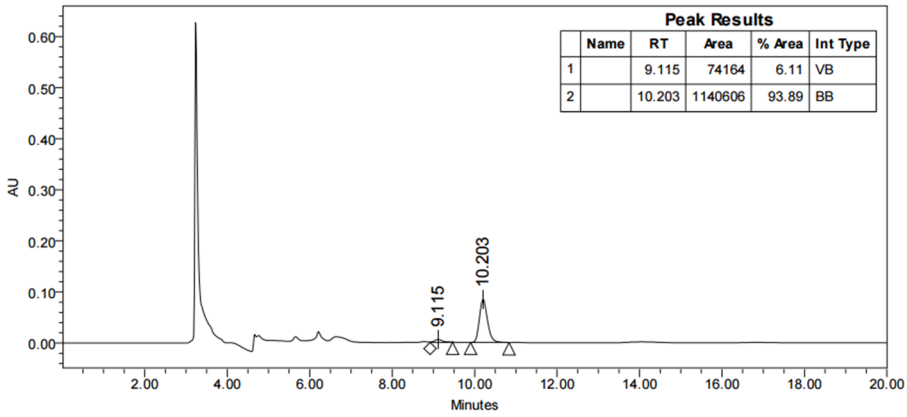


With catalyst **1i** (**Table 5, entry 6** of the body of the article).

Compound **4i**. HPLC: Chiralpak IC3, hexane/ethanol 85/15, 0.6 mL/min, λ = 220 nm, retention times 9.1 min (R), 10.6 (S).

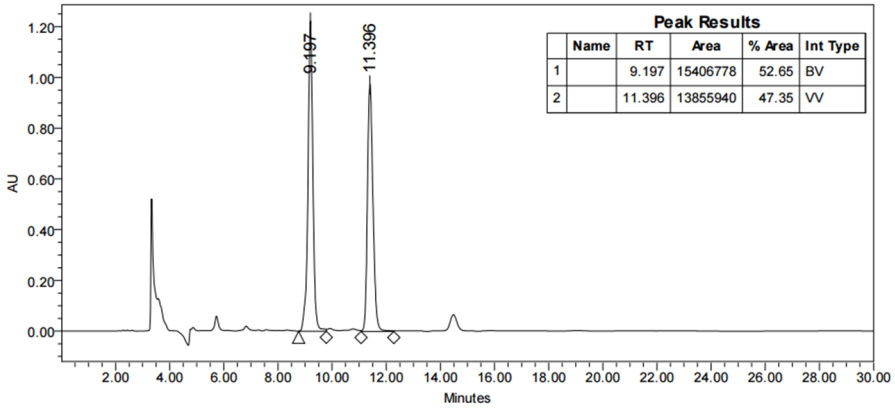


Racemic (**Fig. 7** of the body of the article).

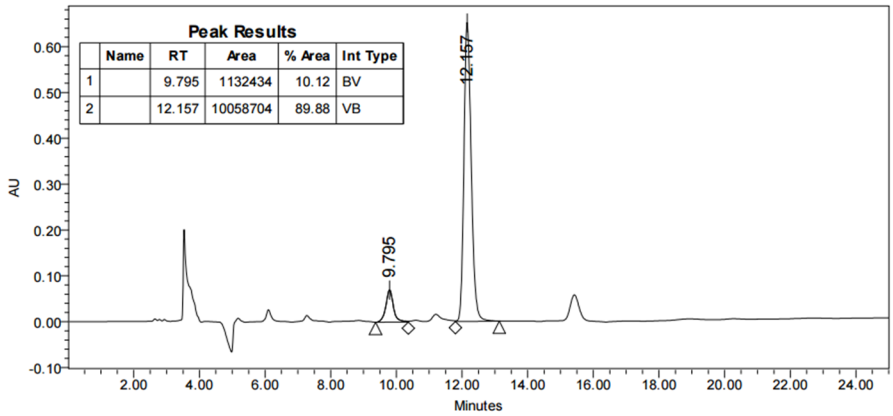


With catalyst **1i** (**Fig. 7** of the body of the article).

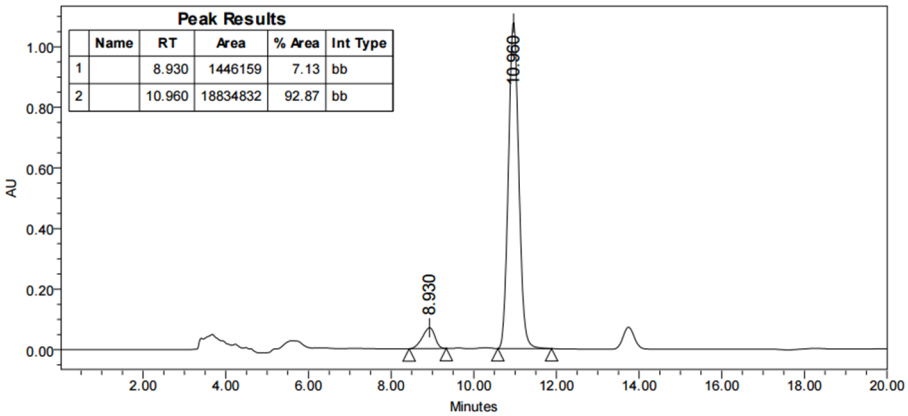
Compound **4k**. HPLC: Chiralpak IC3, hexane/ethanol 85/15, 0.6 mL/min, λ = 220 nm, retention times 9.1 min (R), 11.3 (S).



Racemic (**Fig. 7** of the body of the article).

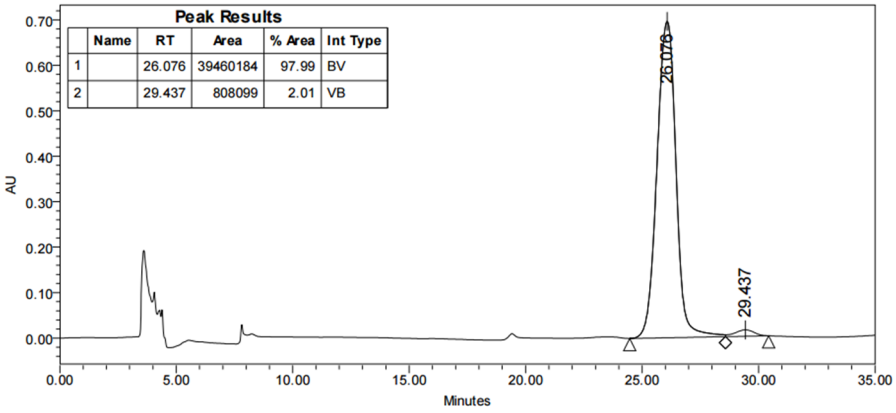


With catalyst **1i** (**Fig. 7** of the body of the article).



With catalyst **1i**, 3°C, 48h (**Fig. 7** of the body of the article).

Compound **4l**. HPLC: Chiralcel OJ, hexane/ethanol 70/30, 0.8 mL/min, λ = 220 nm, retention times 26.0 min (S), 29.43 (R).



With catalyst **1i** (**Fig. 7** of the body of the article).

3. References

1 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 and Others, *Gaussian Inc., Wallingford, CT*, 2009.

2 S. Kossmann and F. Neese, *J. Chem. Theory Comput.*, 2010, **6**, 2325–2338.

3 F. Neese, *WIREs Comput Mol Sci*, 2012, **2**, 73–78.

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