

Electronic Supporting Information

Atropisomerism about aryl-C(sp<sup>3</sup>) bonds: chemically driven  
rotational pathway in cannabidiol derivatives

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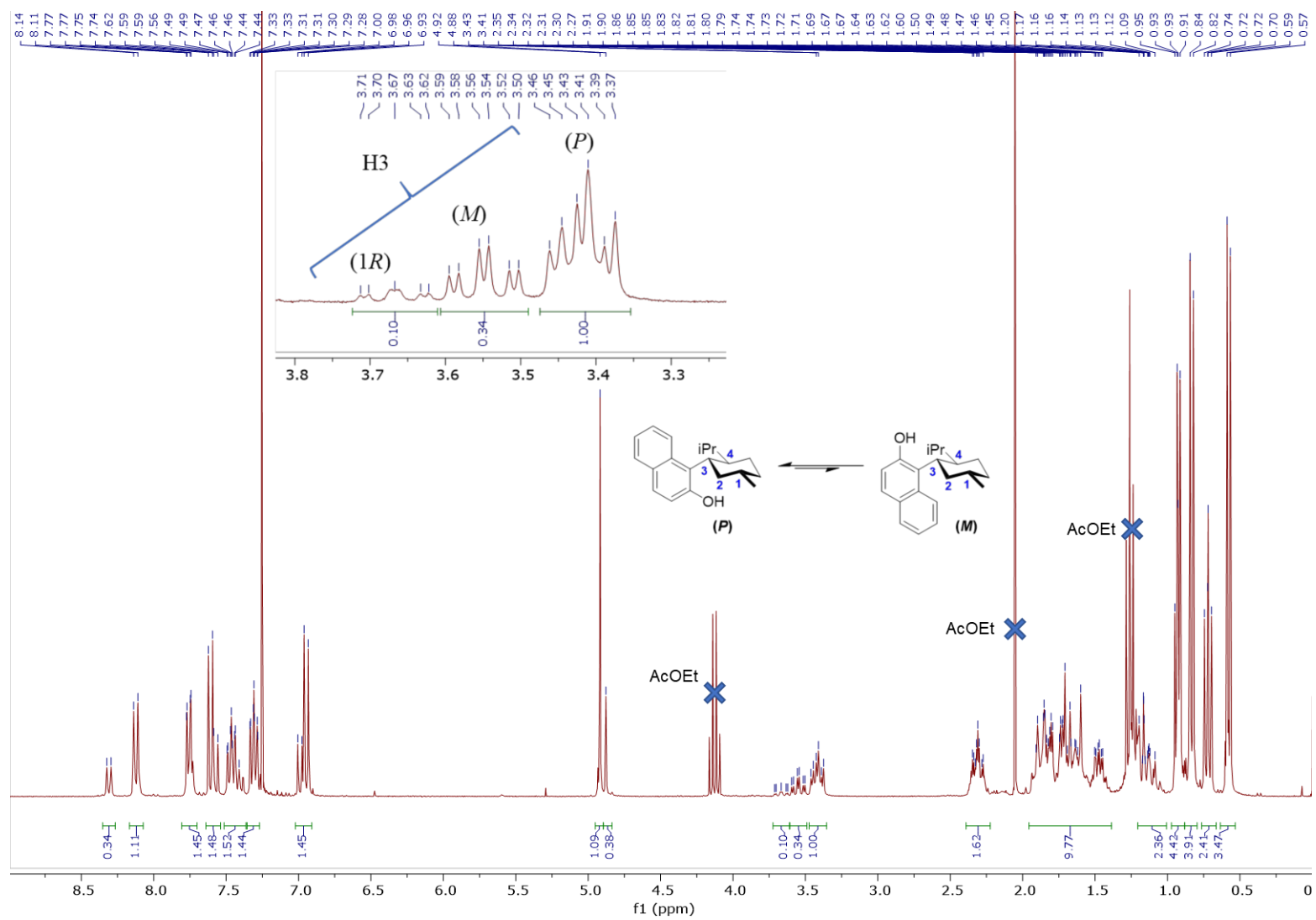
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## Table of Contents

<sup>1</sup> H and <sup>13</sup> C NMR Spectra of Naphthylcyclohexanes <b>2a-c</b>	S4-S25
<sup>1</sup> H and <sup>13</sup> C NMR Spectra of Naphthylcyclohexene oxides <b>3b,c</b>	S26-S41
Table S1,S2	S42
VT- NMR Experiments and Determination of Kinetic Parameters	S43-S51
VT-2D EXSY Spectra of <b>2a-c</b> and <b>3b,c</b>	S52-S56
X-Ray Crystal Structure data of ( <i>P</i> )- <b>2c</b>	S57-S58
Quantum chemical calculations	S59-S188

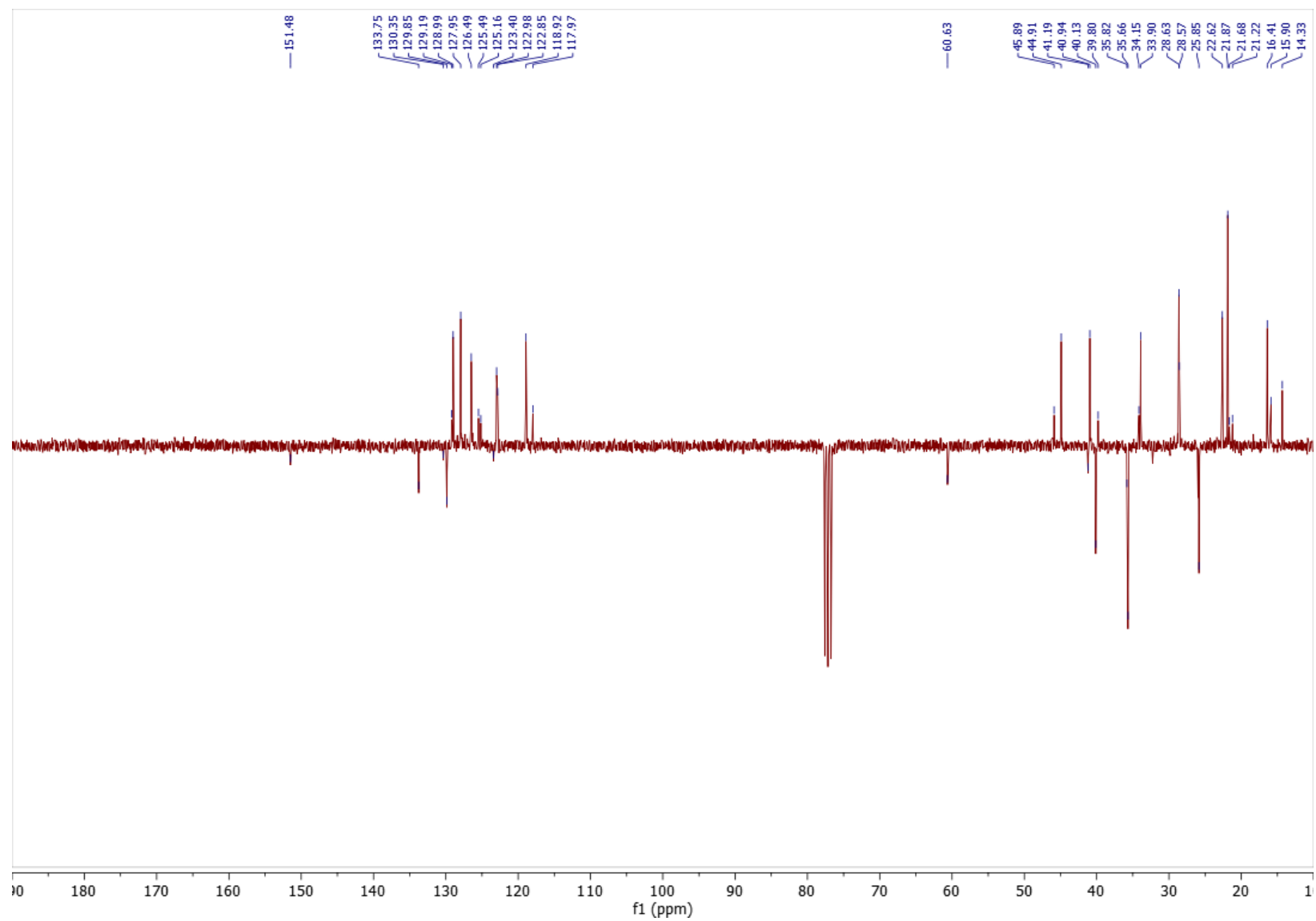
*<sup>1</sup>H and <sup>13</sup>C NMR Spectra of Naphthylcyclohexanes 2a-c and Naphthylcyclohexene oxides 3b,c:*

300 MHz  $^1\text{H}$  spectrum of **2a** in  $\text{CDCl}_3$  at 298 K

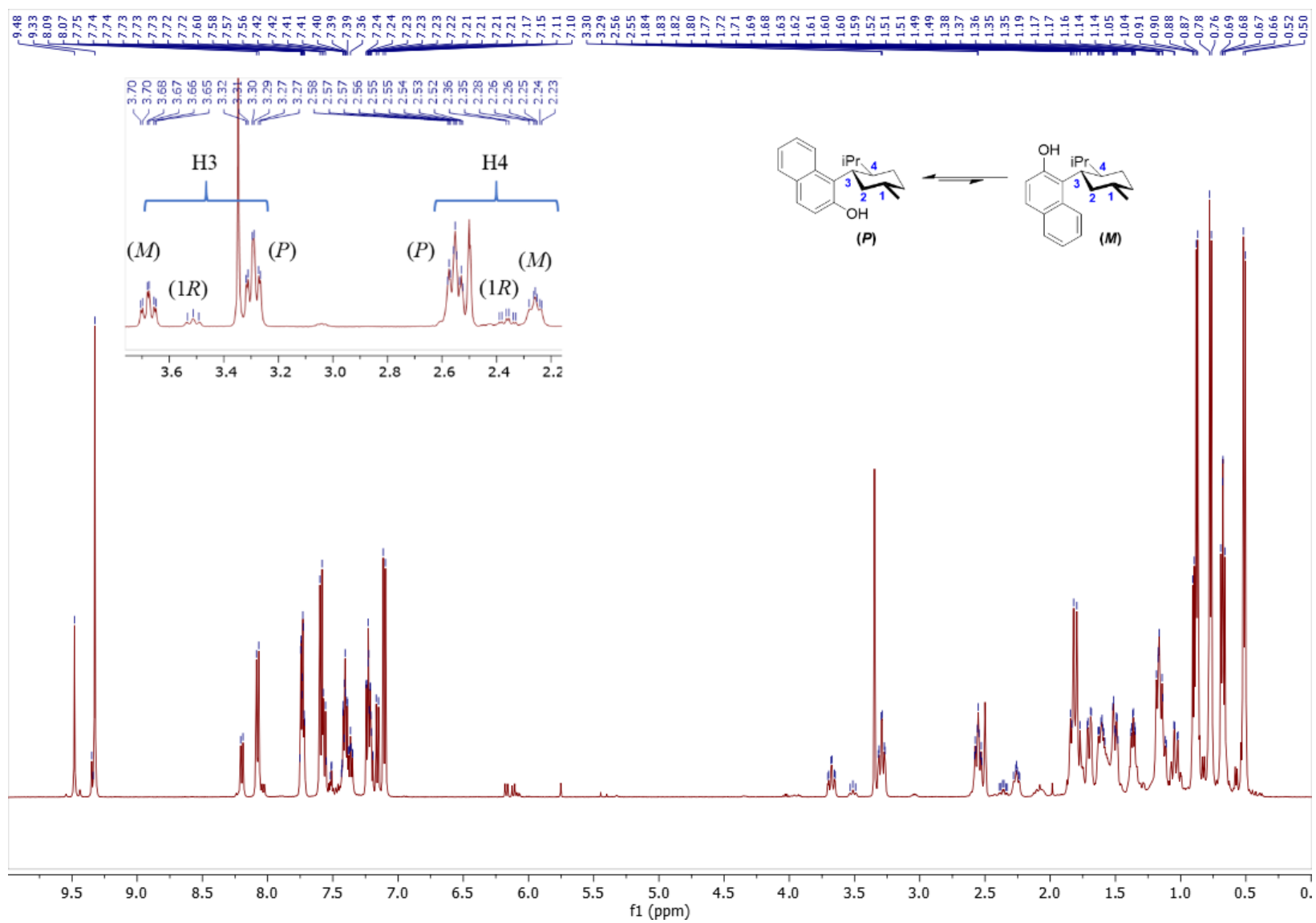




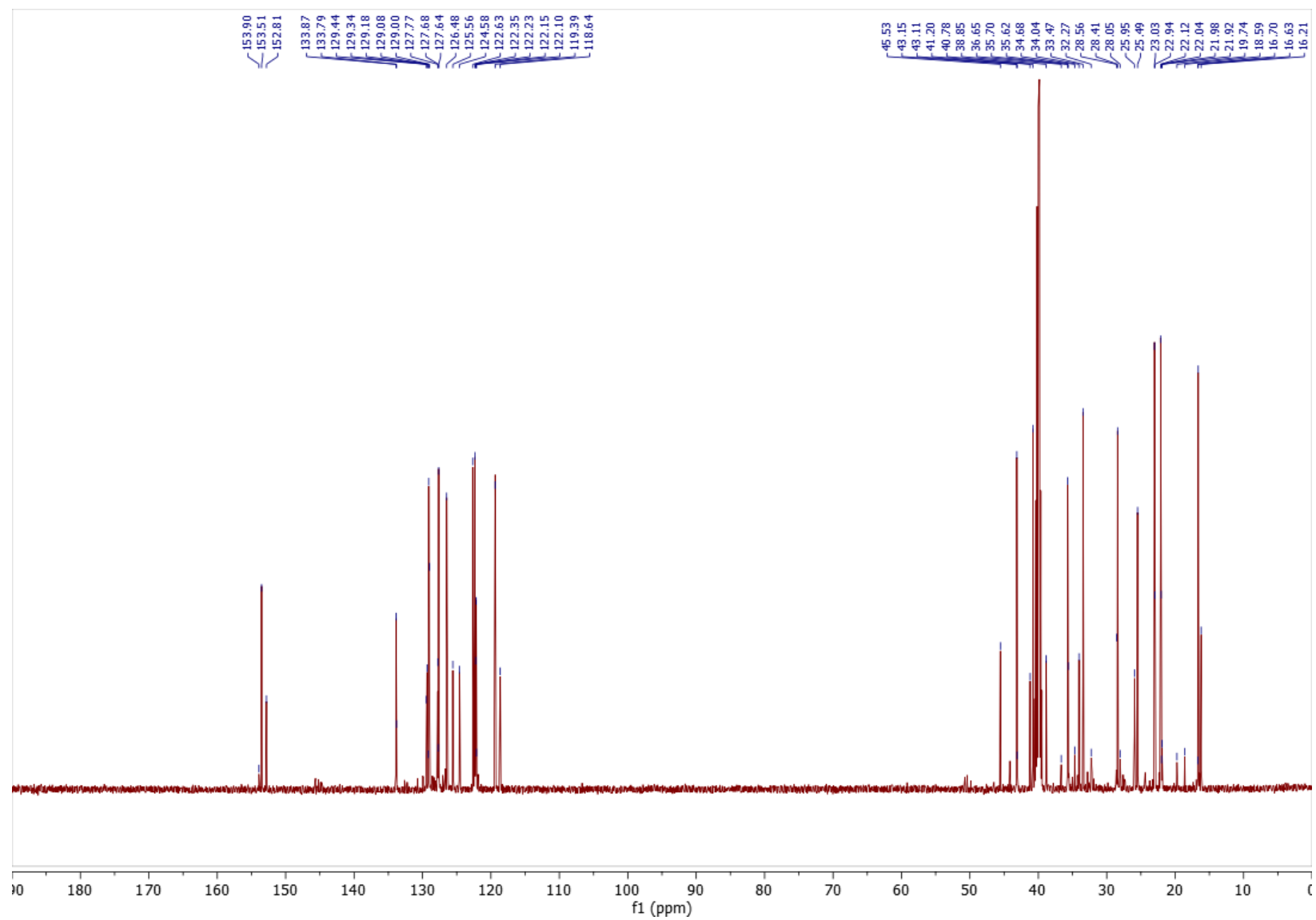
75 MHz  $^{13}\text{C}$  spectrum of **2a** in  $\text{CDCl}_3$  at 298 K



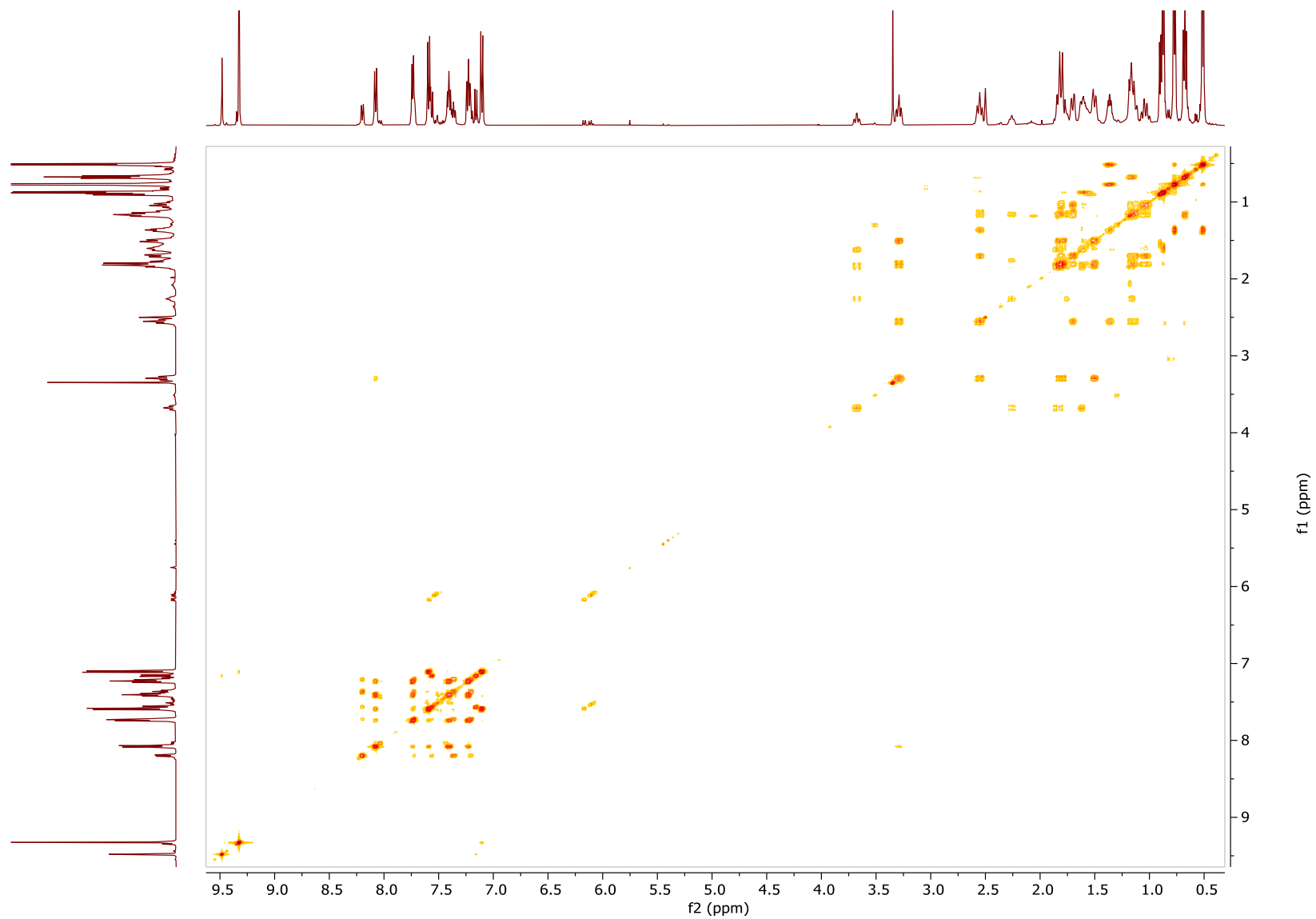
500 MHz  $^1\text{H}$  spectrum of **2a** in  $\text{DMSO-}d_6$  at 298 K



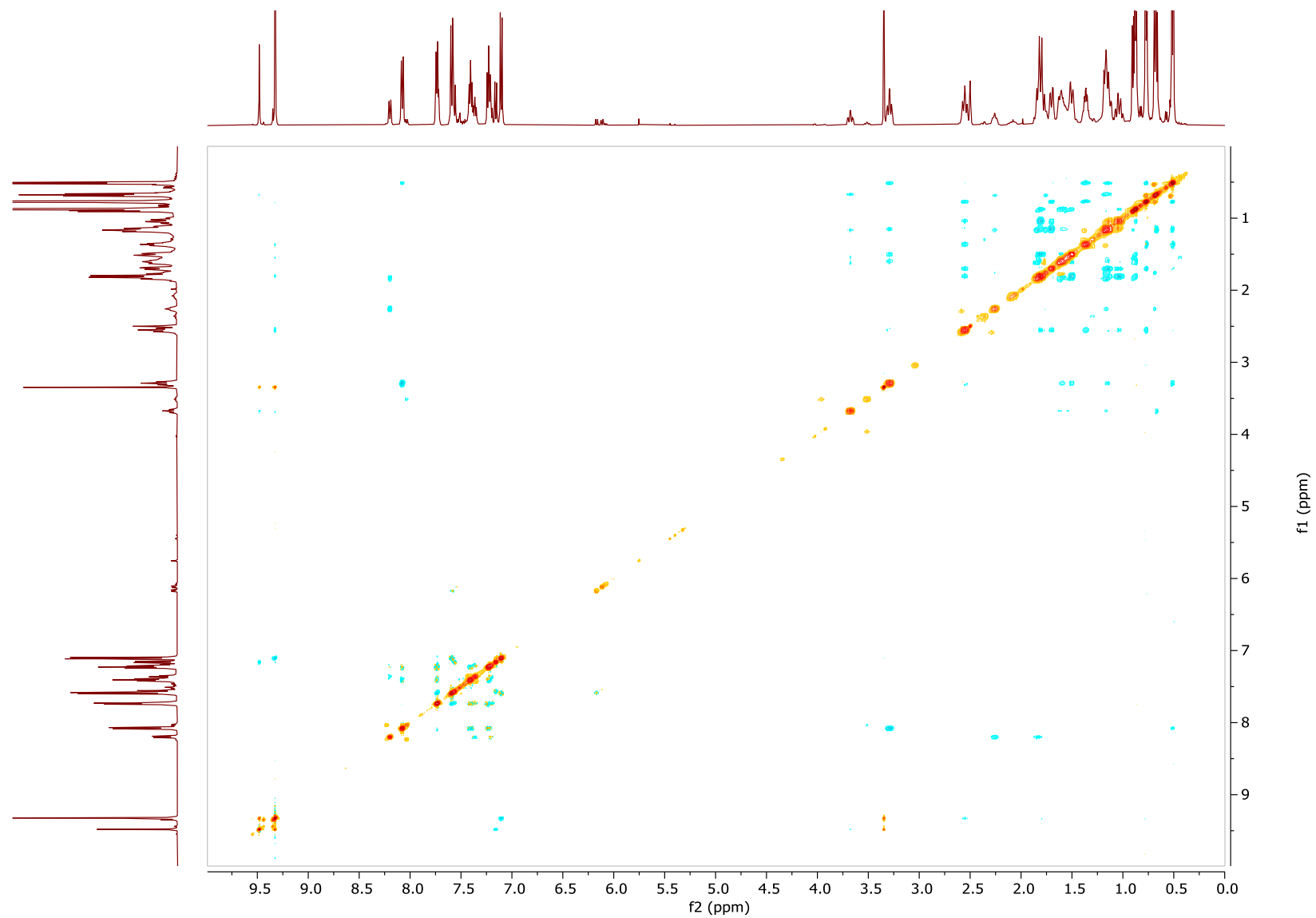
150 MHz  $^{13}\text{C}$  spectrum of **2a** in DMSO-*d*<sub>6</sub> at 298 K



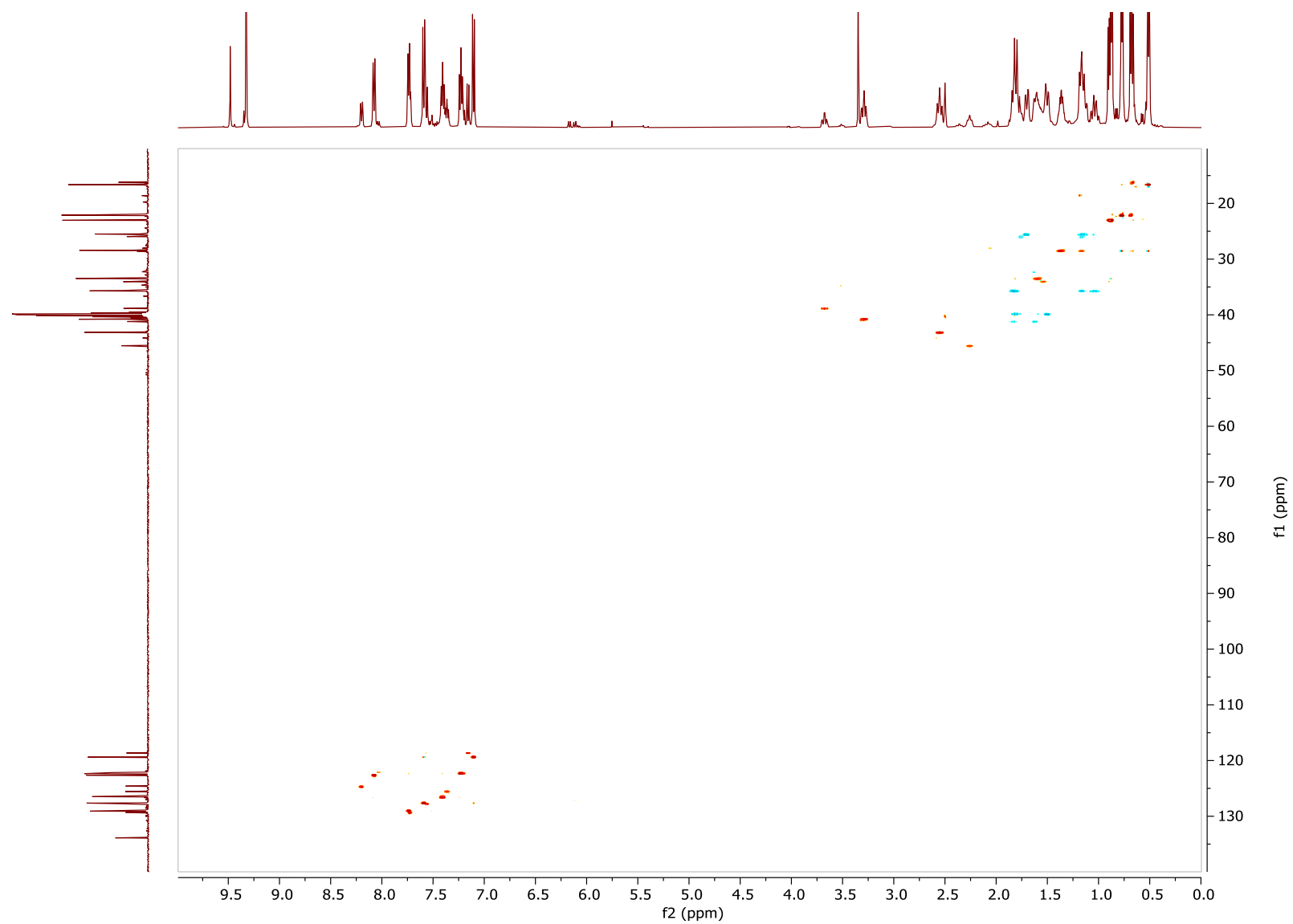
COSY spectrum of **2a** in DMSO-*d*<sub>6</sub> at 298 K



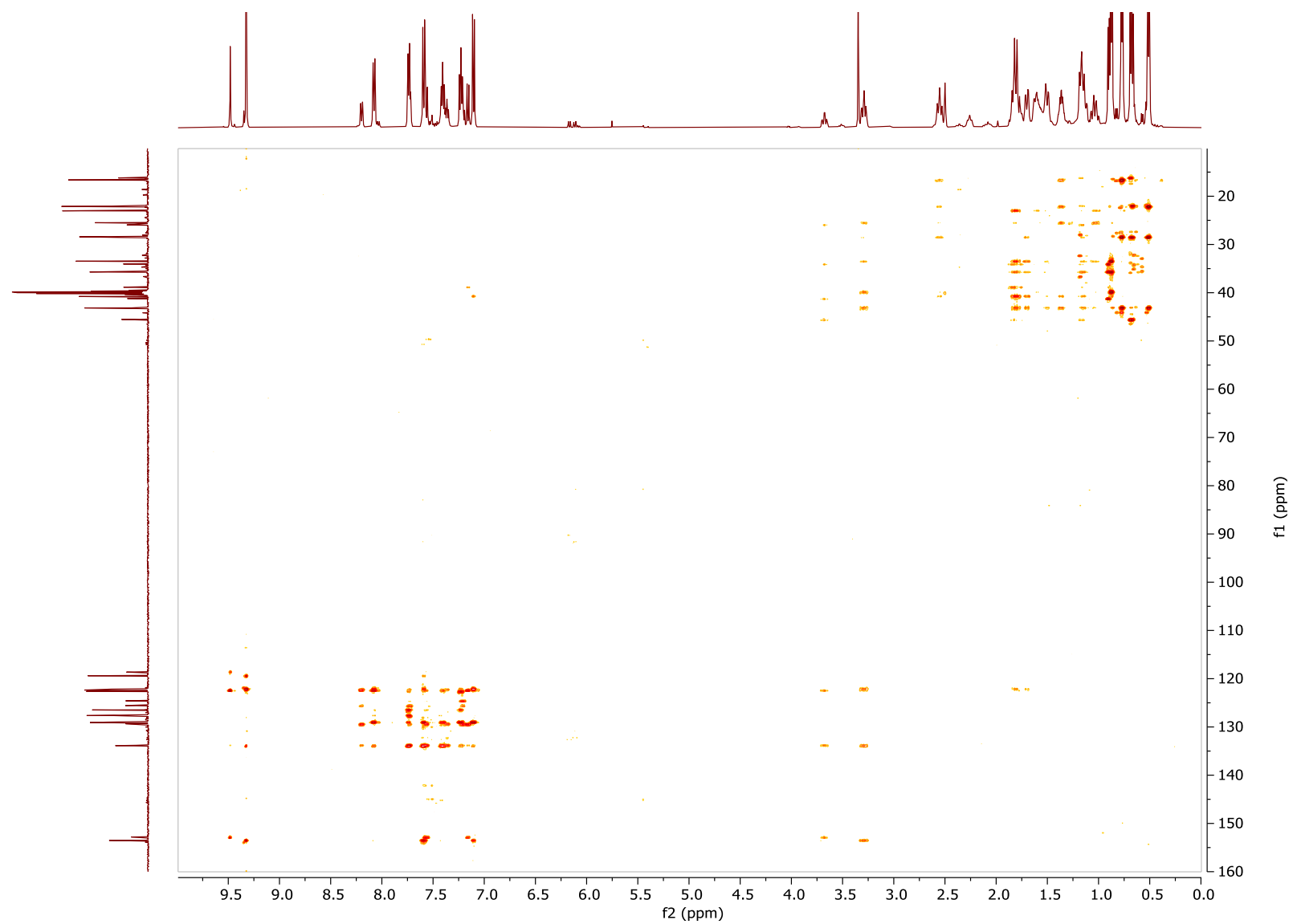
NOESY spectrum of **2a** in DMSO-*d*<sub>6</sub> at 298 K



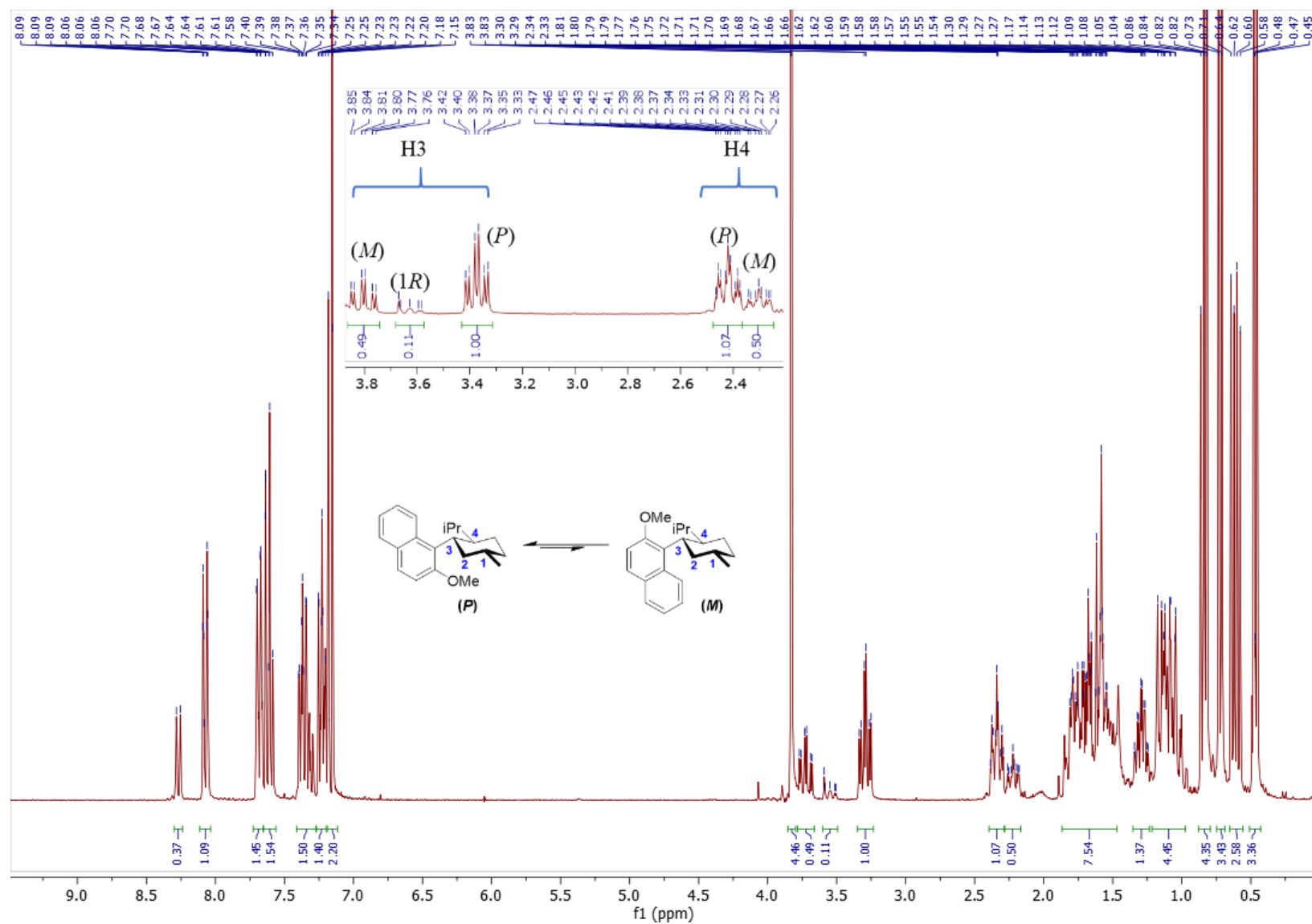
HSQC spectrum of **2a** in DMSO-*d*<sub>6</sub> at 298 K



HMBC spectrum of **2a** in DMSO-*d*<sub>6</sub> at 298 K

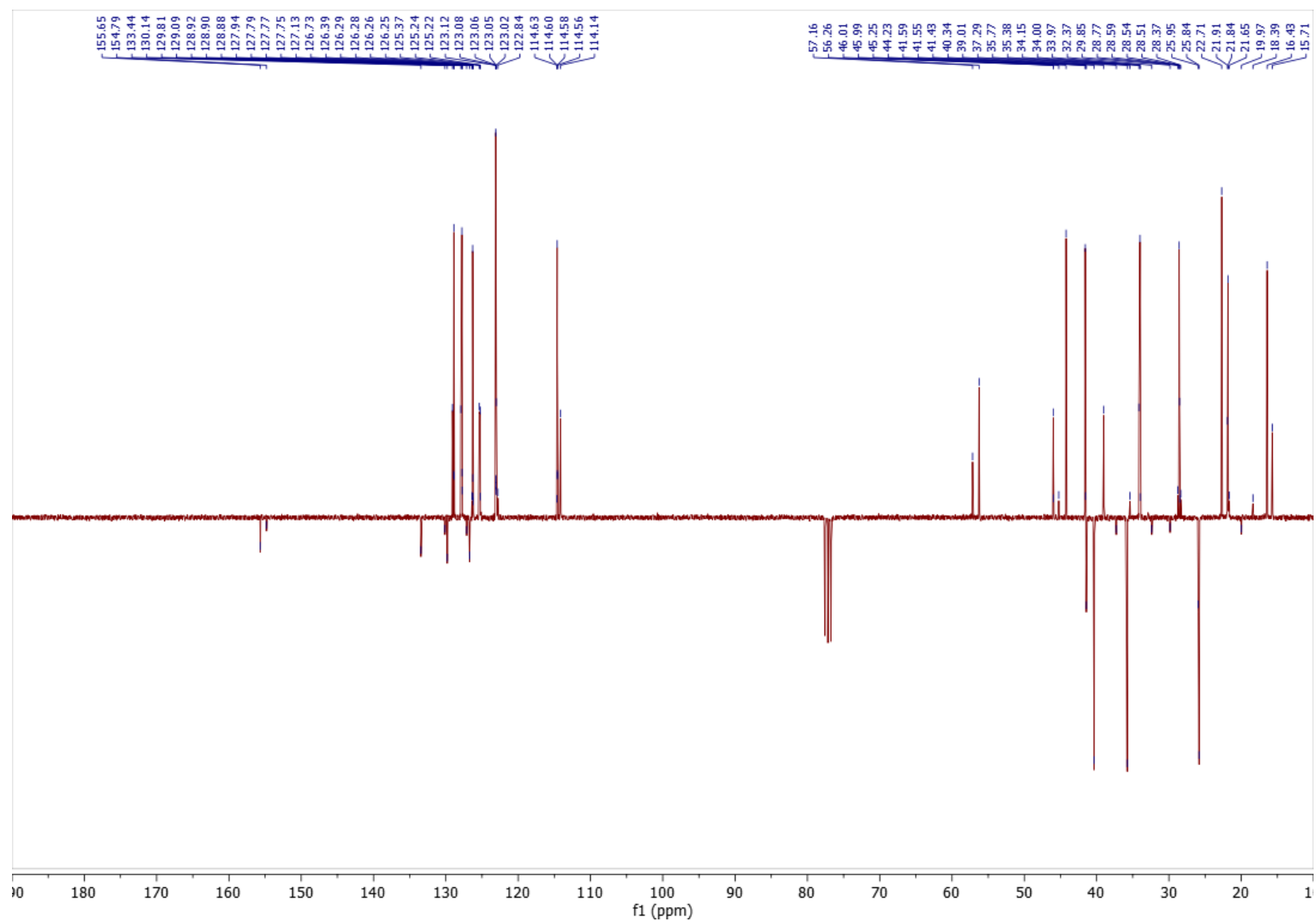


300 MHz  $^1\text{H}$  spectrum of **2b** in  $\text{CDCl}_3$  at 298 K

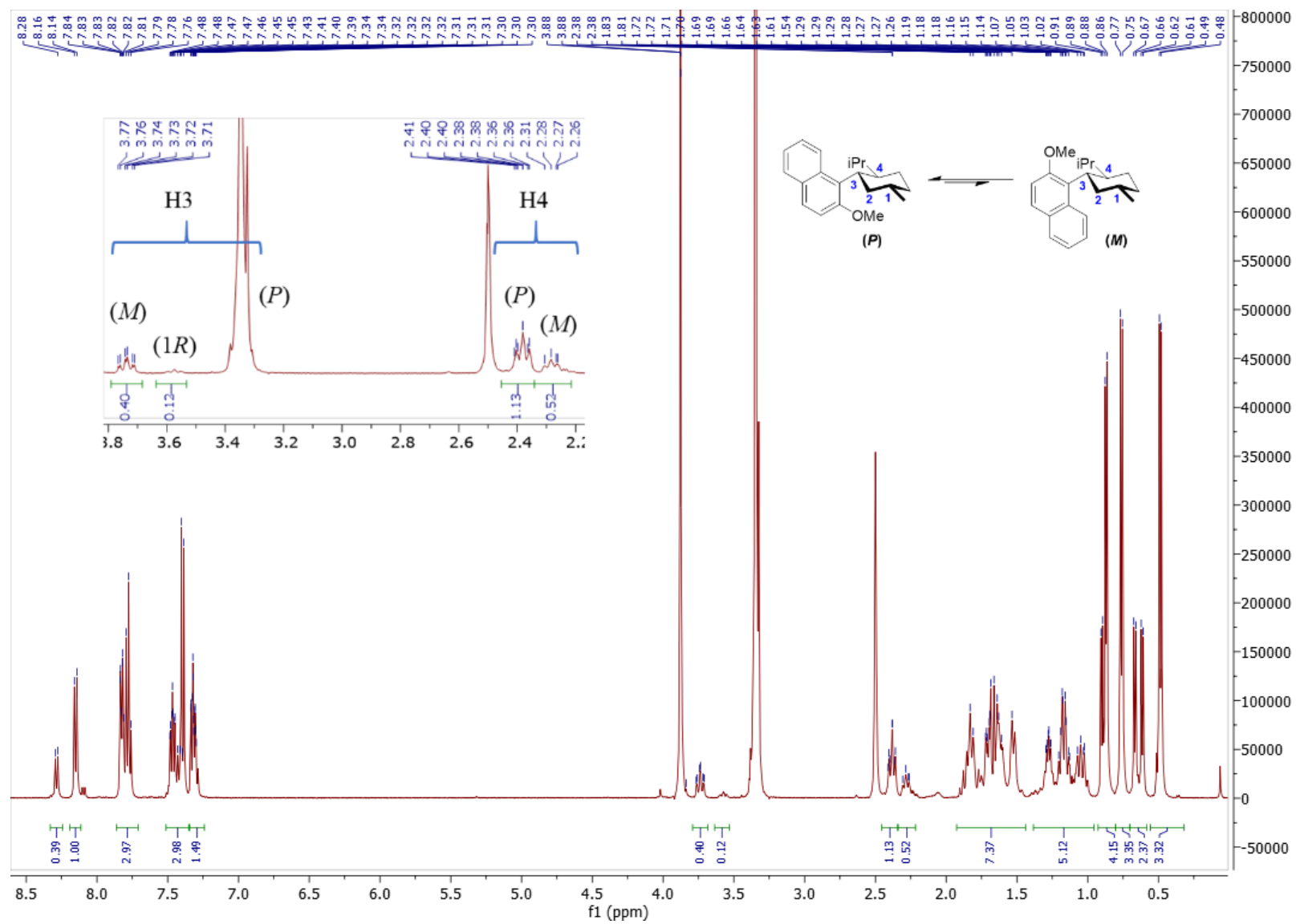




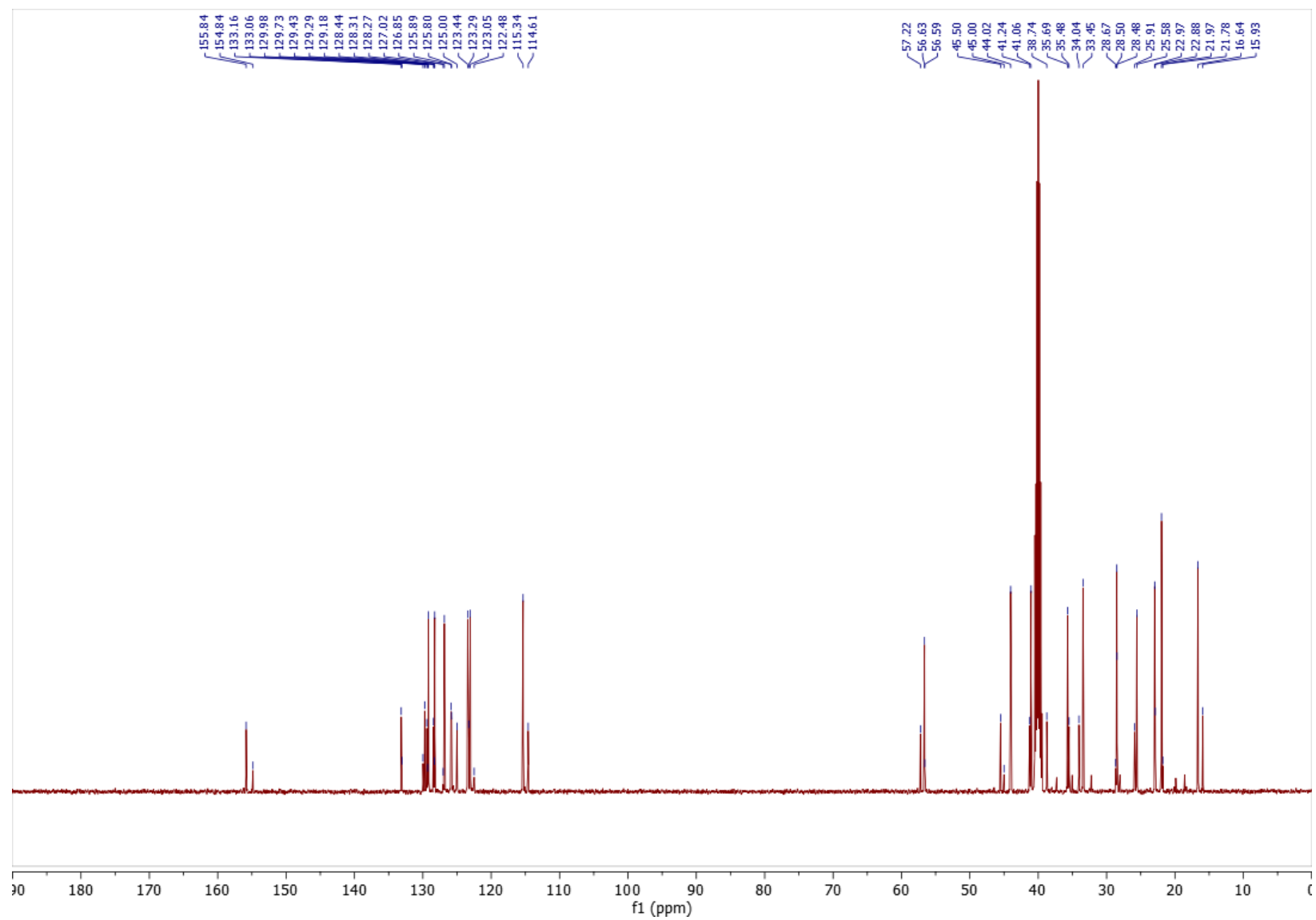
75 MHz  $^{13}\text{C}$  spectrum of **2b** in  $\text{CDCl}_3$  at 298 K



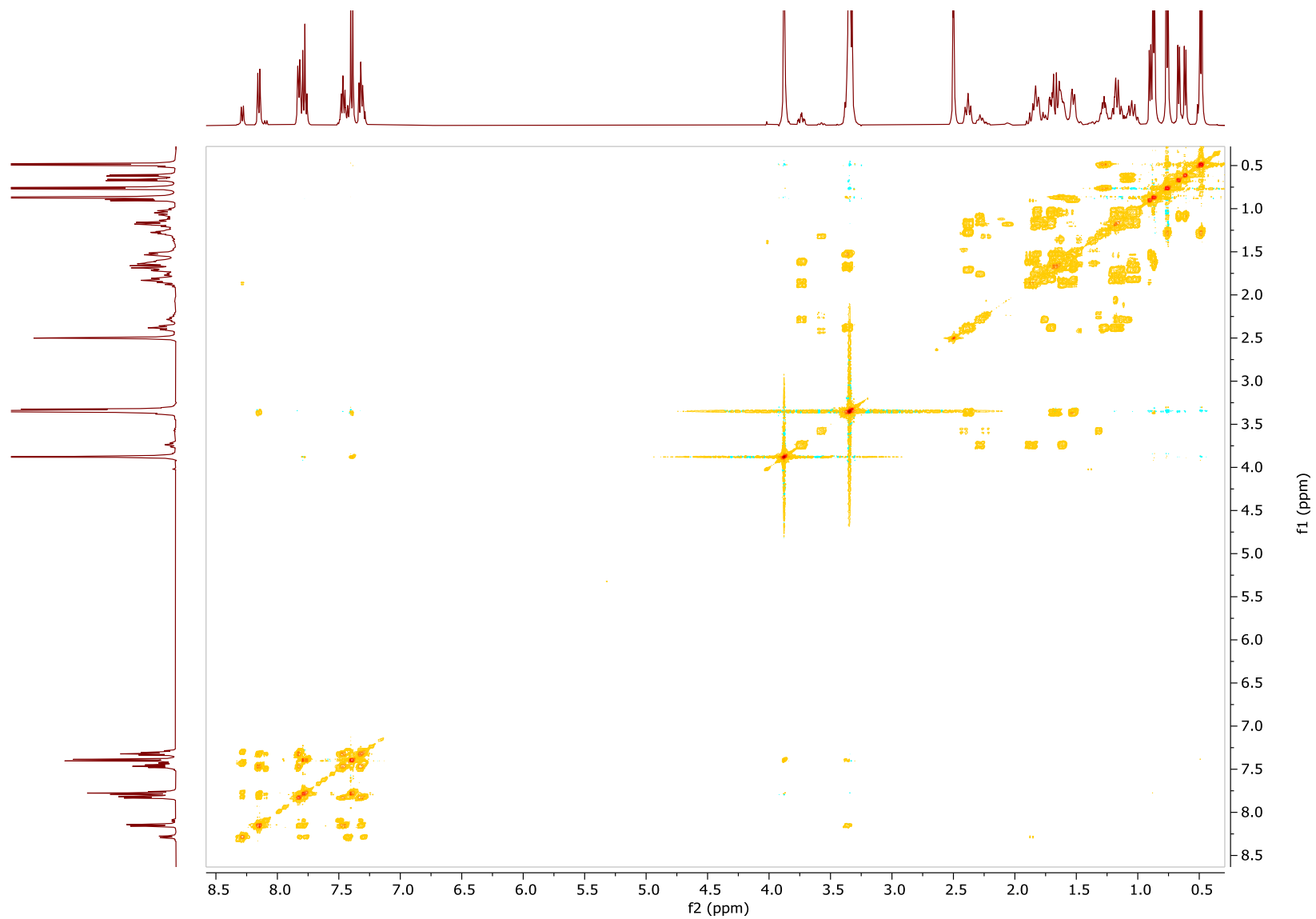
500 MHz  $^1\text{H}$  spectrum of **2b** in  $\text{DMSO-}d_6$  at 298 K



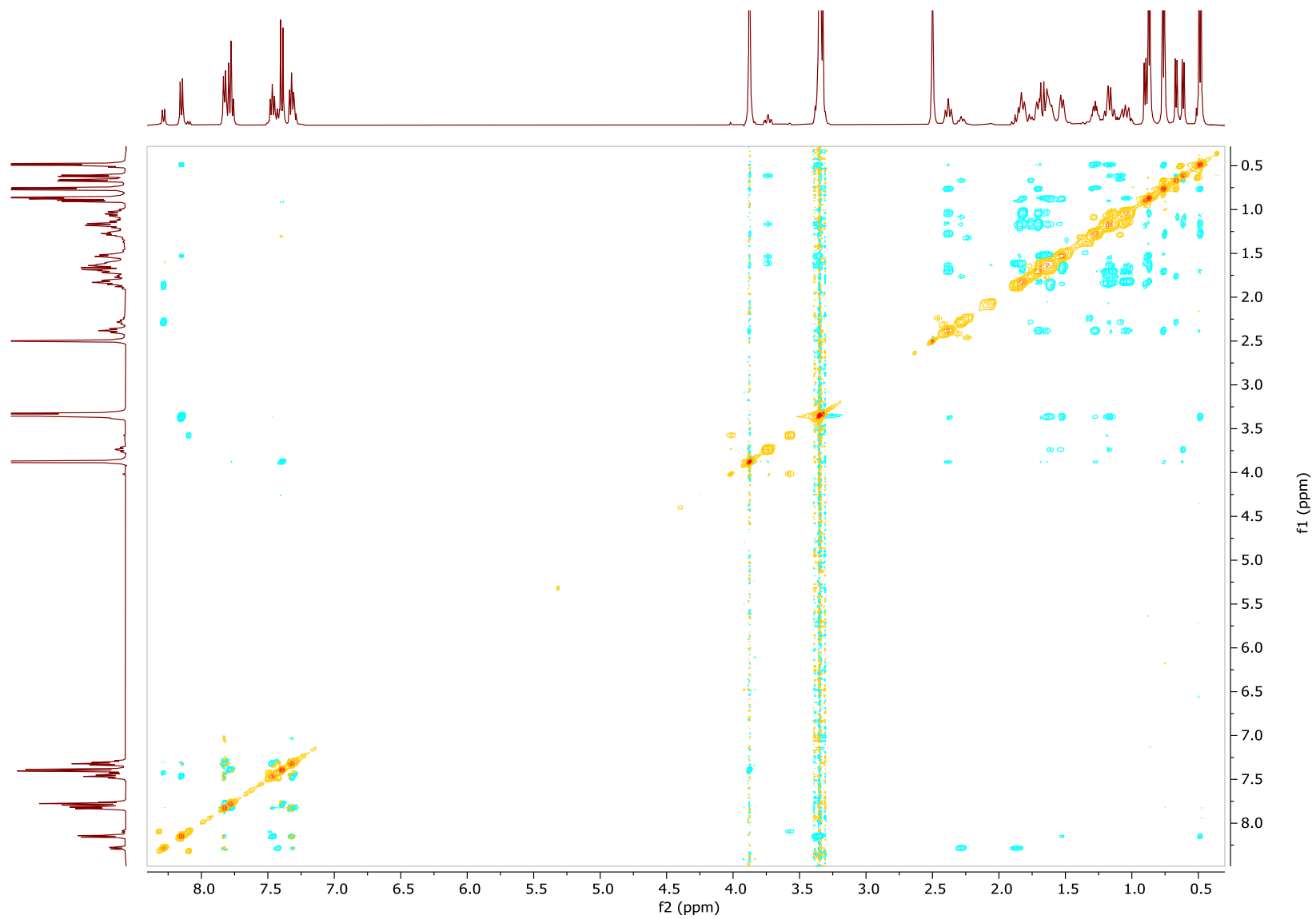
150 MHz  $^{13}\text{C}$  spectrum of **2b** in DMSO-*d*<sub>6</sub> at 298 K



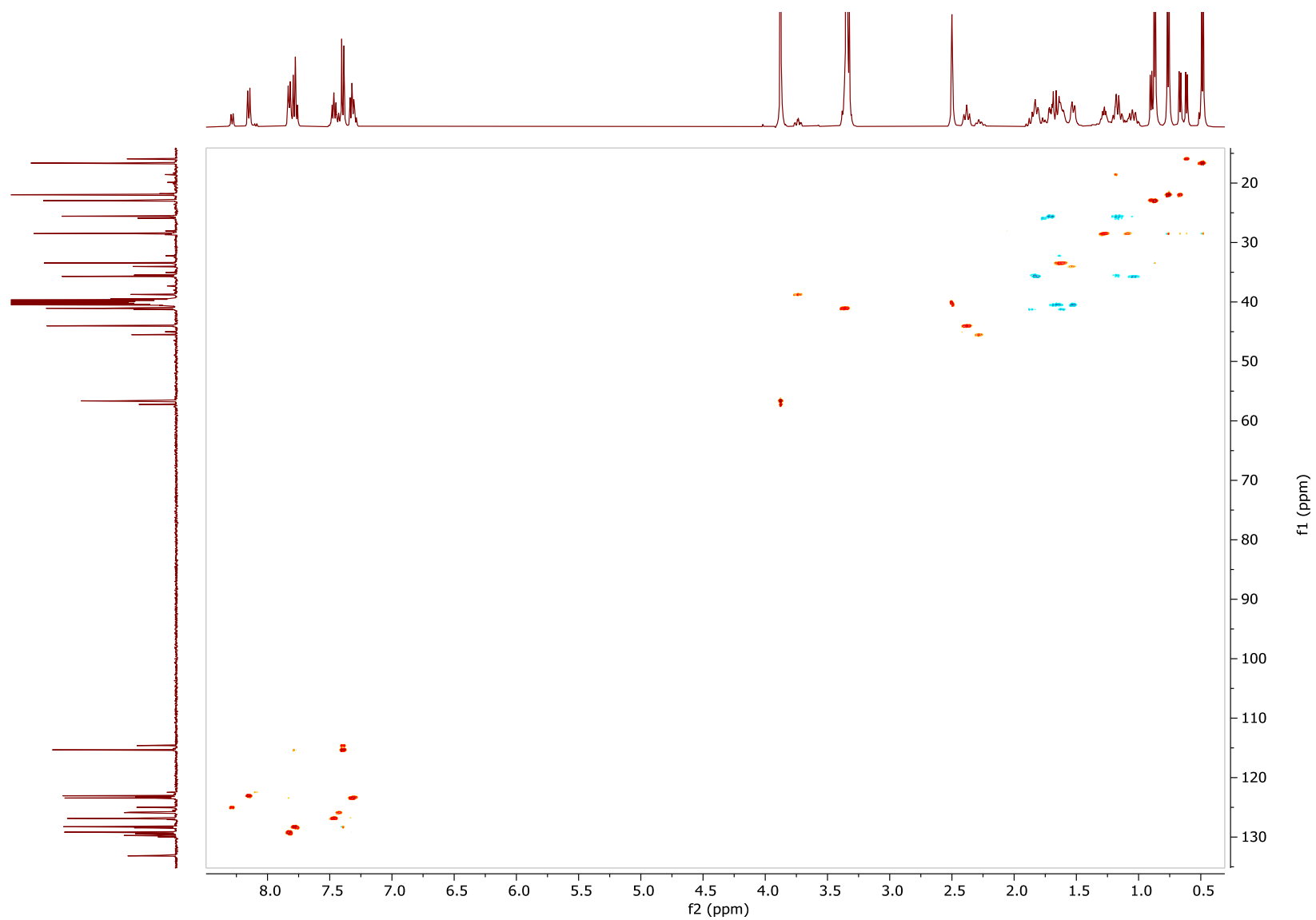
COSY spectrum of **2b** in DMSO-*d*<sub>6</sub> at 298 K



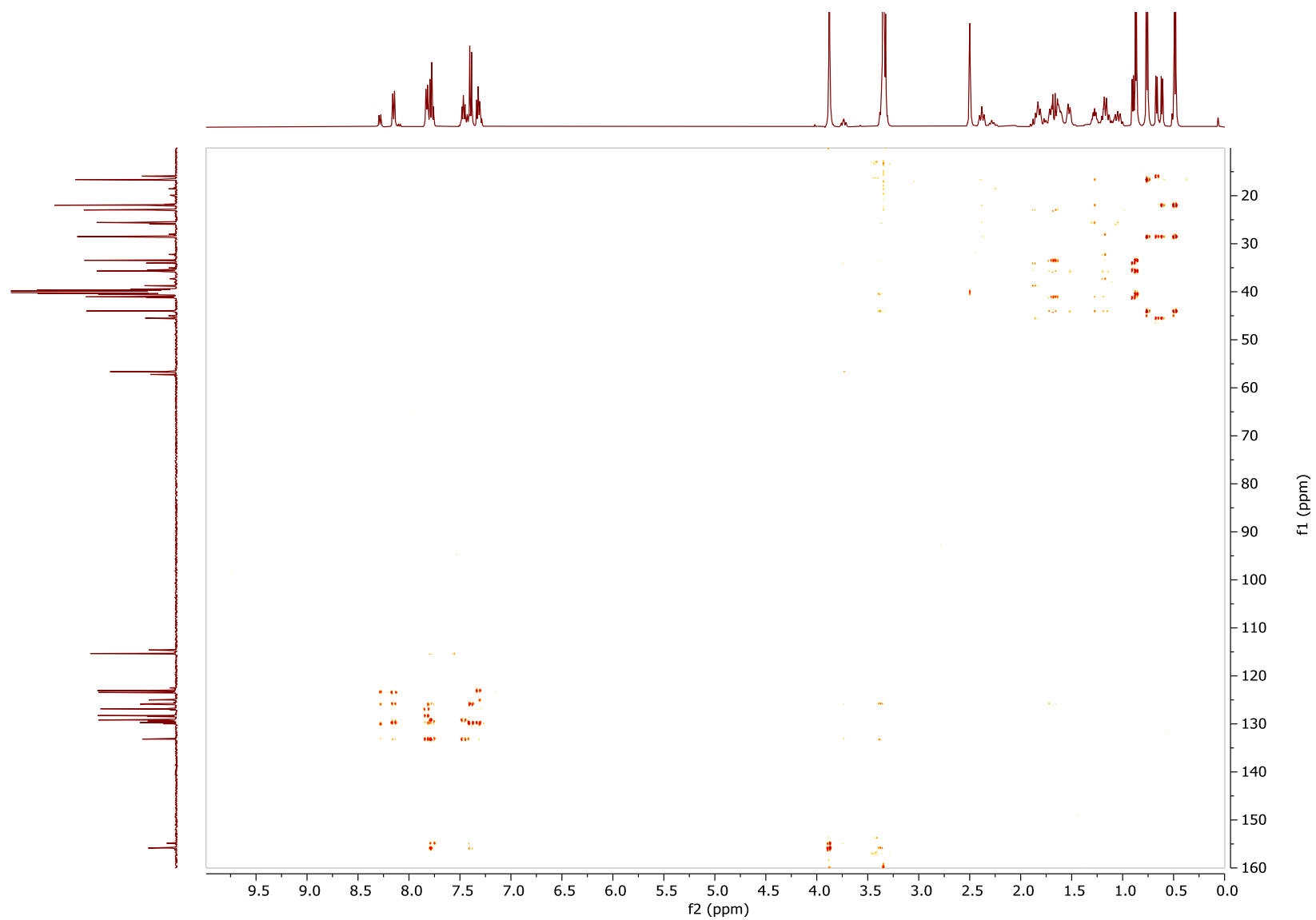
NOESY spectrum of **2b** in DMSO-*d*<sub>6</sub> at 298 K



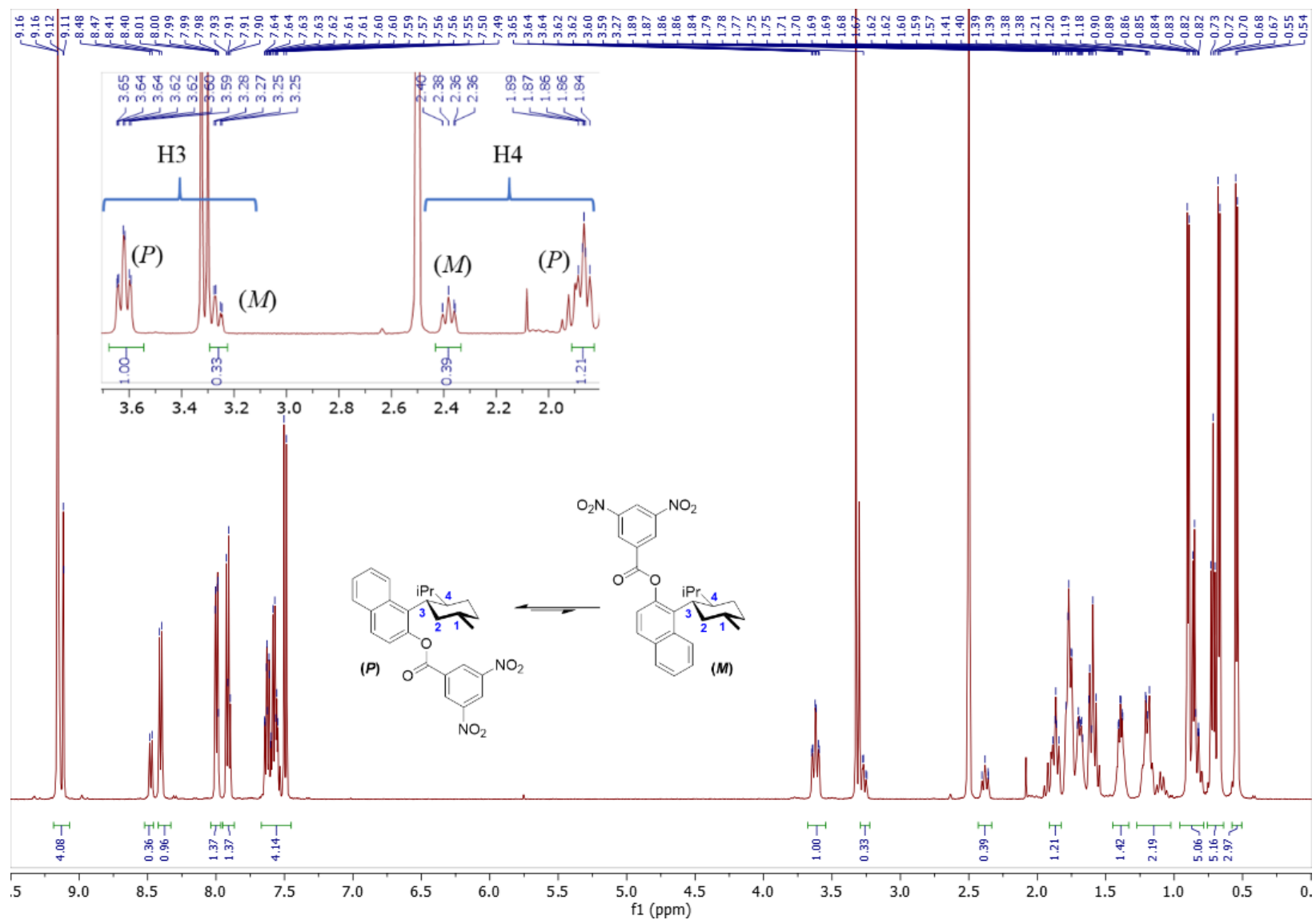
HSQC spectrum of **2b** in DMSO-*d*<sub>6</sub> at 298 K



HMBC spectrum of **2b** in DMSO-*d*<sub>6</sub> at 298 K

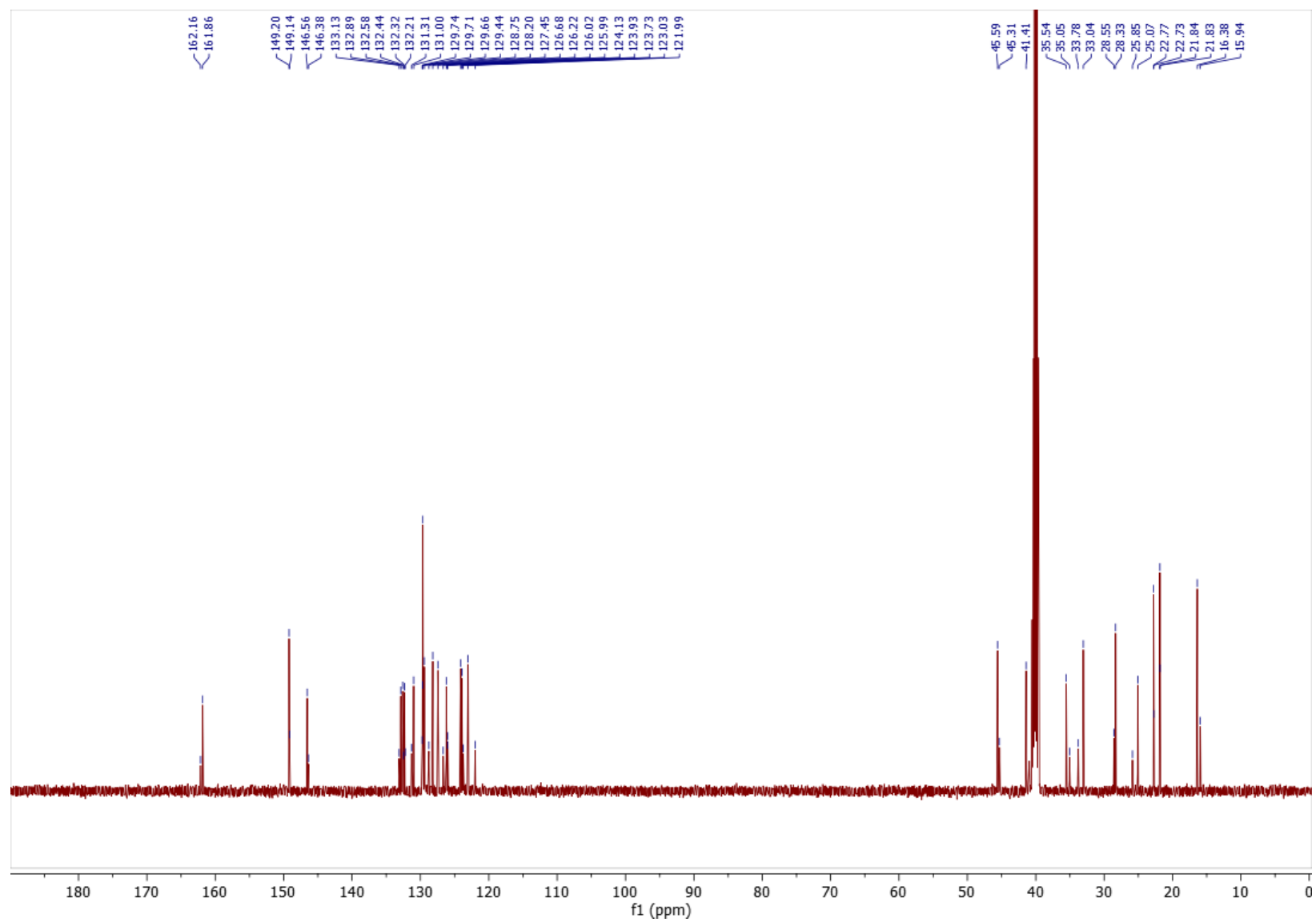


500 MHz  $^1\text{H}$  spectrum of **2c** in  $\text{DMSO-}d_6$  at 298 K



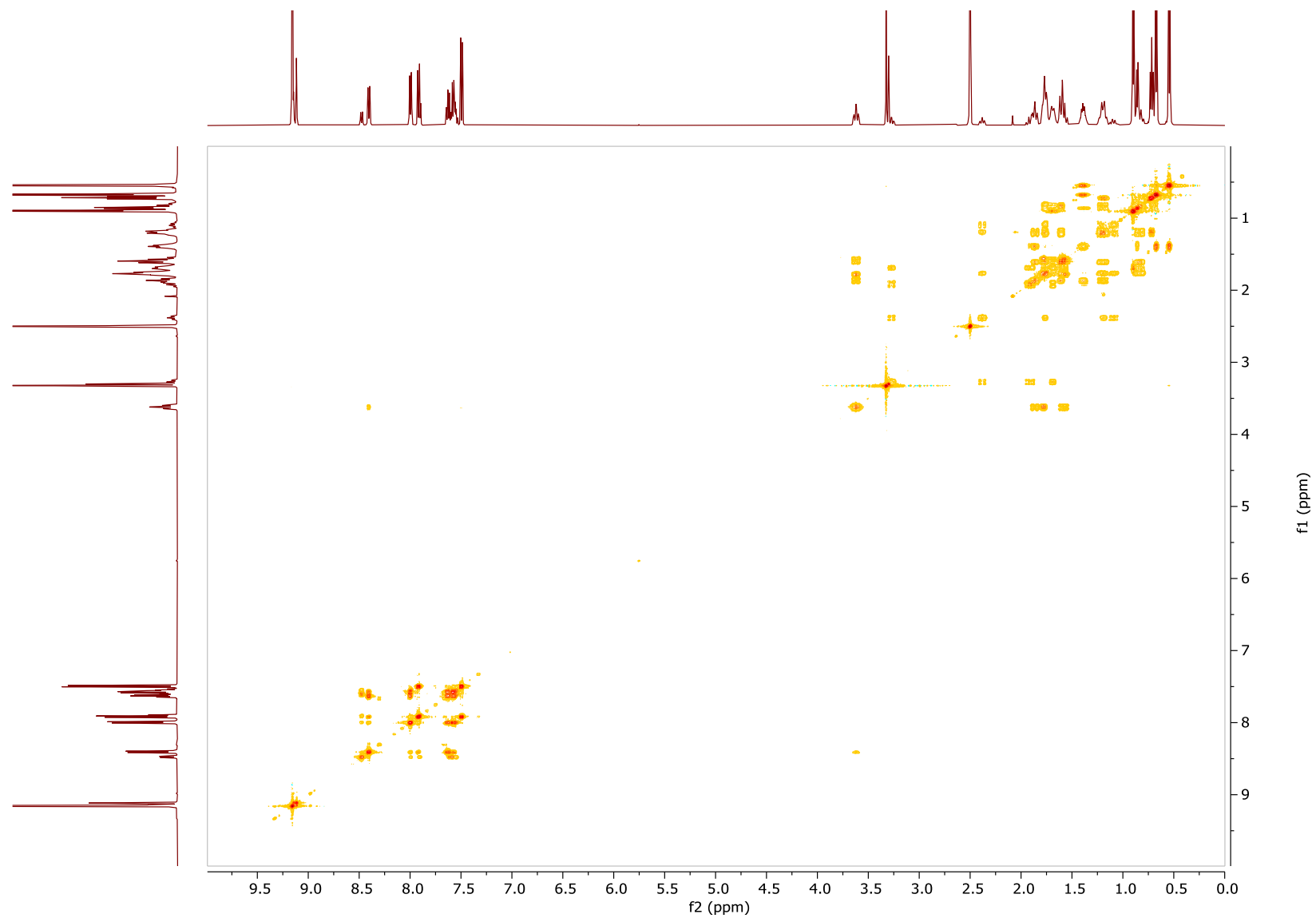


150 MHz  $^{13}\text{C}$  spectrum of **2c** in DMSO-*d*<sub>6</sub> at 298 K

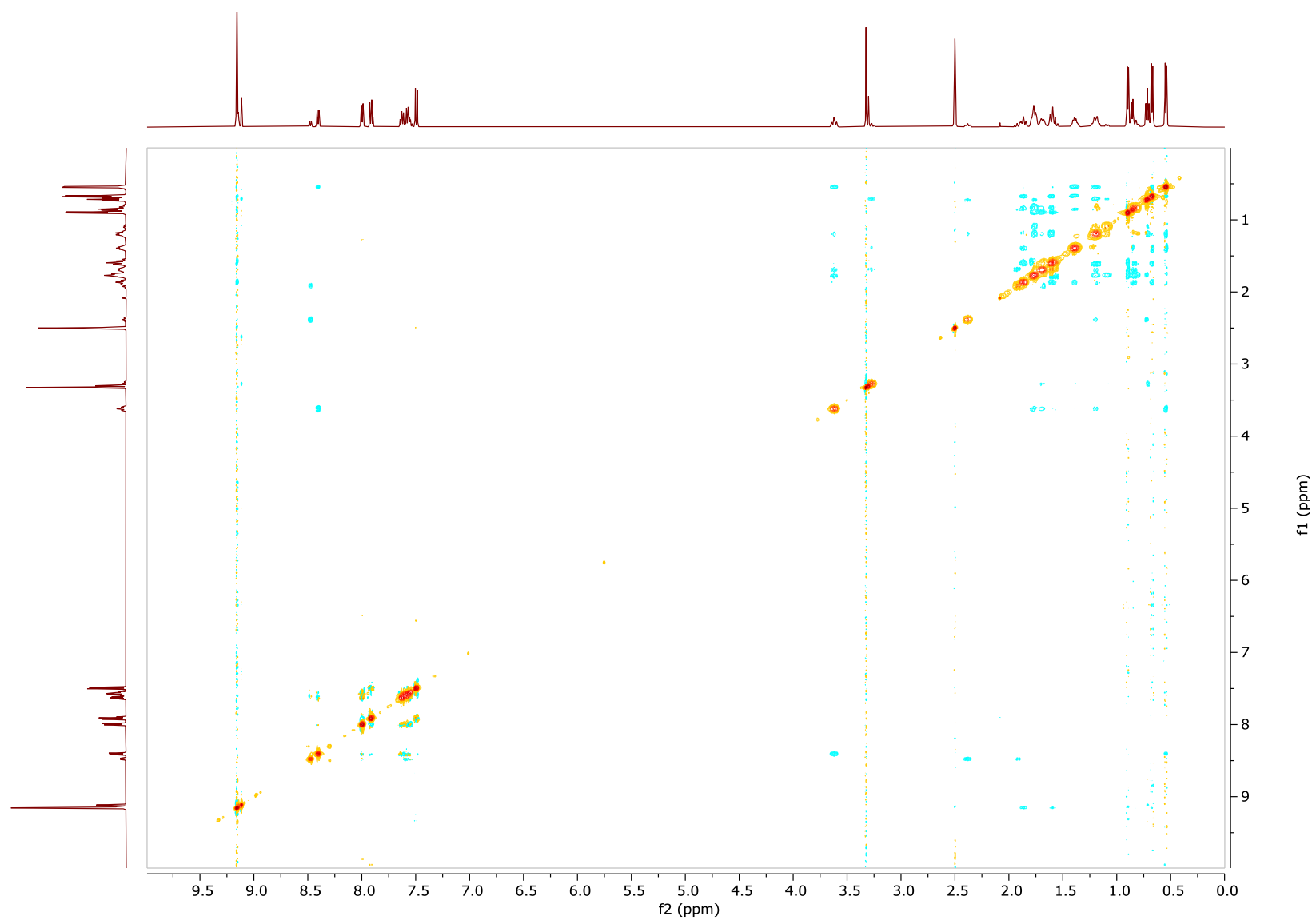


S21

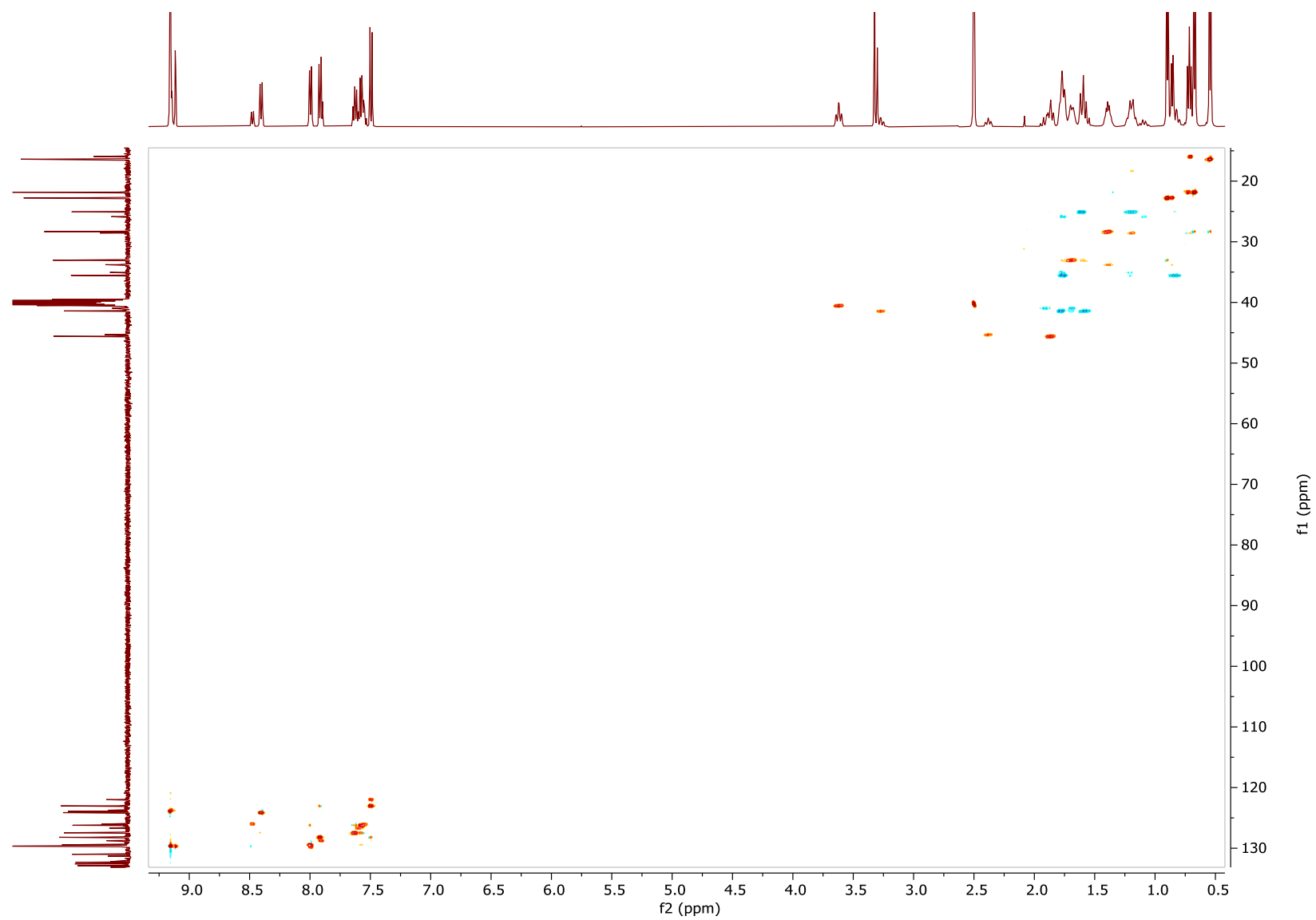
COSY spectrum of **2c** in DMSO-*d*<sub>6</sub> at 298 K



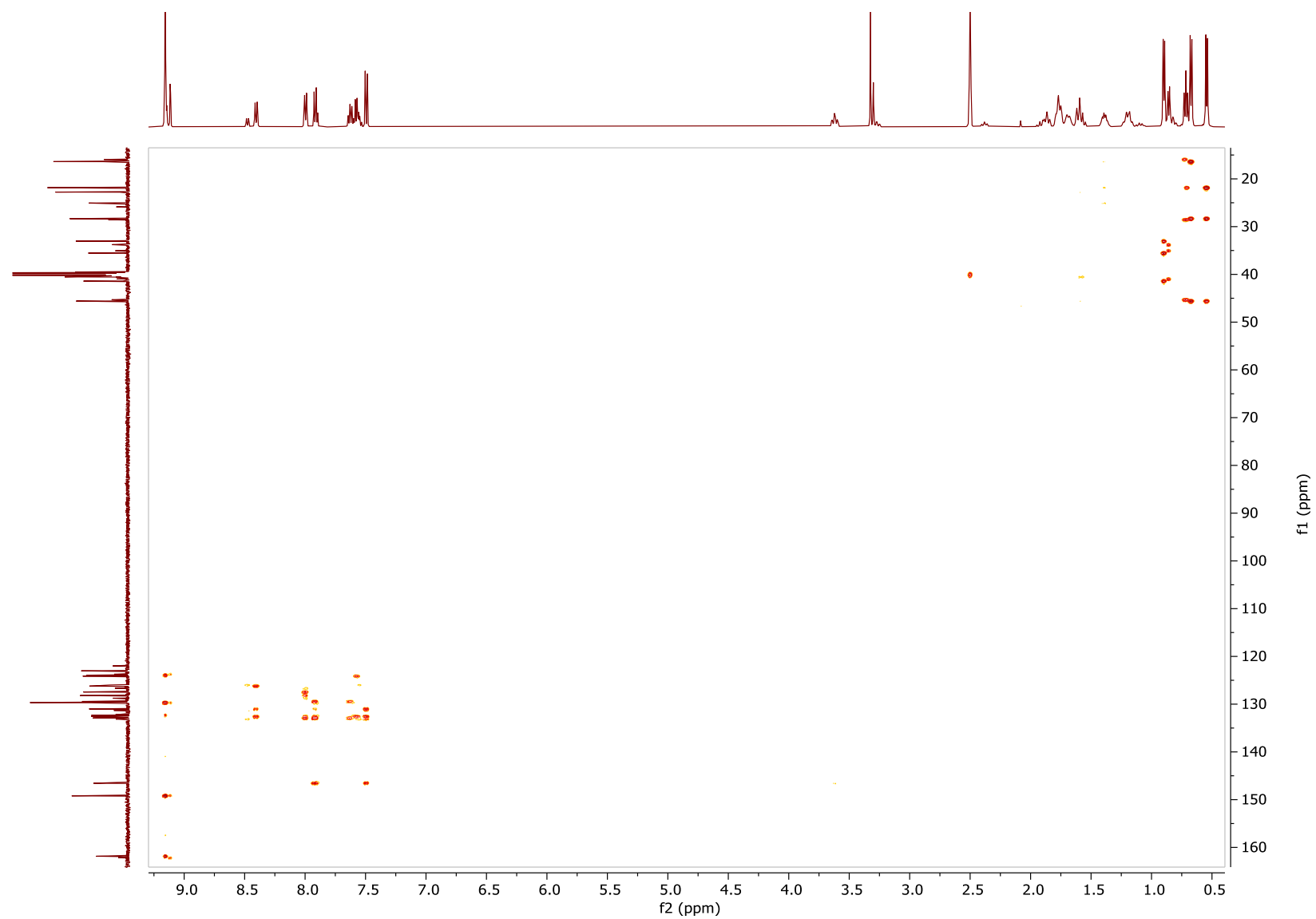
NOESY spectrum of **2c** in DMSO-*d*<sub>6</sub> at 298 K



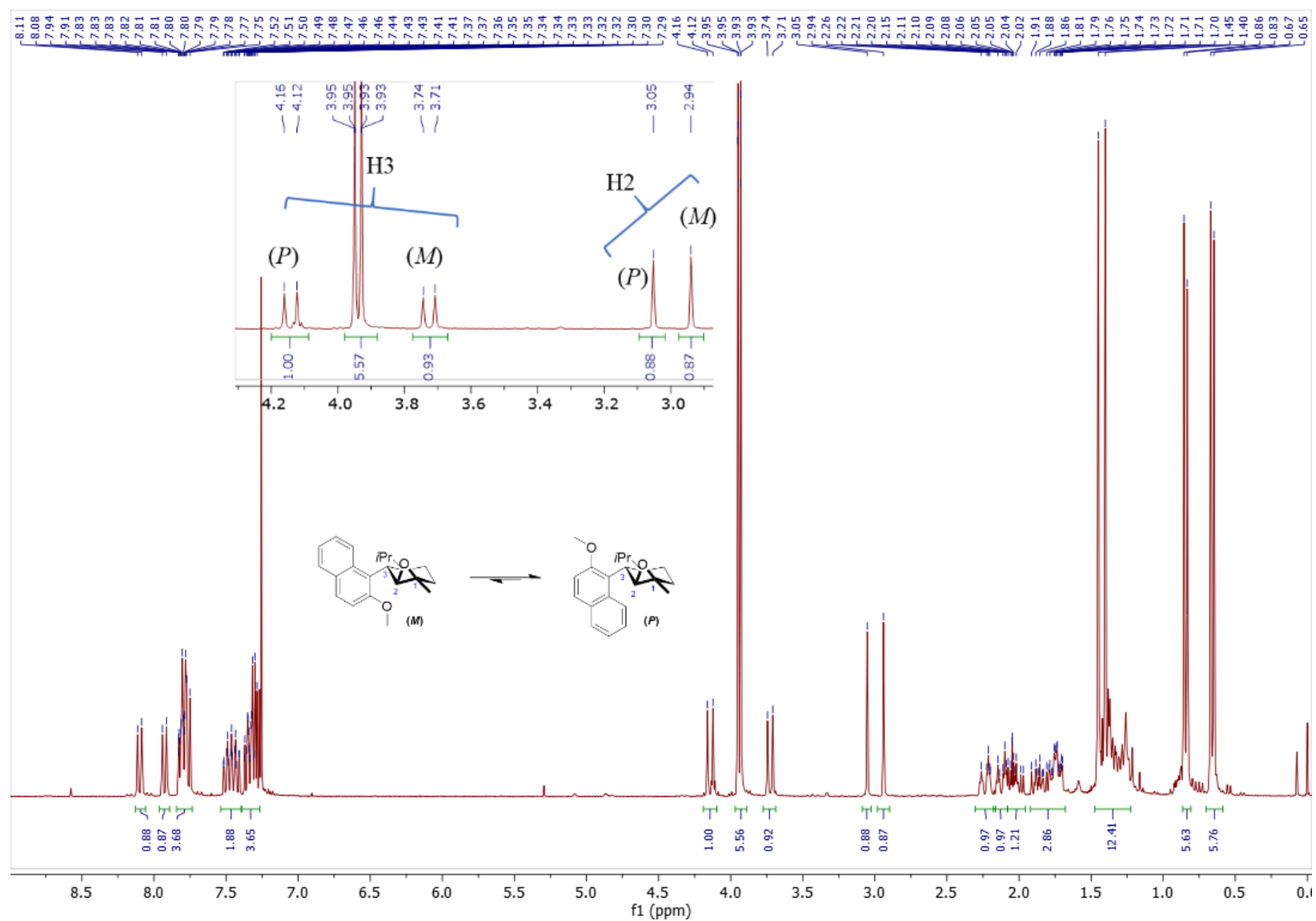
HSQC spectrum of **2c** in DMSO-*d*<sub>6</sub> at 298 K



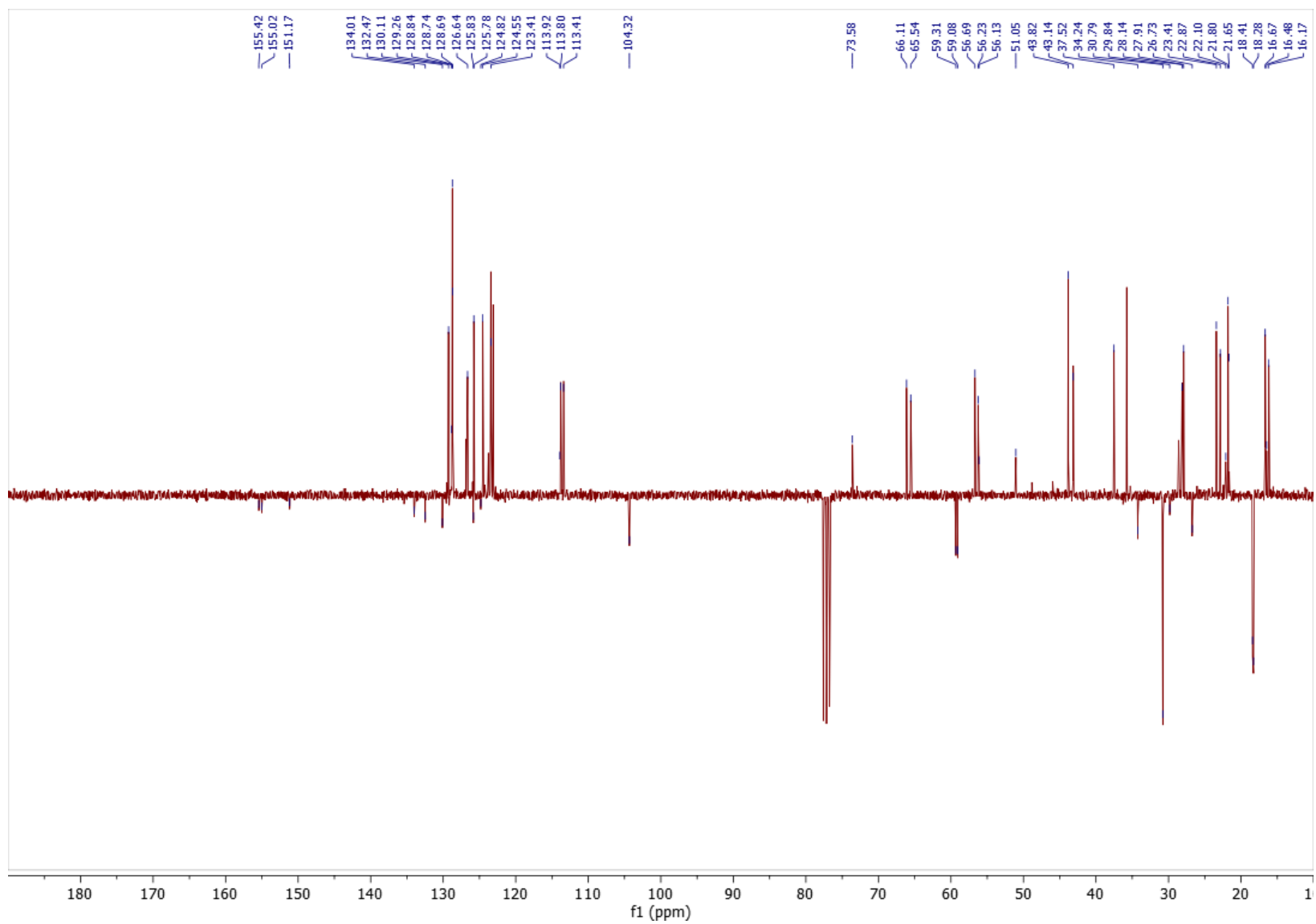
HMBC spectrum of **2c** in DMSO-*d*<sub>6</sub> at 298 K



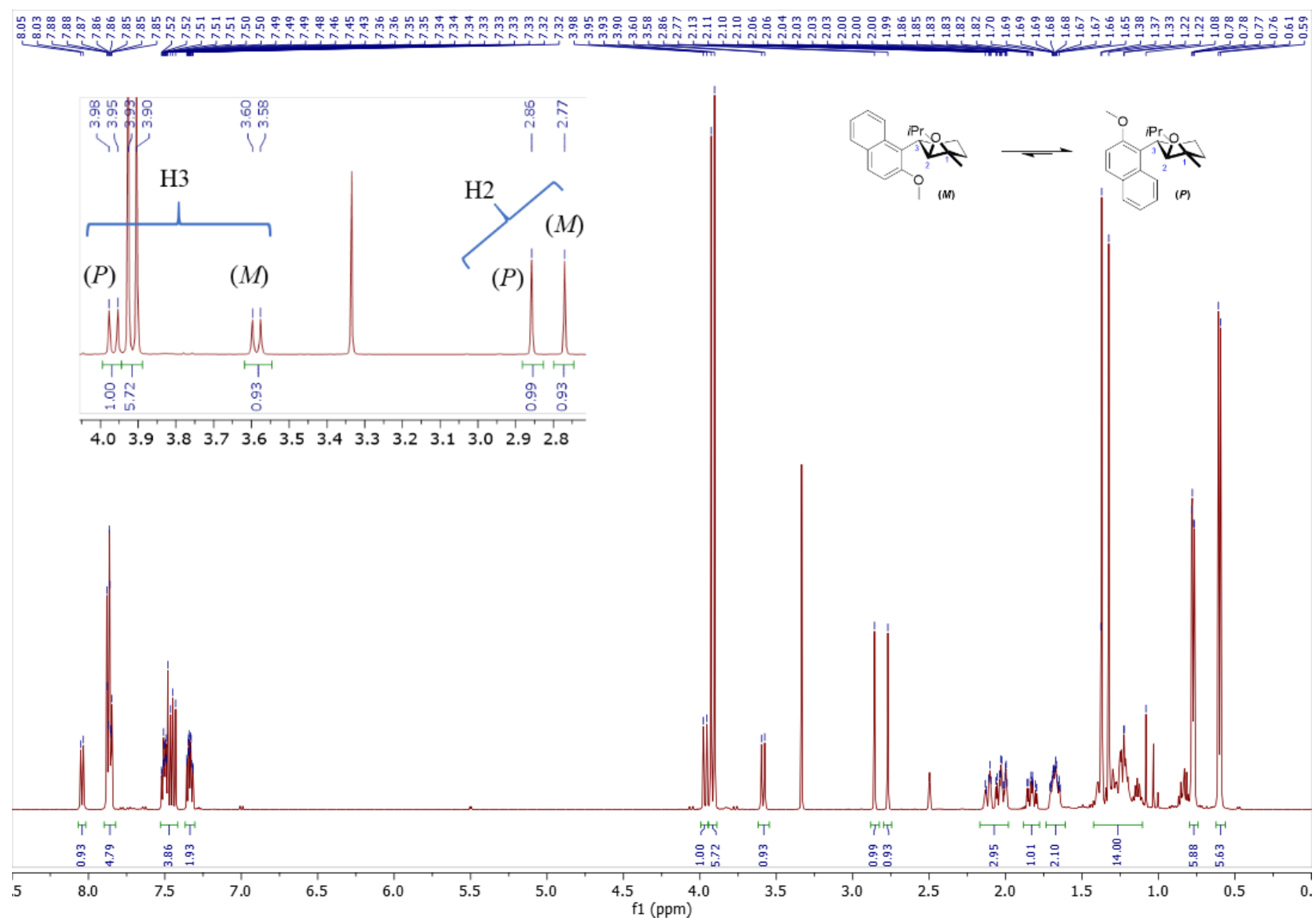
300 MHz  $^1\text{H}$  spectrum of **3b** in  $\text{CDCl}_3$  at 298 K



75 MHz  $^{13}\text{C}$  spectrum of **3b** in  $\text{CDCl}_3$  at 298 K

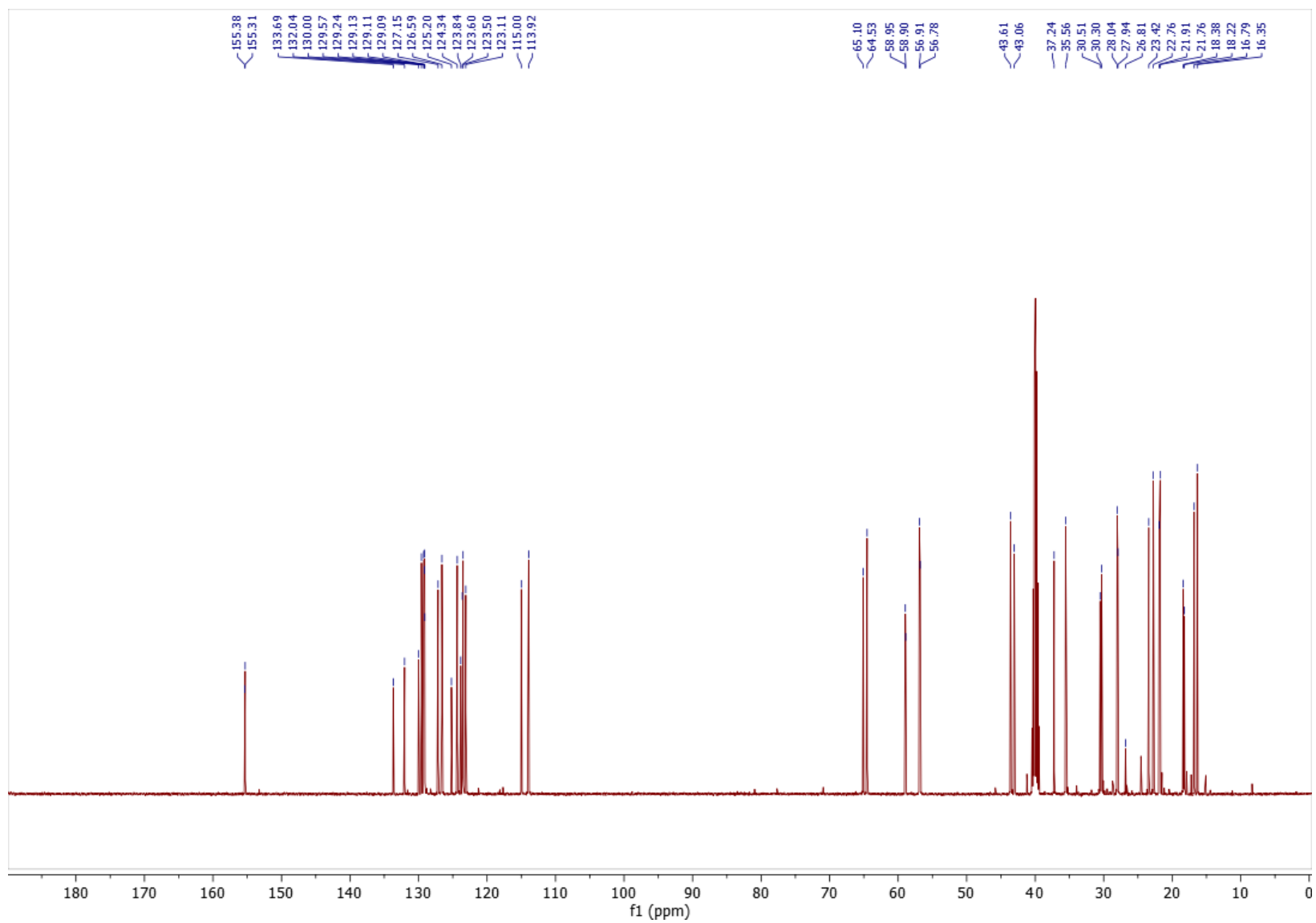


500 MHz  $^1\text{H}$  spectrum of **3b** in DMSO- $d_6$  at 298 K

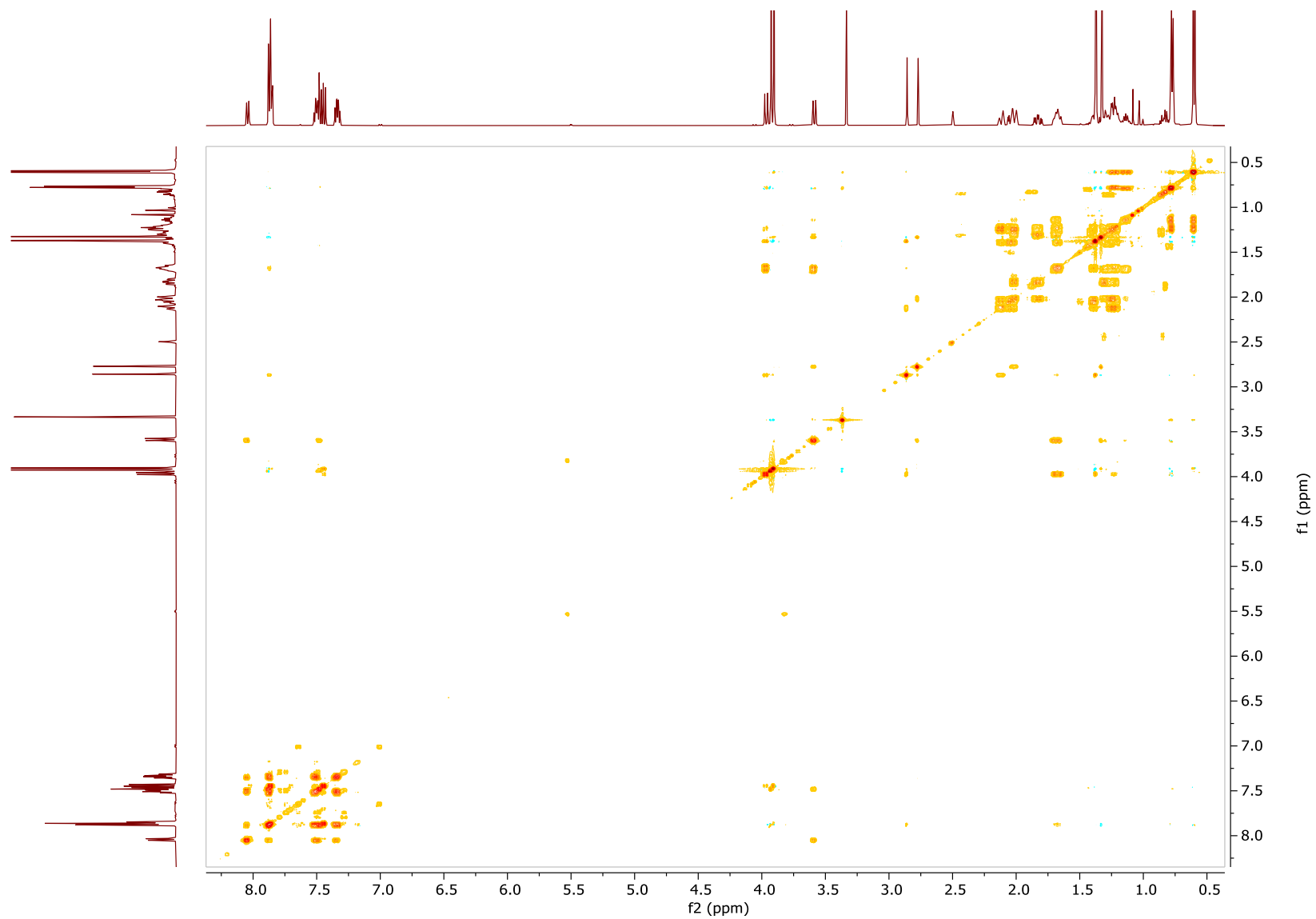




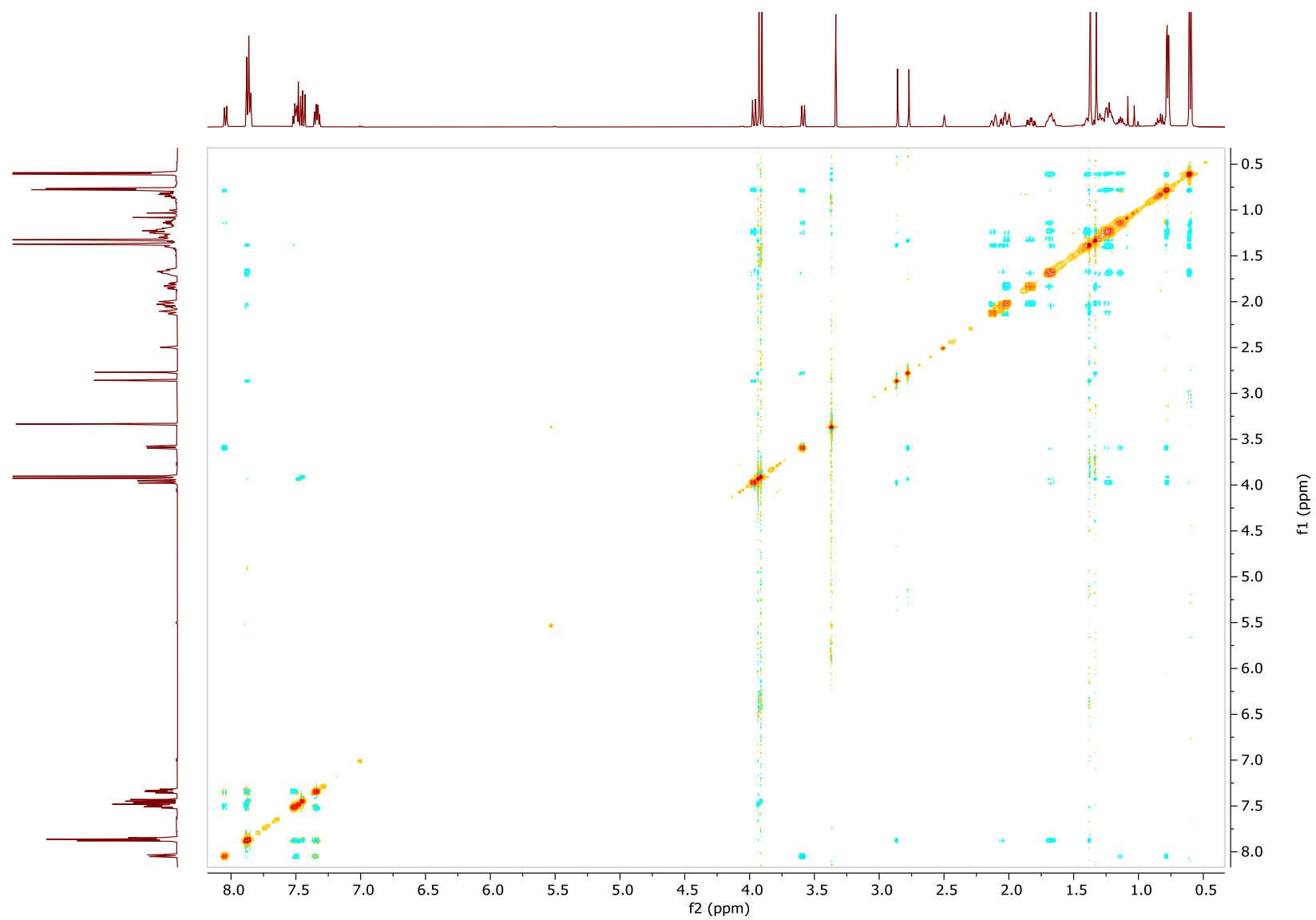
150 MHz  $^{13}\text{C}$  spectrum of **3b** in DMSO-*d*<sub>6</sub> at 298 K



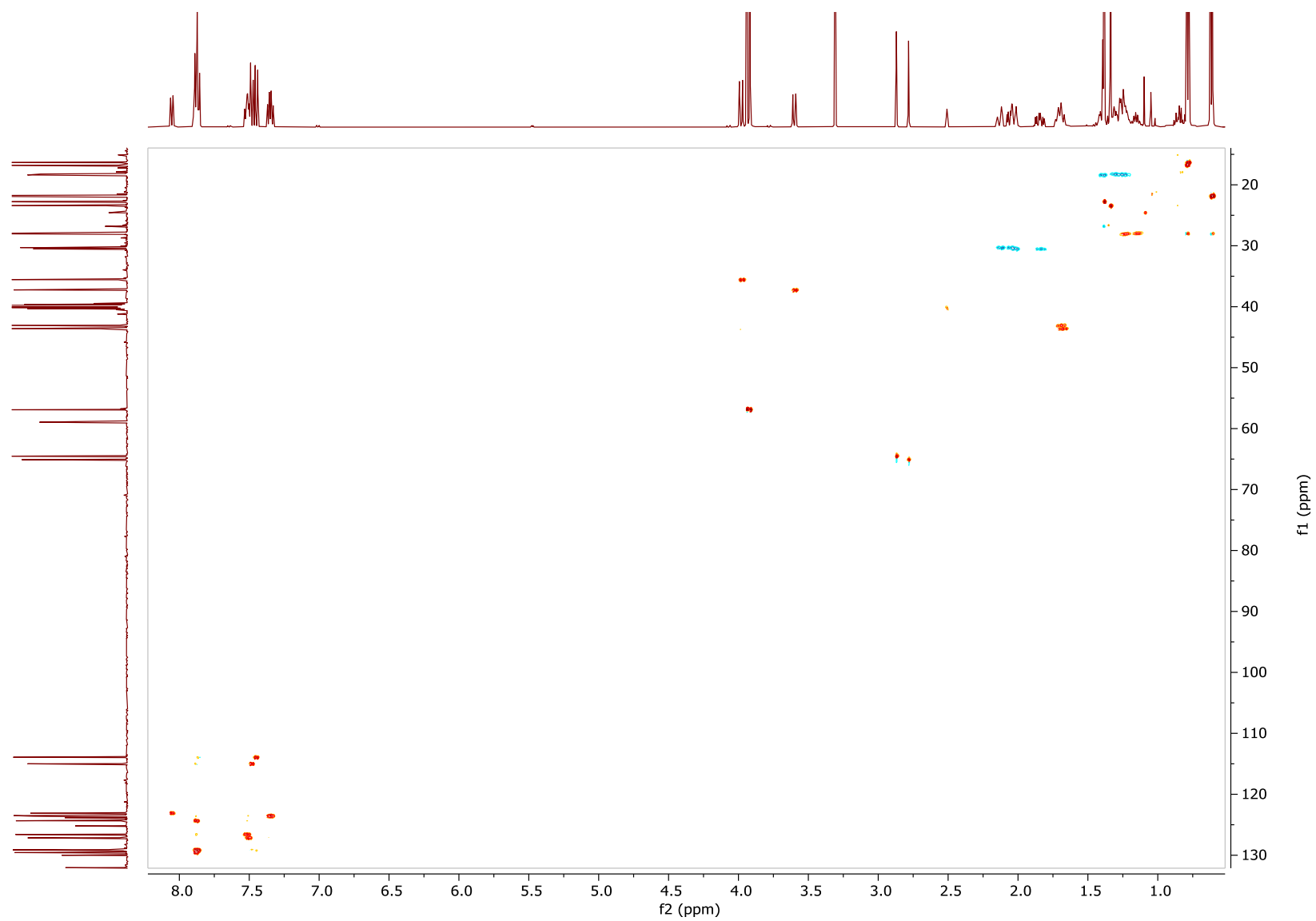
COSY spectrum of **3b** in DMSO-*d*<sub>6</sub> at 298 K



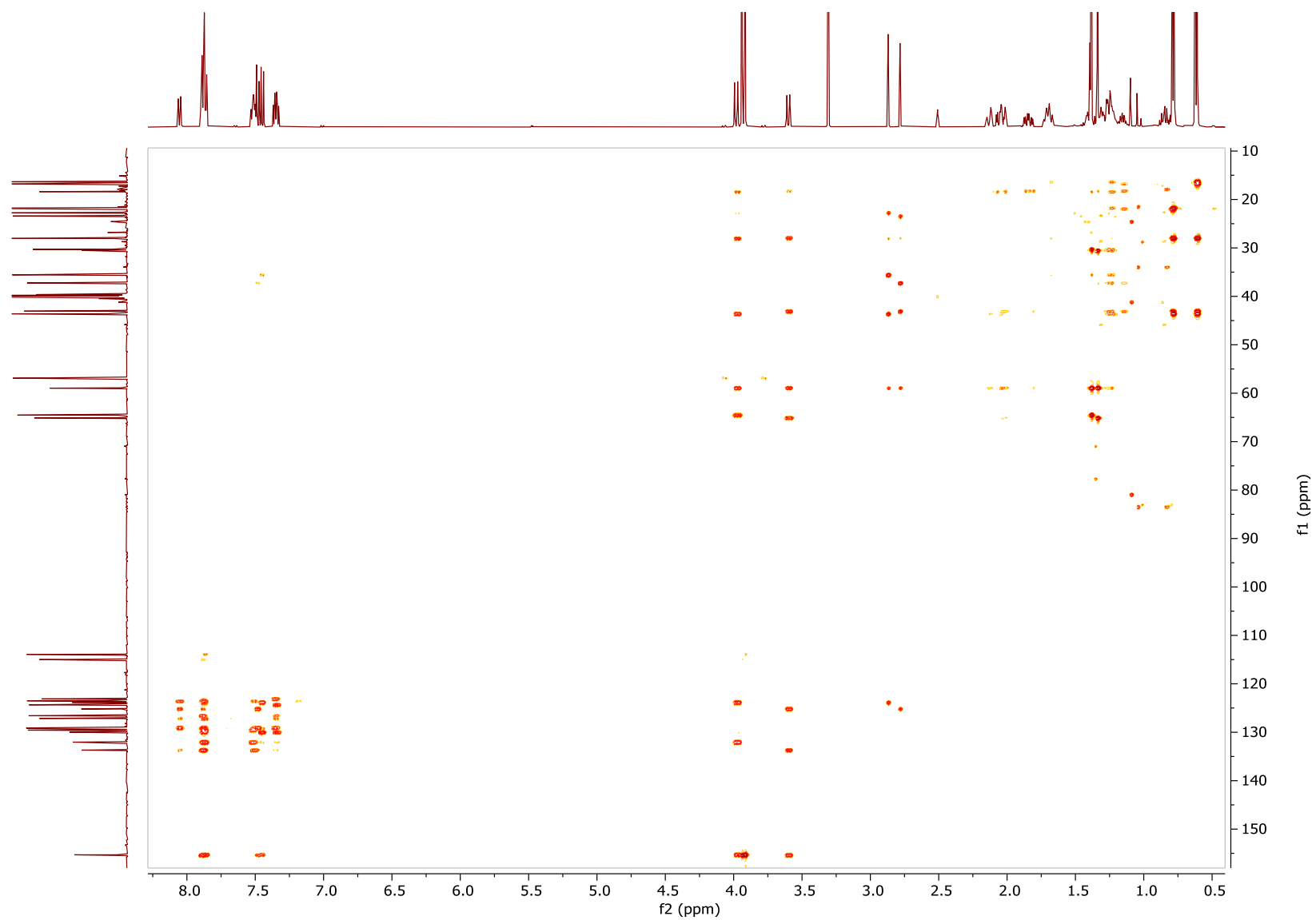
NOESY spectrum of **3b** in DMSO-*d*<sub>6</sub> at 298 K



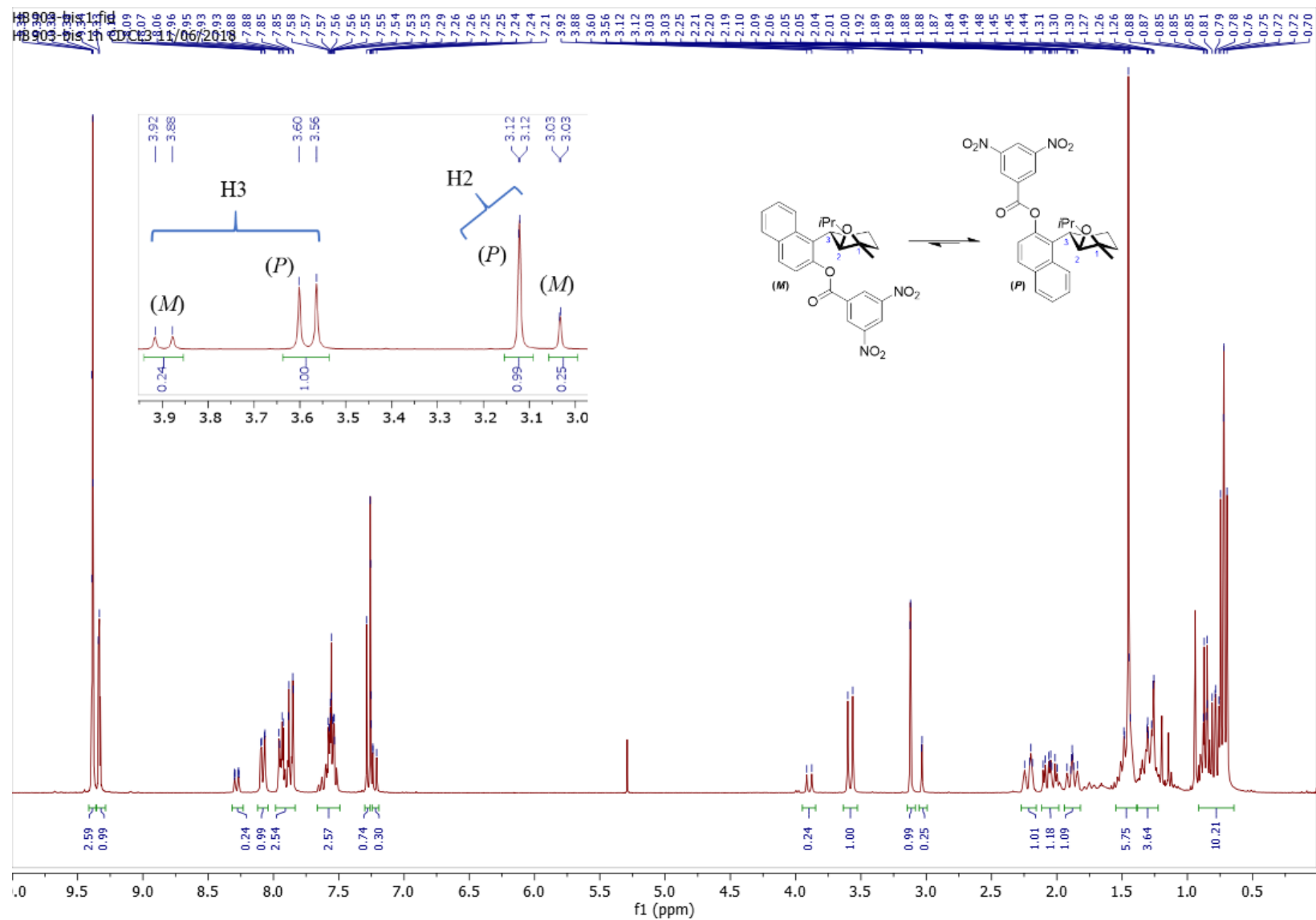
HSQC spectrum of **3b** in DMSO-*d*<sub>6</sub> at 298 K



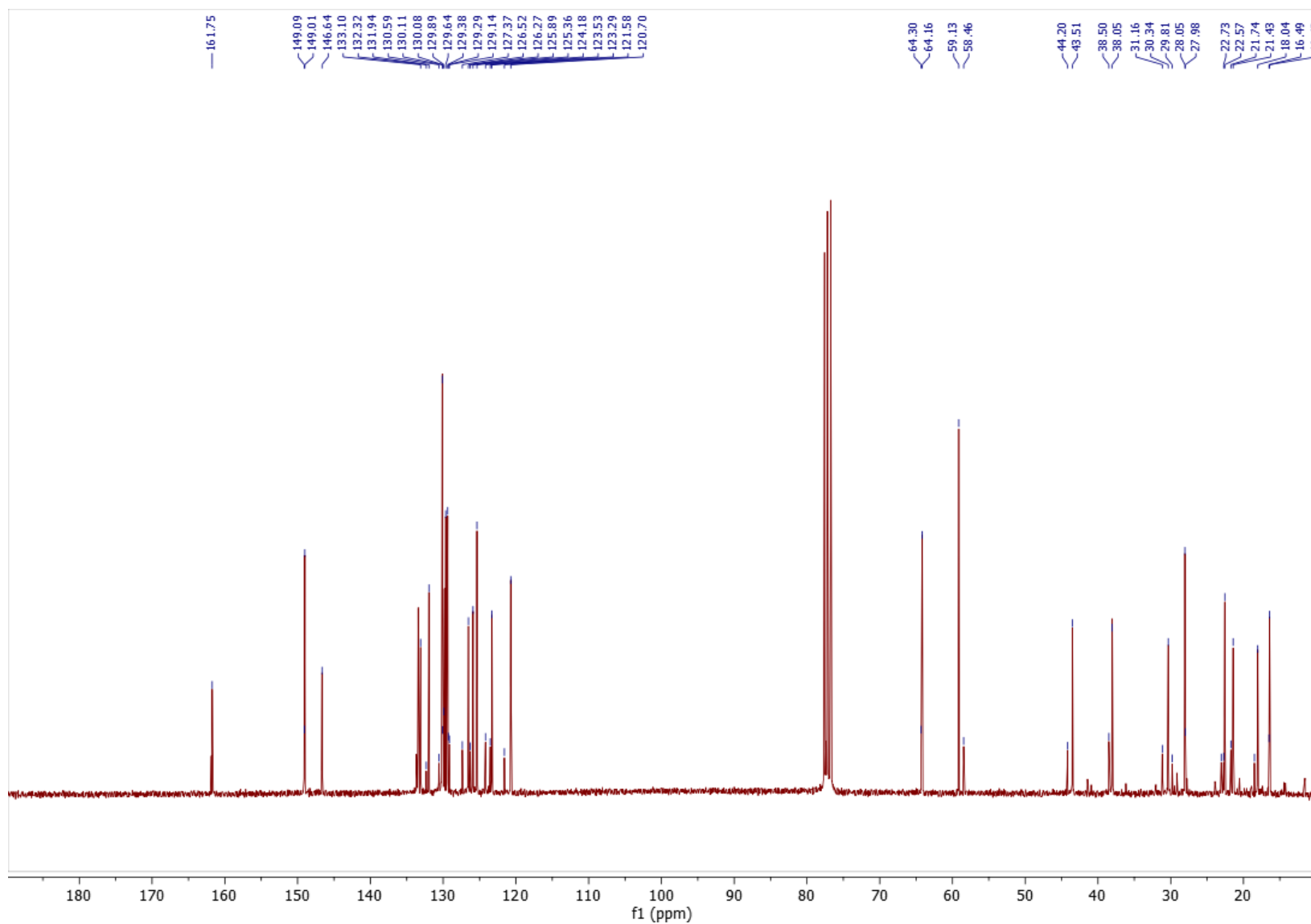
HMBC spectrum of **3b** in DMSO-*d*<sub>6</sub> at 298 K



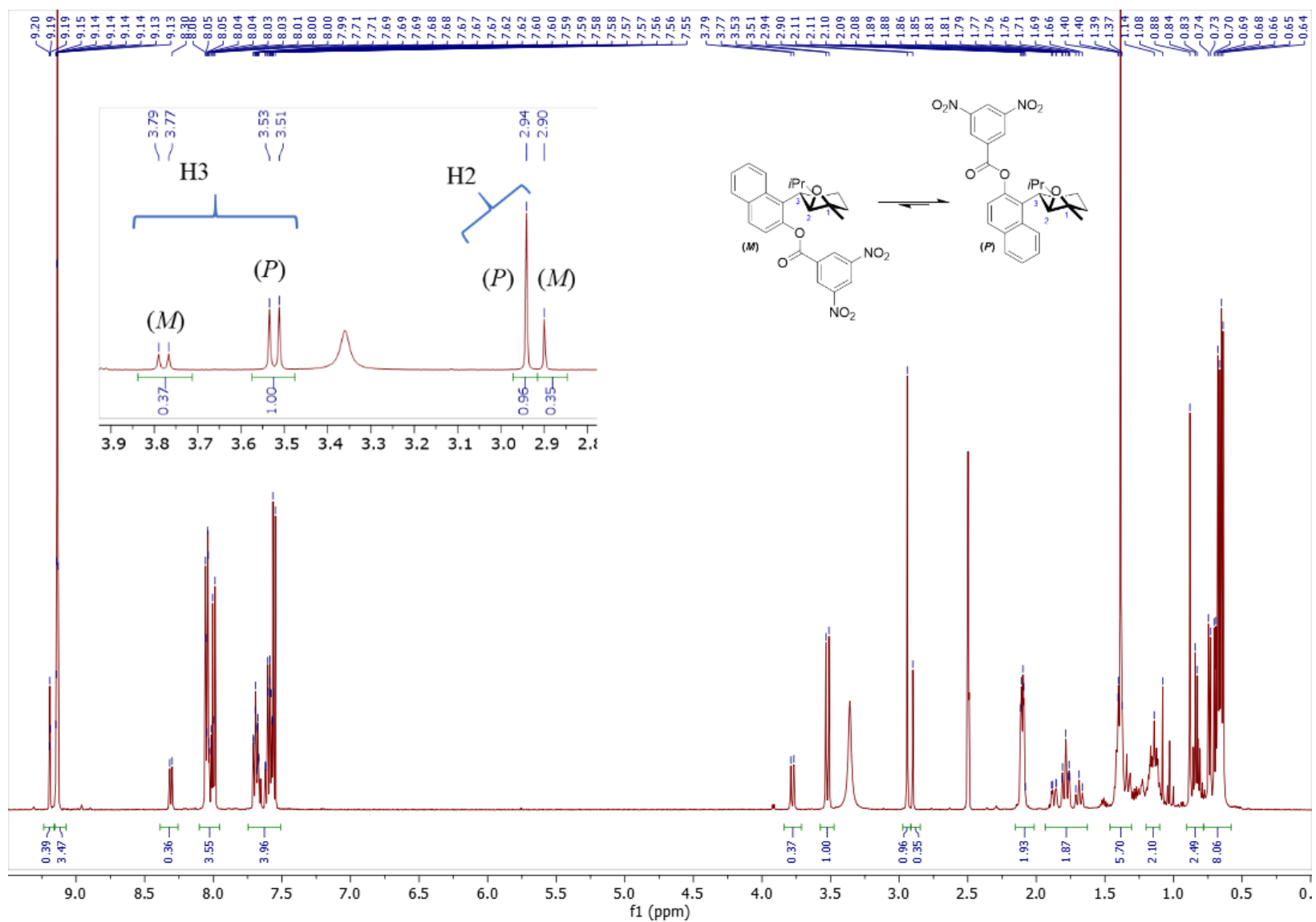
300 MHz  $^1\text{H}$  spectrum of **3c** in  $\text{CDCl}_3$  at 298 K



75 MHz  $^{13}\text{C}$  spectrum of **3c** in  $\text{CDCl}_3$  at 298 K

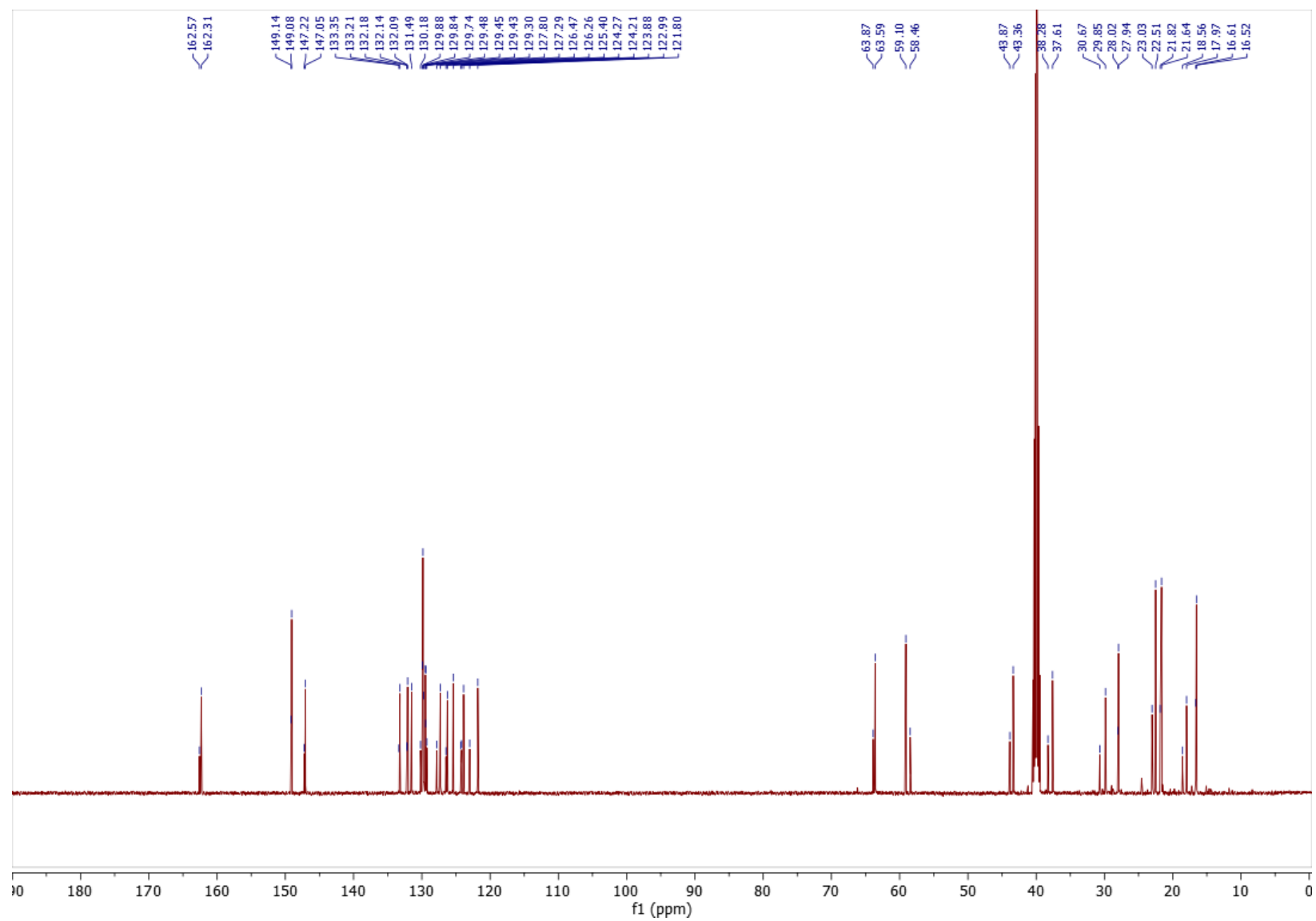


500 MHz  $^1\text{H}$  spectrum of **3c** in DMSO- $d_6$  at 298 K

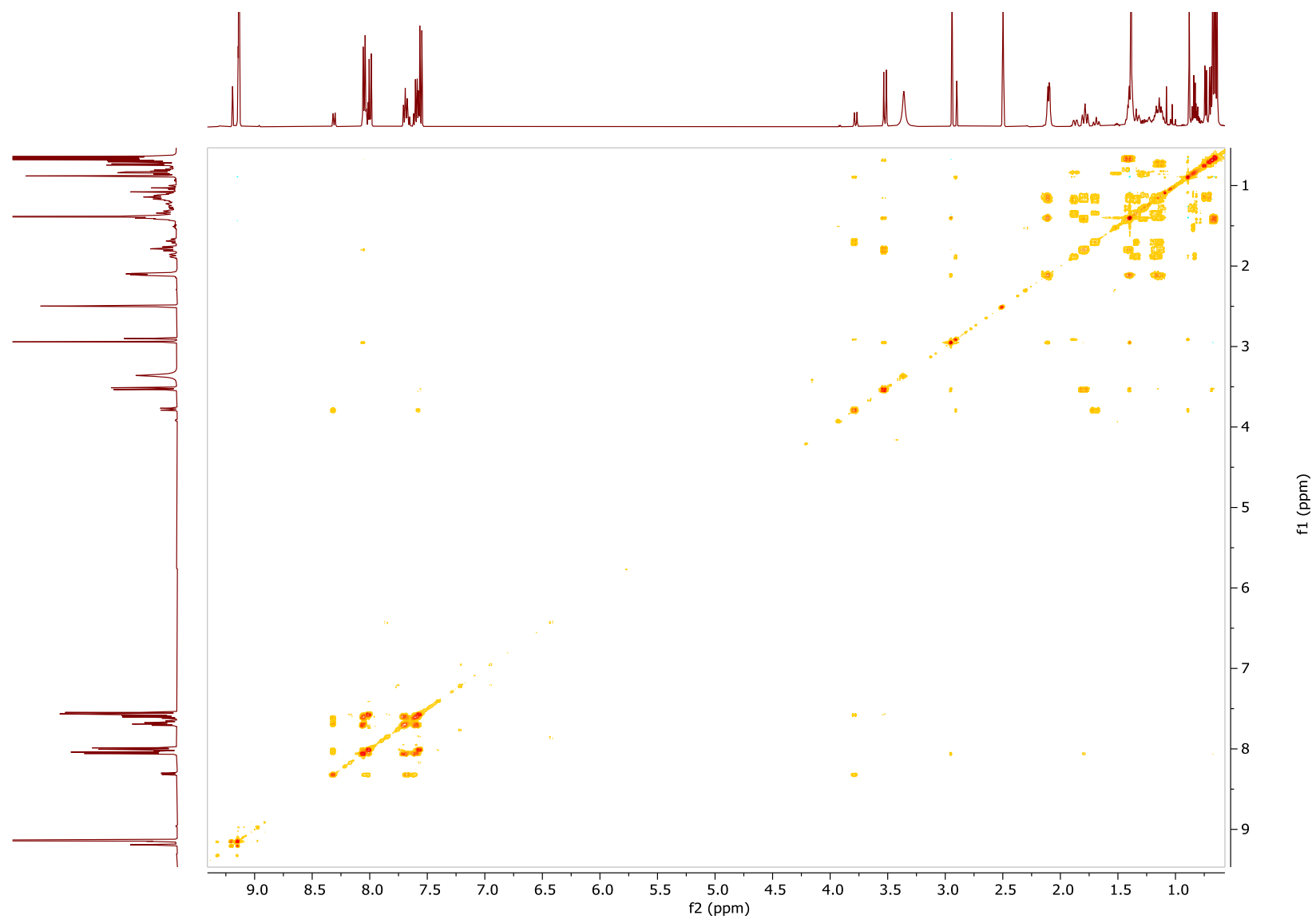




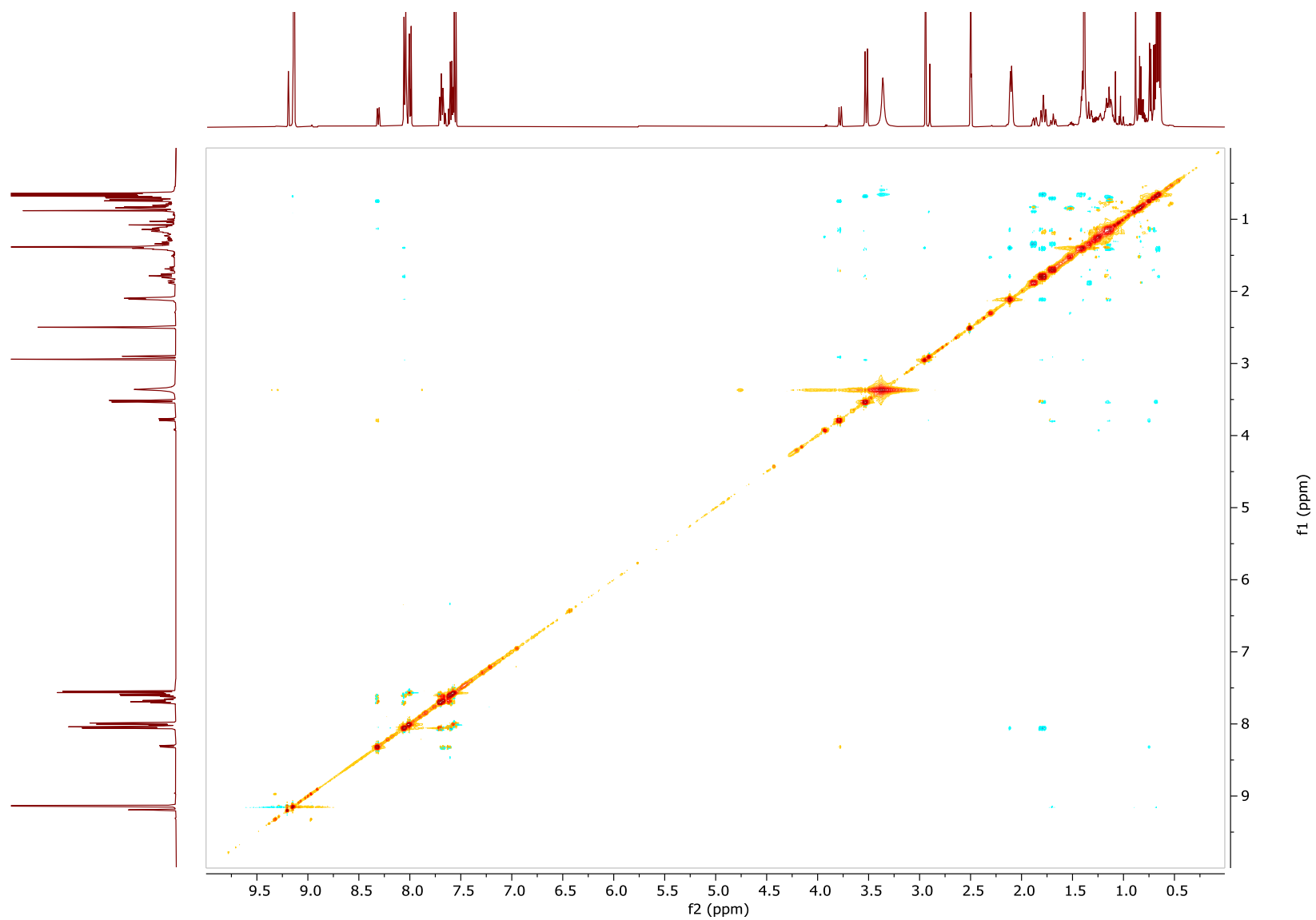
150 MHz  $^{13}\text{C}$  spectrum of **3c** in DMSO-*d*<sub>6</sub> at 298 K



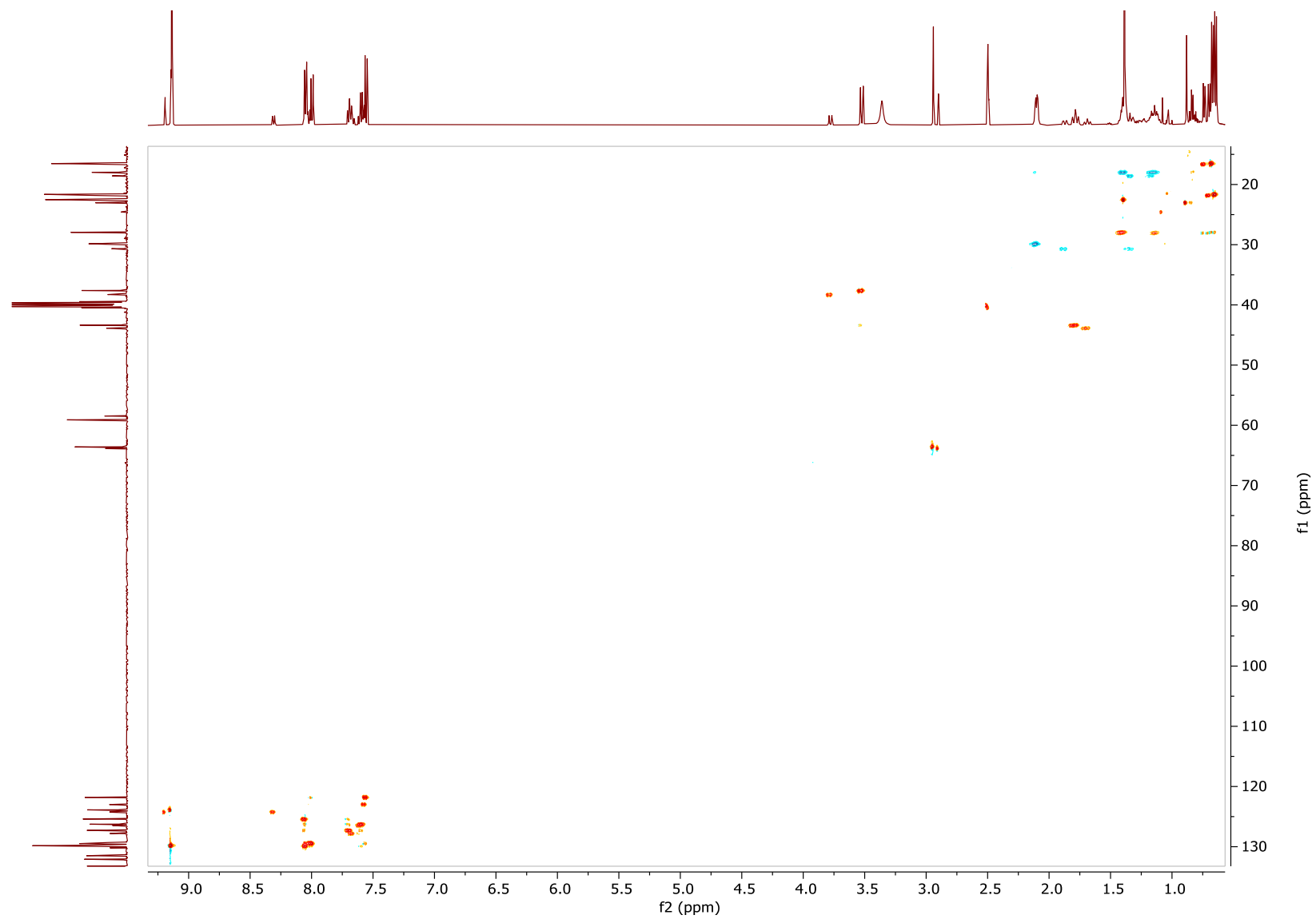
COSY spectrum of **3c** in DMSO-*d*<sub>6</sub> at 298 K



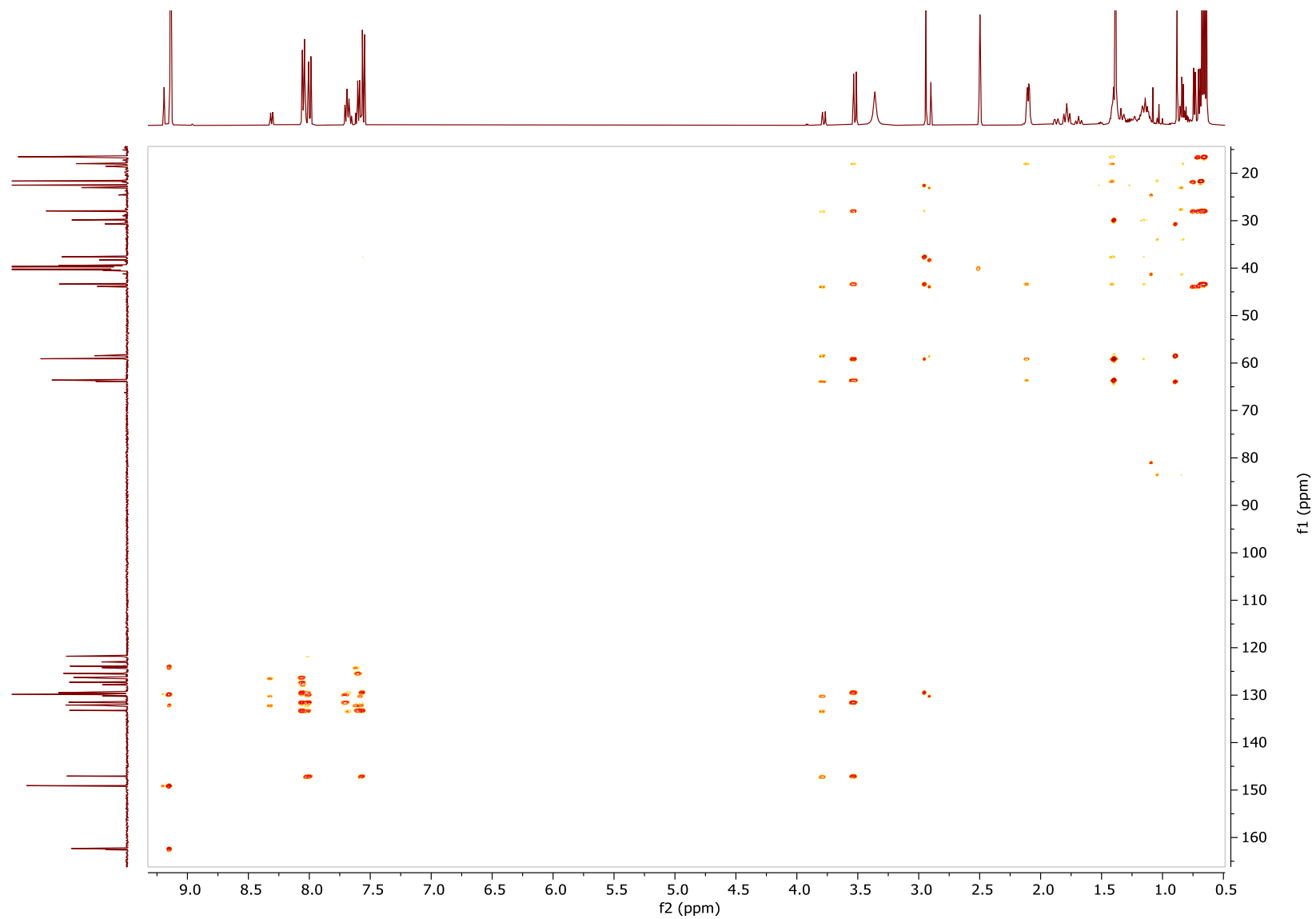
NOESY spectrum of **3c** in DMSO-*d*<sub>6</sub> at 298 K



HSQC spectrum of **3c** in DMSO-*d*<sub>6</sub> at 298 K



HMBC spectrum of **3c** in DMSO-*d*<sub>6</sub> at 298 K



**Table S1.** Conformational Analysis Based on the  $^1\text{H}$  NMR and NOESY Spectra Data for Naphthylcyclohexanes **2a-c** at 298 K.

<i>Sub.</i>	<i>Solvent</i>	<i>Ratio</i> <sup>[a]</sup>	$\delta_{\text{C3-H}}$ <sup>[b]</sup> (ppm)	$\Delta\delta$ <sup>[c]</sup> (ppm)
<i>(M,P)</i> - <b>2a</b>	$\text{CDCl}_3$	25:75	3.55, 3.42	0.13
	$\text{DMSO-}d_6$	28:72	3.66, 3.30	0.36
<i>(M,P)</i> - <b>2b</b>	$\text{CDCl}_3$	30:70	3.81, 3.38	0.43
	$\text{DMSO-}d_6$	28:72	3.68, 3.29	0.39
<i>(M,P)</i> - <b>2c</b>	$\text{CDCl}_3$	25:75	3.24, 3.58	0.34
	$\text{DMSO-}d_6$	27:73	3.27, 3.62	0.35

[a] Ratio of conformers. [b] C3-H chemical shift of conformers. [c] Chemical shift variation between conformers.

**Table S2.** Conformational Analysis Based on the  $^1\text{H}$  NMR and NOESY Spectra Data for Naphthylcyclohexene oxides **3b,c** at 298 K.

<i>Sub.</i>	<i>Solvent</i>	<i>Ratio</i> <sup>[a]</sup>	$\delta_{\text{C3-H}}$ <sup>[b]</sup> (ppm)	$\Delta\delta$ <sup>[c]</sup> (ppm)
<i>(M,P)</i> - <b>3b</b>	$\text{CDCl}_3$	45:55	3.74, 4.15	0.41
	$\text{DMSO-}d_6$	45:55	3.59, 3.97	0.38
<i>(M,P)</i> - <b>3c</b>	$\text{CDCl}_3$	20:80	3.90, 3.58	0.32
	$\text{DMSO-}d_6$	25:75	3.79, 3.53	0.26

[a] Ratio of conformers. [b] C3-H chemical shift of conformers. [c] Chemical shift variation between conformers.

### VT-NMR Experiments and Determination of Activation/Kinetic Parameters:

VT- 2D EXSY:

EXSY spectra of naphthylcyclohexanes **2a-c** and naphthylcyclohexene oxides **3b,c** in DMSO-*d*<sub>6</sub> were implemented on a Bruker AVIII500 spectrometer. All data matrixes were recorded in States-TPPI mode using the Bruker pulse sequence noesygpqh; their size was 2k × 128 with 4 scans per FID, a 10s relaxation delay and mixing times of 10 and 200 ms were used in the temperature range of 353-393 K for **2a**, 353-413 K for **2b**, 363-423 K for **2c** and 373-423 K for **2'c** (recalculated), and 343-373 K for **3b,c**. For a given temperature *T*, exchange rate constants *k* were determined from a single spectrum in which the crosspeaks had 5-10% of the intensity of the diagonal peaks using the program EXSYCalc.<sup>[3]</sup>

[3] J. C. Cobas, M. Martin-Pastor, *EXSYCalc Version 1.0*, Mestrelab Research.

EXSY determined rates were directly fitted using the Eyring equation:

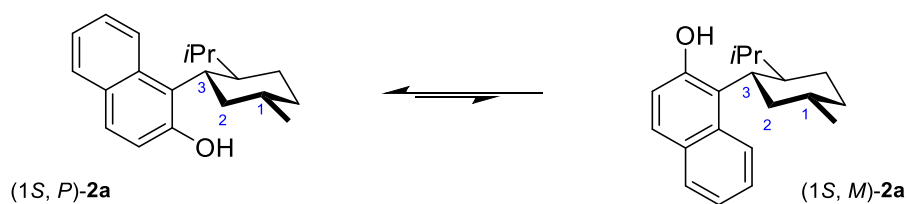
$$k = \frac{k_B \cdot T}{h} \cdot e^{(-\Delta G^\ddagger / R \cdot T)}$$

with *R*, *k<sub>B</sub>* and *h* are gas, Boltzmann's, and Planck's constants, respectively.

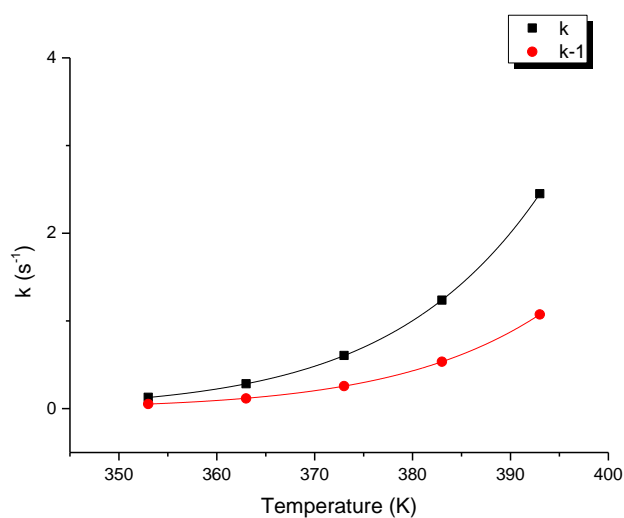
$\Delta G^\ddagger$  was calculated at 298.15 K using  $\Delta G^\ddagger = \Delta H^\ddagger - T\Delta S^\ddagger$

*k* was calculated at 298.15 K using  $k = (k_B T/h) e^{-\Delta G^\ddagger / RT}$

*t*<sub>1/2</sub> was calculated at 298.15 K using  $t_{1/2} = \ln 2/k$

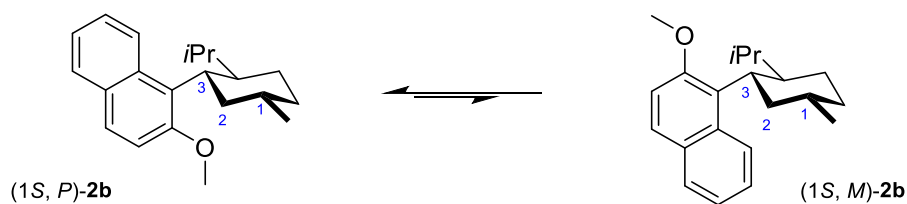
**Table S3.** Rotational Barrier Data for **2a** in DMSO-*d*<sub>6</sub>:

<i>T</i> (K)	$k_{(M) \rightarrow (P)}$ (s <sup>-1</sup> )	$k_{(P) \rightarrow (M)}$ (s <sup>-1</sup> )
353	0.130	0.053
363	0.284	0.116
373	0.606	0.258
383	1.237	0.536
393	2.451	1.074

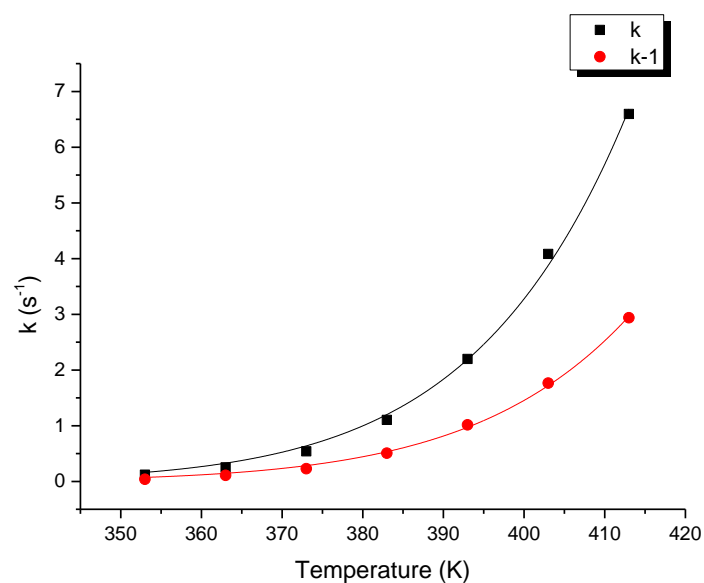
**Graph S1.** Eyring fitting of EXSY rates for **2a** in DMSO-*d*<sub>6</sub>:

	<i>(M)</i> → <i>(P)</i>		<i>(P)</i> → <i>(M)</i>	
	<i>Value</i>	<i>SD</i>	<i>Value</i>	<i>SD</i>
$\Delta G^\ddagger$ (kJ/mol)	91.30	0.05	93.80	0.09
$\Delta H^\ddagger$ (kJ/mol)	82.08	0.16	83.96	0.32
$\Delta S^\ddagger$ (J/mol.K)	-30.92	0.38	-32.97	0.75
<i>Correlation coefficient</i>	1		0.99998	



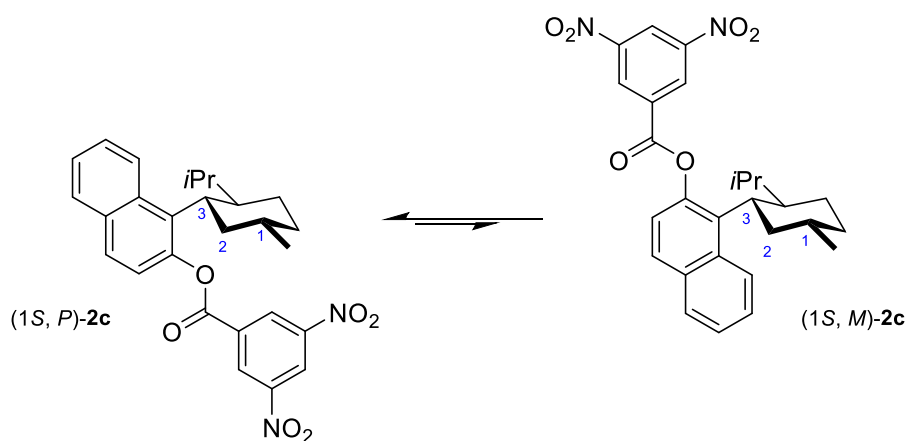
**Table S4.** Rotational Barrier Data for **2b** in DMSO-*d*<sub>6</sub>:

<i>T</i> (K)	$k_{(M) \rightarrow (P)}$ (s <sup>-1</sup> )	$k_{(P) \rightarrow (M)}$ (s <sup>-1</sup> )
353	0.120	0.038
363	0.252	0.109
373	0.540	0.229
383	1.104	0.506
393	2.197	1.016
403	4.084	1.764
413	6.596	2.938

**Graph S2.** Eyring fitting of EXSY rates for **2b** in DMSO-*d*<sub>6</sub>:

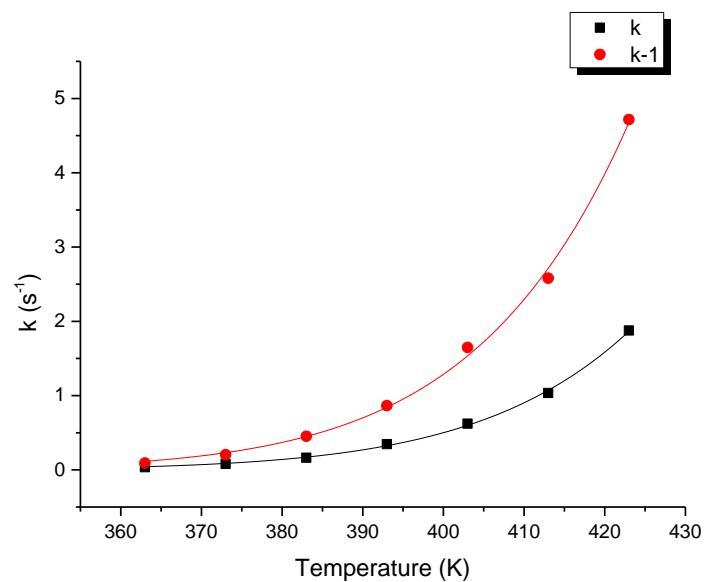
	<i>(M)</i> → <i>(P)</i>		<i>(P)</i> → <i>(M)</i>	
	<i>Value</i>	<i>SD</i>	<i>Value</i>	<i>SD</i>
$\Delta G^\ddagger$ (kJ/mol)	89.13	0.89	91.12	0.76
$\Delta H^\ddagger$ (kJ/mol)	71.95	2.81	71.86	2.36
$\Delta S^\ddagger$ (J/mol.K)	-57.63	6.42	-64.61	5.39
<i>Correlation coefficient</i>	0.99736		0.99812	

**Table S5.** Rotational Barrier Data for **2c** in DMSO-*d*<sub>6</sub>:



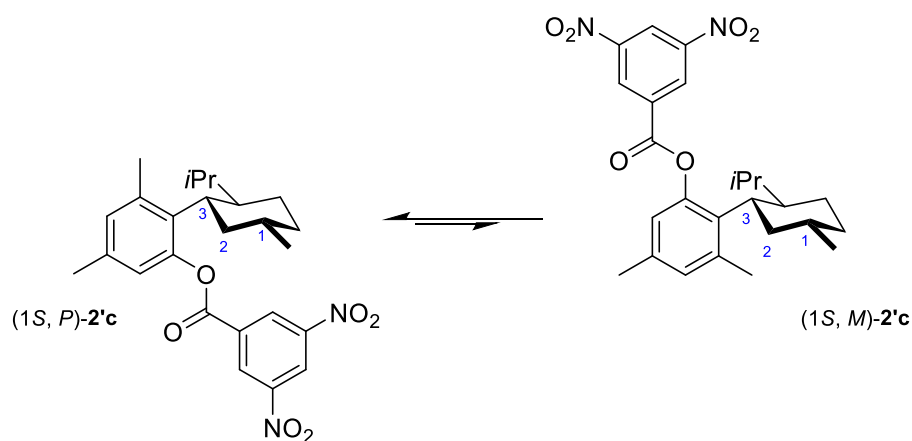
<i>T</i> (K)	$k_{(M) \rightarrow (P)}$ (s <sup>-1</sup> )	$k_{(P) \rightarrow (M)}$ (s <sup>-1</sup> )
363	0.092	0.035
373	0.205	0.080
383	0.452	0.164
393	0.865	0.347
403	1.648	0.623
413	2.581	1.036
423	4.716	1.877

**Graph S3.** Eyring fitting of EXSY rates for **2c** in DMSO-*d*<sub>6</sub>:



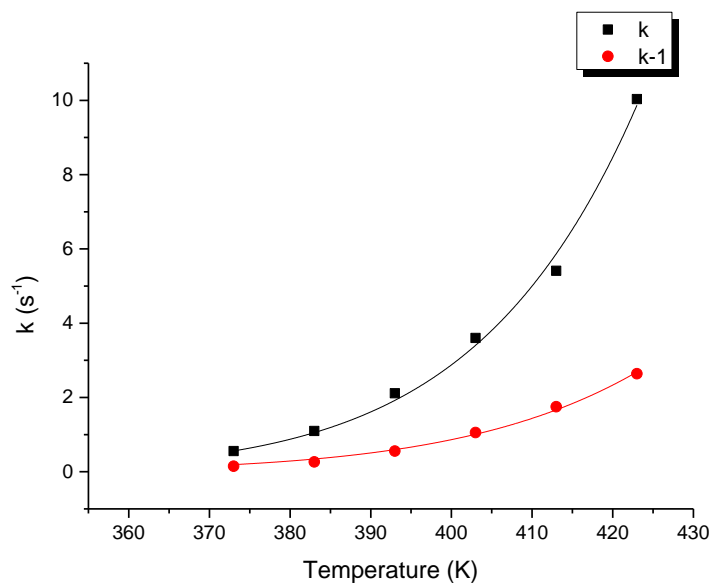
	<i>(M) → (P)</i>		<i>(P) → (M)</i>	
	<i>Value</i>	<i>SD</i>	<i>Value</i>	<i>SD</i>
$\Delta G^\ddagger$ (kJ/mol)	92.36	0.94	95.08	0.67
$\Delta H^\ddagger$ (kJ/mol)	75.53	2.80	77.02	1.99
$\Delta S^\ddagger$ (J/mol.K)	-56.45	6.24	-60.57	4.43
<i>Correlation coefficient</i>	0.99756		0.99883	

**Table S6.** Rotational Barrier Data for **2'c** in DMSO-*d*<sub>6</sub>:



<i>T</i> (K)	$k_{(M) \rightarrow (P)}$ (s <sup>-1</sup> )	$k_{(P) \rightarrow (M)}$ (s <sup>-1</sup> )
373	0.556	0.150
393	1.096	0.265
393	2.114	0.557
403	3.602	1.055
413	5.411	1.750
423	10.035	2.640

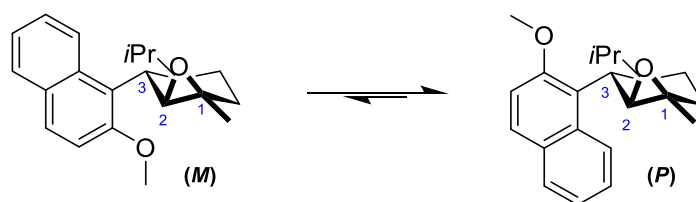
**Graph S4.** Eyring fitting of EXSY rates for **2'c** in DMSO-*d*<sub>6</sub>:



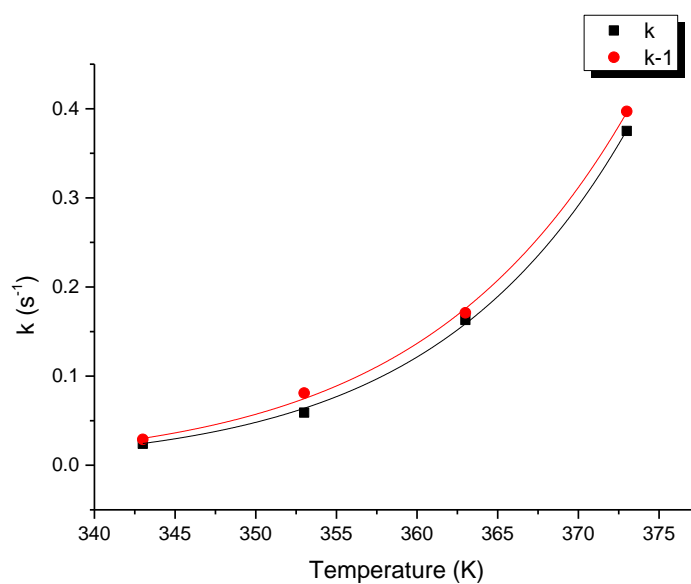
	<i>(M) → (P)</i>		<i>(P) → (M)</i>	
	<i>Value</i>	<i>SD</i>	<i>Value</i>	<i>SD</i>
$\Delta G^\ddagger$ (kJ/mol)	89.46	1.44	90.91	1.22
$\Delta H^\ddagger$ (kJ/mol)	71.97	4.31	65.97	3.64
$\Delta S^\ddagger$ (J/mol.K)	-58.64	9.63	-83.66	8.13
<i>Correlation coefficient</i>	0.99365		0.99446	

**Table S7.** Activation and Kinetic Parameters of Naphthylcyclohexane **2a-c** conformers in DMSO-*d*6 at 298 K.

	<i>Sub.</i>	<i>k</i> ( <i>ms</i> <sup>-1</sup> )	$\Delta G^\ddagger$ ( <i>kJ/mol</i> )	$\Delta H^\ddagger$ ( <i>kJ/mol</i> )	$\Delta S^\ddagger$ ( <i>J/mol.K</i> )	<i>t</i> <sub>1/2</sub> ( <i>s</i> )
<b>2a</b>	( <i>M</i> )→( <i>P</i> )	0.63	91.30 ± 0.05	82.08 ± 0.16	-30.92 ± 0.38	1097.13
	( <i>P</i> )→( <i>M</i> )	0.23	93.80 ± 0.09	83.96 ± 0.32	-32.97 ± 0.75	3006.42
<b>2b</b>	( <i>M</i> )→( <i>P</i> )	1.51	89.13 ± 0.89	71.95 ± 2.81	-57.63 ± 6.42	457.75
	( <i>P</i> )→( <i>M</i> )	0.68	91.12 ± 0.76	71.86 ± 2.36	-64.61 ± 5.39	1021.56
<b>2c</b>	( <i>M</i> )→( <i>P</i> )	0.41	92.36 ± 0.94	75.53 ± 2.80	-56.45 ± 6.24	1684.62
	( <i>P</i> )→( <i>M</i> )	0.14	95.08 ± 0.67	77.02 ± 1.99	-60.57 ± 4.43	5046.91

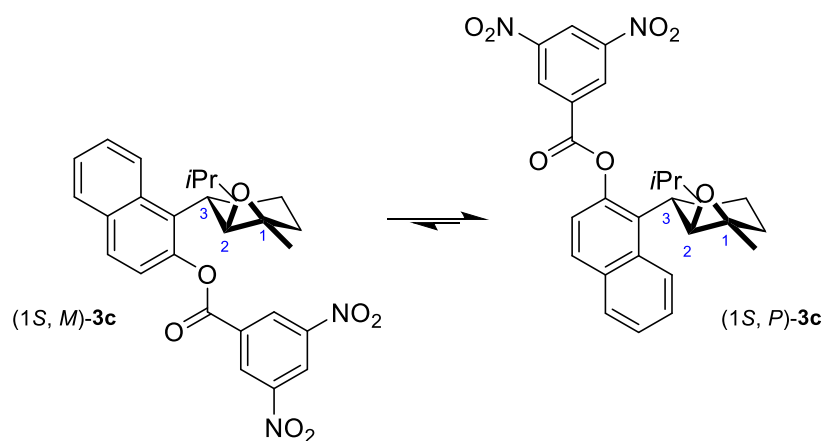
**Table S8.** Rotational Barrier Data for **3b** in **DMSO-*d*<sub>6</sub>**:

<i>T</i> (K)	$k_{(M) \rightarrow (P)}$ ( $s^{-1}$ )	$k_{(P) \rightarrow (M)}$ ( $s^{-1}$ )
343	0.029	0.024
353	0.081	0.059
363	0.171	0.163
373	0.397	0.375

**Graph S5.** Eyring fitting of EXSY rates for **3b** in **DMSO-*d*<sub>6</sub>**:

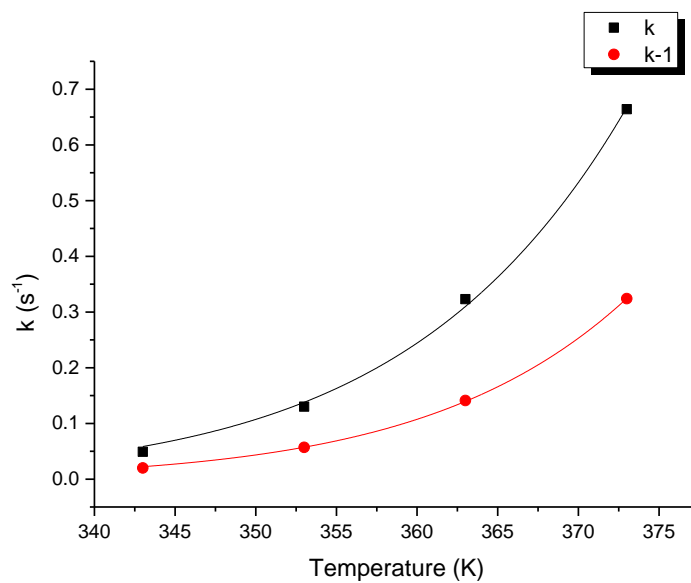
	<i>(P) → (M)</i>		<i>(M) → (P)</i>	
	<i>Value</i>	<i>SD</i>	<i>Value</i>	<i>SD</i>
$\Delta G^\ddagger$ (kJ/mol)	94.86	0.77	93.59	0.83
$\Delta H^\ddagger$ (kJ/mol)	93.99	3.01	88.29	3.25
$\Delta S^\ddagger$ (J/mol.K)	-2.95	7.51	-17.78	8.14
<i>Correlation coefficient</i>	0.99914		0.99875	

**Table S9.** Rotational Barrier Data for **3c** in **DMSO-*d*<sub>6</sub>**:



<i>T</i> (K)	$k_{(M) \rightarrow (P)}$ (s <sup>-1</sup> )	$k_{(P) \rightarrow (M)}$ (s <sup>-1</sup> )
343	0.049	0.020
353	0.130	0.057
363	0.323	0.141
373	0.664	0.324

**Graph S6.** Eyring fitting of EXSY rates for **3c** in **DMSO-*d*<sub>6</sub>**:

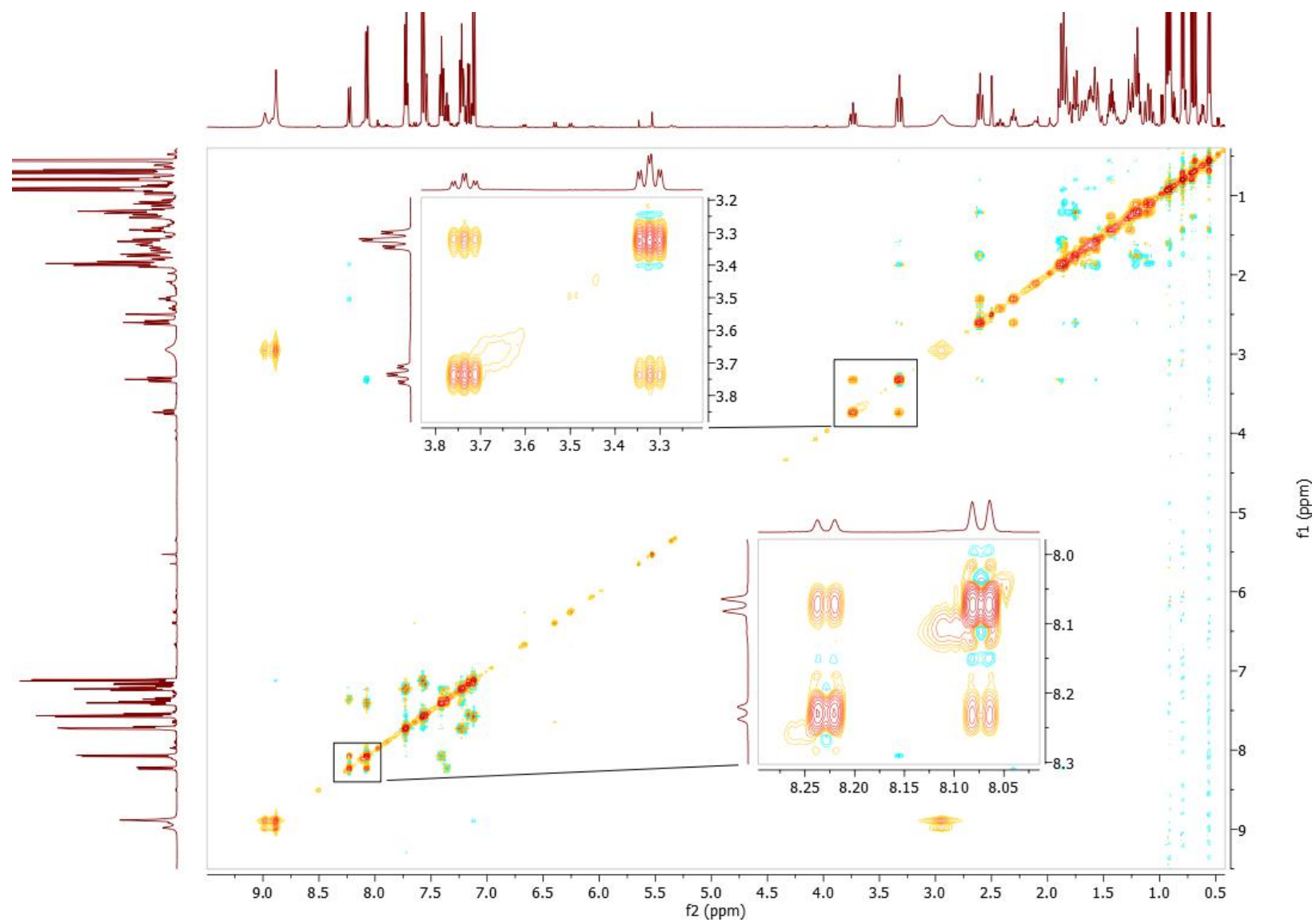


	<i>(P) → (M)</i>		<i>(M) → (P)</i>	
	<i>Value</i>	<i>SD</i>	<i>Value</i>	<i>SD</i>
$\Delta G$ (kJ/mol)	94.81	0.37	91.30	1.02
$\Delta H$ (kJ/mol)	91.89	1.44	83.30	4.03
$\Delta S$ (J/mol.K)	-9.79	3.59	-26.83	10.09
<i>Correlation coefficient</i>	0.99979		0.99775	

**Table S10.** Activation and Kinetic Parameters of Naphthylcyclohexene oxide **3b,c** conformers in DMSO-*d*<sub>6</sub> at 298.15 K.

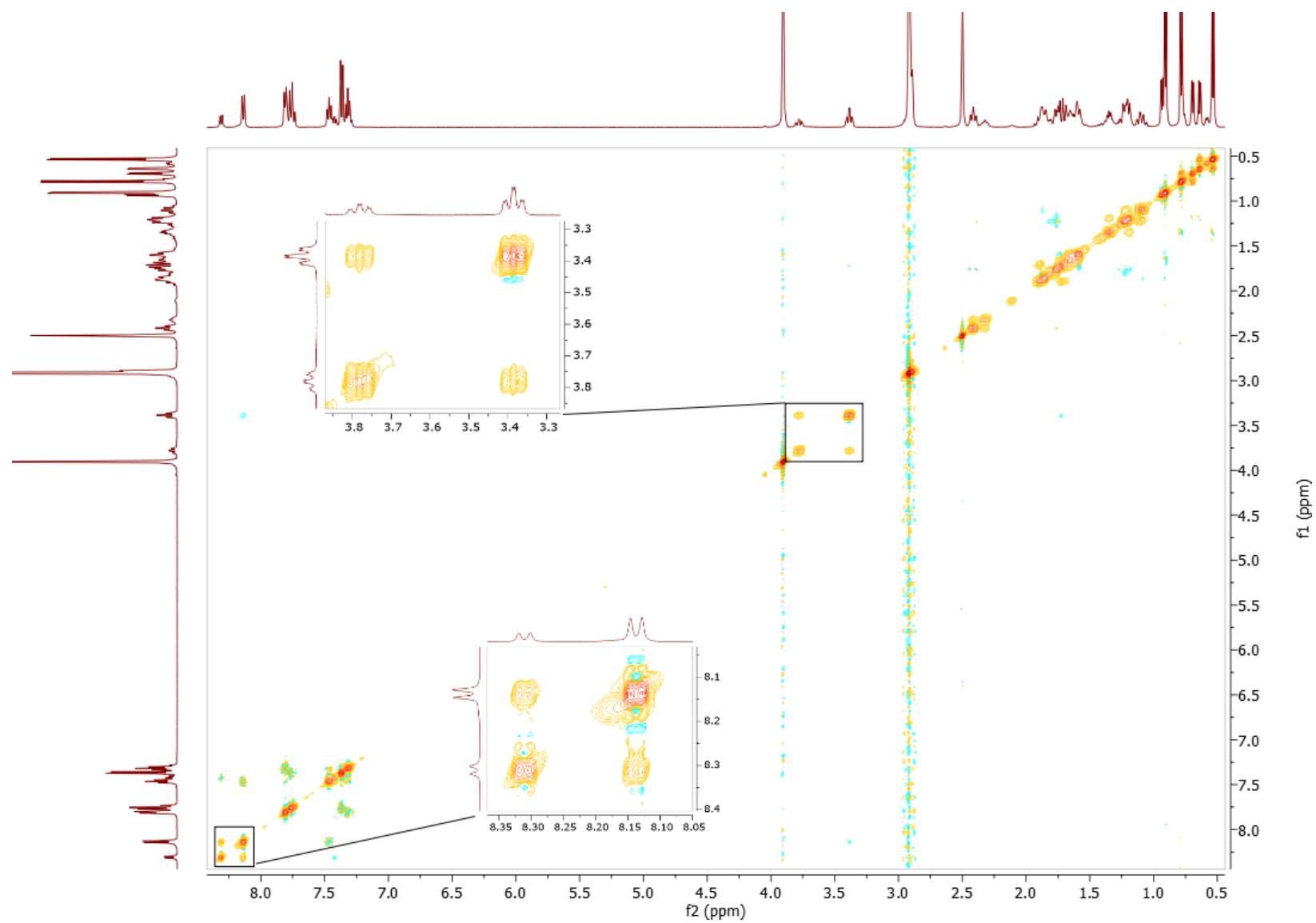
	<i>Sub.</i>	<i>k</i> ( <i>ms</i> <sup>-1</sup> )	$\Delta G^\ddagger$ ( <i>kJ/mol</i> )	$\Delta H^\ddagger$ ( <i>kJ/mol</i> )	$\Delta S^\ddagger$ ( <i>J/mol.K</i> )	<i>t</i> <sub>1/2</sub> ( <i>s</i> )
<b>3b</b>	( <i>M</i> )→( <i>P</i> )	0.25	93.59 ± 0.83	88.29 ± 3.25	-17.78 ± 8.14	2766.87
	( <i>P</i> )→( <i>M</i> )	0.15	94.86 ± 0.77	93.99 ± 3.01	-2.95 ± 7.51	4618.31
<b>3c</b>	( <i>M</i> )→( <i>P</i> )	0.63	91.30 ± 1.02	83.30 ± 4.03	-26.83 ± 10.09	1098.49
	( <i>P</i> )→( <i>M</i> )	0.15	94.81 ± 0.37	91.89 ± 1.44	-9.79 ± 3.59	4526.09

VT-EXSY Spectra at 500 MHz for 2a in DMSO-d<sub>6</sub> at 383 K with d8 = 200 ms

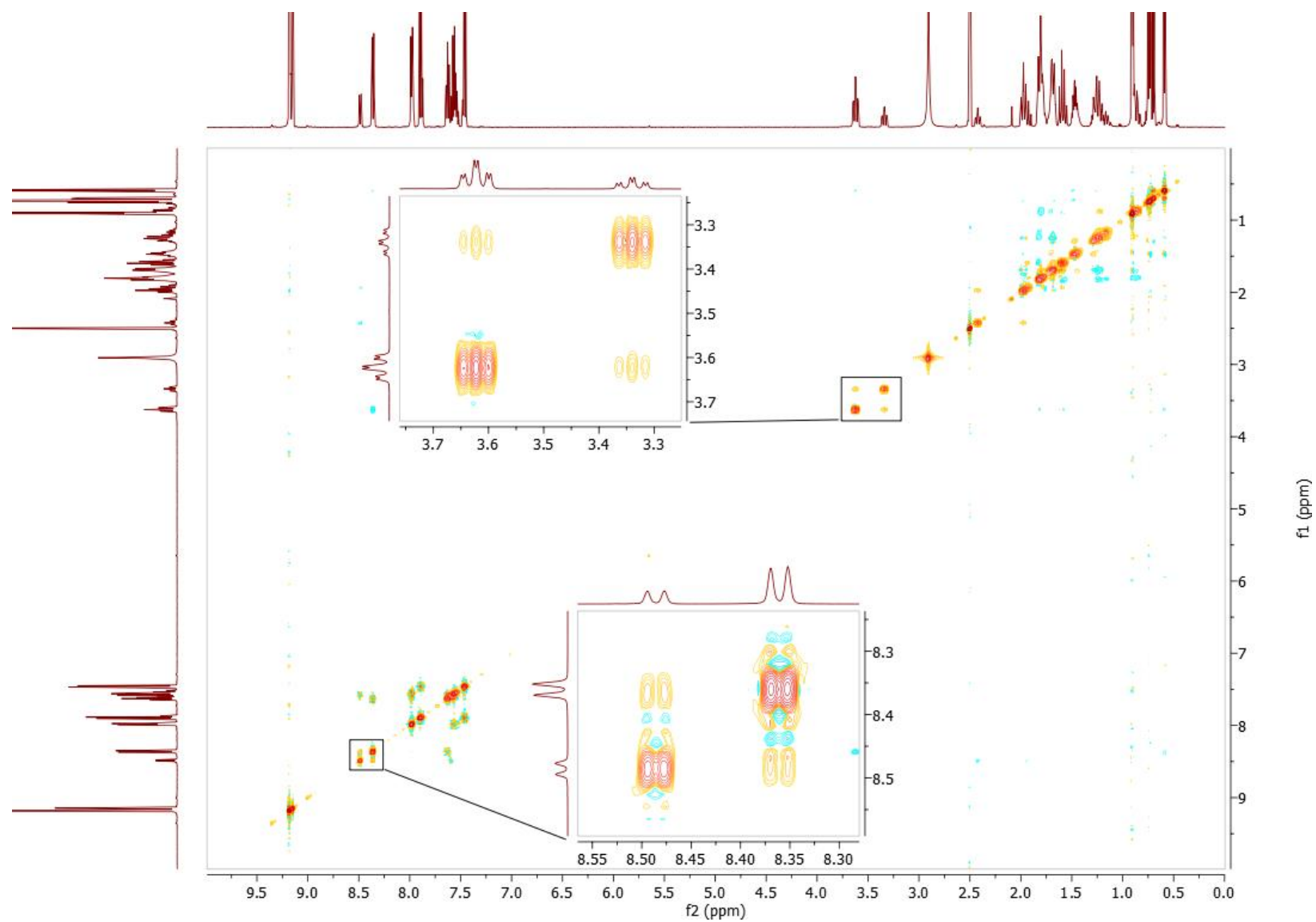




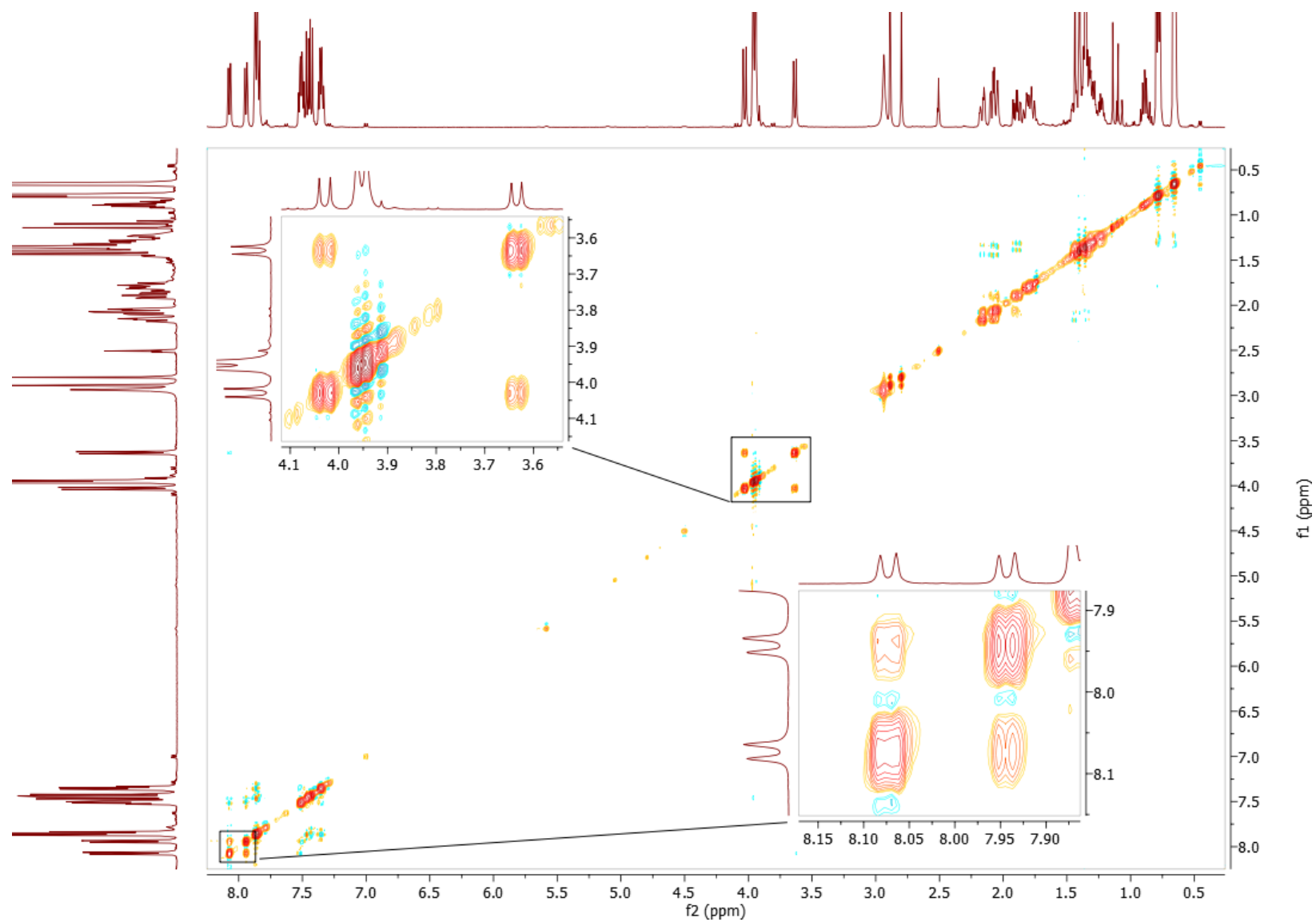
VT-EXSY Spectra at 500 MHz for **2b** in DMSO-*d*<sub>6</sub> at 383 K with d8 = 200 ms



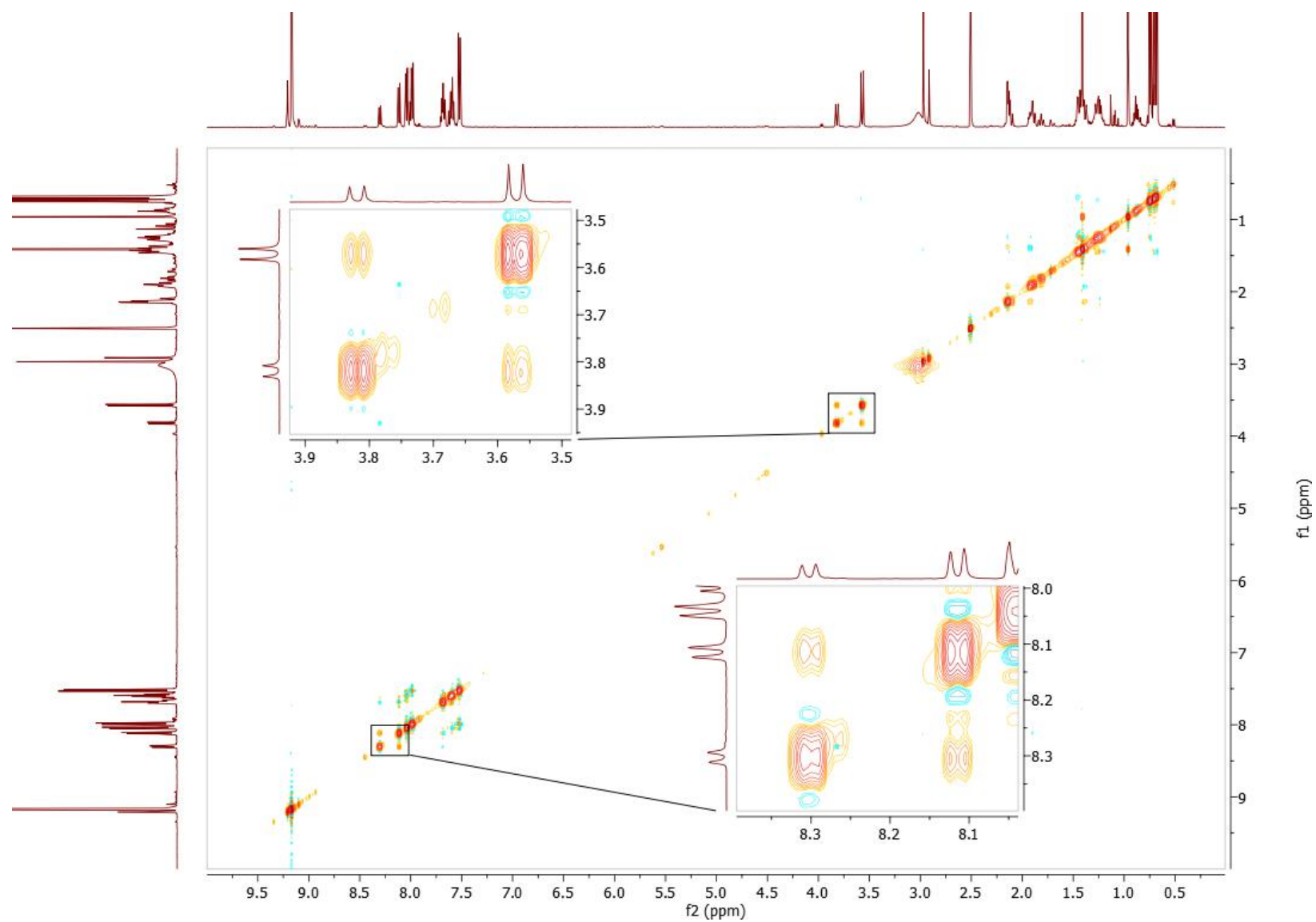
VT-EXSY Spectra at 500 MHz for **2c** in DMSO-*d*<sub>6</sub> at 383 K with d8 = 200 ms



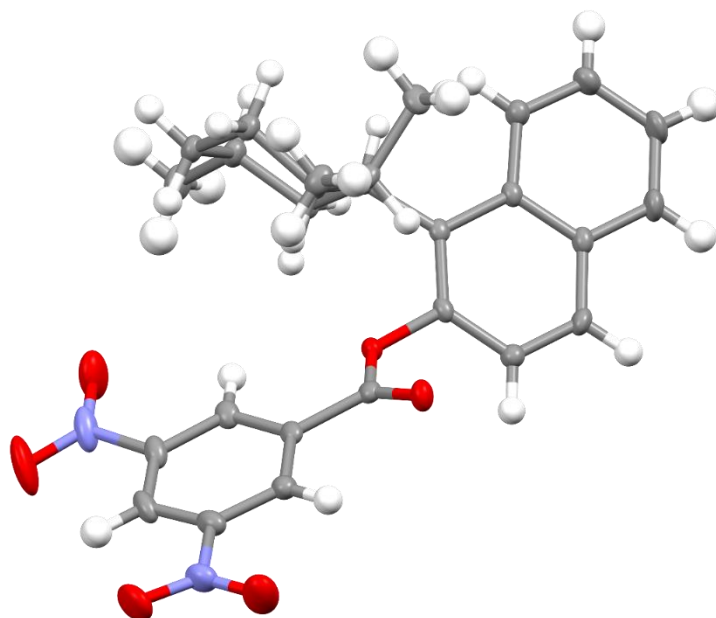
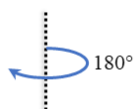
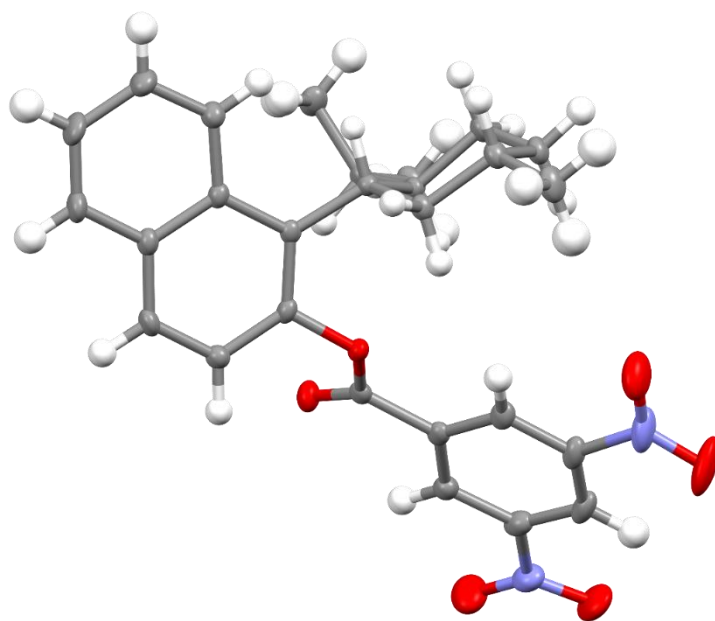
VT-EXSY Spectra at 500 MHz for **3b** in DMSO- $d_6$  at 383 K with  $d_8 = 200$  ms



VT-EXSY Spectra at 500 MHz for **3c** in DMSO-*d*<sub>6</sub> at 383 K with d8 = 200 ms



Single-crystal X-ray structure of (P)-2c:



**Table S11:** Crystal data and structure refinement for (*P*)-**2c** ([CCDC-2226732](#)).

Empirical formula  $C_{27}H_{28}N_2O_6$

Formula weight 476.51

Temperature/K 103

Crystal system monoclinic

Space group P21

$a/\text{\AA}$  11.6688(4)

$b/\text{\AA}$  7.6572(2)

$c/\text{\AA}$  13.4891(4)

$\alpha/^\circ$  90

$\beta/^\circ$  101.345(2)

$\gamma/^\circ$  90

Volume/ $\text{\AA}^3$  1181.71(6)

Z 2

$\rho_{\text{calc}}/\text{cm}^3$  1.339

$\mu/\text{mm}^{-1}$  0.751

F(000) 536.0

Crystal size/ $\text{mm}^3$   $0.4 \times 0.3 \times 0.3$

Radiation  $\text{CuK}\alpha$  ( $\lambda = 1.54184$ )

$2\theta$  range for data collection/ $^\circ$  10.542 to 146.628

Index ranges  $-6 \leq h \leq 8$ ,  $-11 \leq k \leq 11$ ,  $-24 \leq l \leq 24$

Reflections collected 4948

Independent reflections 2428 [ $R_{\text{int}} = 0.0215$ ,  $R_{\text{sigma}} = 0.0204$ ]

Data/restraints/parameters 2428/0/173

Goodness-of-fit on  $F_2$  1.141

Final R indexes [ $I \geq 2\sigma(I)$ ]  $R_1 = 0.0443$ ,  $wR_2 = 0.1214$

Final R indexes [all data]  $R_1 = 0.0548$ ,  $wR_2 = 0.1490$

Largest diff. peak/hole /  $e \text{\AA}^{-3}$  0.21/-0.20

### Quantum Chemical Calculations:

All structures were fully optimized with the M06-2X<sup>1</sup> DFT method with 6-311+G(2d,p) basis set for all atoms. D3 version of Grimme's dispersion with the original D3 damping function<sup>2</sup> is added for all calculations. The nature of all extrema as minimum or transition state was characterized with analytical calculations of frequencies at 298.15 K and 1 Atm, and the transition states were connected to reactants and products with IRC calculations. Transition states were located using synchronous Transit-Guided Quasi-Newton method (STQN)<sup>3</sup> and fully optimized using Berny algorithm. The solvent effect (dimethyl sulfoxide with  $\epsilon$  of 46.7 or THF with  $\epsilon$  of 7.58) was taken in account using the IEFPCM formalism during optimization and frequency calculations. All calculations were done with the Gaussian16 revision B.01 program packages. Graphical representations were done using ChimeraX 1.6.1 software.<sup>4</sup> Noncovalent interaction analysis were performed with NCIPLLOT 4.0 software<sup>5</sup> and visualizations were done by VMD program.<sup>6</sup>

Full reference of Gaussian16 software:

Gaussian16, Revision B.01

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

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<sup>1</sup> Zhao, Y.; Truhlar, D.G. *Theor. Chem. Acc.* **2008**, *120*, 215.

<sup>2</sup> Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, J. *J. Chem. Phys.* **2010**, *132*, 154104.

<sup>3</sup> a) Peng, C.; Schlegel, H.B. *Israel J. of Chem.* **1993**, *33*, 449; b) Peng, C.; Ayala, P.Y.; Schlegel, H.B.; Frisch, M.J. *J. Comp. Chem.* **1996**, *17*, 49.

<sup>4</sup> E. F. Pettersen, T. D. Goddard, C. C Huang, E. C. Meng, G. S. Couch, T. I. Croll, J. H. Morris, T. E. Ferrin, *Protein Sci.* **2021**, *30*, 70–82.

<sup>5</sup> a) Johnson, E. R.; Keinan, S.; Mori-Sanchez, P.; Contreras-Garcia, J.; J. Cohen, A. J.; Yang, W. *J. Am. Chem. Soc.* **2010**, *132*, 6498-6506, b) Contreras-Garcia, J.; Johnson, E. R.; Keinan, S.; R. Chaudret, Piquemal, J-P.; Beratan, D. N.; Yang, W. *J. Chem. Theory Comput.* **2011**, *7*, 625-632, c) Boto, R. A.; Peccati, F.; Laplaza, R.; Quan, C.; Carbone, A.; Piquemal, J.-P.; Maday, Y.; Contreras-Garcia, J. *J. Chem. Theory Comput.* **2020**, *16*, 4150-4158.

<sup>6</sup> Humphrey, W.; Dalke, A.; Schulten, K. *J. Molec. Graphics*, **1996**, *14*, 33-38.

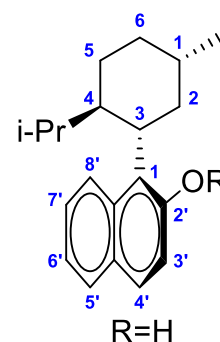
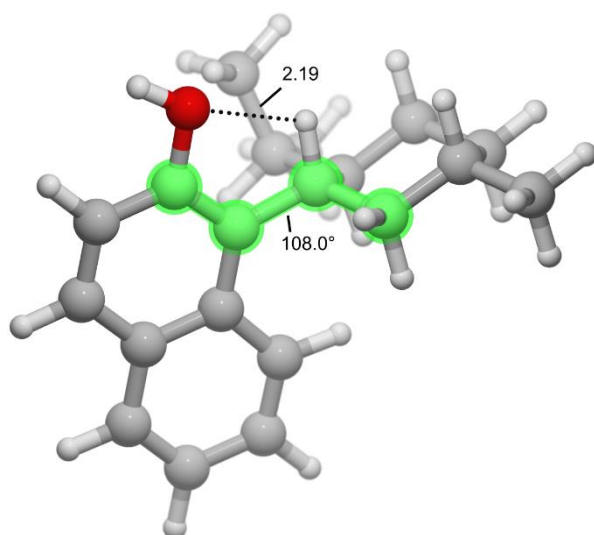
<http://www.ks.uiuc.edu/Research/vmd/>

**Table S12.** Thermodynamic parameters of **2a** conformational equilibrium calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

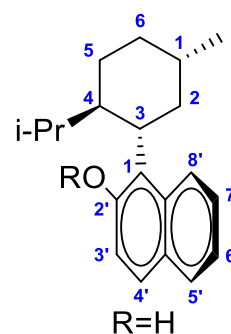
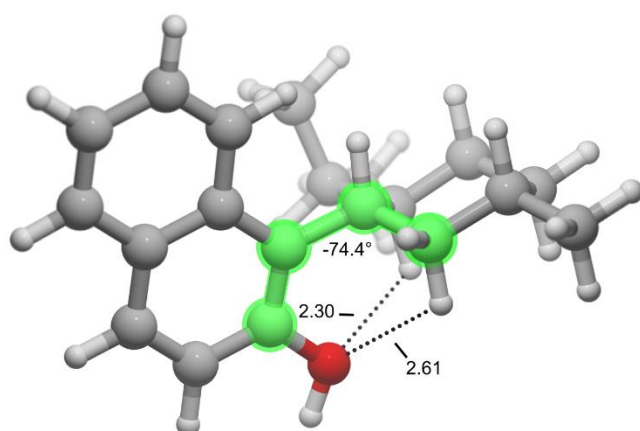
	( <i>M</i> )- <b>2a</b>	( <i>P</i> )- <b>2a</b>	TS1- <b>2a</b>	TS2- <b>2a</b>
$\Delta H^\circ$ (kJ/mol)	2.14	0.00	90.7	85.3
$\Delta G^\circ$ (kJ/mol)	3.73	0.00	98.6	96.4
$\Delta S^\circ$ (J/mol.K)	-5.32	0.00	-26.3	-37.1
$\mu$ (Debye)	1.85	1.95	1.70	1.80

**Figure S1.** Geometrical parameters of (*M*)-**2a** and (*P*)-**2a** atropisomers calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

(*M*)-**2a**



(*P*)-**2a**





**Table S13.** NBO analysis of (*M*)-**2a** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

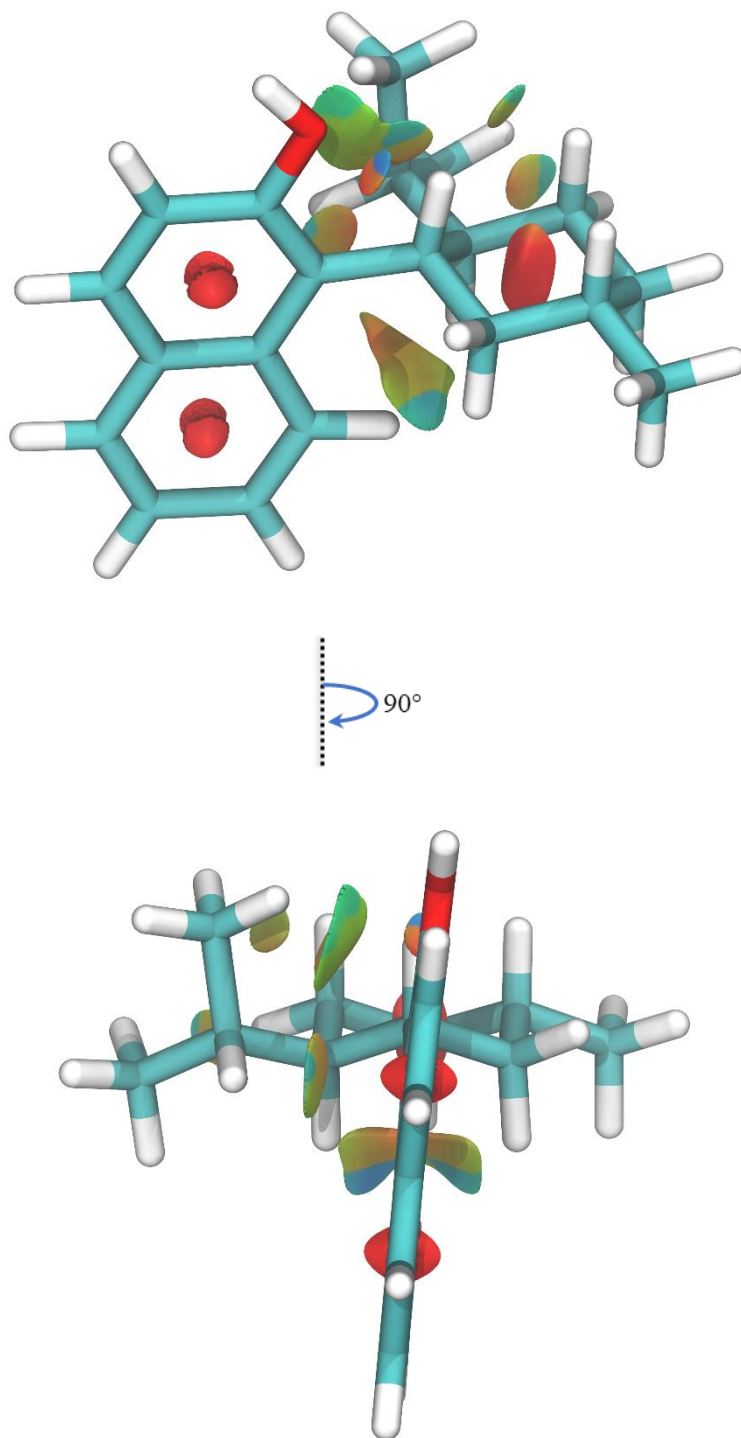
<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C4H4	3.31
$\sigma$ C4H4	$\sigma^*$ C8'H8'	4.10
$\sigma$ C8'H8'	$\sigma^*$ C2H2 $\alpha$	1.59
$\sigma$ C2H2 $\alpha$	$\sigma^*$ C8'H8'	2.18
$\sigma$ C3H3	$\pi^*$ C1'C8a'	25.40
$\pi$ C1'C8a'	$\sigma^*$ C3H3	4.02
$\sigma$ CH i-Pr	$\pi^*$ C1'C2'	2.09
n O2'	$\sigma^*$ C3H3	7.41
n O2'	$\sigma^*$ CH Me $\beta$ i-Pr	5.44
	<b>Total</b>	<b>55.52</b>

**Table S14.** NBO analysis of (*P*)-**2a** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C3H3	6.07
$\sigma$ C3H3	$\sigma^*$ C8'H8'	2.64
$\sigma$ C3H3	$\pi^*$ C1'C2'	20.42
$\pi$ C1'C2'	$\sigma^*$ C3H3	4.81
$\pi$ C1'C2'	$\sigma^*$ CH i-Pr	2.13
n O2'	$\sigma^*$ C4H4	5.77
n O2'	$\sigma^*$ C2H2 $\alpha$	1.38
	<b>Total</b>	<b>43.22</b>

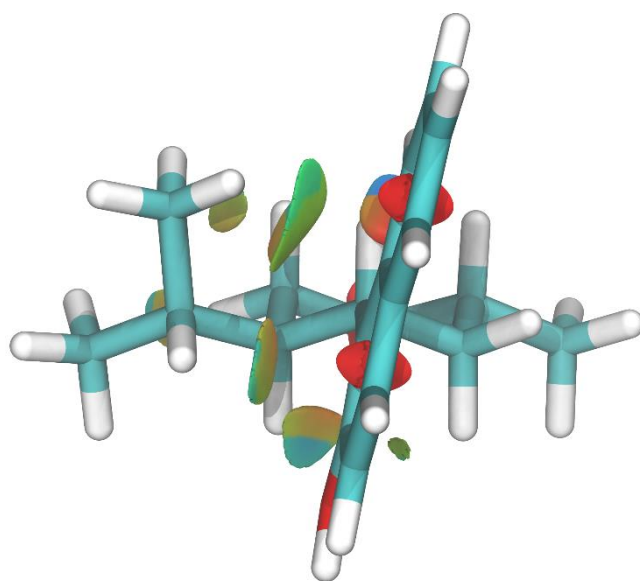
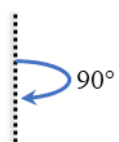
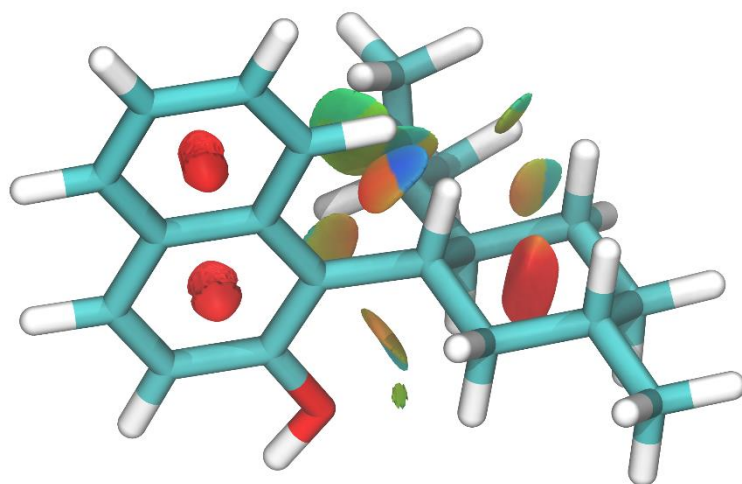
**Figure S2.** NCI analysis of (*M*)-**2a** and (*P*)-**2a** atropisomers implied in **2a** conformational equilibrium.

(*M*)-**2a**

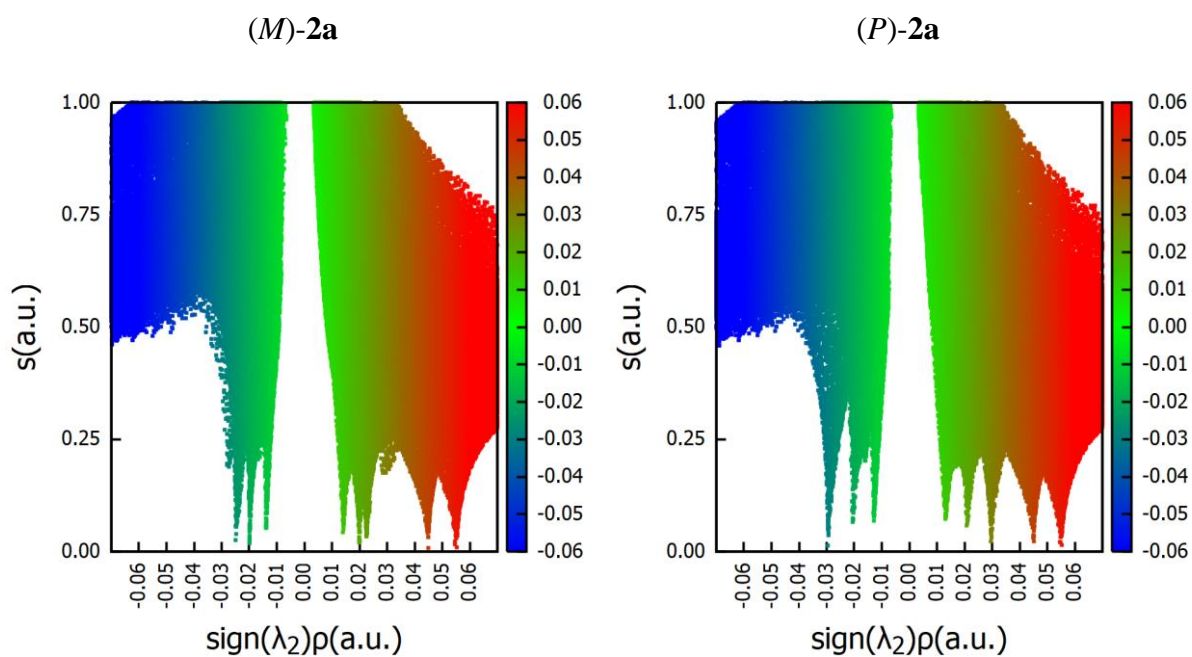


(P)-2a

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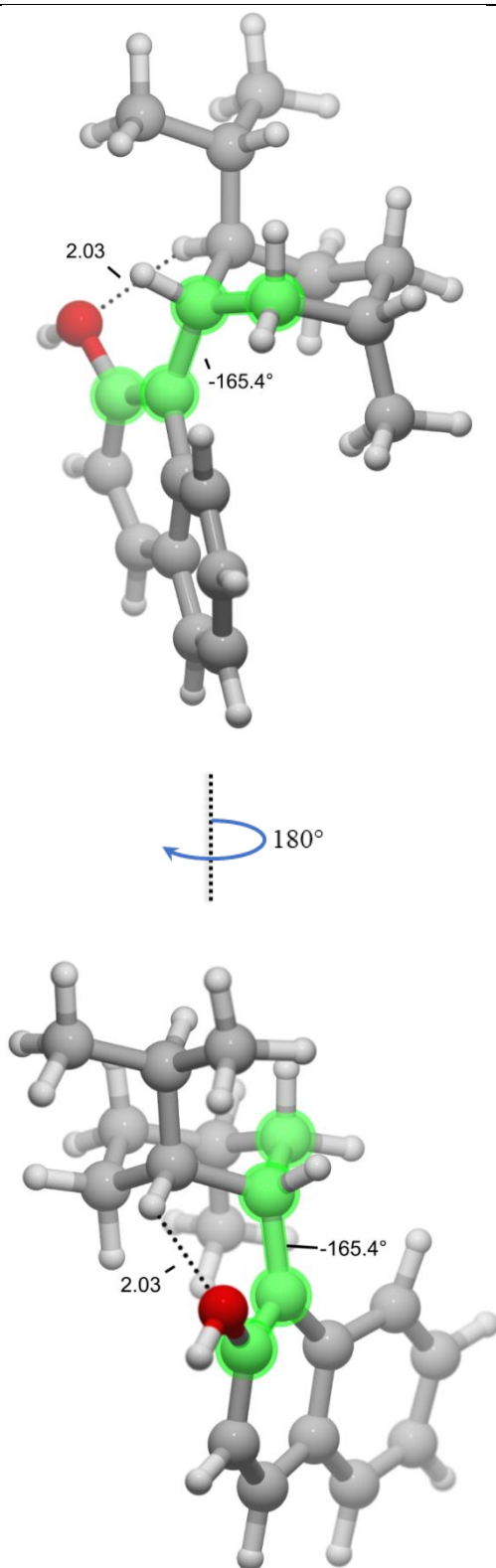
**Figure S3.** Plots of RDG vs  $\text{sign}(\lambda_2)\rho$  of (*M*)-**2a** and (*P*)-**2a** atropisomers and quantitative analysis in the attractive ( $\text{sign}(\lambda_2)\rho < 0$ ), VDW ( $\text{sign}(\lambda_2)\rho \approx 0$ ) and repulsive regions ( $\text{sign}(\lambda_2)\rho > 0$ ).



	<i>Attractive region</i>	<i>VDW region</i>	<i>Repulsive region</i>
( <i>M</i> )- <b>2a</b>	-0.1523	0.0027	0.2845
( <i>P</i> )- <b>2a</b>	-0.1526	0.0027	0.2845
( <i>M</i> ) versus ( <i>P</i> )	3.25E-04	-2.10E-07	-4.50E-05

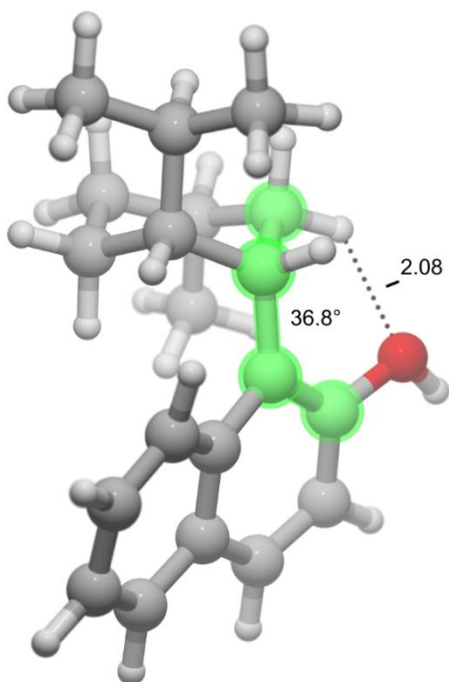
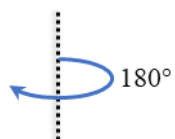
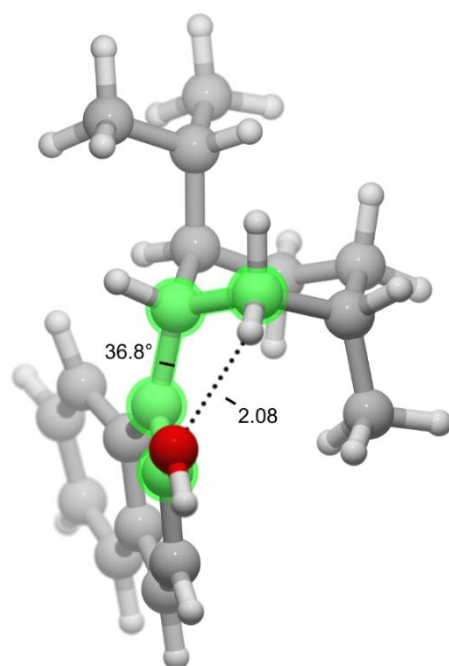
**Figure S4.** Geometrical parameters of located transition states implied in **2a** conformational equilibrium calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

TS1-2a



TS2-2a

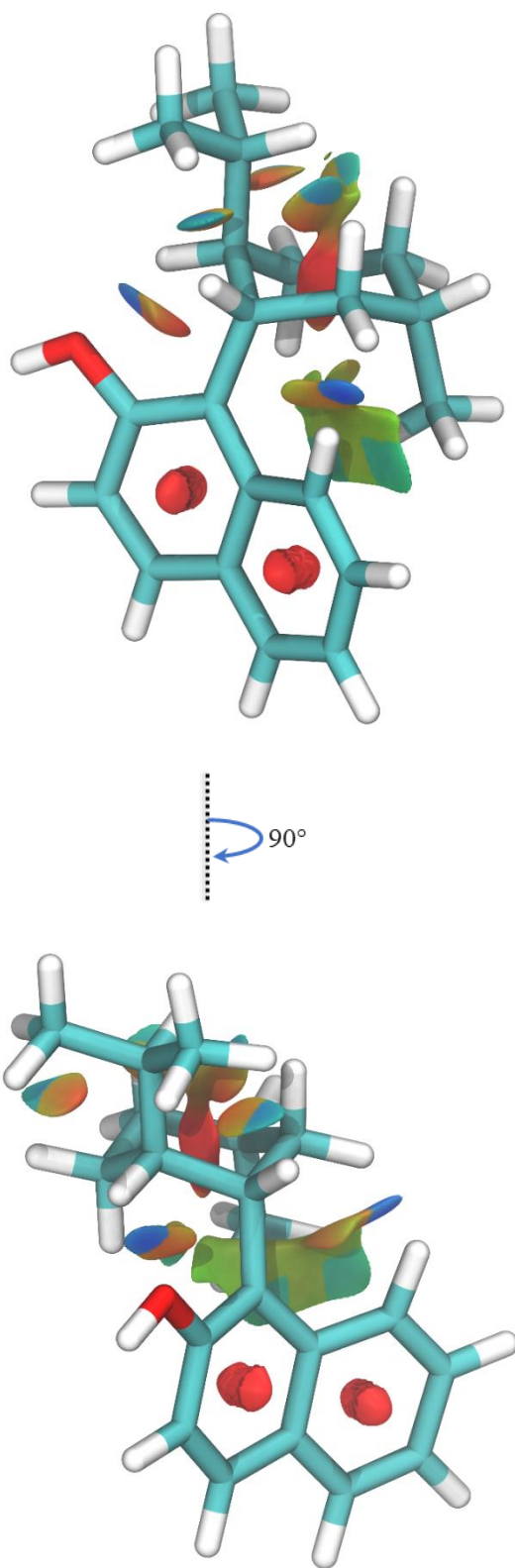
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**Figure S5.** NCI analysis of located transition states implied in **2a** conformational equilibrium.

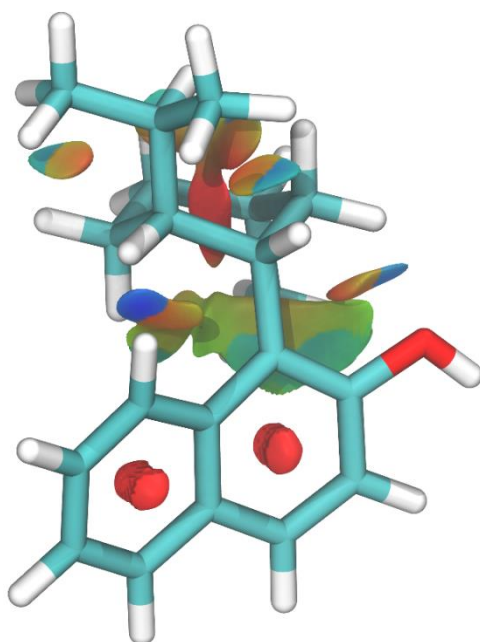
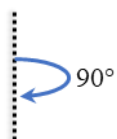
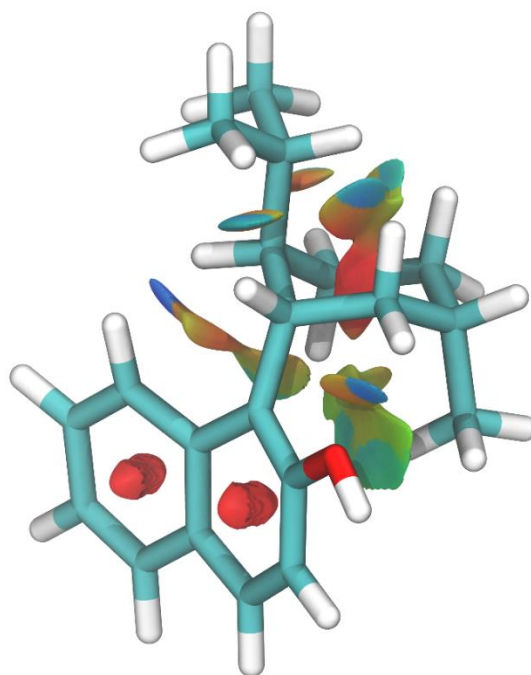
TS1-2a

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TS2-2a

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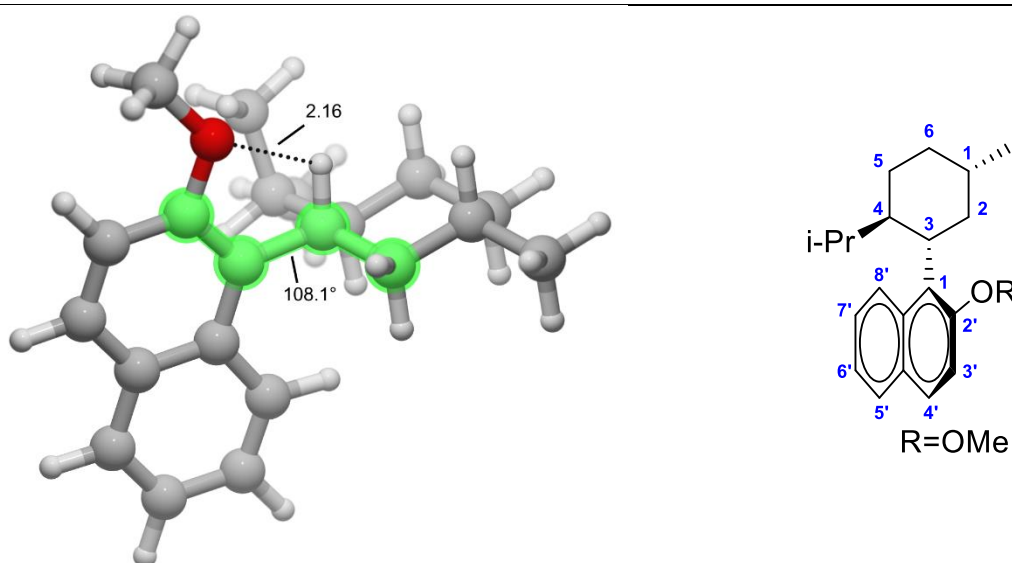


**Table S15.** Thermodynamic parameters of **2b** conformational equilibrium calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

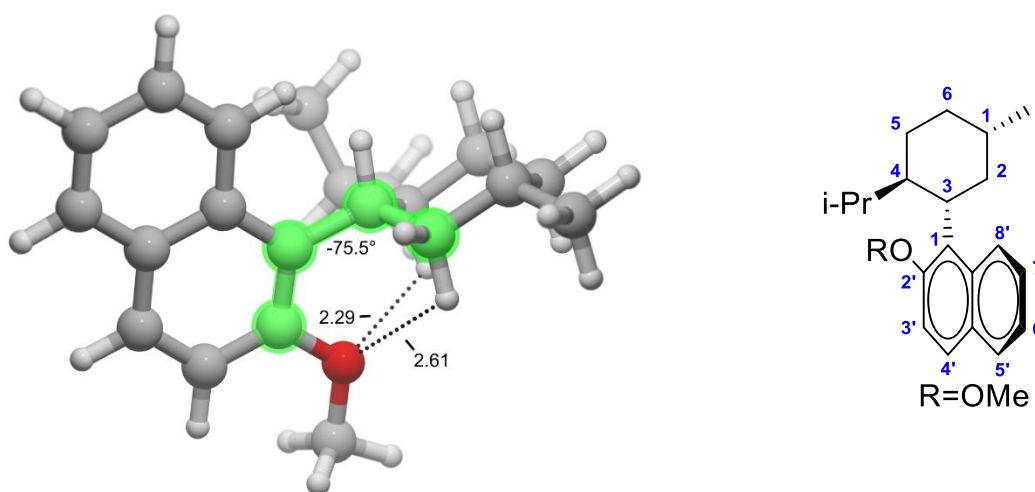
	( <i>M</i> )- <b>2b</b>	( <i>P</i> )- <b>2b</b>	TS1- <b>2b</b>	TS2- <b>2b</b>
$\Delta H^\circ$ (kJ/mol)	2.51	0.00	90.6	86.0
$\Delta G^\circ$ (kJ/mol)	4.38	0.00	101.0	98.6
$\Delta S^\circ$ (J/mol.K)	-6.28	0.00	-34.8	-42.6
$\mu$ (debye)	2.11	2.21	1.92	2.24

**Figure S6.** Geometrical parameters of (*M*)-**2b** and (*P*)-**2b** atropisomers calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

(*M*)-**2b**



(*P*)-**2b**



**Table S16.** NBO analysis of (*M*)-**2b** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C4H4	3.31
$\sigma$ C4H4	$\sigma^*$ C8'H8'	4.02
$\sigma$ C8'H8'	$\sigma^*$ C2H2 $\alpha$	1.63
$\sigma$ C2H2 $\alpha$	$\sigma^*$ C8'H8'	2.26
$\sigma$ C3H3	$\pi^*$ C1'C8a'	24.89
$\pi$ C1'C8a'	$\sigma^*$ C3H3	4.10
$\sigma$ CH i-Pr	$\pi^*$ C1'C2'	1.97
n O2'	$\sigma^*$ C3H3	8.37
n O2'	$\sigma^*$ CH Me $\beta$ i-Pr	3.89
	<b>Total</b>	<b>54.43</b>

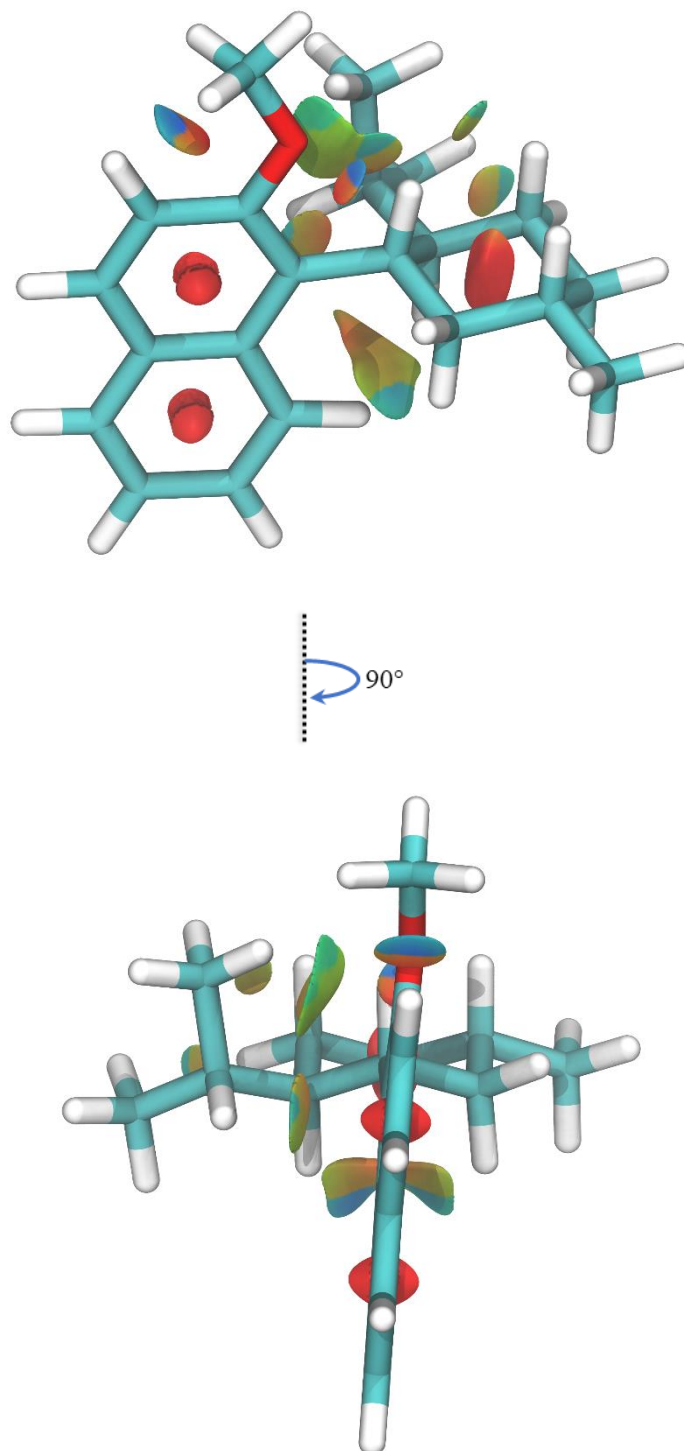
**Table S17.** NBO analysis of (*P*)-**2b** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C3H3	6.28
$\sigma$ C3H3	$\sigma^*$ C8'H8'	2.59
$\sigma$ C3H3	$\pi^*$ C1'C2'	21.55
$\pi$ C1'C2'	$\sigma^*$ C3H3	4.73
$\pi$ C1'C2'	$\sigma^*$ CH i-Pr	2.26
n O2'	$\sigma^*$ C4H4	5.02
n O2'	$\sigma^*$ C3H3	1.55
n O2'	$\sigma^*$ C2H2 $\alpha$	1.30
	<b>Total</b>	<b>19.00</b>

**Figure S7.** NCI analysis of (*M*)-**2b** and (*P*)-**2b** atropisomers implied in **2b** conformational equilibrium.

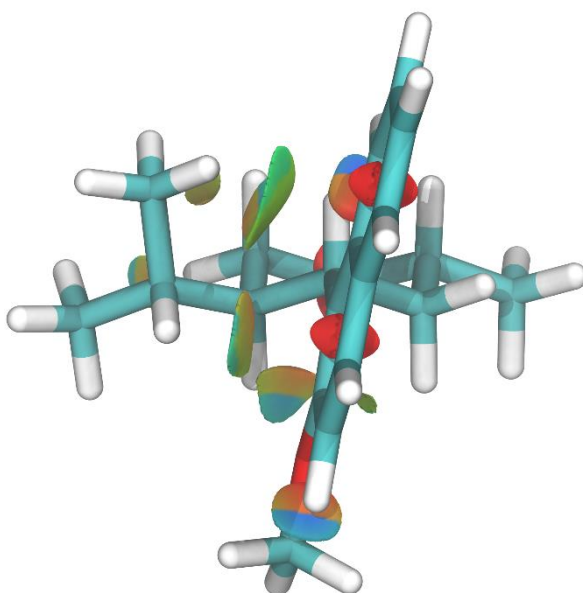
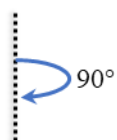
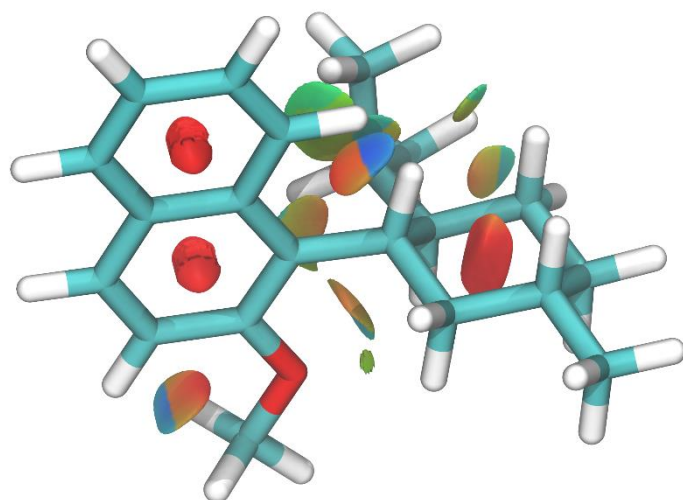
(*M*)-**2b**

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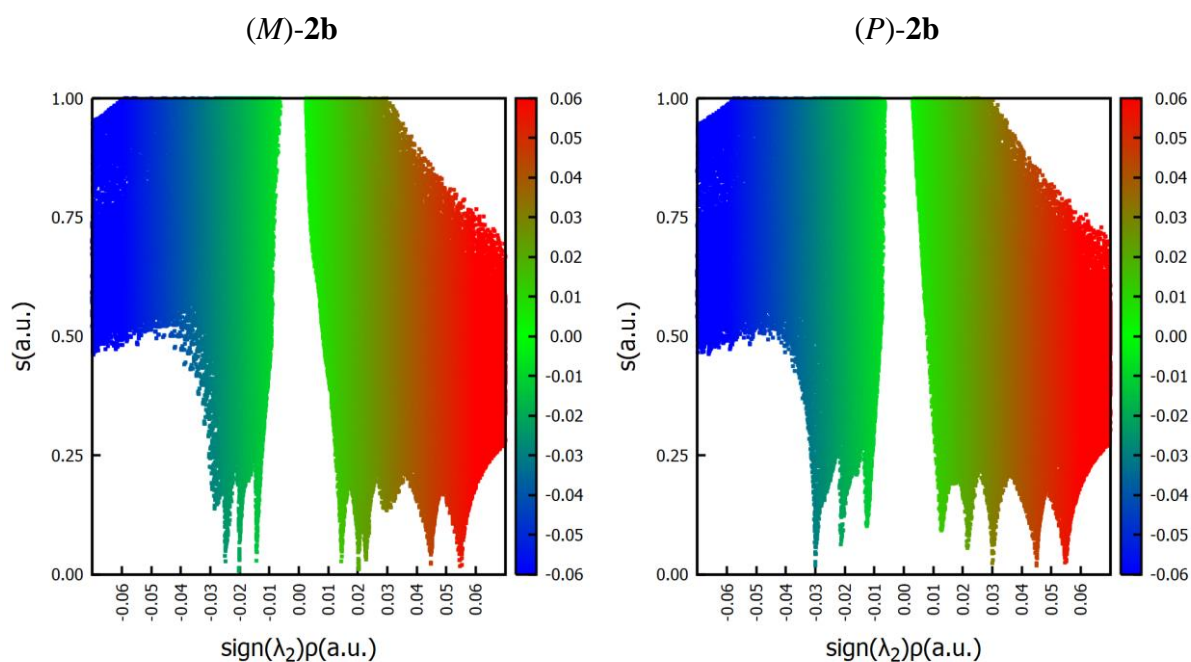


(P)-2b

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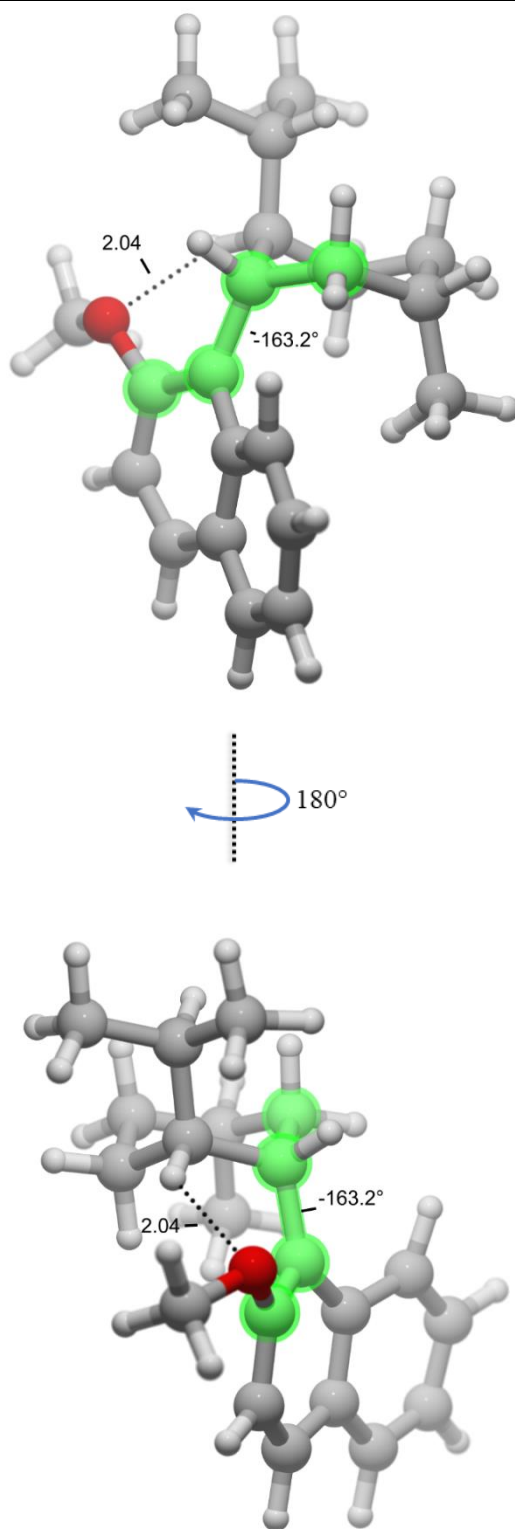
**Figure S8.** Plots of RDG vs  $\text{sign}(\lambda_2)\rho$  of (*M*)-**2b** and (*P*)-**2b** atropisomers and quantitative analysis in the attractive ( $\text{sign}(\lambda_2)\rho < 0$ ), VDW ( $\text{sign}(\lambda_2)\rho \approx 0$ ) and repulsive regions ( $\text{sign}(\lambda_2)\rho > 0$ ).



	<i>Attractive region</i>	<i>VDW region</i>	<i>Repulsive region</i>
( <i>M</i> )- <b>2b</b>	-0.1628	0.0027	0.2997
( <i>P</i> )- <b>2b</b>	-0.1625	0.0027	0.2994
( <i>M</i> ) versus ( <i>P</i> )	-2.82E-04	8.92E-06	3.57E-04

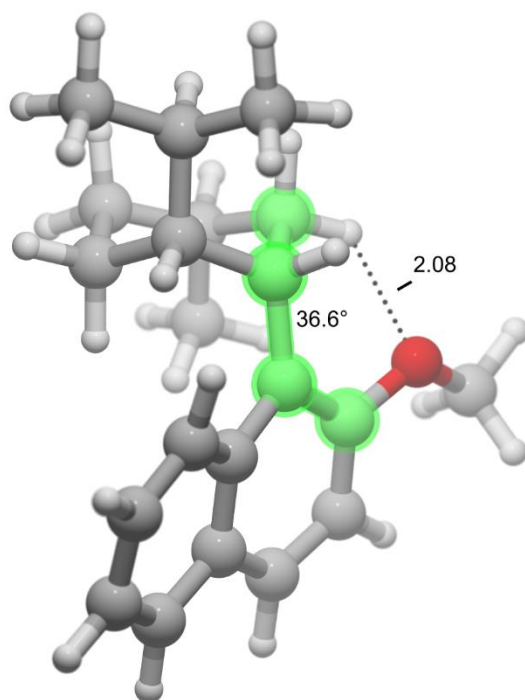
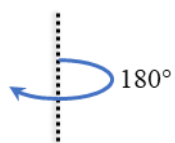
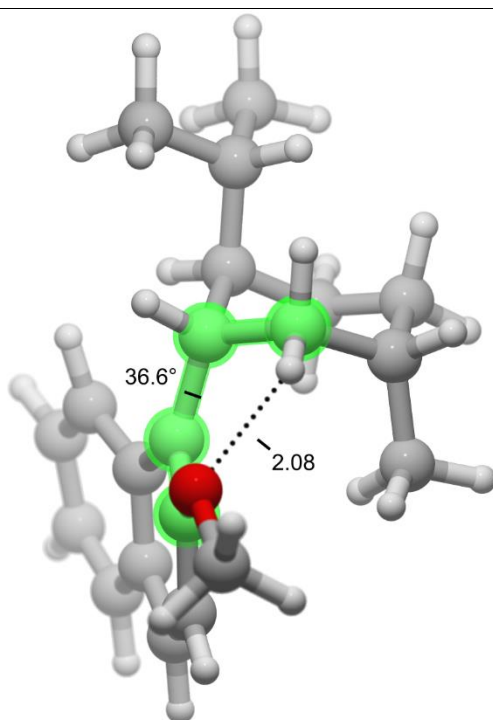
**Figure S9.** Geometrical parameters of located transition states implied in **2b** conformational equilibrium calculated in DMSO @ the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

TS1-2b



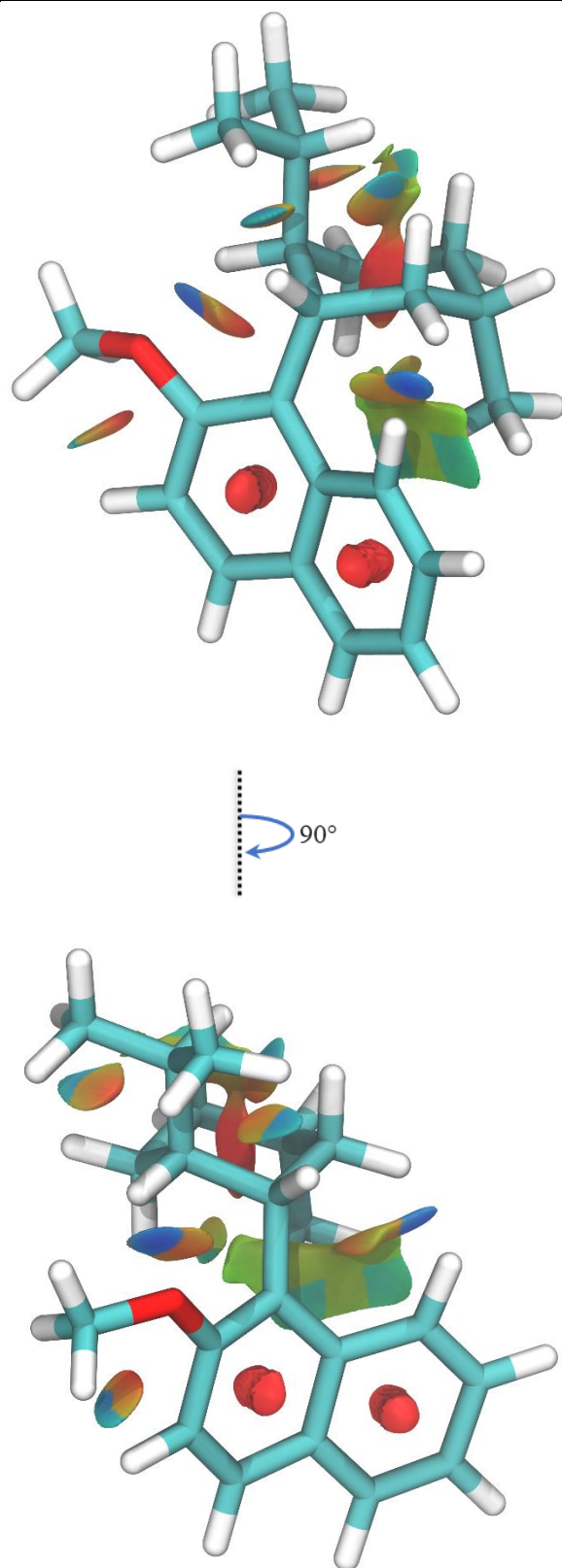
TS2-2b

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**Figure S10.** NCI analysis of located transition states implied in **2b** conformational equilibrium.

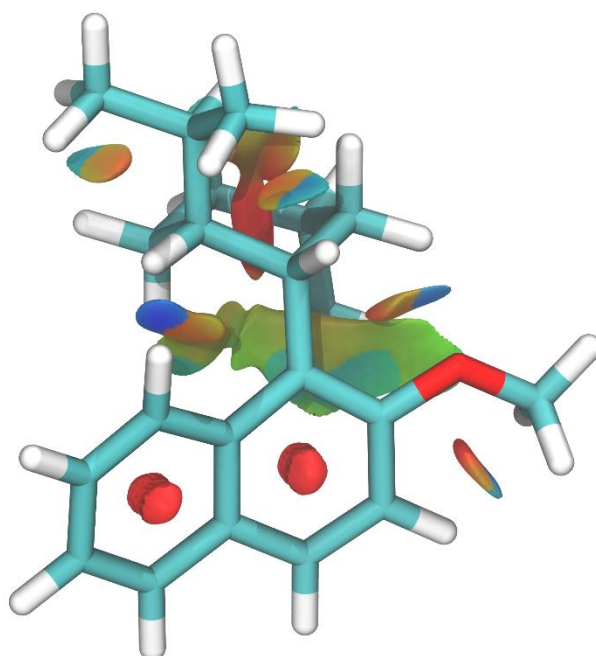
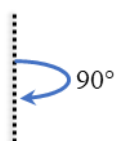
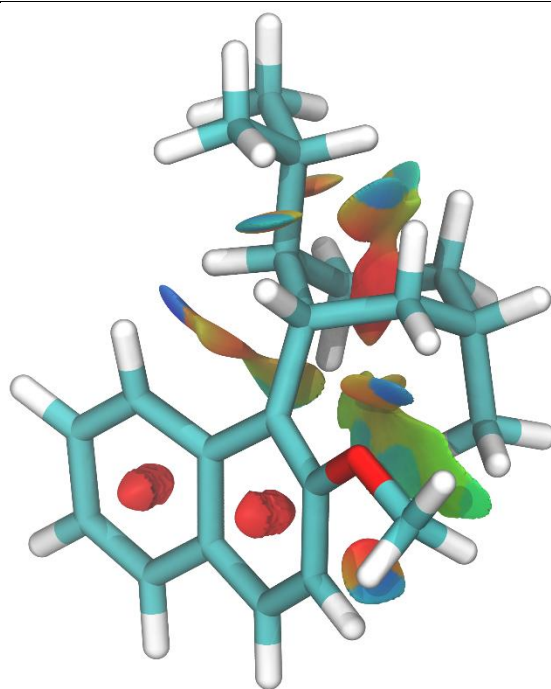
TS1-2b





TS2-2b

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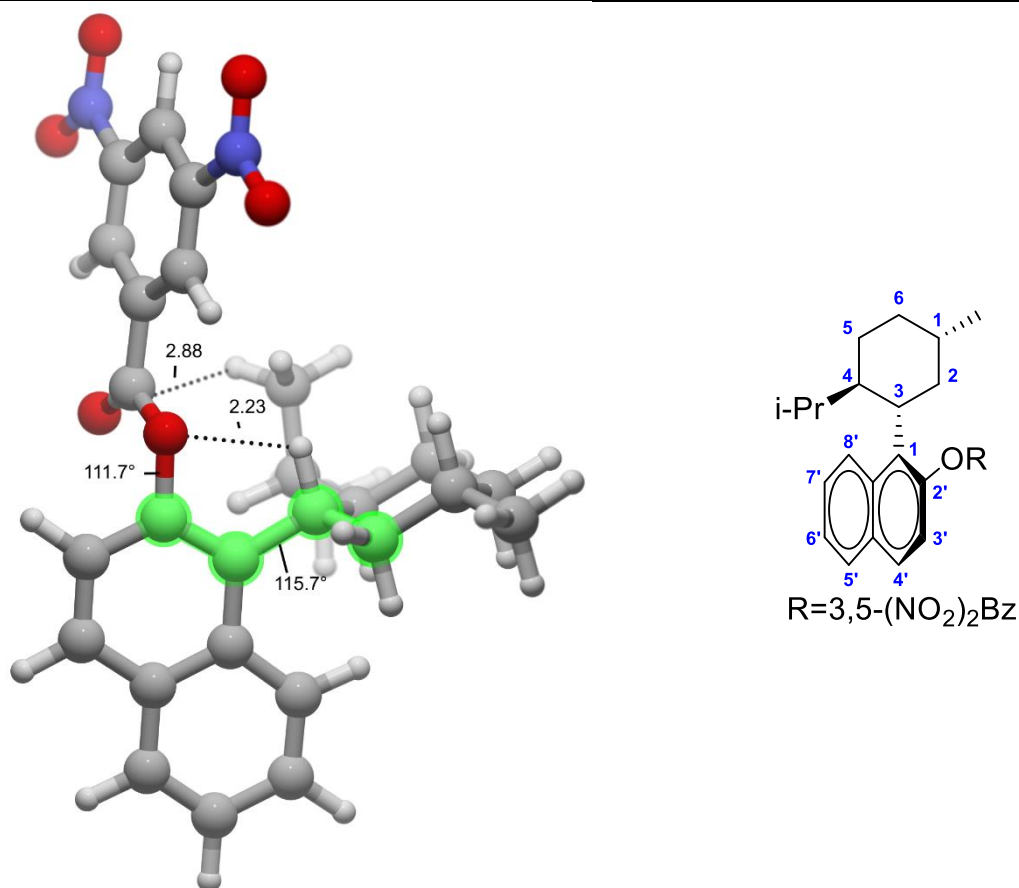


**Table S18.** Thermodynamic parameters of **2c** conformational equilibrium calculated in DMSO @ the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

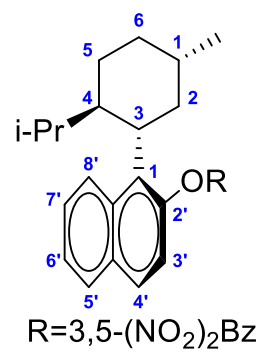
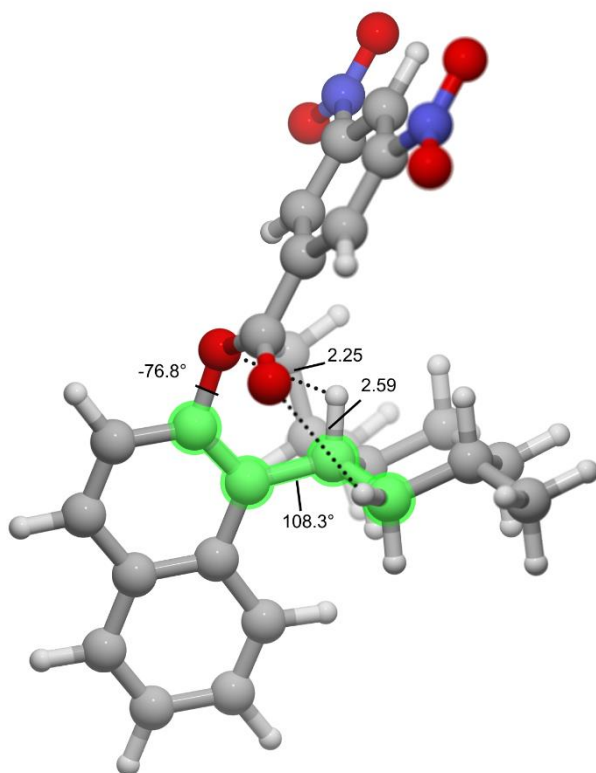
	( <i>M</i> )- <b>2c bis</b>	( <i>M</i> )- <b>2c</b>	( <i>P</i> )- <b>2c</b>	( <i>P</i> )- <b>2cbis</b>	TS1- <b>2c</b>	TS1'- <b>2c</b>	TS2- <b>2c</b>	TS2'- <b>2c</b>
$\Delta H^\circ$ (kJ/mol)	10.23	7.11	0.00	3.27	94.44	98.93	91.6	102.43
$\Delta G^\circ$ (kJ/mol)	9.82	3.53	0.00	0.82	104.66	107.16	99.1	109.84
$\Delta S^\circ$ (J/mol.K)	1.37	12.01	0.00	8.23	-34.26	-27.61	-25.1	-24.86
$\mu$ (Debye)	5.01	5.06	5.13	5.12	4.88	4.78	4.71	4.71

**Figure S11.** Geometrical parameters of (*M*)-**2c** and (*P*)-**2c** atropisomers calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

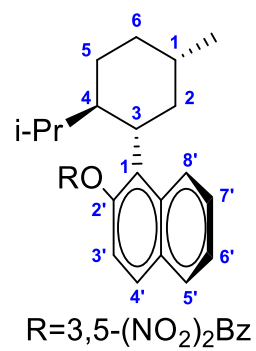
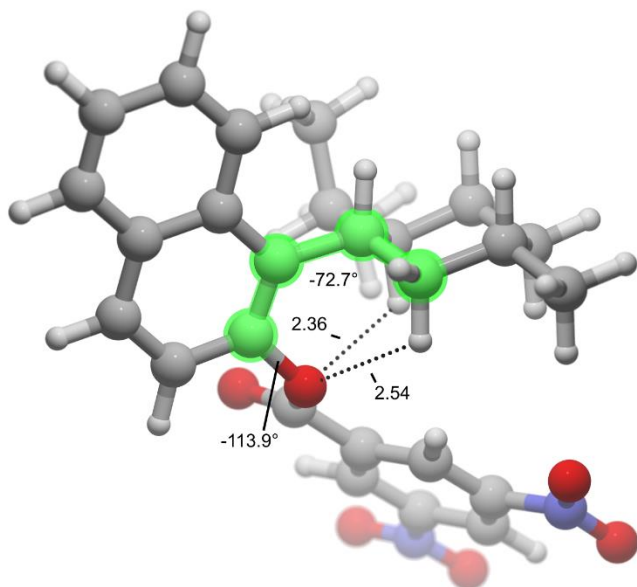
(*M*)-**2c bis**



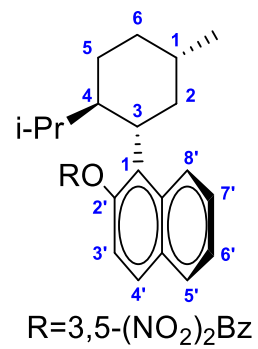
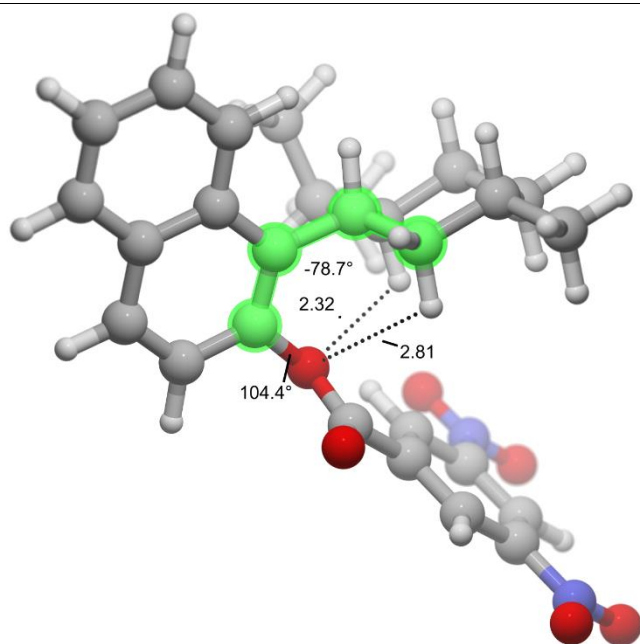
(*M*)-2c



(*P*)-2c



(P)-2c bis



**Table S19.** NBO analysis of (*M*)-**2c** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) of theory.

<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C4H4	3.01
$\sigma$ C4H4	$\sigma^*$ C8'H8'	3.51
$\sigma$ C8'H8'	$\sigma^*$ C2H2 $\alpha$	1.51
$\sigma$ C2H2 $\alpha$	$\sigma^*$ C8'H8'	2.43
$\sigma$ C3H3	$\pi^*$ C1'C8a'	25.86
$\pi$ C1'C8a'	$\sigma^*$ C3H3	3.81
$\sigma$ CH i-Pr	$\pi^*$ C1'C2'	2.09
$\sigma$ C3H3	$\pi^*$ C1''O	3.31
$\pi$ C1''O	$\sigma^*$ C2H2 $\beta$	1.55
n O2'	$\sigma^*$ C3H3	2.85
	<b>Total</b>	<b>49.92</b>

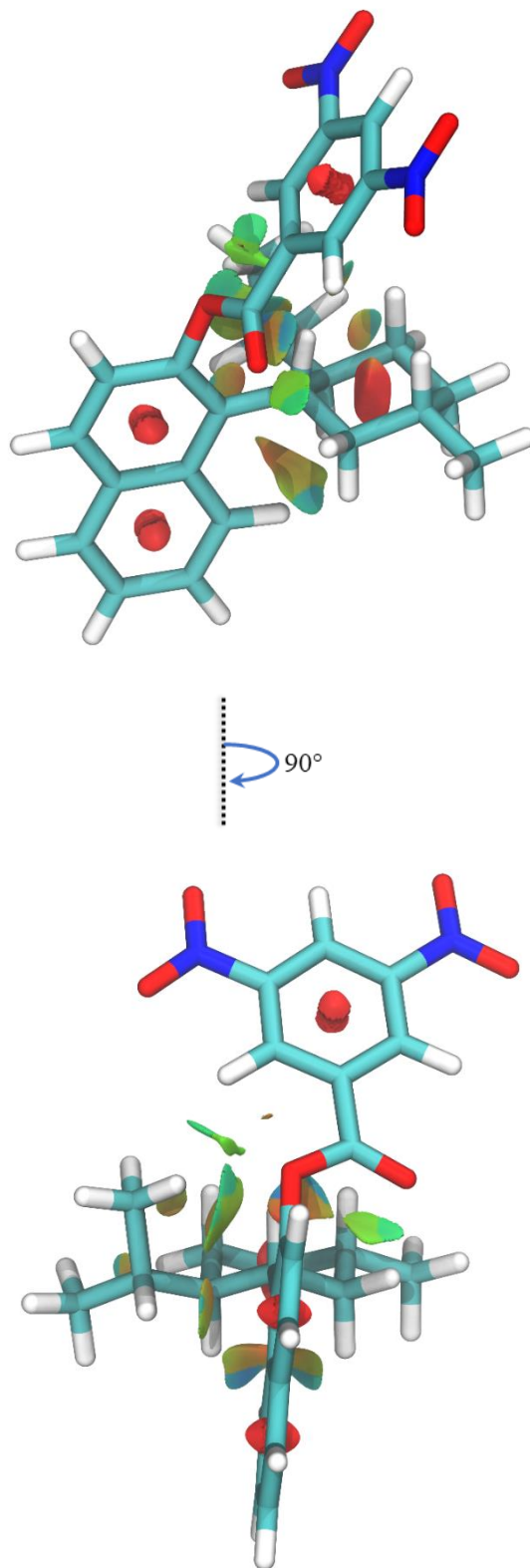
**Table S20.** NBO analysis of (*P*)-**2c** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C3H3	5.90
$\sigma$ C3H3	$\sigma^*$ C8'H8'	2.13
$\sigma$ C3H3	$\pi^*$ C1'C2'	21.80
$\pi$ C1'C2'	$\sigma^*$ C3H3	4.27
$\sigma$ CH Me $\beta$ i-Pr	$\pi^*$ C7'C8'	1.51
$\pi$ C1'C2'	$\sigma^*$ CH i-Pr	2.80
$\sigma$ C4H4	$\pi^*$ C1''O	1.92
$\pi$ C1''O	$\sigma^*$ CH i-Pr	1.59
n O2'	$\sigma^*$ C4H4	1.34
n O2'	$\sigma^*$ C2H2 $\alpha$	1.92
	<b>Total</b>	<b>51.17</b>

**Figure S12.** NCI analysis of (*M*)-**2c** and (*P*)-**2c** atropisomers implied in **2c** conformational equilibrium.

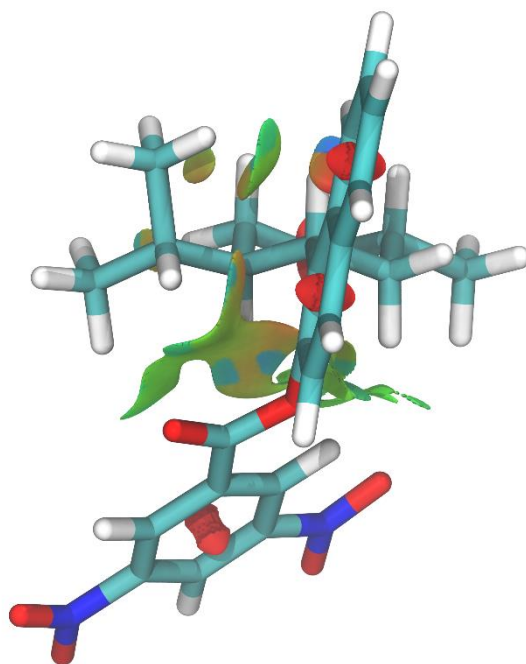
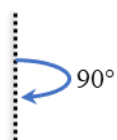
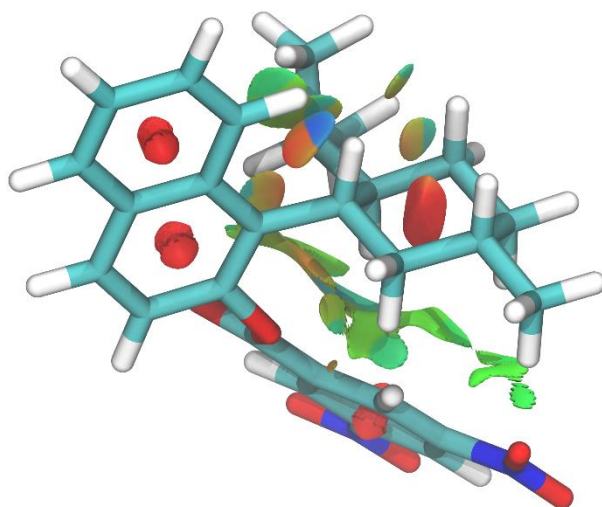
(*M*)-**2c**

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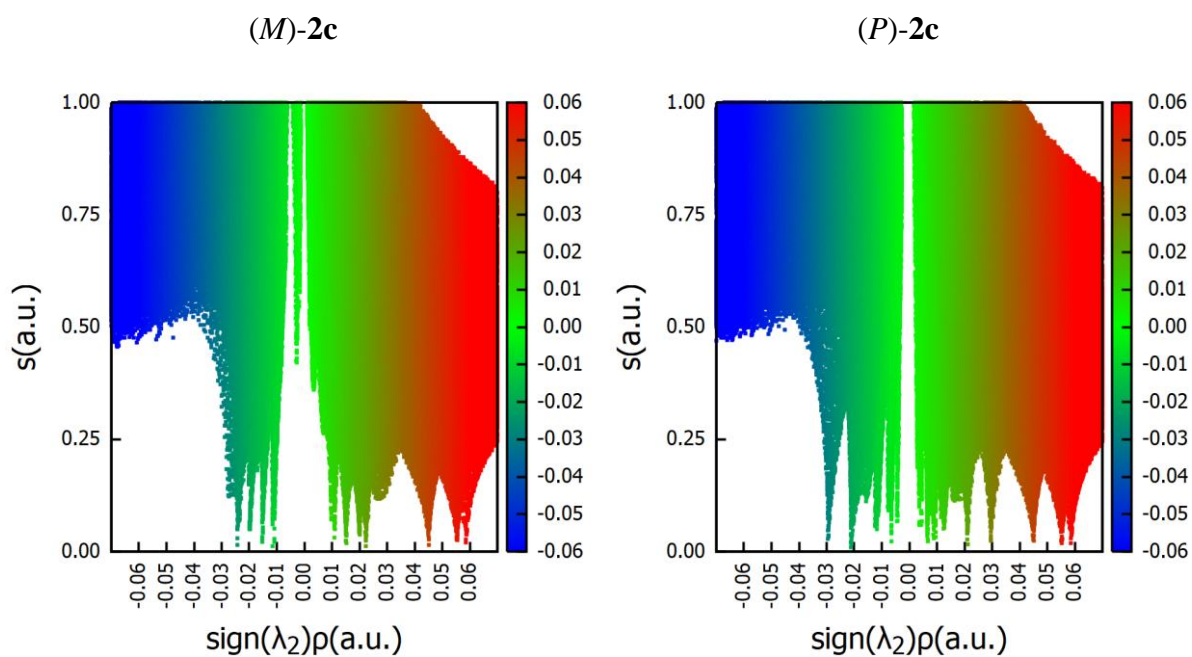


(P)-2c

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**Figure S13.** Plots of RDG vs  $\text{sign}(\lambda_2)\rho$  of (*M*)-**2c** and (*P*)-**2c** atropisomers and quantitative analysis in the attractive ( $\text{sign}(\lambda_2)\rho < 0$ ), VDW ( $\text{sign}(\lambda_2)\rho \approx 0$ ) and repulsive regions ( $\text{sign}(\lambda_2)\rho > 0$ ).

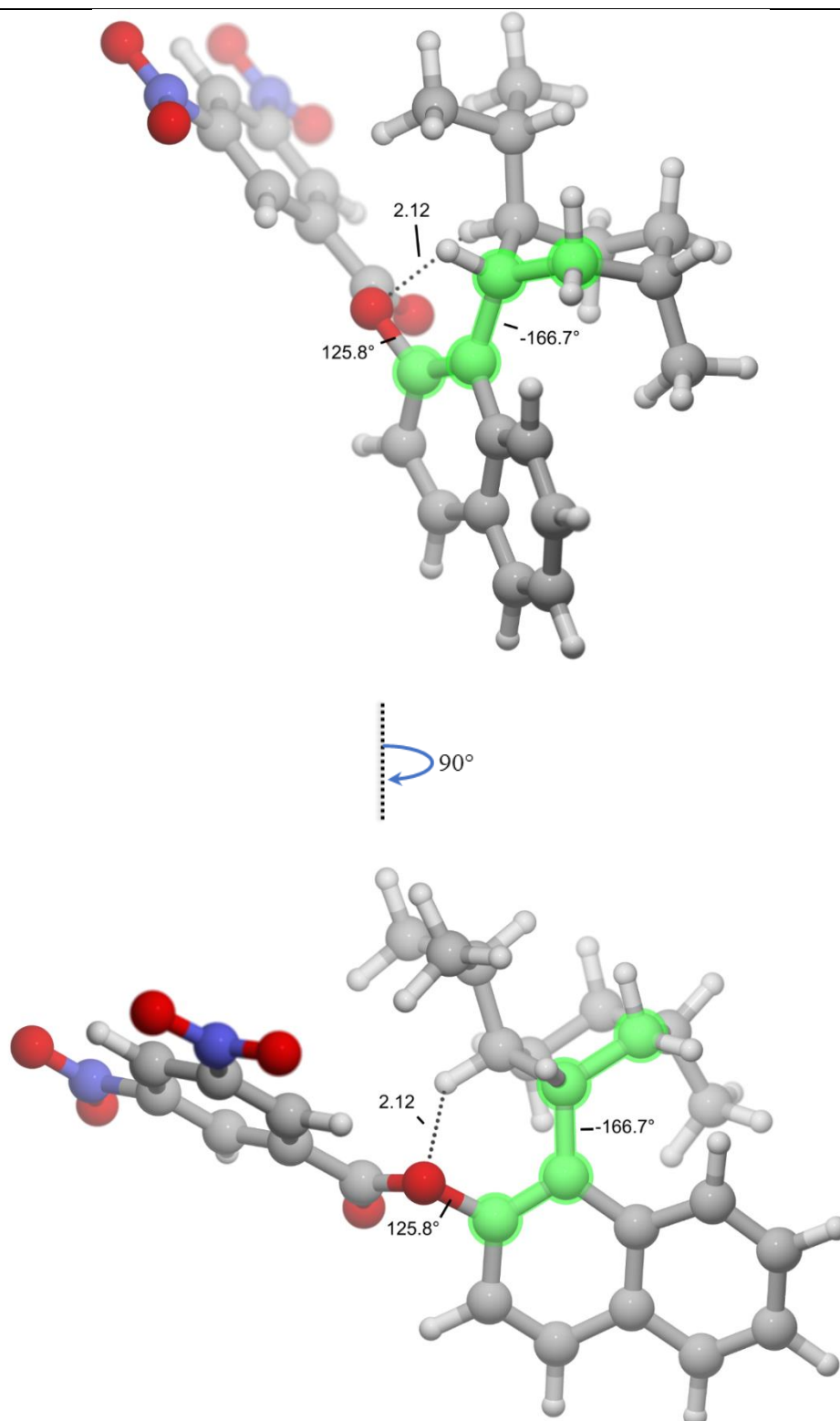


	<i>Attractive region</i>	<i>VDW region</i>	<i>Repulsive region</i>
( <i>M</i> )- <b>2c</b>	-0.2108	0.0035	0.3841
( <i>P</i> )- <b>2c</b>	-0.2119	0.0035	0.3841
( <i>M</i> ) versus ( <i>P</i> )	1.06E-03	-6.43E-06	2.63E-05

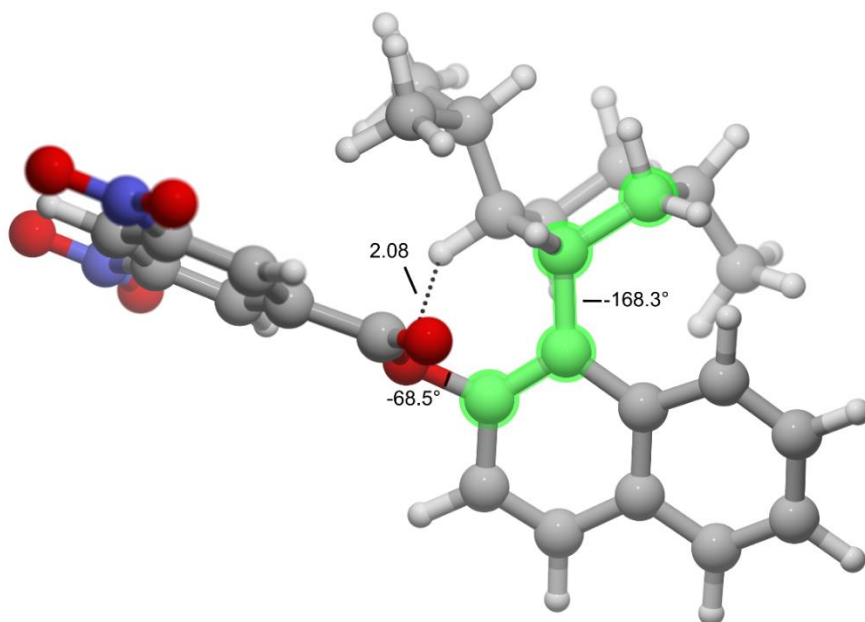
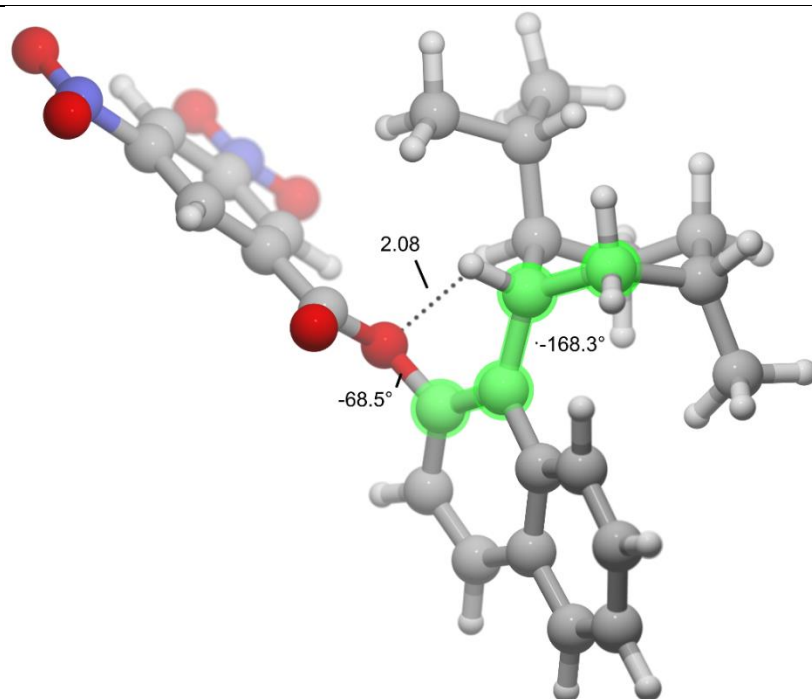


**Figure S14.** Geometrical parameters of located transition states implied in **2c** conformational equilibrium calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

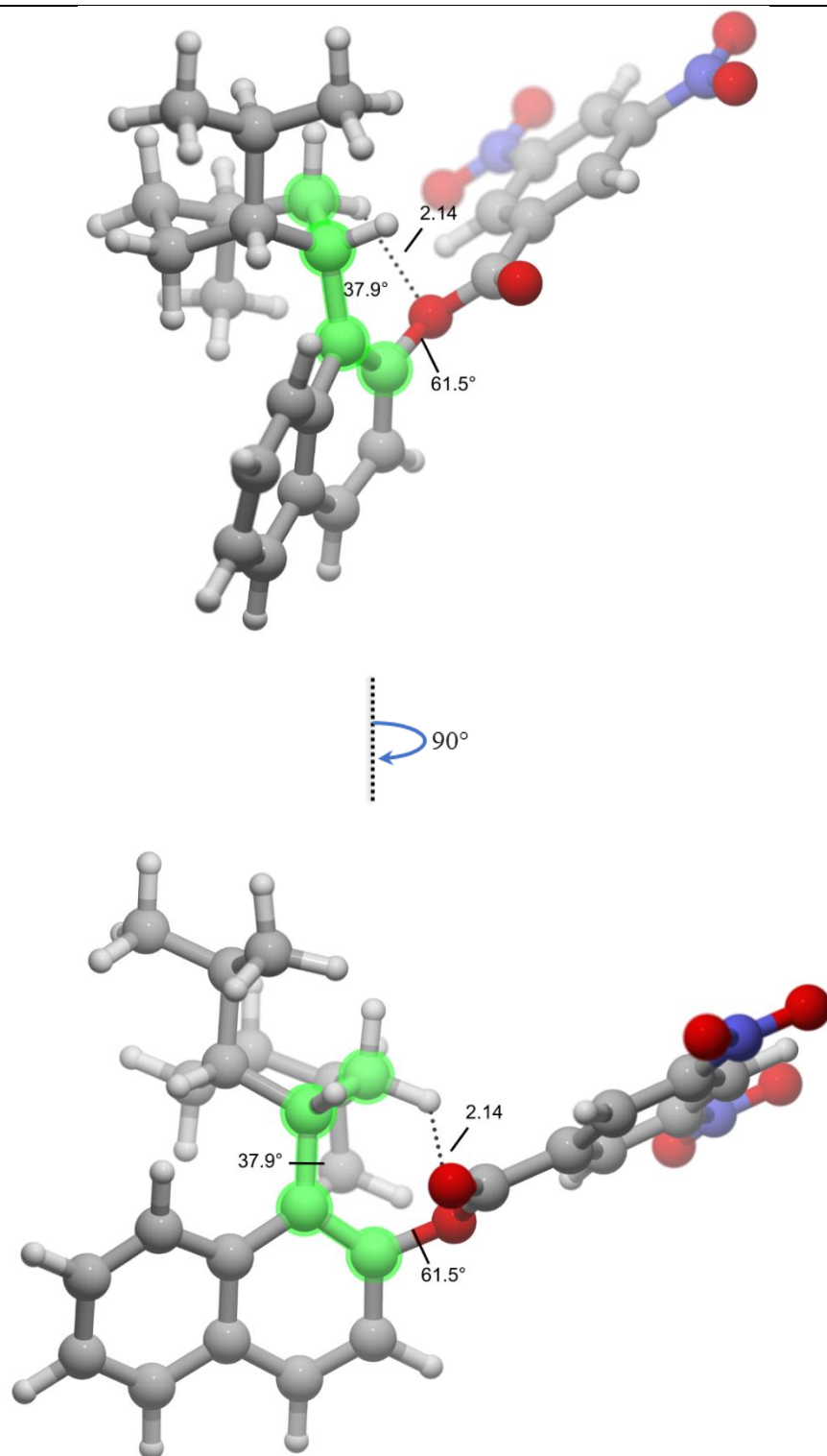
TS1-**2c**



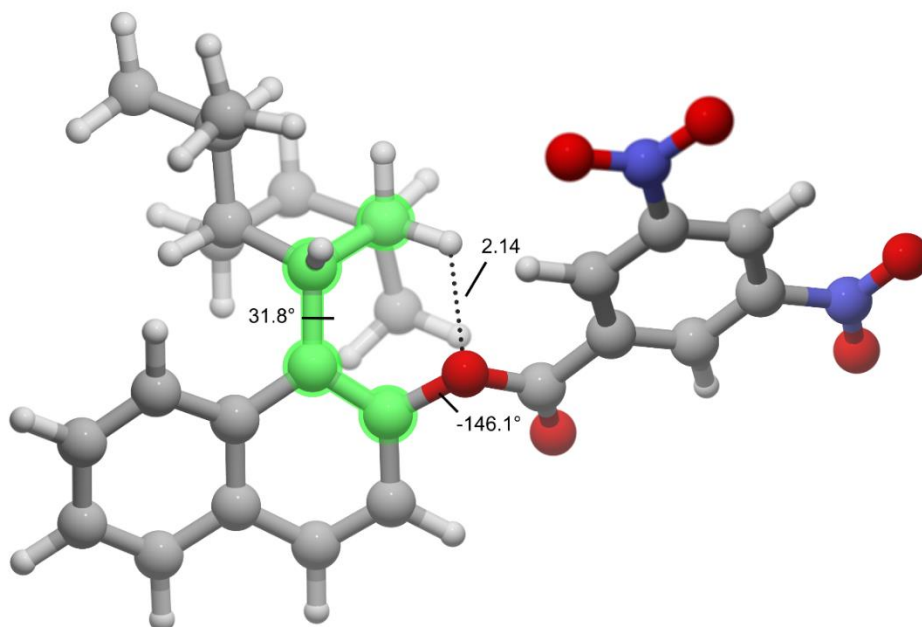
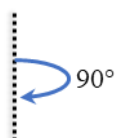
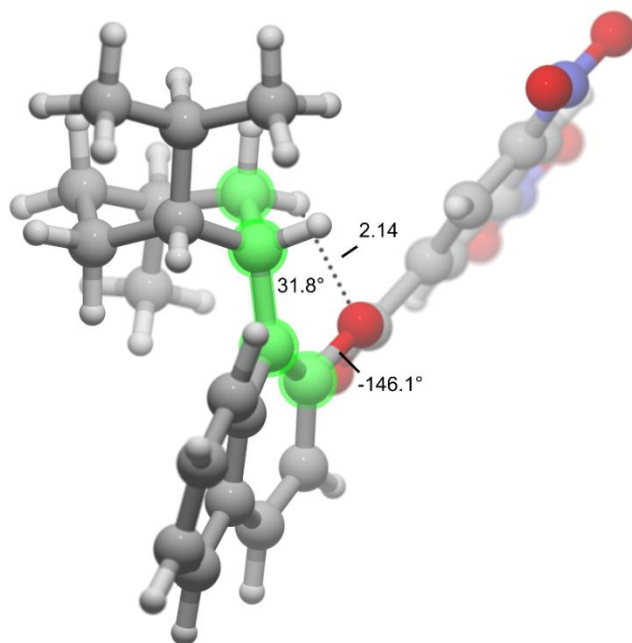
TS1'-2c



TS2-2c

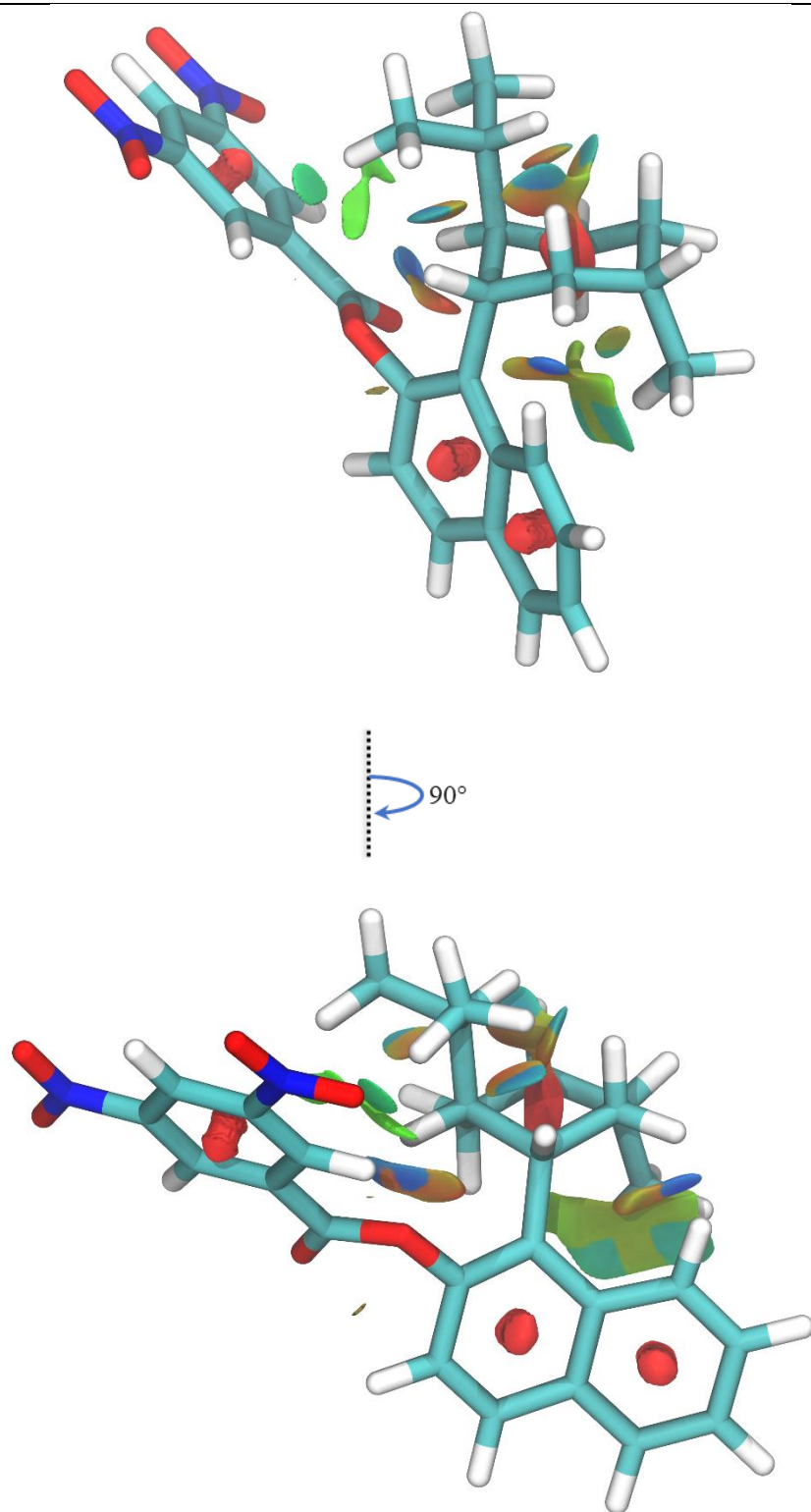


TS2'-2c



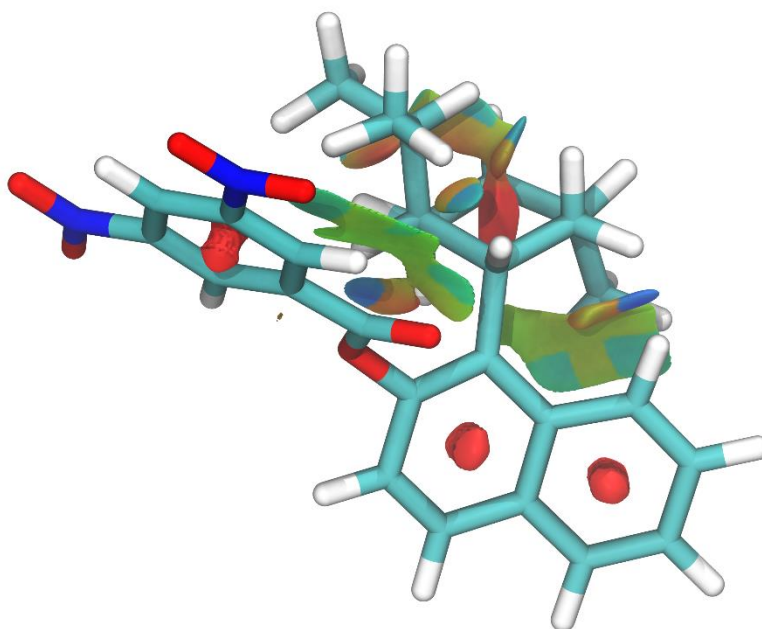
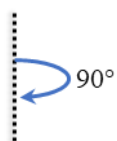
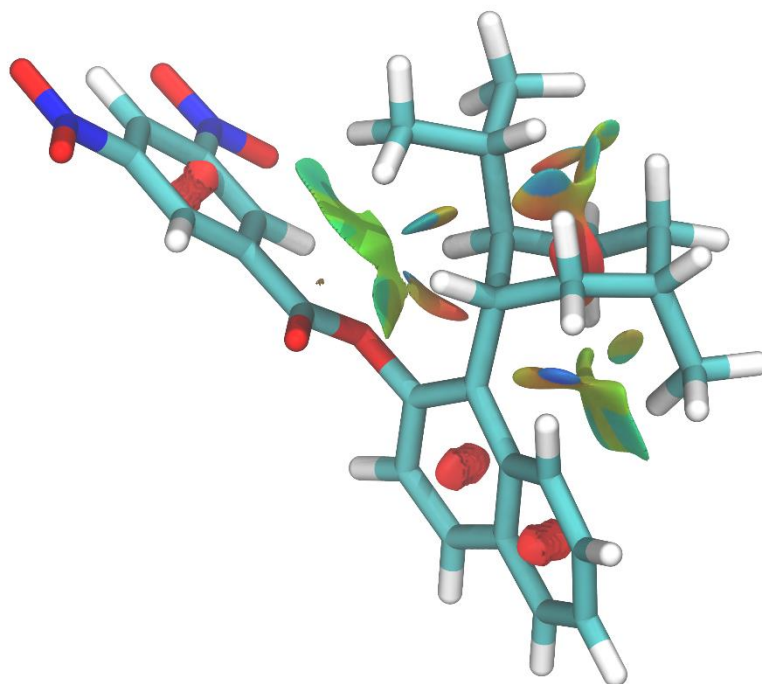
**Figure S15.** NCI analysis of located transition states implied in **2c** conformational equilibrium.

TS1-2c



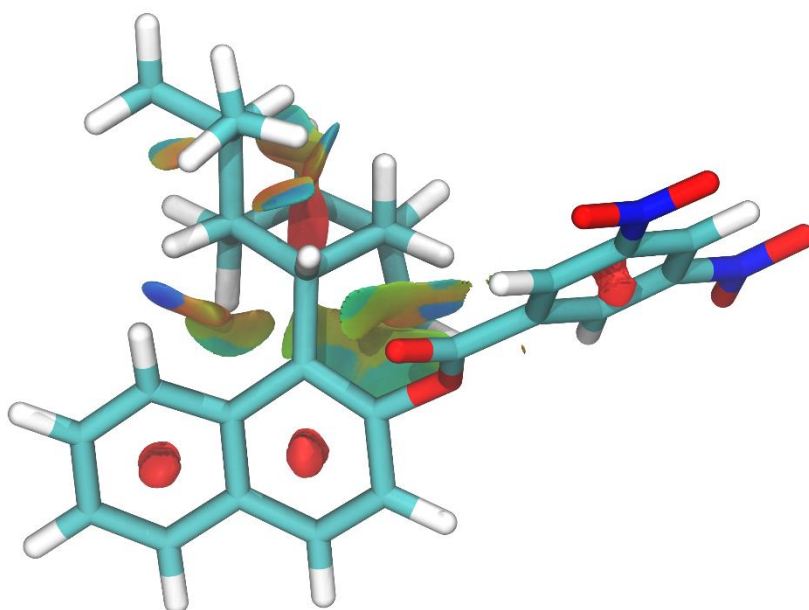
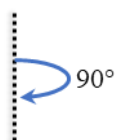
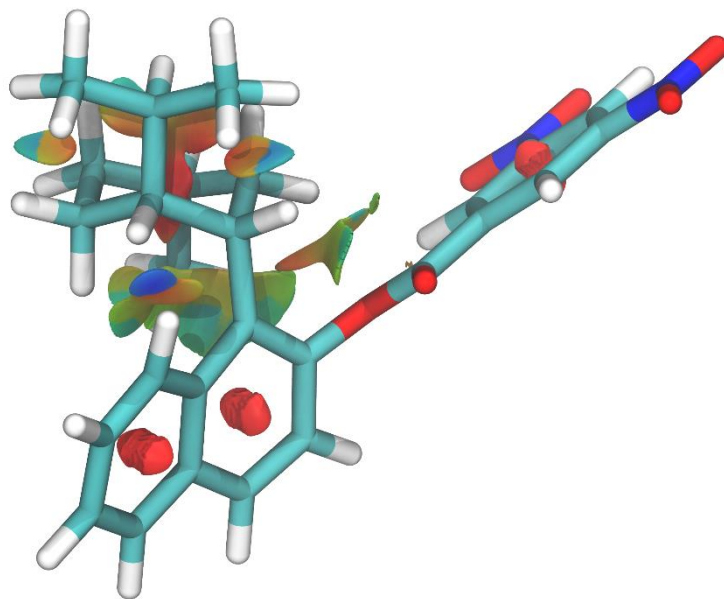
TS1'-2c

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TS2-2c

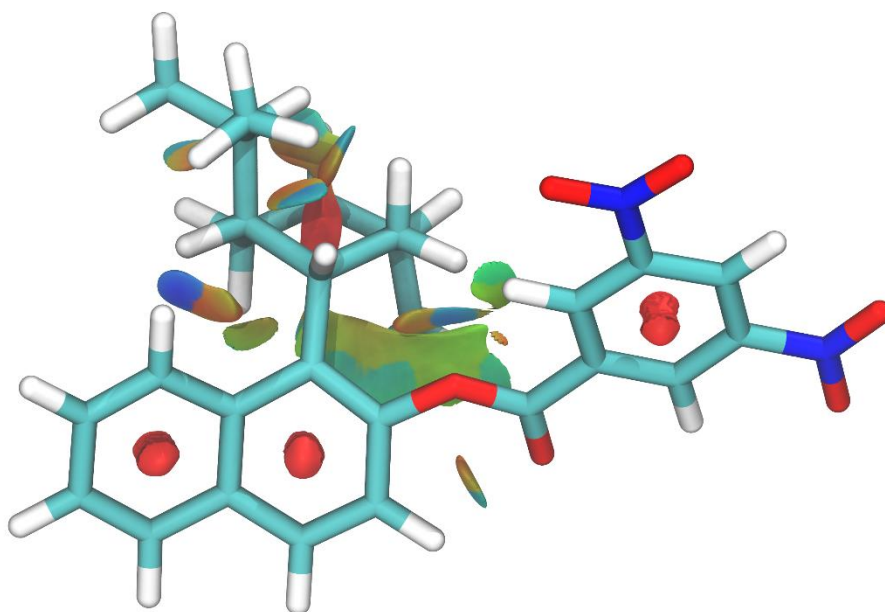
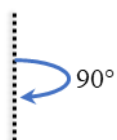
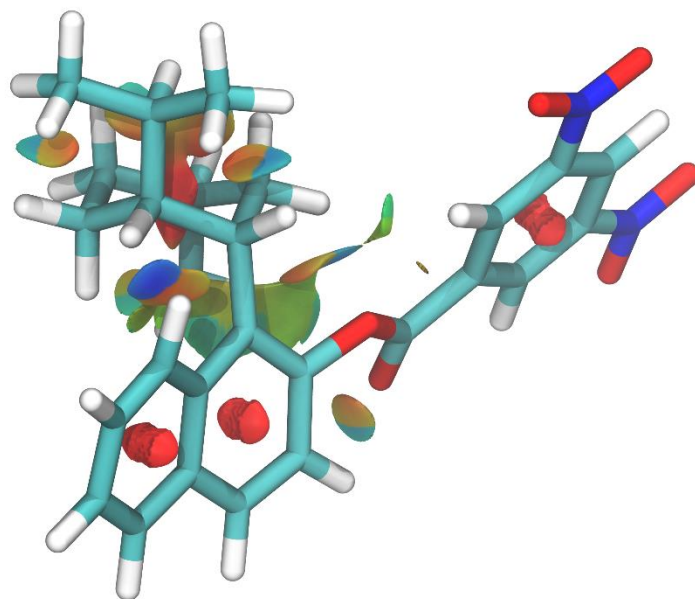
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TS2'-2c

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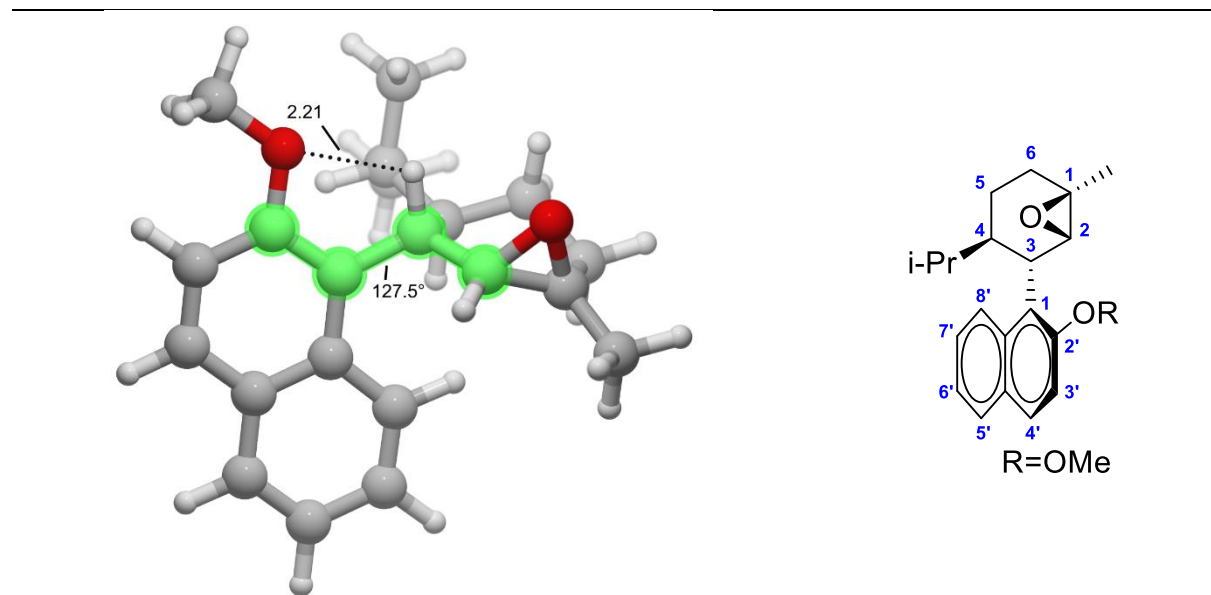
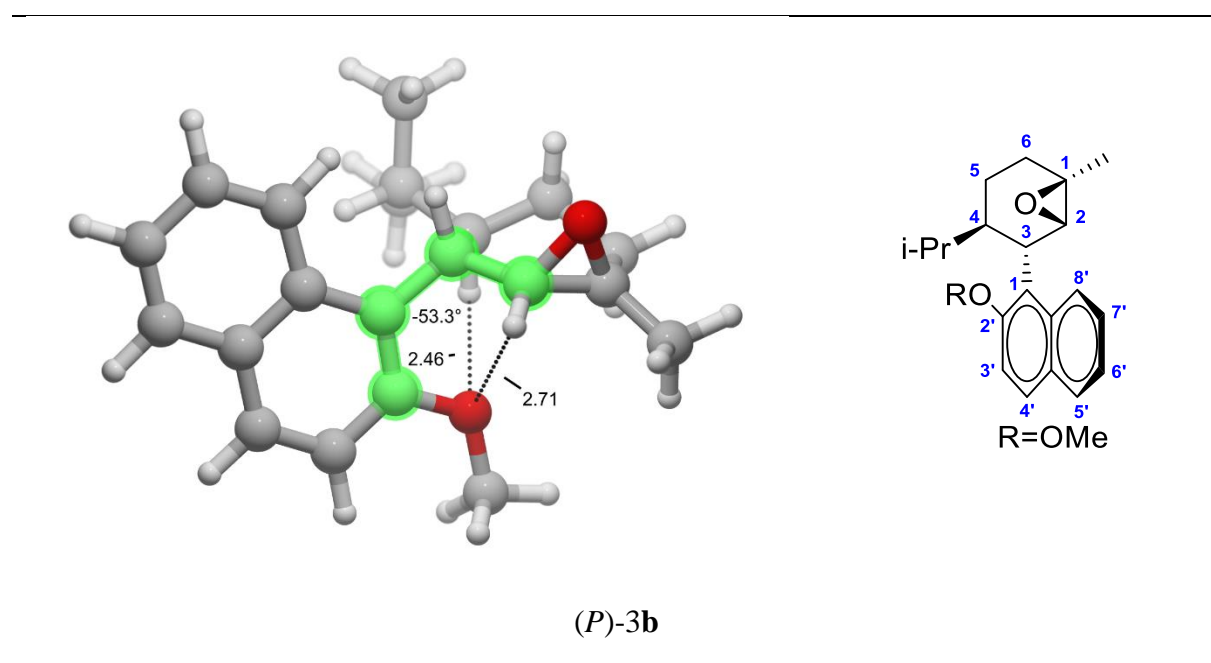


**Table S21.** Thermodynamic parameters of **3b** conformational equilibrium calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

	( <i>M</i> )- <b>3b</b>	( <i>P</i> )- <b>3b</b>	TS1- <b>3b</b>	TS2- <b>3b</b>
$\Delta H^\circ$ (kJ/mol)	1.88	0.00	92.1	93.6
$\Delta G^\circ$ (kJ/mol)	2.43	0.00	99.7	102.2
$\Delta S^\circ$ (J/mol.K)	-1.85	0.00	-25.2	-29.1
$\mu$ (Debye)	4.89	3.10	3.62	3.66

**Figure S16.** Geometrical parameters of (*M*)-**3b** and (*P*)-**3b** atropisomers calculated in DMSO @ the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

(*M*)-**3b**



**Table S22.** NBO analysis of (*M*)-**3b** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

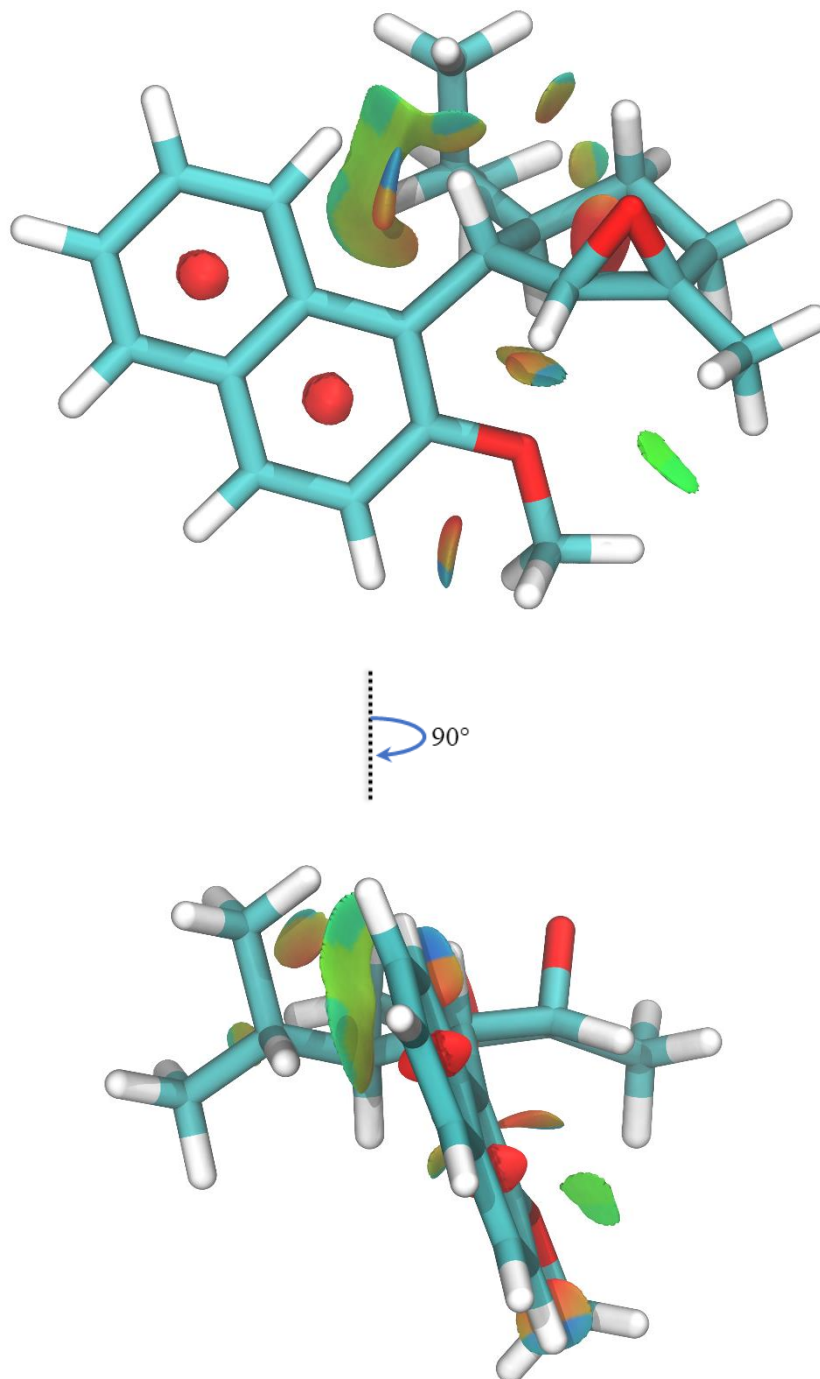
<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C3H3	3.31
$\sigma$ C3H3	$\sigma^*$ C8'H8'	2.64
$\sigma$ CH Me $\beta$ i-Pr	$\sigma^*$ C8'H8'	1.55
$\sigma$ C3H3	$\pi^*$ C1'C2'	19.66
$\pi$ C1'C2'	$\sigma^*$ C3H3	5.40
n O2'	$\sigma^*$ C3H3	1.88
n O2'	$\sigma^*$ C4H4	3.43
n O2'	$\sigma^*$ C2O1	7.45
	<b>Total</b>	<b>39.71</b>

**Table S23.** NBO analysis of (*P*)-**3b** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C2O1	3.43
$\sigma$ C3H3	$\pi^*$ C1'C8a'	22.84
$\pi$ C1'C8a'	$\sigma^*$ C3H3	4.56
$\pi$ C1'C2'	$\sigma^*$ CH i-Pr	2.97
n O2'	$\sigma^*$ C3H3	5.98
	<b>Total</b>	<b>39.79</b>

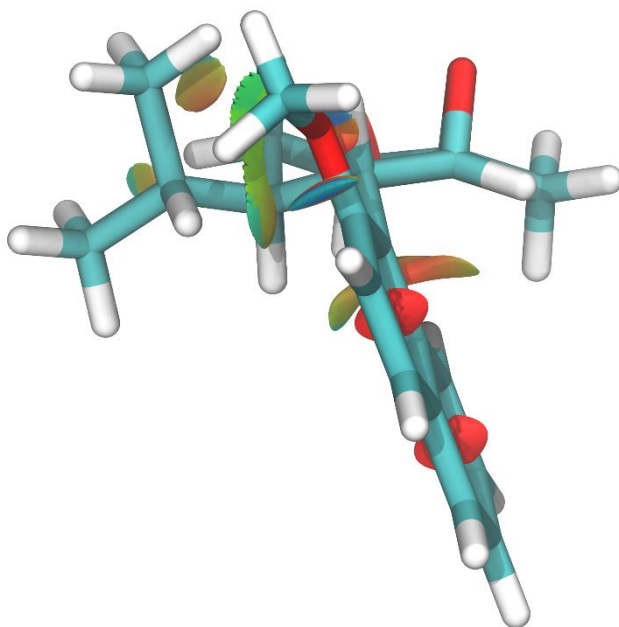
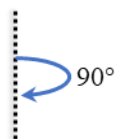
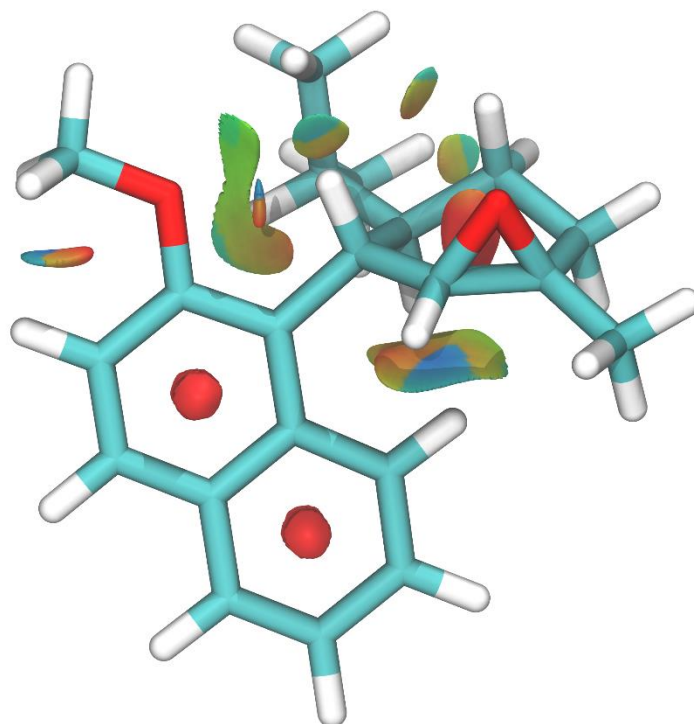
**Figure S17.** NCI analysis of (*M*)-**3b** and (*P*)-**3b** atropisomers implied in **3b** conformational equilibrium.

(*M*)-**3b**

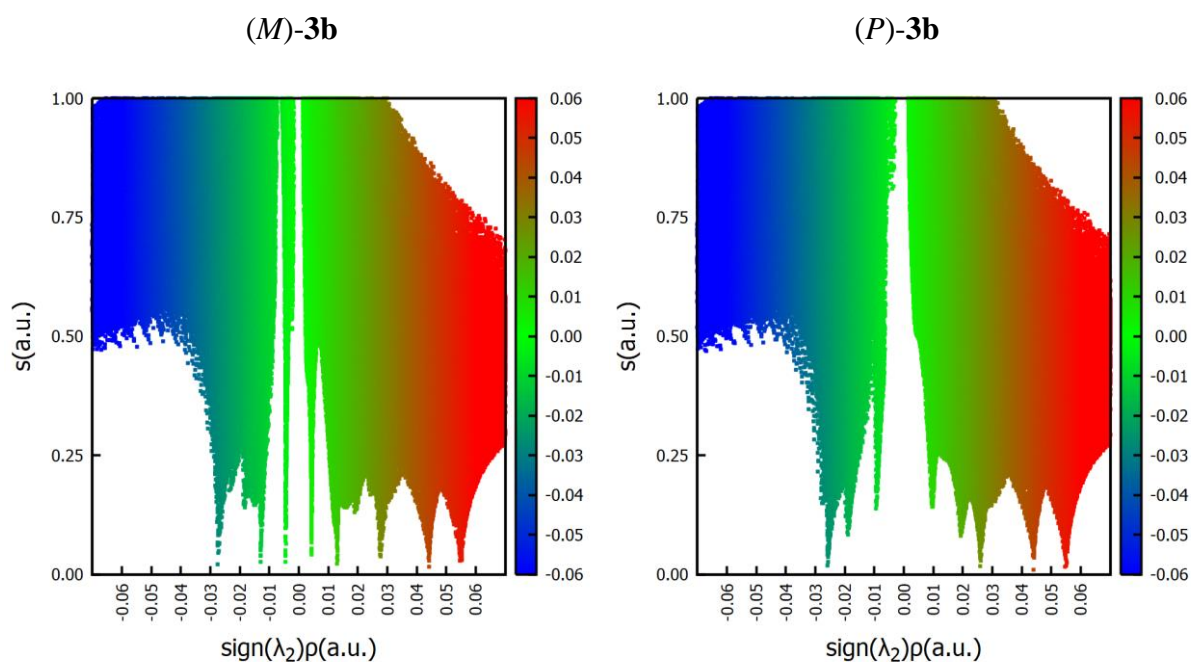


*(P)*-3b

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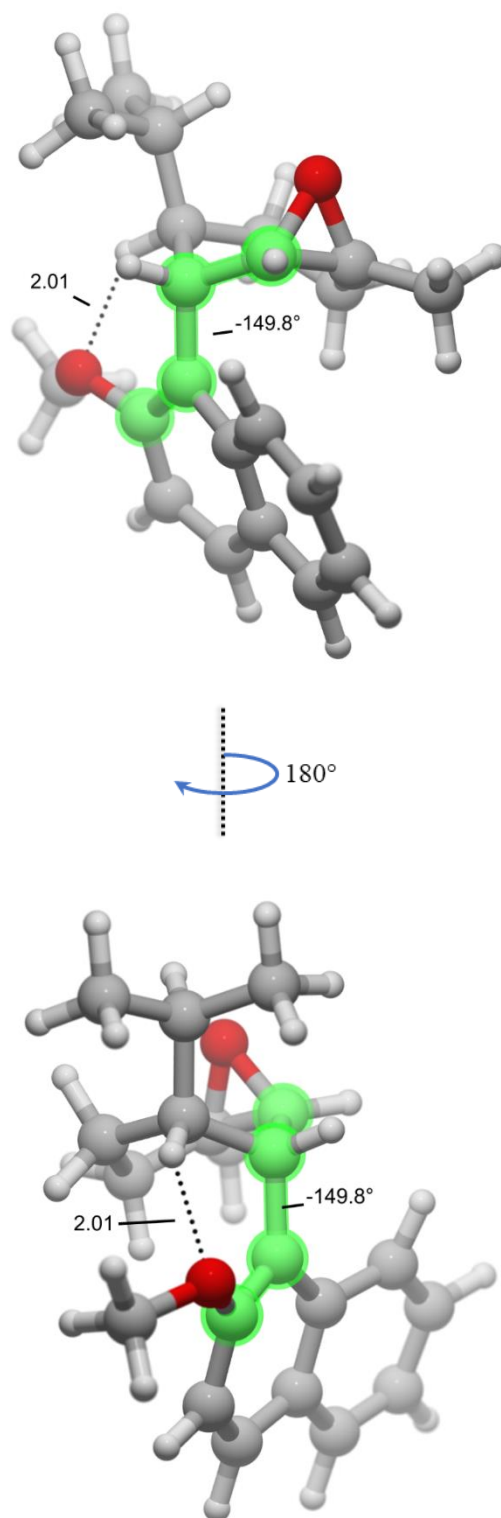
**Figure S18.** Plots of RDG vs  $\text{sign}(\lambda_2)\rho$  of (*M*)-**3b** and (*P*)-**3b** atropisomers and quantitative analysis in the attractive ( $\text{sign}(\lambda_2)\rho < 0$ ), VDW ( $\text{sign}(\lambda_2)\rho \approx 0$ ) and repulsive regions ( $\text{sign}(\lambda_2)\rho > 0$ ).



	<i>Attractive region</i>	<i>VDW region</i>	<i>Repulsive region</i>
( <i>M</i> )- <b>3b</b>	-0.1615	0.0026	0.2936
( <i>P</i> )- <b>3b</b>	-0.1616	0.0025	0.2942
( <i>M</i> ) versus ( <i>P</i> )	1.84E-04	8.43E-05	-5.32E-04

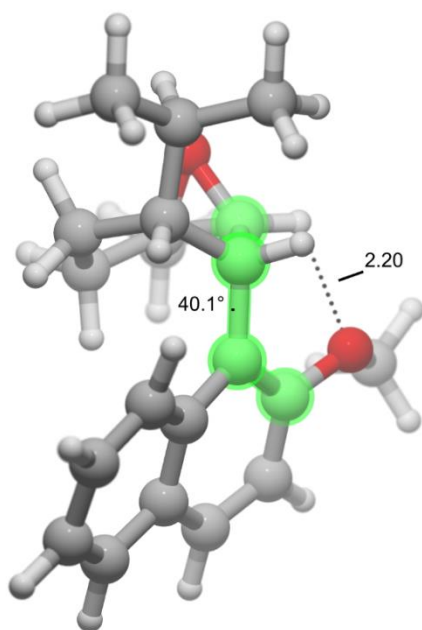
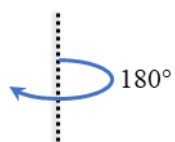
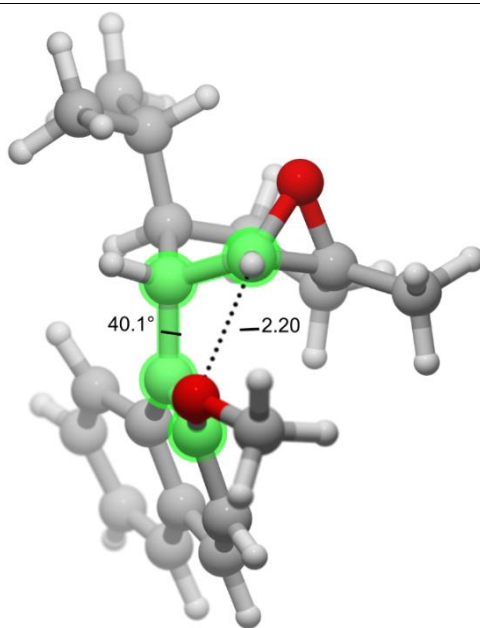
**Figure S19.** Geometrical parameters of located transition states implied in **3b** conformational equilibrium calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

TS1-**3b**



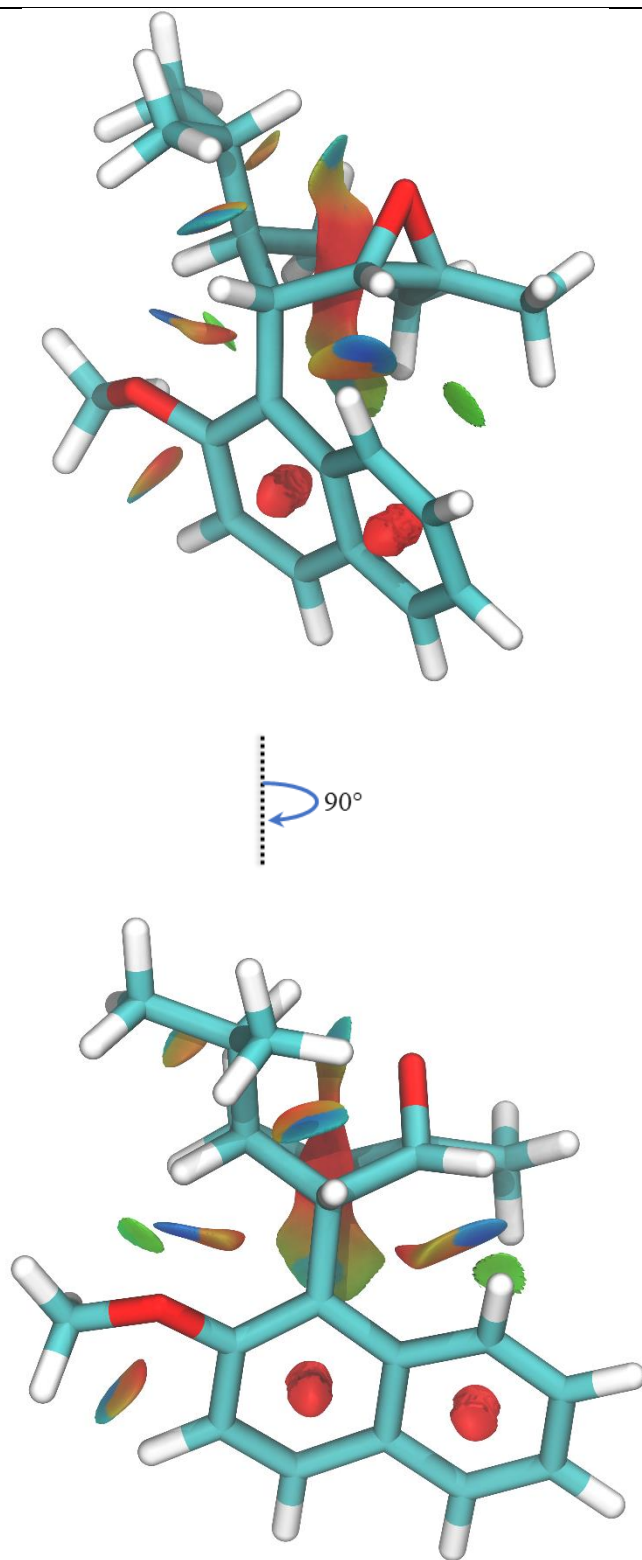
TS2-3b

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**Figure S20.** NCI analysis of located transition states implied in **3b** conformational equilibrium.

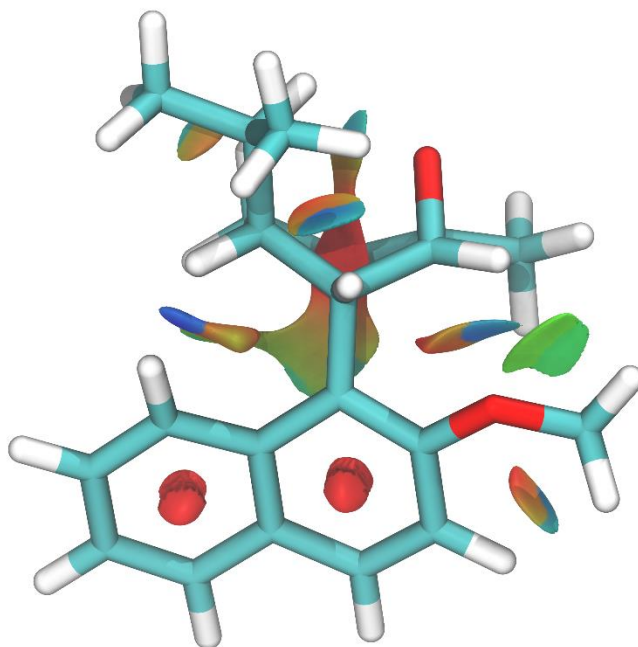
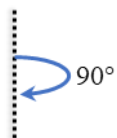
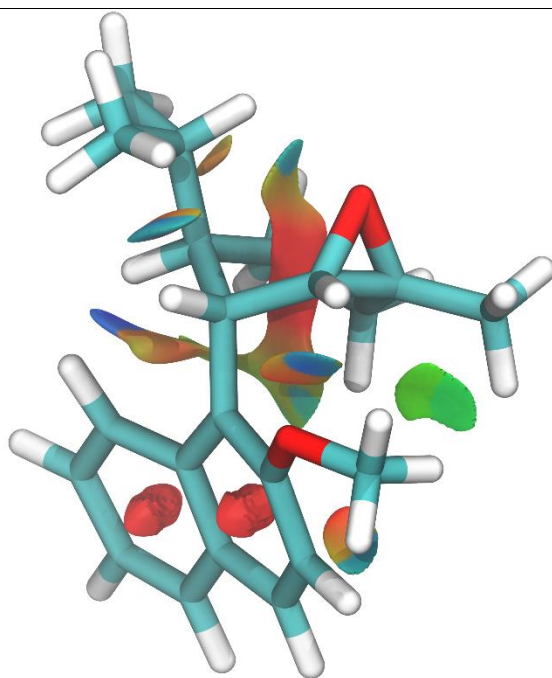
TS1-3b





TS2-3b

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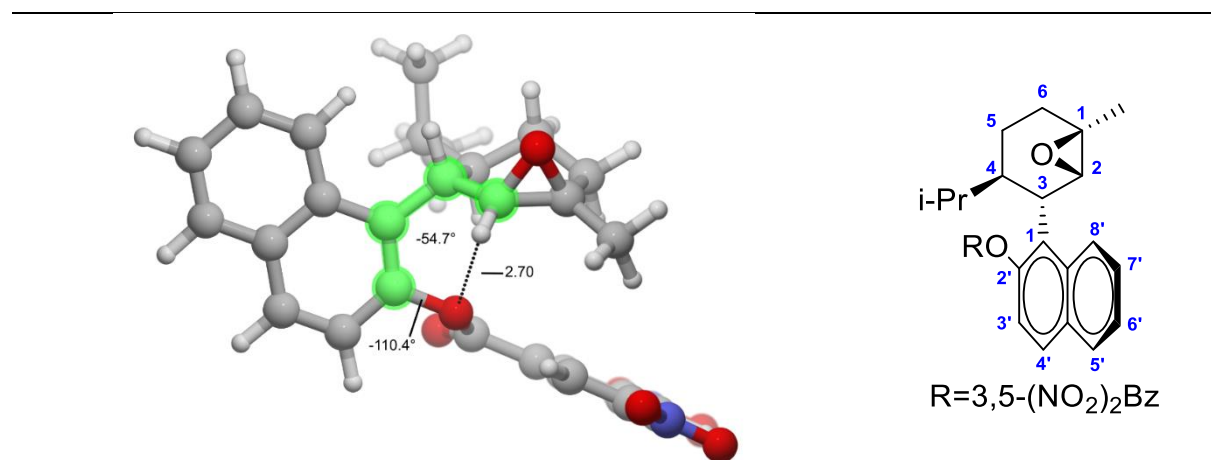


**Table S24.** Thermodynamic parameters of **3c** conformational equilibrium calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

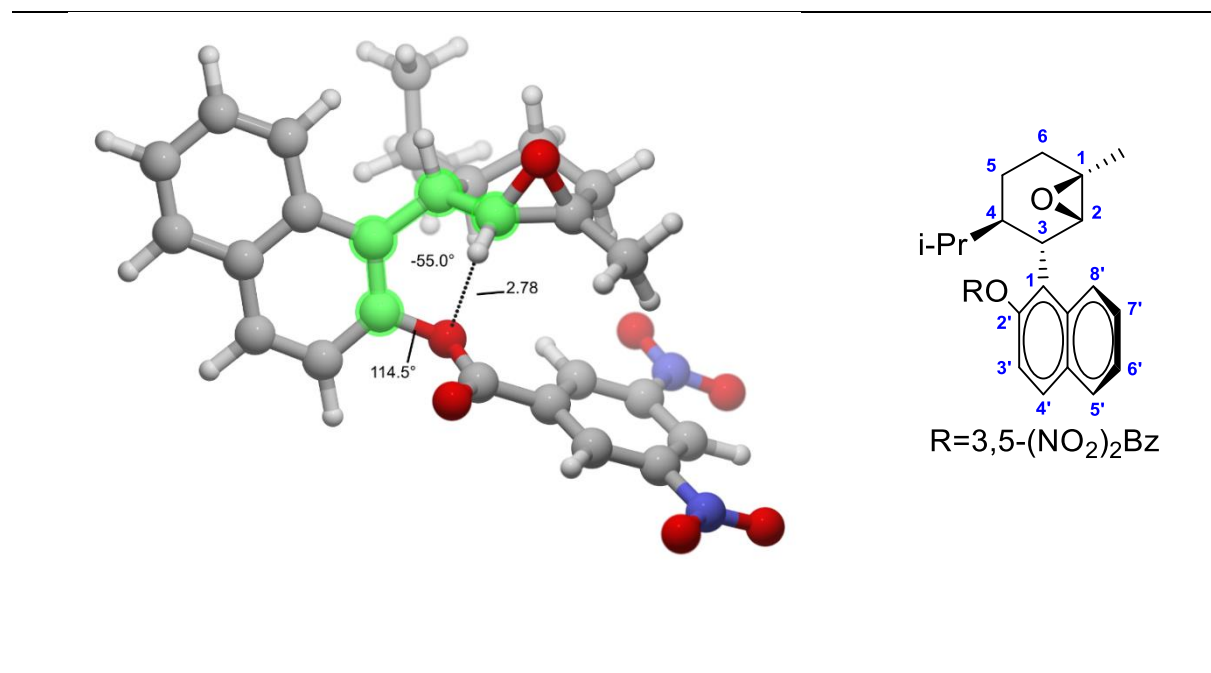
	( <i>M</i> )- <b>3c bis</b>	( <i>M</i> )- <b>3c</b>	( <i>P</i> )- <b>3c</b>	( <i>P</i> )- <b>3c bis</b>	TS1- <b>3c</b>	TS1'- <b>3c</b>	TS2- <b>3c</b>	TS2'- <b>3c</b>
$\Delta H^\circ$ (kJ/mol)	1.54	-2.96	0.00	-1.30	84.76	90.63	97.40	99.53
$\Delta G^\circ$ (kJ/mol)	2.01	2.01	0.00	2.07	95.82	101.23	104.66	109.02
$\Delta S^\circ$ (J/mol.K)	-1.56	-16.68	0.00	-11.32	-37.13	-35.55	-24.37	-31.83
$\mu$ (Debye)	5.24	4.18	7.84	7.23	6.45	6.32	6.40	6.13

**Figure S21.** Geometrical parameters of (*M*)-**3c** and (*P*)-**3c** atropisomers calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

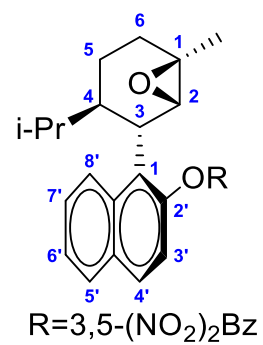
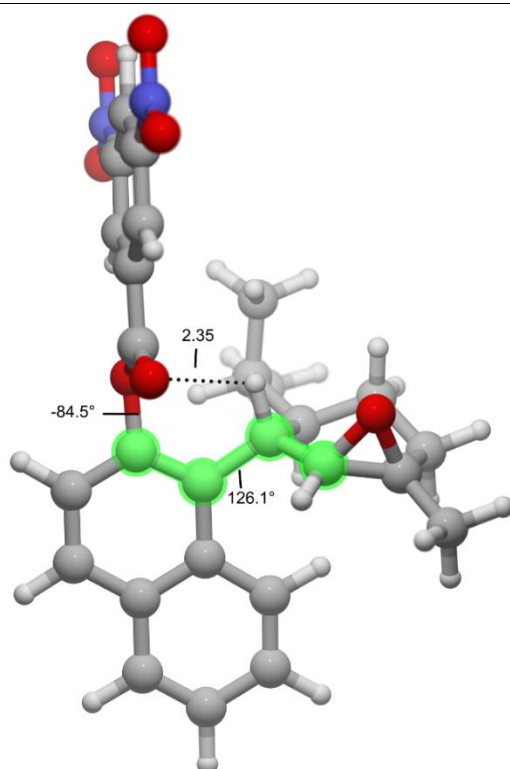
(*M*)-**3c bis**



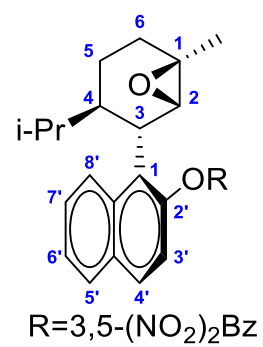
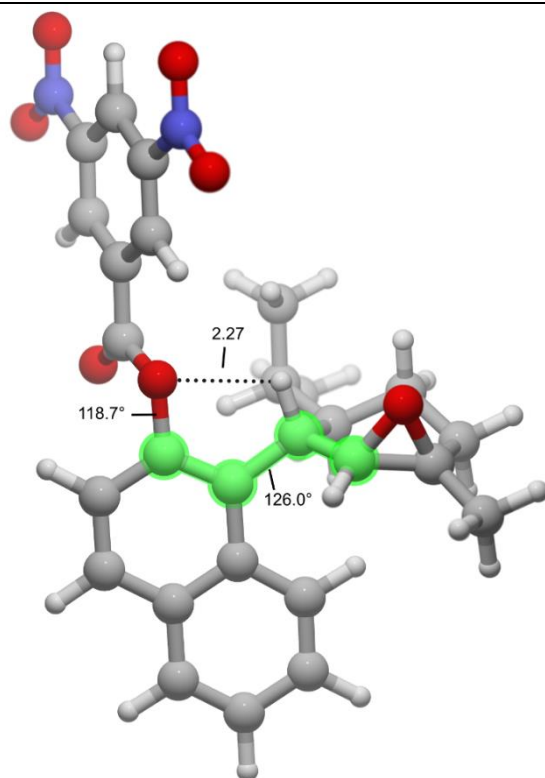
(*M*)-**3c**



(*P*)-**3c**



(*P*)-**3c'**



**Table S25.** NBO analysis of (*M*)-**3c** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C3H3	4.56
$\sigma$ C3H3	$\sigma^*$ C8'H8'	2.72
$\sigma$ C3H3	$\pi^*$ C1'C2'	20.59
$\pi$ C1'C2'	$\sigma^*$ C3H3	4.90
$\sigma^*$ CH Me $\beta$ i-Pr	$\sigma^*$ C8'H8'	1.63
$\sigma$ CH i-Pr	$\pi^*$ C1'C2'	1.80
$\pi$ C1''O	$\sigma^*$ C2H2	1.55
n O2'	$\sigma^*$ C4H4	3.64
n O2'	$\sigma^*$ C3H3	1.42
n O2'	$\sigma^*$ C2O1	2.93
	<b>Total</b>	<b>45.73</b>

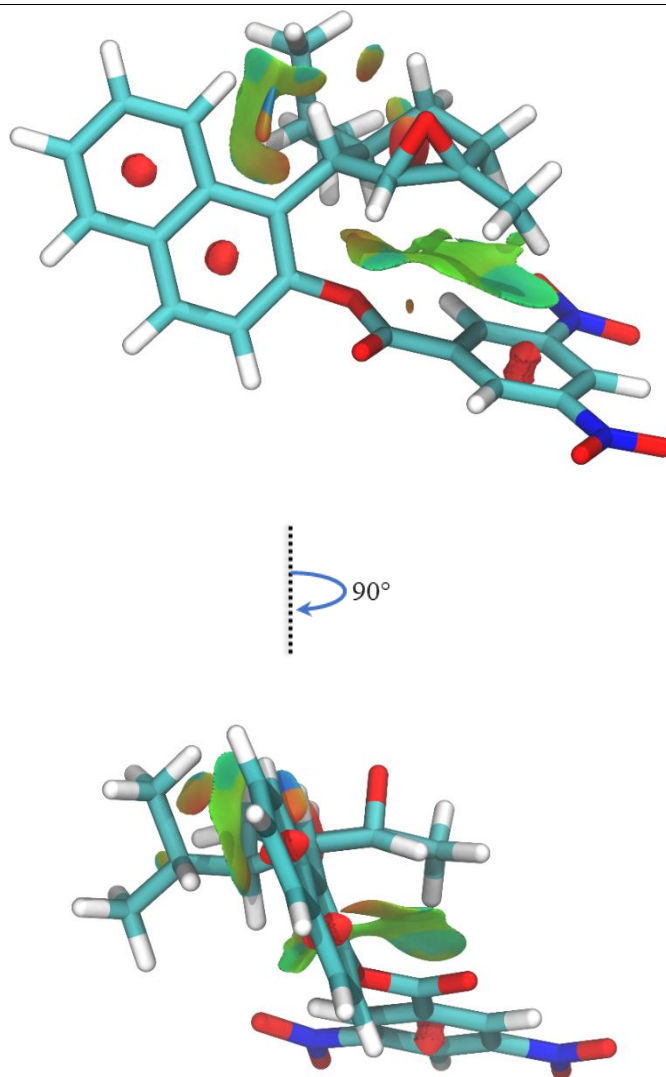
**Table S26.** NBO analysis of (*P*)-**3c** atropisomer in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
$\sigma$ C8'H8'	$\sigma^*$ C2O1	2.93
$\sigma$ C3H3	$\pi^*$ C1'C8a'	23.47
$\pi$ C1'C8a'	$\sigma^*$ C3H3	4.94
$\pi$ C1'C2'	$\sigma^*$ CH i-Pr	2.43
	<b>Total</b>	<b>35.98</b>

**Figure S22.** NCI analysis of (*M*)-**3c** and (*P*)-**3c** atropisomers implied in **3c** conformational equilibrium.

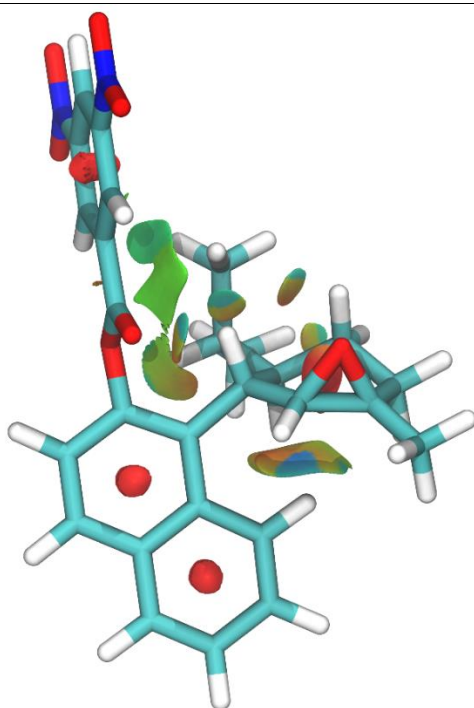
(*M*)-**3c**

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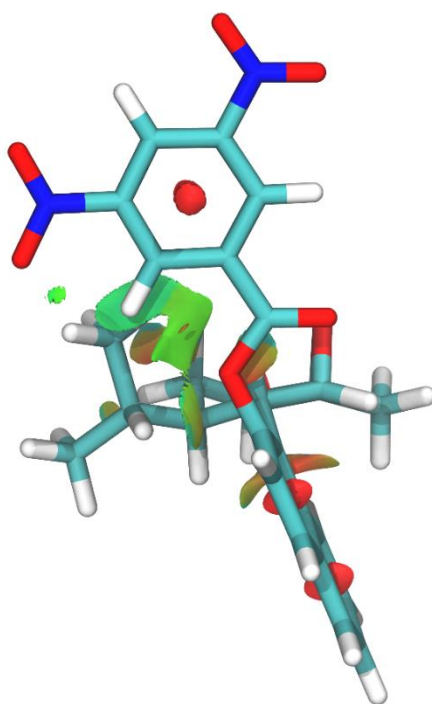


(P)-3c

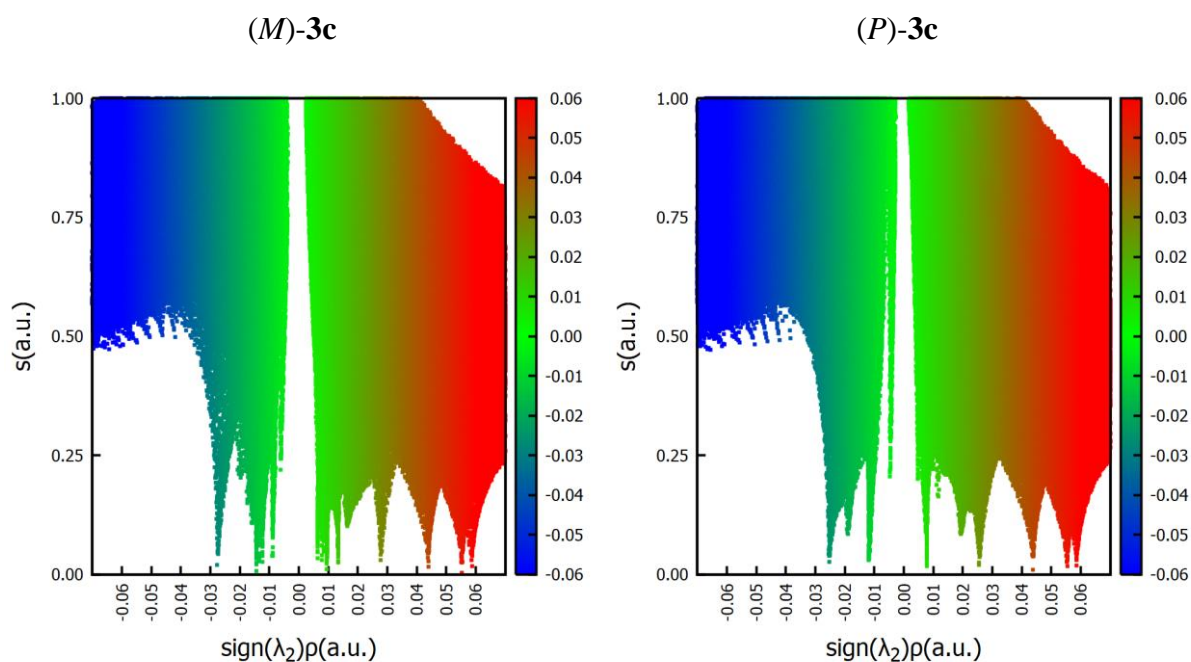
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90°



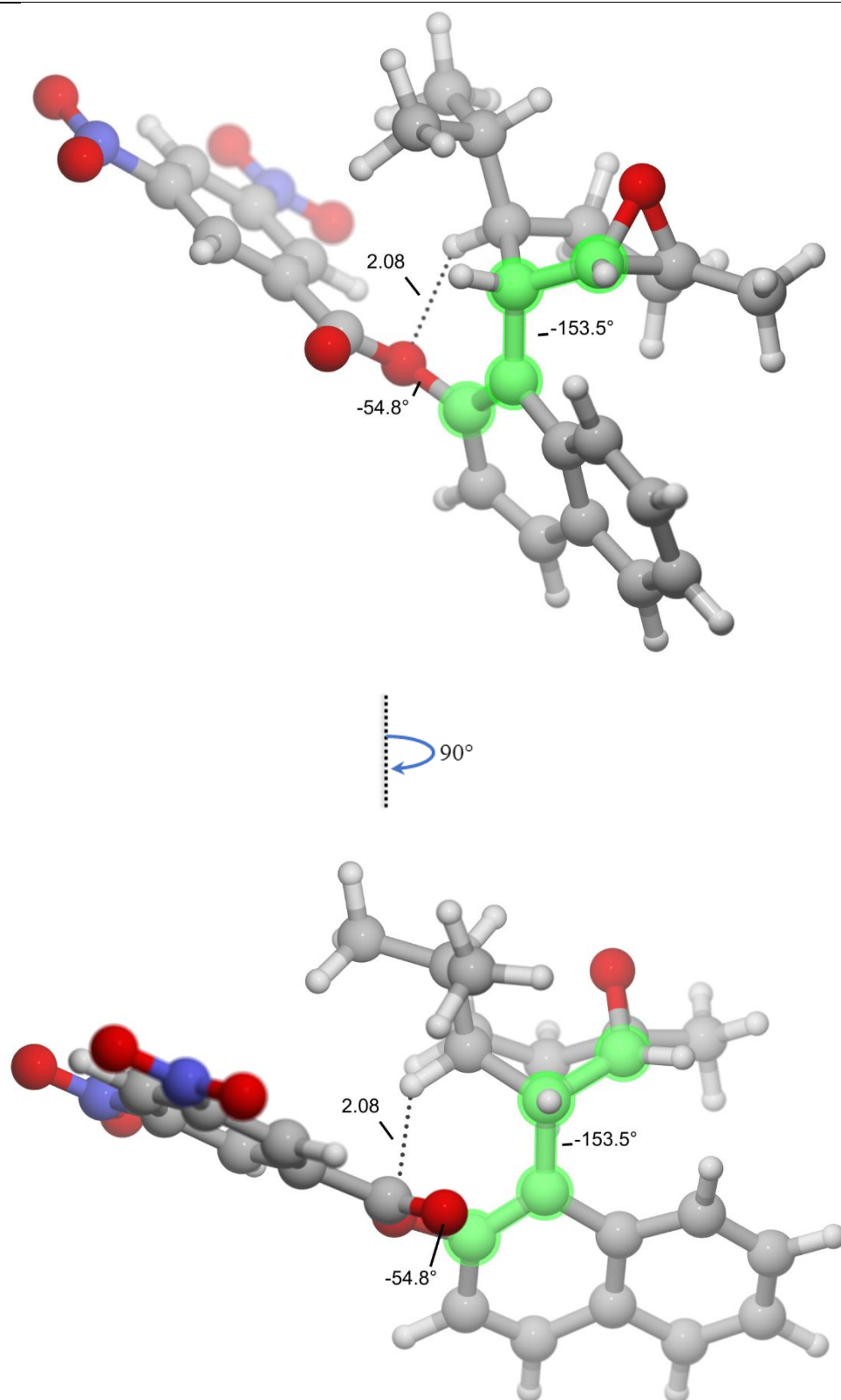
**Figure S23.** Plots of RDG vs  $\text{sign}(\lambda_2)\rho$  of (*M*)-**3c** and (*P*)-**3c** atropisomers and quantitative analysis in the attractive ( $\text{sign}(\lambda_2)\rho < 0$ ), VDW ( $\text{sign}(\lambda_2)\rho \approx 0$ ) and repulsive regions ( $\text{sign}(\lambda_2)\rho > 0$ ).



	<i>Attractive region</i>	<i>VDW region</i>	<i>Repulsive region</i>
( <i>M</i> )- <b>3b</b>	-0.2108	0.0035	0.3786
( <i>P</i> )- <b>3b</b>	-0.2097	0.0032	0.3785
( <i>M</i> ) versus ( <i>P</i> )	-1.05E-03	2.63E-04	1.62E-04

**Figure S24.** Geometrical parameters of located transition states implied in **3c** conformational equilibrium calculated in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

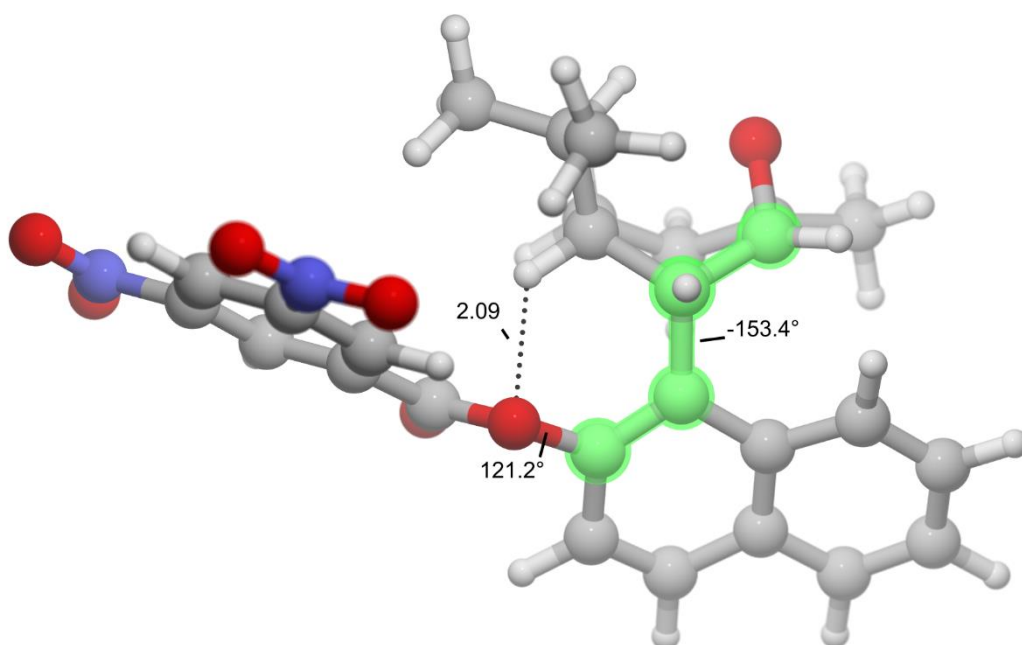
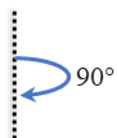
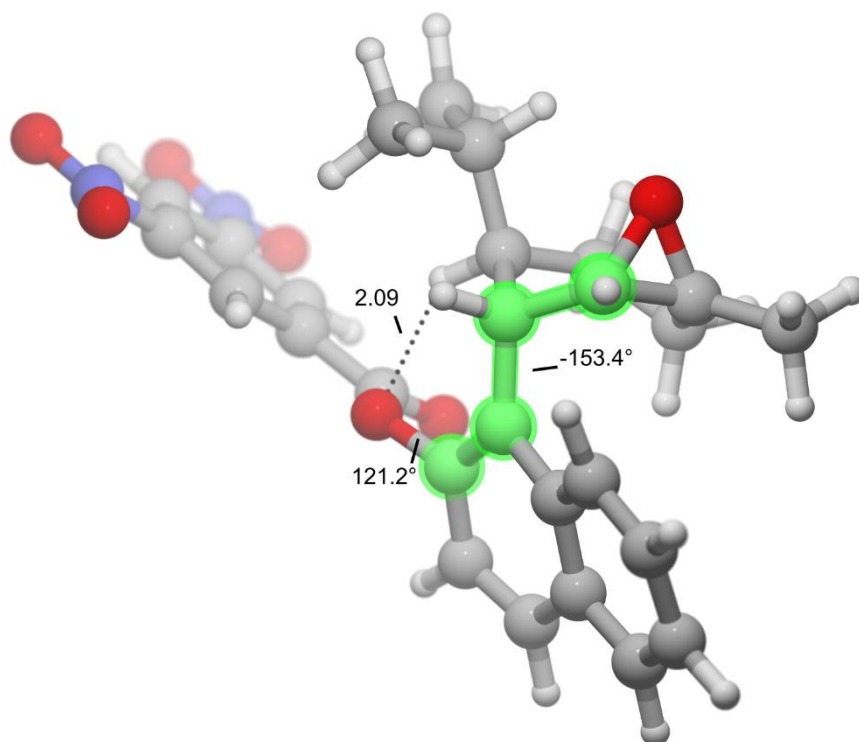
TS1-**3c**



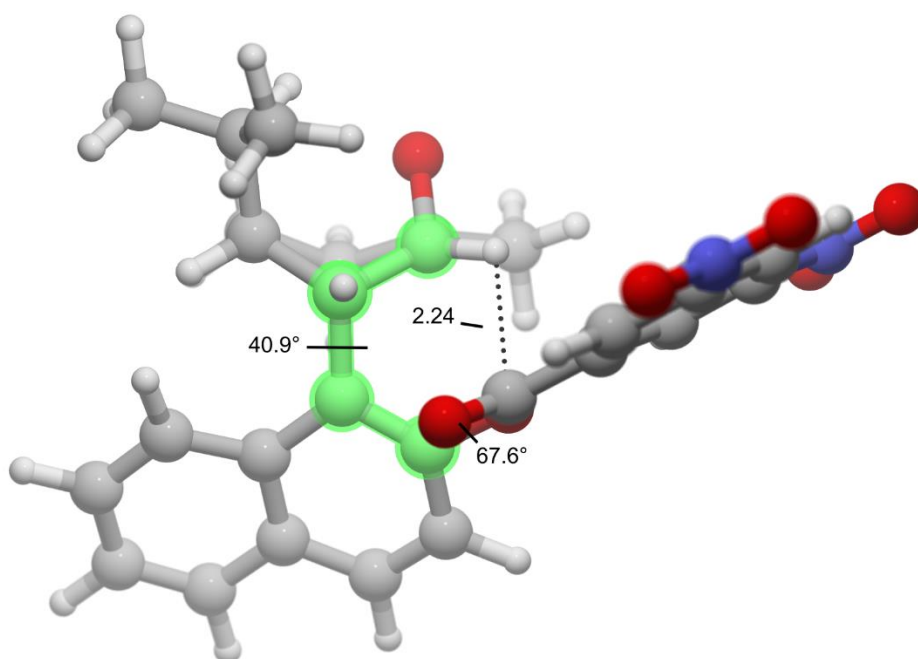
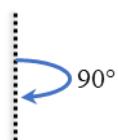
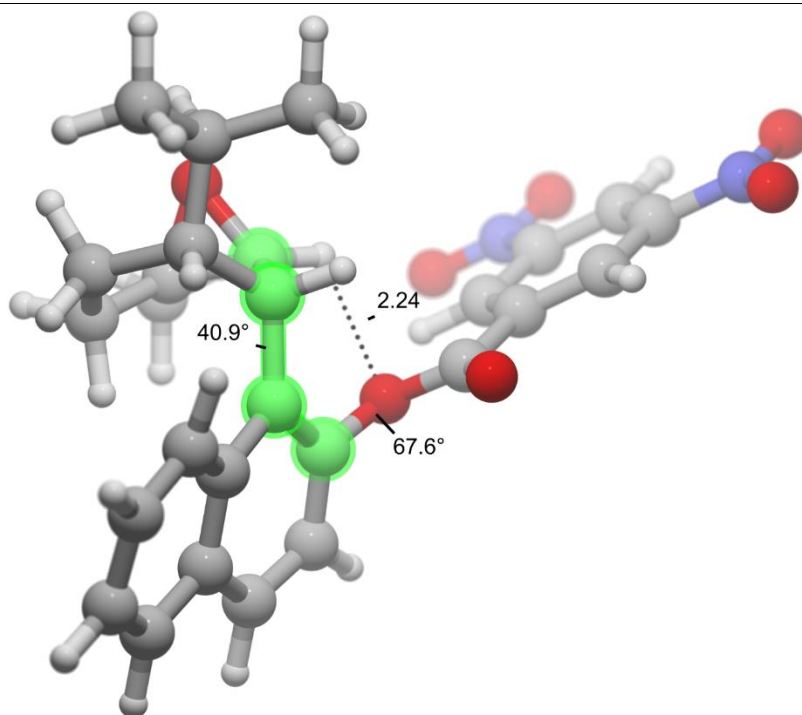


TS1'-3c

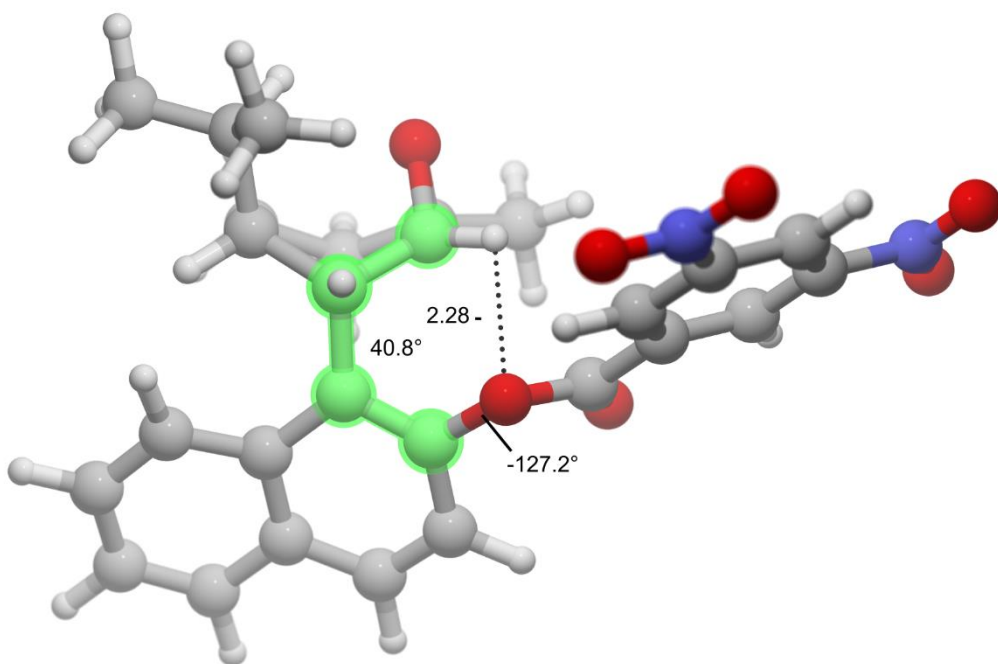
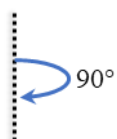
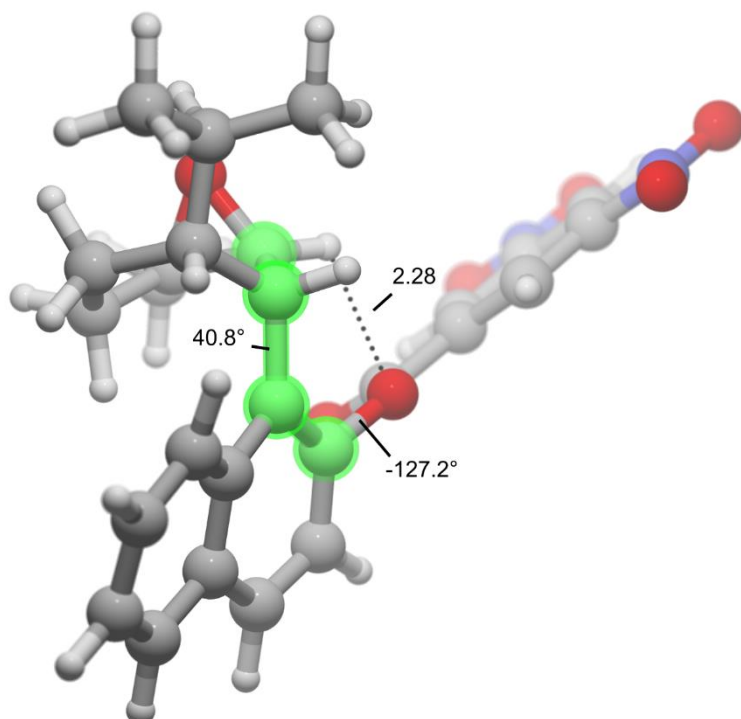
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TS2-3c

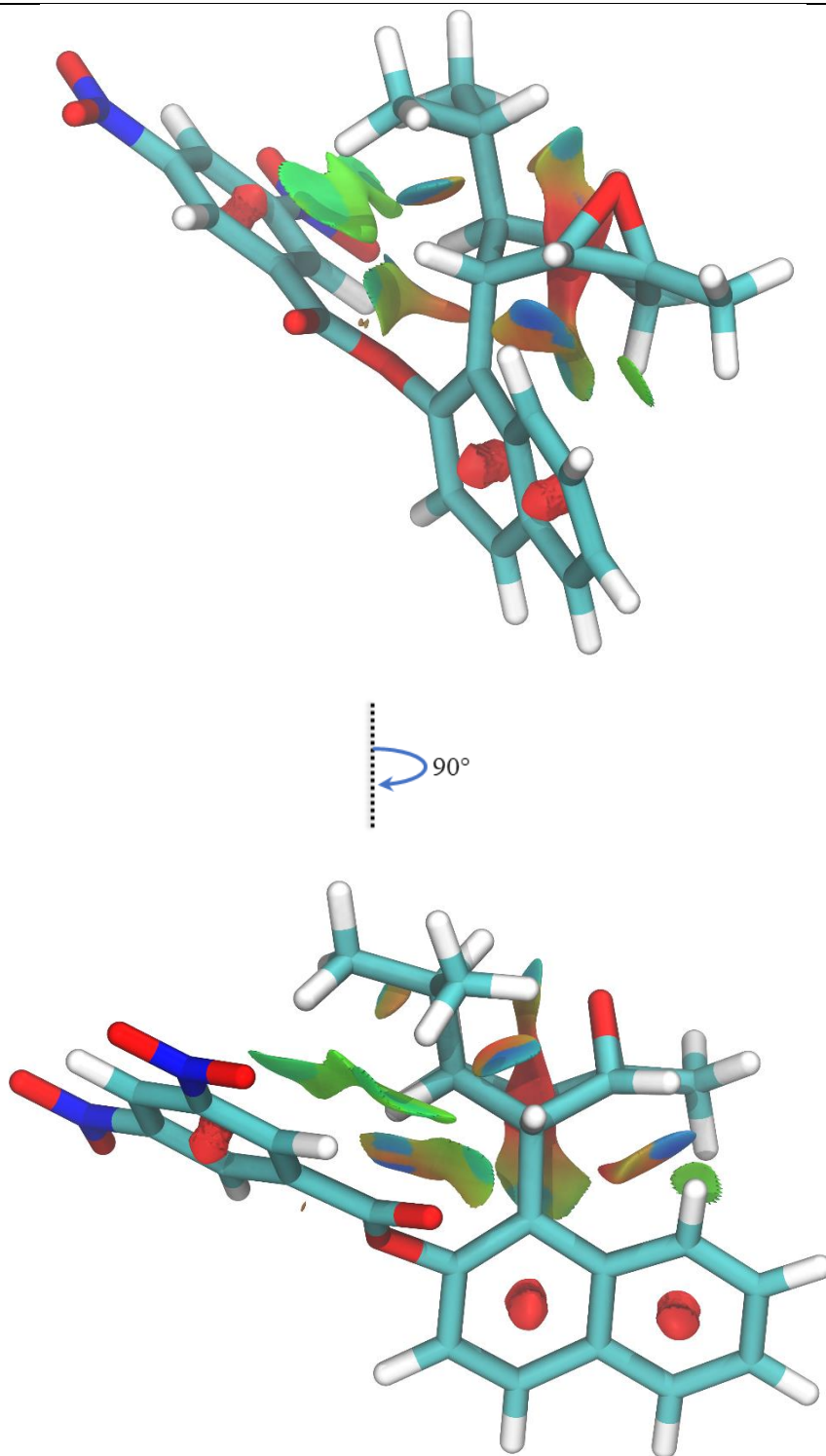


TS2'-3c



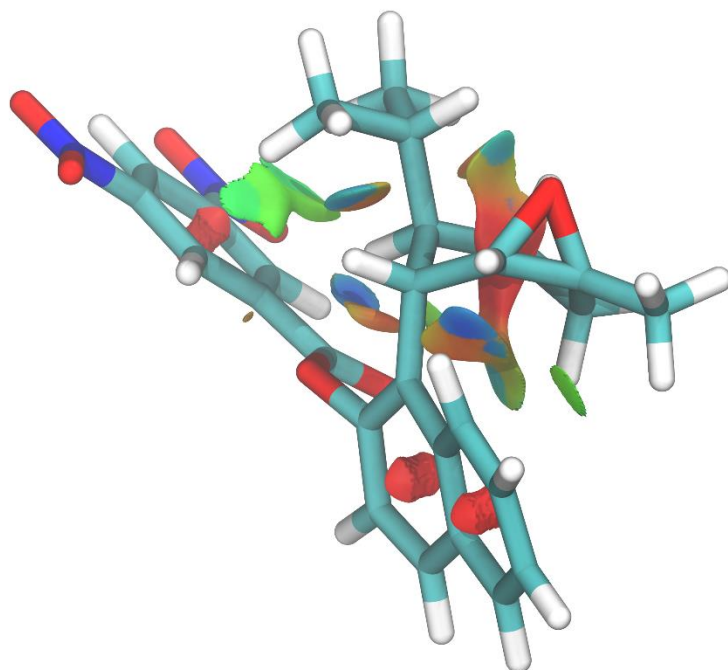
**Figure S25.** NCI analysis of located transition states implied in **3c** conformational equilibrium.

TS1-3c

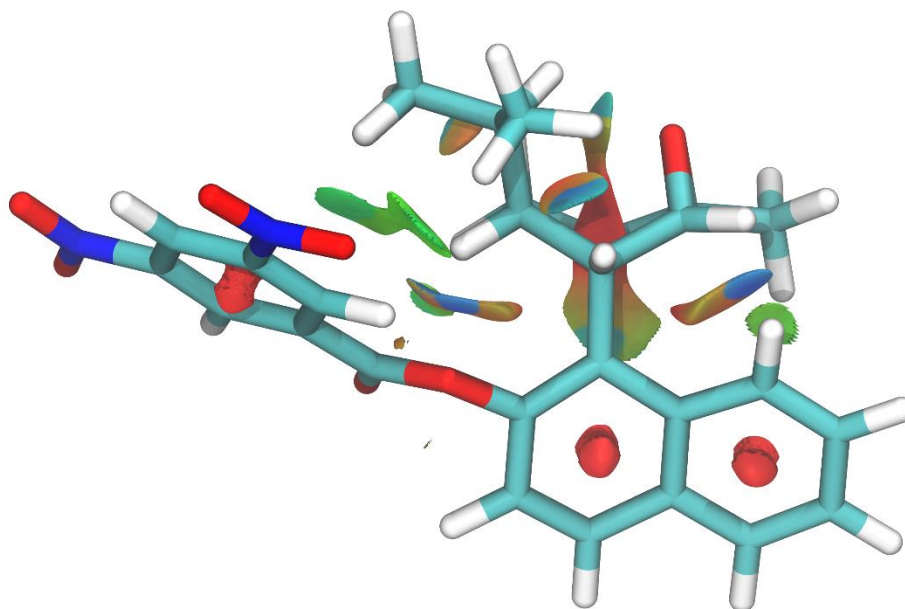


TS1'-3c

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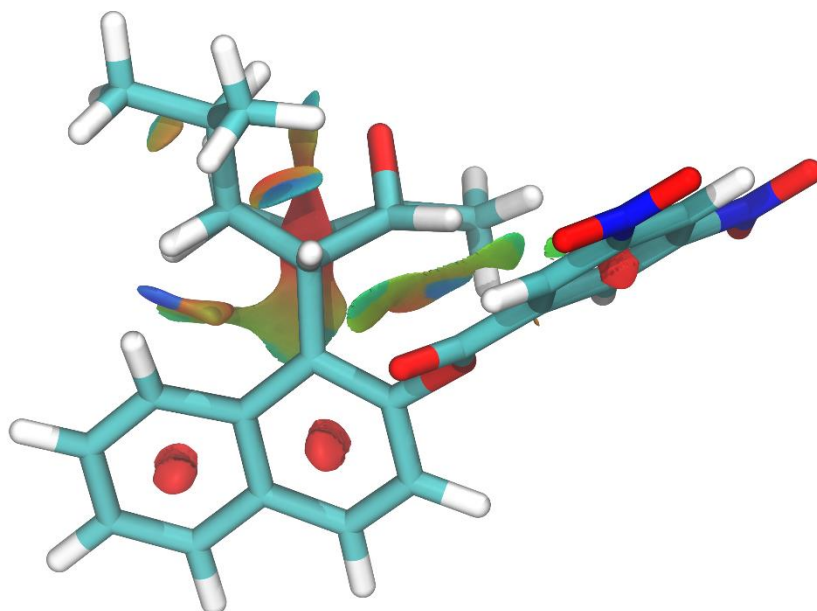
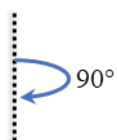
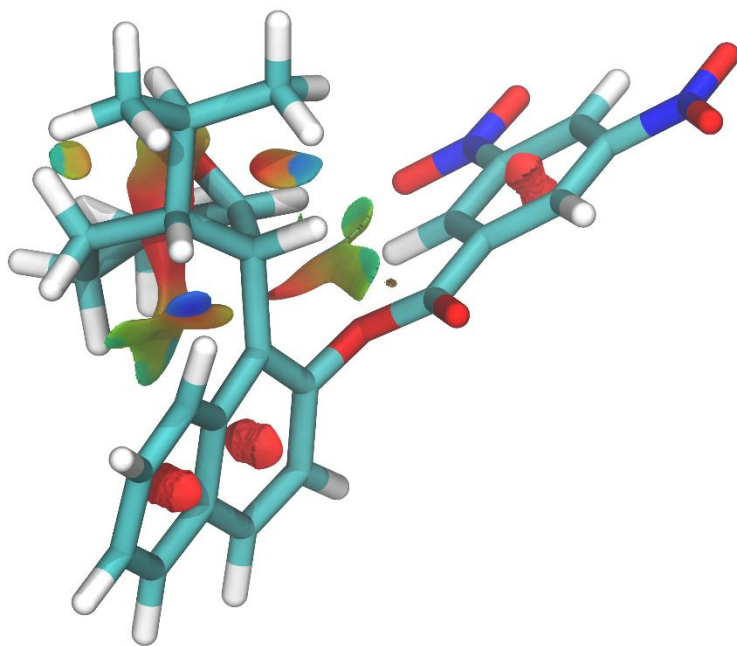


90°



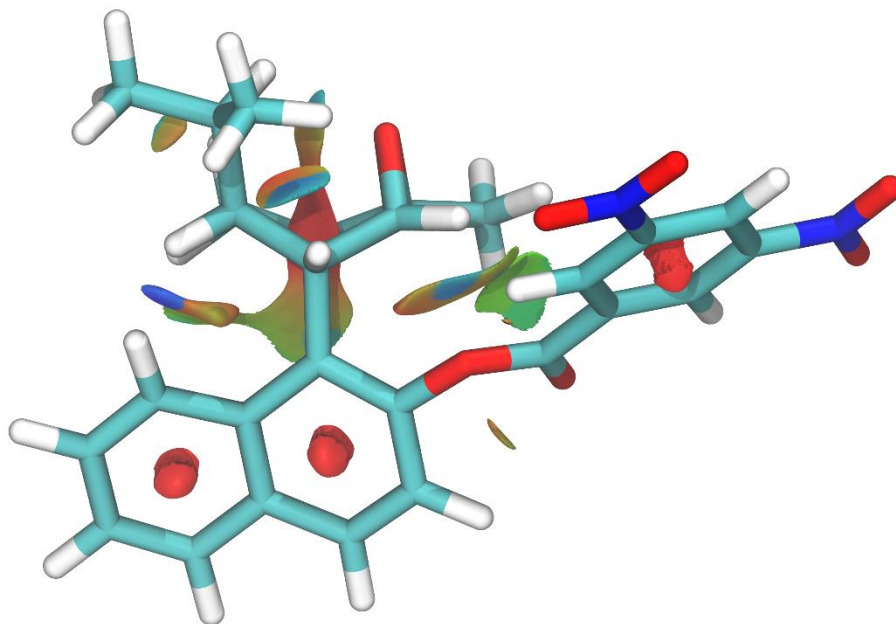
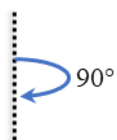
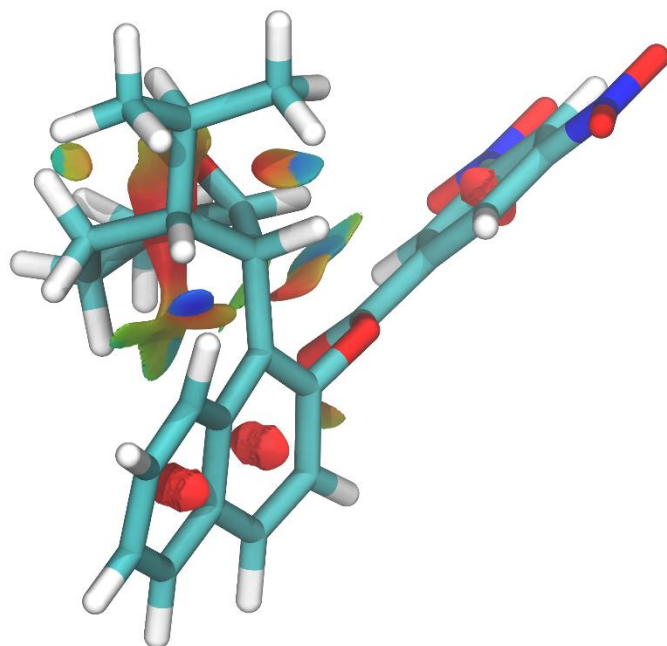
TS2-3c

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TS2'-3c

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**Table S27.** Updated thermodynamic parameters of previously published structures **1a-c** and **1'a-c** calculated in implicit THF at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

	<b>(M)-1a</b>	<b>(P)-1a</b>	<b>TS1-1a</b>	<b>TS2-1a</b>
$\Delta H^\circ$ (kJ/mol)	6.6	0.0	64.5	70.6
$\Delta G^\circ$ (kJ/mol)	5.4	0.0	68.8	76.7
$\Delta S^\circ$ (J/mol.K)	4.2	0.0	-14.3	-20.4
	<b>(M)-1b</b>	<b>(P)-1b</b>	<b>TS1-1b</b>	<b>TS2-1b</b>
$\Delta H^\circ$ (kJ/mol)	6.8	0.0	66.5	70.1
$\Delta G^\circ$ (kJ/mol)	6.3	0.0	71.5	76.0
$\Delta S^\circ$ (J/mol.K)	1.5	0.0	-16.7	-19.9
	<b>(M)-1c</b>	<b>(P)-1c</b>	<b>TS1-1c</b>	<b>TS2-1c</b>
$\Delta H^\circ$ (kJ/mol)	0.0	11.2	64.1	75.6
$\Delta G^\circ$ (kJ/mol)	0.0	6.0	66.8	78.7
$\Delta S^\circ$ (J/mol.K)	0.0	17.6	-9.0	-10.4
	<b>(M)-1'a</b>	<b>(P)-1'a</b>	<b>TS1-1'a</b>	<b>TS2-1'a</b>
$\Delta H^\circ$ (kJ/mol)	0.0	0.0	54.0	56.9
$\Delta G^\circ$ (kJ/mol)	0.0	0.8	61.3	66.1
$\Delta S^\circ$ (J/mol.K)	0.0	-2.8	-24.3	-30.7
	<b>(M)-1'b</b>	<b>(P)-1'b</b>	<b>TS1-1'b</b>	<b>TS2-1'b</b>
$\Delta H^\circ$ (kJ/mol)	0.7	0.0	57.4	58.9
$\Delta G^\circ$ (kJ/mol)	2.5	0.0	65.7	66.4
$\Delta S^\circ$ (J/mol.K)	-6.3	0.0	-27.9	-24.9
	<b>(M)-1'c</b>	<b>(P)-1'c</b>	<b>TS1-1'c</b>	<b>TS2-1'c</b>
$\Delta H^\circ$ (kJ/mol)	0.0	11.5	59.3	63.7
$\Delta G^\circ$ (kJ/mol)	0.0	7.6	65.7	71.0
$\Delta S^\circ$ (J/mol.K)	0.0	13.1	-21.6	-24.6



**Table S28.** Updated thermodynamic parameters of previously published structures **2'a-c** and **3'b-c** calculated in implicit DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

	<i>(M)</i> -2'a	<i>(P)</i> -2'a	TS1-2'a	TS2-2'a
$\Delta H^\circ$ (kJ/mol)	5.1	0.0	90.7	89.2
$\Delta G^\circ$ (kJ/mol)	7.5	0.0	97.4	96.7
$\Delta S^\circ$ (J/mol.K)	-8.1	0.0	-22.6	-25.3
	<i>(M)</i> -2'b	<i>(P)</i> -2'b	TS1-2'b	TS2-2'b
$\Delta H^\circ$ (kJ/mol)	5.0	0.0	92.6	83.5
$\Delta G^\circ$ (kJ/mol)	6.5	0.0	102.3	95.9
$\Delta S^\circ$ (J/mol.K)	-4.8	0.0	-32.4	-41.4
	<i>(M)</i> -2'c	<i>(P)</i> -2'c	TS1-2'c	TS2-2'c
$\Delta H^\circ$ (kJ/mol)	8.4	0.0	88.2	89.6
$\Delta G^\circ$ (kJ/mol)	5.1	0.0	99.7	98.4
$\Delta S^\circ$ (J/mol.K)	11.1	0.0	-38.5	-29.3
	<i>(M)</i> -3'b	<i>(P)</i> -3'b	TS1-3'b	TS2-3'b
$\Delta H^\circ$ (kJ/mol)	0.0	3.8	91.2	87.3
$\Delta G^\circ$ (kJ/mol)	0.0	5.0	99.5	94.6
$\Delta S^\circ$ (J/mol.K)	0.0	-4.0	-28.0	-24.6
	<i>(M)</i> -3'c	<i>(P)</i> -3'c	TS1-3'c	TS2-3'c
$\Delta H^\circ$ (kJ/mol)	0.0	7.7	76.0	81.3
$\Delta G^\circ$ (kJ/mol)	0.0	1.6	87.3	89.0
$\Delta S^\circ$ (J/mol.K)	0.0	20.5	-37.9	-26.0

**Table S29.** NBO analysis of located transition states TS1-3'b and TS2-3'b involved in 3'b conformational equilibrium in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.

<i>Transition state</i>	<i>Donnor</i>	<i>Acceptor</i>	<i>Energy</i>
TS1-3'b	n O2'	$\sigma^*$ C4H4	9.0
TS2-3'b	n O2'	$\sigma^*$ C2O2	36.5

**Cartesian coordinates of calculated minima and located transition states in DMSO at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.**

**(M)-2a**

C	1.056642000	1.127989000	-1.676493000
C	0.608329000	0.241095000	-0.718892000
C	3.373243000	0.697373000	-1.187235000
C	2.432226000	1.362605000	-1.909760000
H	4.427844000	0.879798000	-1.356361000
H	2.721881000	2.082235000	-2.667604000
C	1.597413000	-0.490782000	0.016339000
C	2.983380000	-0.250515000	-0.211093000
C	3.962283000	-0.958433000	0.528984000
C	3.604024000	-1.888873000	1.463518000
C	2.235716000	-2.151379000	1.684667000
C	1.268522000	-1.478350000	0.986740000
H	5.007310000	-0.745740000	0.333186000
H	4.358151000	-2.426049000	2.024280000
H	1.944403000	-2.898964000	2.412177000
H	0.235988000	-1.723165000	1.175026000
C	-2.951393000	0.385565000	0.857610000
C	-1.418559000	0.388564000	0.906534000
C	-0.890550000	0.088822000	-0.518432000
C	-1.425246000	-1.255749000	-1.042525000
C	-2.954131000	-1.291365000	-1.044787000
C	-3.489360000	-0.950257000	0.345585000
H	-3.301545000	1.188895000	0.199947000
H	-3.358408000	0.585484000	1.851131000
H	-1.137292000	-0.428642000	1.577941000
H	-1.348915000	0.847300000	-1.156359000
H	-3.194500000	-1.747729000	1.039807000
H	-4.582848000	-0.935901000	0.326976000
H	-1.050650000	-1.419995000	-2.057697000
C	-0.814989000	1.668693000	1.515620000
H	0.271168000	1.525133000	1.521304000
C	-3.472574000	-2.641333000	-1.527275000
H	-4.564131000	-2.656081000	-1.558064000
H	-3.144374000	-3.437547000	-0.853177000
H	-3.100432000	-2.873276000	-2.527512000
C	-1.108056000	2.930524000	0.702671000
H	-2.180291000	3.141433000	0.679358000
H	-0.615243000	3.792172000	1.158438000
H	-0.753878000	2.846598000	-0.325972000
C	-1.251026000	1.862395000	2.968517000
H	-2.305342000	2.140013000	3.035024000
H	-1.103319000	0.950601000	3.552621000
H	-0.672214000	2.661417000	3.436175000
H	-1.054886000	-2.087300000	-0.433491000
H	-3.304080000	-0.514998000	-1.737465000
O	0.141232000	1.808512000	-2.432425000
H	0.600394000	2.406673000	-3.032034000

**SCF Done: E(RM062X) = -852.922201721**

**# of imaginary frequencies = 0**

**(P)-2a**

C	0.705766000	0.611372000	1.751103000
C	0.591304000	-0.000815000	0.520423000
C	3.112033000	0.608958000	1.678831000
C	1.957881000	0.925229000	2.327305000

H	4.073295000	0.852172000	2.115648000
H	1.982577000	1.423211000	3.290689000
C	1.804856000	-0.370547000	-0.149148000
C	3.068276000	-0.053487000	0.430200000
C	4.269214000	-0.406826000	-0.234079000
C	4.246162000	-1.067842000	-1.429370000
C	3.002898000	-1.406247000	-2.005036000
C	1.826623000	-1.071131000	-1.389806000
H	5.211087000	-0.142747000	0.233745000
H	5.167721000	-1.336182000	-1.929750000
H	2.976819000	-1.941480000	-2.946233000
H	0.903118000	-1.363751000	-1.867806000
C	-3.016182000	0.366668000	-0.904660000
C	-1.771313000	0.851696000	-0.151730000
C	-0.769604000	-0.324256000	-0.069361000
C	-1.404071000	-1.526925000	0.648708000
C	-2.682090000	-1.997154000	-0.045991000
C	-3.656528000	-0.830611000	-0.201938000
H	-2.748457000	0.082369000	-1.928878000
H	-3.746721000	1.174979000	-0.979335000
H	-2.094209000	1.097168000	0.863054000
H	-0.616924000	-0.633508000	-1.103831000
H	-3.994784000	-0.522063000	0.795398000
H	-4.544245000	-1.161712000	-0.748648000
H	-0.682077000	-2.349029000	0.688036000
C	-1.143801000	2.131888000	-0.734923000
H	-0.330987000	2.412161000	-0.055977000
C	-3.320200000	-3.161357000	0.703388000
H	-4.218031000	-3.514973000	0.191789000
H	-2.627326000	-4.000662000	0.794483000
H	-3.607809000	-2.851449000	1.712001000
C	-0.535068000	1.939218000	-2.125110000
H	-1.292159000	1.621829000	-2.846817000
H	0.266385000	1.197853000	-2.122505000
H	-0.112821000	2.880188000	-2.484710000
C	-2.137911000	3.293853000	-0.750995000
H	-2.900291000	3.155491000	-1.521011000
H	-1.623504000	4.232951000	-0.964695000
H	-2.644656000	3.395573000	0.211943000
H	-1.631927000	-1.247328000	1.683655000
H	-2.406573000	-2.339472000	-1.052282000
O	-0.431194000	0.931746000	2.436819000
H	-0.197423000	1.354357000	3.270636000

**SCF Done: E(RM062X) = -852.922712587**

**# of imaginary frequencies = 0**

#### TS1-2a

C	1.876811000	-1.974788000	-1.324827000
C	0.810186000	-1.589549000	0.934655000
C	2.039393000	0.273117000	-0.160456000
C	1.839831000	-0.460716000	-1.494461000
C	0.835656000	-0.040472000	0.795028000
C	0.781373000	-2.434721000	-0.356620000
H	-1.360281000	-2.839686000	-0.390866000
H	-0.878554000	-1.531777000	-1.465512000
H	-1.226295000	3.646141000	-1.194155000
H	1.086137000	0.348292000	1.786359000
H	2.857944000	-2.273825000	-0.942639000
H	1.750320000	-2.474490000	-2.289330000
H	0.872666000	-0.159400000	-1.910588000

H	3.482774000	1.939091000	1.466558000
H	-0.512942000	-3.203613000	-1.899048000
C	-0.449571000	0.703114000	0.360231000
C	-2.586026000	2.018662000	-1.008792000
C	-1.405267000	2.653973000	-0.793572000
C	-0.367257000	2.020024000	-0.066905000
H	2.590386000	-0.136073000	-2.216965000
C	3.418790000	0.003752000	0.489486000
H	2.052936000	1.333656000	-0.383857000
C	4.547168000	0.259937000	-0.513568000
H	2.962891000	0.637232000	2.542292000
H	4.656546000	0.775137000	2.094176000
H	3.500250000	-1.038967000	0.806359000
C	-0.573409000	-2.500075000	-1.065132000
H	4.456731000	1.261674000	-0.945386000
H	5.517745000	0.194735000	-0.018193000
H	4.544188000	-0.461379000	-1.331430000
C	3.636223000	0.886446000	1.721842000
H	1.015929000	-3.457371000	-0.042583000
H	0.040562000	-1.948425000	1.606825000
H	1.745285000	-1.836467000	1.444012000
O	0.743377000	2.763743000	0.217975000
H	-3.365780000	2.476515000	-1.605324000
C	-1.791825000	0.170652000	0.396221000
C	-2.832064000	0.784102000	-0.363520000
C	-4.127354000	0.211675000	-0.404912000
C	-4.447705000	-0.869912000	0.366505000
C	-3.475579000	-1.384742000	1.247391000
C	-2.199439000	-0.887649000	1.256218000
H	-4.873328000	0.681777000	-1.036024000
H	-5.444582000	-1.291035000	0.343765000
H	-3.741754000	-2.174057000	1.939796000
H	-1.515490000	-1.270568000	1.992542000
H	0.659095000	3.635959000	-0.183463000

**SCF Done: E(RM062X) = -852.887509426**

**# of imaginary frequencies = 1 (-47.0610)**

### TS2-2a

C	-2.092460000	-0.781538000	1.948921000
C	-1.624323000	-1.707094000	-0.366285000
C	-1.598523000	0.740825000	-0.023198000
C	-1.408078000	0.501885000	1.483364000
C	-0.905812000	-0.404506000	-0.824382000
C	-1.600811000	-1.993867000	1.147488000
H	0.161441000	-3.274089000	1.043495000
H	0.494193000	-1.678507000	1.714451000
H	3.053616000	-2.891344000	-0.715369000
H	-1.135573000	-0.272262000	-1.885688000
H	-3.175546000	-0.677640000	1.833839000
H	-1.907052000	-0.943452000	3.014752000
H	-0.335779000	0.444771000	1.693421000
H	-2.558403000	1.957557000	-2.270311000
H	-0.364135000	-2.875447000	2.685227000
C	0.637035000	-0.477775000	-0.710599000
C	3.339484000	-0.942082000	0.089015000
C	2.631988000	-1.904459000	-0.556563000
C	1.304204000	-1.659097000	-0.985385000
H	-1.778234000	1.356786000	2.051456000
C	-3.083266000	0.950477000	-0.418434000
H	-1.145661000	1.698296000	-0.249868000

C	-3.669821000	2.146418000	0.337003000
H	-3.041391000	0.272523000	-2.503235000
H	-4.259452000	1.492394000	-2.156341000
H	-3.679958000	0.077170000	-0.147906000
C	-0.246029000	-2.479869000	1.673609000
H	-3.063951000	3.042624000	0.170759000
H	-4.681981000	2.356725000	-0.013339000
H	-3.723852000	1.969380000	1.411448000
C	-3.241160000	1.174836000	-1.924275000
H	-2.309074000	-2.813768000	1.306840000
H	-1.253903000	-2.575992000	-0.895451000
H	-2.669244000	-1.599683000	-0.667025000
H	4.331856000	-1.142454000	0.474578000
C	1.491962000	0.618825000	-0.316600000
C	2.806385000	0.365990000	0.175915000
C	3.609809000	1.426225000	0.663531000
C	3.194726000	2.725232000	0.578267000
C	1.970902000	3.004174000	-0.063134000
C	1.155233000	1.991619000	-0.494935000
H	4.583690000	1.182398000	1.073154000
H	3.818979000	3.531618000	0.941002000
H	1.682157000	4.031954000	-0.245986000
H	0.281705000	2.256218000	-1.067242000
O	0.674273000	-2.659330000	-1.669369000
H	1.252681000	-3.428454000	-1.721644000

**SCF Done: E(RM062X) = -852.889889417**

**# of imaginary frequencies = 1 (-39.3652)**

**(M)-2b**

C	1.115782000	1.666725000	-0.569335000
C	0.606208000	0.390957000	-0.373607000
C	3.393270000	0.896233000	-0.428778000
C	2.508066000	1.921275000	-0.589358000
H	4.459317000	1.091054000	-0.436922000
H	2.877633000	2.926314000	-0.730105000
C	1.536569000	-0.687002000	-0.248239000
C	2.938230000	-0.428988000	-0.262522000
C	3.864319000	-1.493265000	-0.115992000
C	3.438924000	-2.782275000	0.029926000
C	2.053060000	-3.055857000	0.024933000
C	1.137308000	-2.048187000	-0.109395000
H	4.922603000	-1.257294000	-0.125790000
H	4.151521000	-3.589591000	0.140401000
H	1.709176000	-4.078195000	0.123186000
H	0.091028000	-2.305470000	-0.126281000
C	-2.992976000	-0.315598000	0.941568000
C	-1.462822000	-0.410741000	0.986863000
C	-0.902929000	0.215089000	-0.314751000
C	-1.467746000	-0.482414000	-1.564951000
C	-2.996074000	-0.438811000	-1.591450000
C	-3.559340000	-1.016043000	-0.293491000
H	-3.297071000	0.736931000	0.927253000
H	-3.422878000	-0.760451000	1.841603000
H	-1.228006000	-1.479273000	1.011041000
H	-1.316259000	1.224457000	-0.341539000
H	-3.310441000	-2.084189000	-0.248274000
H	-4.650826000	-0.945936000	-0.300927000
H	-1.068979000	0.007058000	-2.459083000
C	-0.837319000	0.192238000	2.259795000
H	0.242441000	0.023751000	2.182141000

C	-3.546730000	-1.167570000	-2.812023000
H	-4.636751000	-1.109786000	-2.847104000
H	-3.266862000	-2.224401000	-2.781935000
H	-3.153184000	-0.742039000	-3.737669000
C	-1.058608000	1.699502000	2.397966000
H	-2.121837000	1.932339000	2.498174000
H	-0.556716000	2.070420000	3.294378000
H	-0.667786000	2.251506000	1.541461000
C	-1.316101000	-0.529317000	3.520289000
H	-2.361464000	-0.299803000	3.738628000
H	-1.221541000	-1.613238000	3.417632000
H	-0.725515000	-0.218315000	4.384385000
H	-1.145446000	-1.528079000	-1.610509000
H	-3.298260000	0.615003000	-1.647897000
O	0.218762000	2.678440000	-0.753187000
C	0.693376000	4.014002000	-0.776170000
H	1.328795000	4.196069000	-1.645028000
H	-0.191411000	4.641577000	-0.841215000
H	1.241823000	4.252347000	0.137824000

**SCF Done: E(RM062X) = -892.208361531**

**# of imaginary frequencies = 0**

**(P)-2b**

C	-0.698221000	1.437839000	-0.872768000
C	-0.610673000	0.170996000	-0.317056000
C	-3.105894000	1.413725000	-0.816050000
C	-1.943268000	2.064210000	-1.113129000
H	-4.059936000	1.895406000	-0.995625000
H	-1.982118000	3.059395000	-1.531088000
C	-1.829988000	-0.525915000	-0.045163000
C	-3.085073000	0.107182000	-0.286411000
C	-4.297774000	-0.573413000	-0.004523000
C	-4.293542000	-1.847192000	0.485335000
C	-3.058131000	-2.496037000	0.708090000
C	-1.872882000	-1.862448000	0.453947000
H	-5.231944000	-0.056185000	-0.193149000
H	-5.222543000	-2.361098000	0.696370000
H	-3.048087000	-3.512156000	1.082884000
H	-0.958489000	-2.410018000	0.629597000
C	2.969227000	-0.554879000	1.046187000
C	1.762576000	0.344827000	0.752188000
C	0.737285000	-0.480747000	-0.061115000
C	1.366042000	-0.980268000	-1.372673000
C	2.610749000	-1.830770000	-1.118409000
C	3.605495000	-1.064506000	-0.247502000
H	2.660512000	-1.410555000	1.657671000
H	3.715437000	-0.004096000	1.622920000
H	2.125809000	1.159144000	0.120786000
H	0.558855000	-1.368775000	0.545700000
H	3.984957000	-0.209133000	-0.820829000
H	4.466021000	-1.701379000	-0.022742000
H	0.628115000	-1.566243000	-1.930221000
C	1.146239000	0.998709000	2.002643000
H	0.357611000	1.667986000	1.641565000
C	3.247776000	-2.281171000	-2.428229000
H	4.120271000	-2.912440000	-2.246079000
H	2.540115000	-2.846364000	-3.038643000
H	3.575283000	-1.414099000	-3.008752000
C	0.497238000	-0.001838000	2.960795000
H	1.229979000	-0.721799000	3.334292000

H	-0.314672000	-0.556245000	2.485766000
H	0.079589000	0.519955000	3.824705000
C	2.162443000	1.863098000	2.750118000
H	2.904176000	1.250018000	3.267064000
H	1.661887000	2.475429000	3.502951000
H	2.692771000	2.531148000	2.066766000
H	1.631338000	-0.117988000	-1.994801000
H	2.295028000	-2.722047000	-0.560065000
O	0.473328000	2.059333000	-1.177659000
C	0.434035000	3.381333000	-1.686743000
H	1.470943000	3.676720000	-1.823642000
H	-0.082964000	3.421527000	-2.647714000
H	-0.046529000	4.062821000	-0.981624000

**SCF Done: E(RM062X) = -892.208945472**

**# of imaginary frequencies = 0**

### TS1-2b

C	1.643708000	-2.208333000	-1.412390000
C	0.570345000	-1.886518000	0.848431000
C	1.981143000	-0.063860000	-0.096394000
C	1.748066000	-0.689579000	-1.479140000
C	0.742822000	-0.340173000	0.827970000
C	0.483280000	-2.624653000	-0.503339000
H	-1.689059000	-2.786160000	-0.596860000
H	-1.042866000	-1.475189000	-1.576593000
H	-1.020866000	3.557274000	-1.062206000
H	1.015988000	-0.053145000	1.847316000
H	2.581179000	-2.620391000	-1.024993000
H	1.502410000	-2.630163000	-2.411480000
H	0.822954000	-0.273812000	-1.892028000
H	3.610888000	1.428721000	1.543340000
H	-0.852839000	-3.145976000	-2.113098000
C	-0.474577000	0.529247000	0.436550000
C	-2.473137000	2.016106000	-0.940051000
C	-1.256216000	2.571497000	-0.686172000
C	-0.285248000	1.852248000	0.054106000
H	2.542325000	-0.387331000	-2.163598000
C	3.323711000	-0.477714000	0.553980000
H	2.082682000	1.004215000	-0.251554000
C	4.482657000	-0.315221000	-0.433376000
H	2.889619000	0.207981000	2.596732000
H	4.600773000	0.120542000	2.202171000
H	3.298306000	-1.528218000	0.855052000
C	-0.854445000	-2.494514000	-1.235787000
H	4.491370000	0.697405000	-0.849486000
H	5.436675000	-0.478068000	0.071598000
H	4.422015000	-1.020151000	-1.263072000
C	3.615881000	0.364735000	1.799155000
H	0.603907000	-3.686840000	-0.265230000
H	-0.246154000	-2.216697000	1.478542000
H	1.466731000	-2.262909000	1.348031000
O	0.860124000	2.477958000	0.448625000
H	-3.205023000	2.537513000	-1.545410000
C	-1.848401000	0.094819000	0.447129000
C	-2.824628000	0.795647000	-0.320631000
C	-4.156085000	0.314875000	-0.397374000
C	-4.565001000	-0.754165000	0.348570000
C	-3.650463000	-1.351060000	1.241574000
C	-2.343460000	-0.946296000	1.283000000
H	-4.855502000	0.845054000	-1.034140000

H	-5.588090000	-1.104270000	0.299009000
H	-3.988223000	-2.127690000	1.916815000
H	-1.700525000	-1.381188000	2.028999000
C	1.369977000	3.536575000	-0.351055000
H	0.795105000	4.453443000	-0.213478000
H	2.391056000	3.702156000	-0.014411000
H	1.374609000	3.258261000	-1.407497000

**SCF Done: E(RM062X) = -892.173902930**

**# of imaginary frequencies = 1 (-37.5088)**

### TS2-2b

C	-2.101822000	-0.693047000	2.059325000
C	-1.396656000	-1.802905000	-0.109384000
C	-1.787032000	0.636680000	-0.082946000
C	-1.621331000	0.620042000	1.445338000
C	-0.881938000	-0.464621000	-0.718250000
C	-1.386089000	-1.894271000	1.428280000
H	0.563573000	-2.865341000	1.520094000
H	0.606673000	-1.164123000	1.977362000
H	3.451757000	-2.166923000	-0.147989000
H	-1.088585000	-0.506917000	-1.791654000
H	-3.181862000	-0.788899000	1.912605000
H	-1.934189000	-0.688578000	3.140298000
H	-0.563764000	0.771863000	1.681409000
H	-2.837985000	1.380058000	-2.489340000
H	-0.077808000	-2.353891000	3.087151000
C	0.645090000	-0.250667000	-0.565230000
C	3.328143000	-0.120078000	0.372149000
C	2.840041000	-1.276927000	-0.155716000
C	1.518907000	-1.328545000	-0.664349000
H	-2.150745000	1.463347000	1.891590000
C	-3.268725000	0.544999000	-0.530745000
H	-1.488055000	1.621828000	-0.419146000
C	-4.071387000	1.713490000	0.048438000
H	-3.034030000	-0.377242000	-2.505855000
H	-4.445488000	0.659726000	-2.347274000
H	-3.726639000	-0.373386000	-0.158087000
C	0.009241000	-2.075841000	2.034102000
H	-3.613863000	2.669185000	-0.225822000
H	-5.090060000	1.705222000	-0.343617000
H	-4.137119000	1.669891000	1.135861000
C	-3.399640000	0.546318000	-2.055719000
H	-1.954881000	-2.796075000	1.678288000
H	-0.871169000	-2.657504000	-0.517319000
H	-2.432936000	-1.906573000	-0.439895000
H	4.315496000	-0.090256000	0.817483000
C	1.272461000	1.020129000	-0.309237000
C	2.583005000	1.072346000	0.252494000
C	3.166252000	2.315669000	0.607433000
C	2.541115000	3.495816000	0.323971000
C	1.322251000	3.464758000	-0.387339000
C	0.715089000	2.276528000	-0.692094000
H	4.143740000	2.305617000	1.076709000
H	2.998088000	4.441800000	0.584488000
H	0.874945000	4.391260000	-0.726039000
H	-0.157973000	2.301270000	-1.323455000
O	1.063169000	-2.463387000	-1.260173000
C	1.846148000	-3.643888000	-1.200311000
H	1.247027000	-4.419516000	-1.670238000
H	2.781927000	-3.527888000	-1.750346000



H 2.059844000 -3.926762000 -0.167130000  
**SCF Done: E(RM062X) = -892.175933608**  
**# of imaginary frequencies = 1 (-42.8575)**

**(M)-2c bis**

C	1.380271000	-0.865589000	-1.439158000
C	2.171596000	-0.448360000	-0.397670000
C	3.182483000	-1.800198000	-2.692790000
C	1.852415000	-1.533003000	-2.583278000
H	3.575159000	-2.306333000	-3.566150000
H	1.144839000	-1.812185000	-3.353016000
C	3.570889000	-0.755880000	-0.499547000
C	4.069721000	-1.422670000	-1.655342000
C	5.453204000	-1.711529000	-1.763639000
C	6.324033000	-1.367345000	-0.769166000
C	5.838061000	-0.721023000	0.386590000
C	4.507619000	-0.426394000	0.517102000
H	5.804718000	-2.216167000	-2.656177000
H	7.378860000	-1.592577000	-0.860468000
H	6.523650000	-0.458383000	1.182389000
H	4.173155000	0.055167000	1.421312000
O	0.006159000	-0.579626000	-1.439383000
C	1.147004000	2.319566000	2.141120000
C	2.064471000	1.697417000	1.080332000
C	1.540193000	0.270646000	0.782100000
C	1.517092000	-0.593913000	2.055644000
C	0.633602000	0.038807000	3.130904000
C	1.095481000	1.468736000	3.410369000
H	0.133461000	2.420708000	1.737088000
H	1.493253000	3.324623000	2.390182000
H	3.056280000	1.629958000	1.537331000
H	0.490494000	0.422358000	0.517775000
H	2.095863000	1.430422000	3.859947000
H	0.435003000	1.933313000	4.147735000
H	1.146405000	-1.592255000	1.808114000
C	2.231058000	2.559884000	-0.185685000
H	2.924081000	2.019474000	-0.840443000
C	0.623539000	-0.804257000	4.400660000
H	-0.028262000	-0.365048000	5.158710000
H	0.275346000	-1.819255000	4.198034000
H	1.631003000	-0.870922000	4.820705000
C	0.930907000	2.768207000	-0.963767000
H	1.121700000	3.364031000	-1.858690000
H	0.191745000	3.304497000	-0.363564000
H	0.491651000	1.822734000	-1.284372000
C	2.874804000	3.909243000	0.135666000
H	2.184945000	4.560656000	0.676589000
H	3.157746000	4.423733000	-0.784618000
H	3.773196000	3.785474000	0.745175000
H	2.527483000	-0.719074000	2.458067000
H	-0.389862000	0.085778000	2.734676000
C	-0.789987000	-1.366739000	-0.699526000
O	-0.433590000	-2.365063000	-0.140346000
C	-4.797904000	0.127682000	-0.400772000
C	-4.422422000	-1.091486000	0.130725000
C	-3.137199000	-1.587845000	0.034727000
C	-2.182713000	-0.831251000	-0.633130000
C	-2.515634000	0.399569000	-1.184180000
C	-3.816528000	0.848887000	-1.051097000
H	-5.807974000	0.498534000	-0.309958000

H	-2.874817000	-2.542007000	0.469816000
H	-1.782822000	1.000422000	-1.702765000
N	-5.441479000	-1.890445000	0.834319000
O	-5.095699000	-2.954831000	1.298768000
O	-6.561746000	-1.433229000	0.904419000
N	-4.173486000	2.158716000	-1.624263000
O	-5.324698000	2.522198000	-1.517902000
O	-3.292661000	2.791483000	-2.165180000

**SCF Done: E(RM062X) = -1606.27758052**

**# of imaginary frequencies = 0**

**(M)-2c**

C	-1.246194000	-1.156767000	-1.151449000
C	-2.198749000	-0.384116000	-0.539059000
C	-2.792733000	-2.795663000	-1.934634000
C	-1.512494000	-2.345591000	-1.857230000
H	-3.027506000	-3.706904000	-2.470955000
H	-0.691353000	-2.876537000	-2.320981000
C	-3.552875000	-0.868478000	-0.605284000
C	-3.838537000	-2.076471000	-1.304195000
C	-5.167804000	-2.563009000	-1.369042000
C	-6.192834000	-1.895007000	-0.761511000
C	-5.922010000	-0.702499000	-0.060006000
C	-4.648190000	-0.205854000	0.013720000
H	-5.351930000	-3.483227000	-1.911399000
H	-7.204874000	-2.275480000	-0.813898000
H	-6.729903000	-0.171169000	0.427161000
H	-4.488422000	0.709003000	0.560230000
O	0.090434000	-0.731087000	-1.130447000
C	-1.547896000	2.289420000	2.229305000
C	-1.983587000	0.928622000	1.673634000
C	-1.795160000	0.917758000	0.136569000
C	-2.429524000	2.134237000	-0.567213000
C	-1.987068000	3.461013000	0.047587000
C	-2.269053000	3.448964000	1.548543000
H	-0.471578000	2.417540000	2.073475000
H	-1.716332000	2.317289000	3.308800000
H	-3.046526000	0.814225000	1.904323000
H	-0.720017000	1.028357000	-0.024647000
H	-3.351648000	3.360539000	1.706230000
H	-1.958892000	4.398640000	1.993119000
H	-2.154600000	2.104901000	-1.626133000
C	-1.253990000	-0.251701000	2.354132000
H	-1.419987000	-1.138066000	1.732895000
C	-2.668005000	4.634988000	-0.646420000
H	-2.330898000	5.586414000	-0.229997000
H	-3.752332000	4.576048000	-0.517012000
H	-2.457000000	4.637912000	-1.717915000
C	0.258641000	-0.042906000	2.471224000
H	0.492814000	0.669427000	3.265766000
H	0.756264000	-0.985354000	2.708017000
H	0.698236000	0.346578000	1.549204000
C	-1.845911000	-0.549807000	3.731755000
H	-1.733066000	0.305408000	4.402683000
H	-2.909409000	-0.787173000	3.659425000
H	-1.339087000	-1.400021000	4.193121000
H	-3.520704000	2.090029000	-0.531788000
H	-0.901734000	3.555684000	-0.087701000
C	0.953189000	-1.454371000	-0.400413000
O	0.669561000	-2.444239000	0.213302000

C	4.907787000	0.202614000	-0.369342000
C	4.583998000	-0.951961000	0.317446000
C	3.315735000	-1.498688000	0.308869000
C	2.323876000	-0.860706000	-0.424986000
C	2.603091000	0.303769000	-1.128997000
C	3.890950000	0.805385000	-1.082866000
H	5.905763000	0.614267000	-0.347290000
H	3.093506000	-2.400770000	0.861710000
H	1.839083000	0.813443000	-1.697968000
N	5.640888000	-1.621674000	1.095982000
O	5.340831000	-2.632283000	1.693407000
O	6.744225000	-1.120060000	1.090421000
N	4.195247000	2.042733000	-1.823336000
O	3.285475000	2.575947000	-2.420578000
O	5.335883000	2.450789000	-1.788333000

**SCF Done: E(RM062X) = -1606.27651937**

**# of imaginary frequencies = 0**

**(P)-2c**

C	1.640571000	-0.954913000	-1.104148000
C	2.453969000	-0.132774000	-0.367422000
C	3.426578000	-2.309521000	-1.921766000
C	2.094252000	-2.035161000	-1.882388000
H	3.802657000	-3.138098000	-2.509285000
H	1.373524000	-2.625739000	-2.432564000
C	3.865158000	-0.402579000	-0.431282000
C	4.340975000	-1.502458000	-1.202062000
C	5.729727000	-1.779496000	-1.259524000
C	6.631372000	-0.998130000	-0.594704000
C	6.173354000	0.104428000	0.156370000
C	4.837581000	0.393019000	0.235758000
H	6.060815000	-2.626591000	-1.849059000
H	7.690367000	-1.216452000	-0.645338000
H	6.886179000	0.732519000	0.675645000
H	4.537920000	1.253719000	0.815183000
O	0.268927000	-0.670633000	-1.145461000
C	0.449881000	1.977752000	2.226463000
C	0.782995000	0.703326000	1.441919000
C	1.899662000	1.038729000	0.425091000
C	1.461954000	2.171232000	-0.520499000
C	1.045126000	3.430527000	0.238842000
C	-0.012691000	3.091609000	1.287884000
H	1.332213000	2.316477000	2.780233000
H	-0.329682000	1.769630000	2.962190000
H	-0.129002000	0.458230000	0.889894000
H	2.712740000	1.444969000	1.025846000
H	-0.929674000	2.773710000	0.772798000
H	-0.267391000	3.988920000	1.858355000
H	2.281649000	2.407114000	-1.206163000
C	1.113339000	-0.514834000	2.324852000
H	1.333932000	-1.345735000	1.646665000
C	0.551049000	4.506235000	-0.721866000
H	1.313565000	4.756987000	-1.462265000
H	0.283333000	5.418971000	-0.185533000
H	-0.337226000	4.156408000	-1.255572000
C	2.343390000	-0.308604000	3.209658000
H	2.549536000	-1.215270000	3.781972000
H	3.235930000	-0.079899000	2.623326000
H	2.185064000	0.503450000	3.923221000
C	-0.089013000	-0.938376000	3.169219000

H	-0.300712000	-0.213327000	3.958064000
H	0.102791000	-1.899985000	3.649078000
H	-0.988552000	-1.041832000	2.555534000
H	0.624260000	1.827808000	-1.138012000
H	1.929745000	3.809681000	0.766526000
C	-0.579353000	-1.544653000	-0.582575000
O	-0.268814000	-2.605287000	-0.118708000
C	-4.598138000	-0.055337000	-0.410159000
C	-4.270009000	-1.340807000	-0.023403000
C	-2.982521000	-1.838153000	-0.084426000
C	-1.975871000	-1.012562000	-0.568047000
C	-2.261330000	0.285669000	-0.971721000
C	-3.565551000	0.733286000	-0.877860000
H	-5.610338000	0.315209000	-0.345160000
H	-2.758446000	-2.844854000	0.239913000
H	-1.488020000	0.941287000	-1.345333000
N	-5.343512000	-2.212133000	0.487154000
O	-5.036685000	-3.330460000	0.838313000
O	-6.465641000	-1.755766000	0.523810000
N	-3.865556000	2.118231000	-1.281506000
O	-2.936651000	2.809015000	-1.641566000
O	-5.020190000	2.481291000	-1.224256000

**SCF Done: E(RM062X) = -1606.28020802**

**# of imaginary frequencies = 0**

**(P)-2c bis**

C	-1.592807000	-0.888882000	-1.101133000
C	-2.417838000	-0.306795000	-0.176083000
C	-3.349190000	-2.041531000	-2.233966000
C	-2.025875000	-1.742405000	-2.132168000
H	-3.710583000	-2.690825000	-3.021881000
H	-1.294524000	-2.137741000	-2.825391000
C	-3.812814000	-0.651030000	-0.259223000
C	-4.270911000	-1.510546000	-1.298432000
C	-5.646193000	-1.839808000	-1.390482000
C	-6.547117000	-1.358269000	-0.483529000
C	-6.100588000	-0.525256000	0.563290000
C	-4.779630000	-0.182016000	0.672113000
H	-5.966908000	-2.489015000	-2.197050000
H	-7.595482000	-1.616654000	-0.560073000
H	-6.809821000	-0.153930000	1.292262000
H	-4.483375000	0.447950000	1.498098000
O	-0.227271000	-0.576550000	-1.084900000
C	-0.680775000	2.617139000	1.736013000
C	-0.927732000	1.732065000	0.508031000
C	-1.898845000	0.602346000	0.924526000
C	-1.301726000	-0.229334000	2.071973000
C	-0.977578000	0.633173000	3.291469000
C	-0.084996000	1.805361000	2.886062000
H	-1.619518000	3.078018000	2.063242000
H	0.001036000	3.429284000	1.476895000
H	0.041513000	1.289749000	0.260910000
H	-2.760543000	1.124956000	1.340206000
H	0.891179000	1.410074000	2.575518000
H	0.095165000	2.448449000	3.751866000
H	-2.000563000	-1.023531000	2.352619000
C	-1.397627000	2.500973000	-0.740571000
H	-1.415205000	1.778515000	-1.563893000
C	-0.337863000	-0.199874000	4.396239000
H	-0.130122000	0.409884000	5.277910000

H	-0.987655000	-1.024323000	4.697001000
H	0.608434000	-0.625421000	4.050404000
C	-2.808663000	3.076319000	-0.604324000
H	-2.869922000	3.773062000	0.235511000
H	-3.558374000	2.296216000	-0.456020000
H	-3.078953000	3.625714000	-1.508424000
C	-0.411577000	3.602897000	-1.131136000
H	-0.465660000	4.447392000	-0.440608000
H	-0.639781000	3.980237000	-2.129753000
H	0.618686000	3.236943000	-1.135066000
H	-0.384085000	-0.723556000	1.729189000
H	-1.923712000	1.044770000	3.666158000
C	0.619784000	-1.501148000	-0.612672000
O	0.302728000	-2.594738000	-0.236986000
C	4.661663000	-0.080342000	-0.432293000
C	4.291636000	-1.319909000	0.053249000
C	2.995212000	-1.792549000	-0.007028000
C	2.021310000	-0.985110000	-0.580213000
C	2.348519000	0.267806000	-1.084150000
C	3.663028000	0.687820000	-0.997356000
H	5.681281000	0.270213000	-0.373118000
H	2.738607000	-2.766841000	0.384783000
H	1.601721000	0.903459000	-1.538986000
N	5.329594000	-2.169502000	0.663712000
O	4.988676000	-3.252602000	1.086578000
O	6.459141000	-1.732072000	0.704478000
N	4.017313000	2.016460000	-1.526845000
O	5.173983000	2.366116000	-1.436682000
O	3.128240000	2.677557000	-2.018692000

**SCF Done: E(RM062X) = -1606.27883488**

**# of imaginary frequencies = 0**

### TS1-2c

C	-2.995736000	3.361105000	-0.054681000
C	-2.896426000	1.454943000	-1.704493000
C	-1.012841000	1.780167000	-0.100915000
C	-1.993497000	2.570847000	0.777433000
C	-1.803803000	0.686647000	-0.906658000
C	-3.823428000	2.422219000	-0.938443000
H	-5.565153000	1.124744000	-0.755684000
H	-4.569200000	1.163166000	0.695521000
H	-0.845099000	-2.113744000	2.686695000
H	-1.134133000	0.262159000	-1.660660000
H	-2.460909000	4.080637000	-0.682118000
H	-3.659744000	3.940577000	0.592248000
H	-2.524419000	1.863980000	1.424014000
H	1.737904000	1.614605000	-0.868607000
H	-5.586309000	2.547272000	0.291111000
C	-2.205771000	-0.500901000	0.000106000
C	-2.912334000	-2.265610000	2.148892000
C	-1.629572000	-1.847430000	1.990467000
C	-1.299632000	-1.012101000	0.905746000
H	-1.441097000	3.232610000	1.446093000
C	-0.137973000	2.681190000	-1.007623000
H	-0.307693000	1.309166000	0.578218000
C	0.454895000	3.853057000	-0.220130000
H	0.694286000	0.993819000	-2.157987000
H	1.545742000	2.520022000	-2.364237000
H	-0.740902000	3.102144000	-1.814986000
C	-4.946274000	1.768620000	-0.130567000

H	0.978281000	3.487660000	0.669284000
H	1.178417000	4.391318000	-0.835412000
H	-0.303739000	4.566265000	0.102622000
C	1.016290000	1.898808000	-1.639403000
H	-4.311239000	3.028068000	-1.709031000
H	-3.490705000	0.809880000	-2.339651000
H	-2.334568000	2.068891000	-2.411898000
O	0.070583000	-0.712262000	0.861589000
C	0.789598000	-1.204554000	-0.157219000
O	0.341268000	-1.804299000	-1.093426000
C	2.244172000	-0.906747000	0.012491000
C	2.726131000	-0.226946000	1.124055000
C	3.106143000	-1.306395000	-1.000224000
C	4.080471000	0.042859000	1.192026000
H	2.065980000	0.094479000	1.916625000
C	4.449684000	-1.010322000	-0.877478000
H	2.728033000	-1.830718000	-1.866679000
C	4.972779000	-0.333202000	0.207436000
H	6.026341000	-0.108688000	0.281502000
H	-3.205698000	-2.865680000	3.001226000
C	-3.479061000	-1.190778000	0.008018000
C	-3.851596000	-1.995222000	1.126316000
C	-5.131764000	-2.602253000	1.176557000
C	-5.987679000	-2.533081000	0.114868000
C	-5.565667000	-1.877510000	-1.058565000
C	-4.363345000	-1.224859000	-1.104459000
H	-5.396546000	-3.162861000	2.065626000
H	-6.955245000	-3.016850000	0.152838000
H	-6.192910000	-1.896563000	-1.941077000
H	-4.065379000	-0.786829000	-2.039129000
N	4.598740000	0.771484000	2.363642000
O	5.790005000	0.990270000	2.405699000
O	3.800952000	1.107651000	3.211652000
N	5.369853000	-1.427470000	-1.950574000
O	6.544042000	-1.157869000	-1.818134000
O	4.894772000	-2.013856000	-2.898536000

**SCF Done: E(RM062X) = -1606.24378457**

**# of imaginary frequencies = 1 (-38.7279)**

**TS1'-2c**

C	2.703644000	3.265801000	-0.828329000
C	3.023596000	1.878112000	1.270354000
C	0.912707000	1.680081000	0.000667000
C	1.651354000	2.237360000	-1.224543000
C	1.911097000	0.860858000	0.884879000
C	3.728590000	2.650519000	0.132907000
H	5.531261000	1.428218000	0.018786000
H	4.341904000	1.039332000	-1.220472000
H	0.767177000	-2.871312000	-1.698824000
H	1.400662000	0.597890000	1.815522000
H	2.215175000	4.122880000	-0.355809000
H	3.216220000	3.649107000	-1.714513000
H	2.126902000	1.401833000	-1.749321000
H	-1.220500000	1.302275000	1.668535000
H	5.288361000	2.523133000	-1.346156000
C	2.291553000	-0.492851000	0.234472000
C	2.880521000	-2.738751000	-1.445363000
C	1.595216000	-2.362946000	-1.223970000
C	1.326583000	-1.268350000	-0.375105000
H	0.938308000	2.666717000	-1.929852000

C	0.128449000	2.758477000	0.788589000
H	0.134962000	1.032258000	-0.379184000
C	-0.874553000	3.458897000	-0.132302000
H	0.056965000	1.824014000	2.773899000
H	-1.289386000	2.897743000	2.421024000
H	0.806708000	3.524584000	1.169612000
C	4.780329000	1.856827000	-0.645121000
H	-1.533597000	2.726764000	-0.611068000
H	-1.499092000	4.146725000	0.440203000
H	-0.382424000	4.034144000	-0.916868000
C	-0.615870000	2.158594000	1.983760000
H	4.261918000	3.469706000	0.625981000
H	3.770276000	1.470912000	1.940445000
H	2.505502000	2.625036000	1.877502000
O	-0.026133000	-1.062991000	-0.065619000
C	-0.909009000	-0.851857000	-1.053467000
O	-0.623944000	-0.708676000	-2.209214000
C	-2.303311000	-0.759373000	-0.527643000
C	-2.598621000	-1.007042000	0.807233000
C	-3.305220000	-0.390995000	-1.416649000
C	-3.910013000	-0.874716000	1.225034000
H	-1.828955000	-1.294390000	1.508964000
C	-4.597036000	-0.274610000	-0.942376000
H	-3.073233000	-0.196510000	-2.454441000
C	-4.936115000	-0.508773000	0.376614000
H	-5.952695000	-0.409188000	0.726858000
H	3.117060000	-3.542344000	-2.131675000
C	3.610160000	-1.093125000	0.229880000
C	3.914229000	-2.145926000	-0.681682000
C	5.226933000	-2.674887000	-0.753293000
C	6.196168000	-2.277349000	0.123420000
C	5.861326000	-1.358704000	1.137119000
C	4.618979000	-0.784793000	1.182008000
H	5.430160000	-3.438668000	-1.495070000
H	7.191678000	-2.699588000	0.075275000
H	6.588940000	-1.108975000	1.899253000
H	4.395557000	-0.134906000	2.007886000
N	-4.229048000	-1.125503000	2.641765000
O	-5.388700000	-1.030011000	2.980421000
O	-3.310996000	-1.409302000	3.380180000
N	-5.664590000	0.119263000	-1.878959000
O	-6.788440000	0.220265000	-1.436695000
O	-5.351848000	0.317391000	-3.032662000

**SCF Done: E(RM062X) = -1606.24204211**

**# of imaginary frequencies = 1 (-40.3388)**

### TS2-2c

C	2.575886000	1.407791000	2.844170000
C	0.653171000	0.988648000	1.242856000
C	2.781367000	1.867933000	0.355247000
C	3.493474000	1.371516000	1.623582000
C	1.600161000	0.911145000	0.008069000
C	1.285886000	0.614647000	2.597378000
H	0.634881000	-1.465543000	2.513319000
H	2.352707000	-1.255306000	2.173282000
H	0.581434000	-3.639984000	-0.137952000
H	1.060370000	1.327795000	-0.846380000
H	2.329719000	2.446277000	3.083295000
H	3.094458000	1.002438000	3.717433000
H	3.840054000	0.347909000	1.453027000

H	2.140982000	3.537049000	-1.708031000
H	1.760584000	-1.096712000	3.826490000
C	1.977931000	-0.535759000	-0.392056000
C	2.677686000	-3.313802000	-0.425379000
C	1.381484000	-2.928839000	-0.296800000
C	1.058343000	-1.557791000	-0.309449000
H	4.391555000	1.962606000	1.808470000
C	2.348936000	3.354910000	0.447043000
H	3.512374000	1.875117000	-0.443423000
C	3.576777000	4.248727000	0.642224000
H	0.594808000	3.354982000	-0.869124000
H	1.454983000	4.886887000	-0.796688000
H	1.698075000	3.513397000	1.309055000
C	1.523277000	-0.887755000	2.781034000
H	4.302123000	4.088279000	-0.161303000
H	3.285771000	5.300472000	0.625584000
H	4.076802000	4.060847000	1.592568000
C	1.586991000	3.803470000	-0.802262000
H	0.555985000	0.910851000	3.357586000
H	-0.253783000	0.407294000	1.124194000
H	0.319455000	2.026475000	1.303153000
O	-0.309031000	-1.334401000	-0.112357000
C	-0.996261000	-0.668599000	-1.051238000
O	-0.542153000	-0.260484000	-2.082482000
C	-2.423155000	-0.482974000	-0.646512000
C	-2.894068000	-0.910736000	0.588690000
C	-3.271626000	0.153403000	-1.543644000
C	-4.223040000	-0.687125000	0.898538000
H	-2.245690000	-1.405774000	1.297324000
C	-4.590280000	0.346104000	-1.181308000
H	-2.903029000	0.488924000	-2.502879000
C	-5.101252000	-0.061723000	0.036076000
H	-6.135602000	0.101060000	0.299803000
H	2.963233000	-4.356008000	-0.354741000
C	3.286274000	-0.967039000	-0.841207000
C	3.653345000	-2.342139000	-0.754294000
C	4.968971000	-2.753756000	-1.085320000
C	5.877099000	-1.871001000	-1.595862000
C	5.471225000	-0.545086000	-1.847657000
C	4.223963000	-0.111661000	-1.484568000
H	5.223419000	-3.799913000	-0.960234000
H	6.875358000	-2.195756000	-1.859610000
H	6.141161000	0.134479000	-2.359378000
H	3.926552000	0.878424000	-1.784783000
N	-4.728808000	-1.133955000	2.208583000
O	-5.901245000	-0.945322000	2.450741000
O	-3.940557000	-1.661823000	2.962660000
N	-5.497101000	1.016803000	-2.129817000
O	-6.647020000	1.181671000	-1.784182000
O	-5.036588000	1.361414000	-3.196322000

**SCF Done: E(RM062X) = -1606.24487942**

**# of imaginary frequencies = 1 (-34.6321)**

**TS2'-2c**

C	2.379971000	1.287348000	2.981085000
C	0.699392000	1.158551000	1.091268000
C	3.072872000	1.618036000	0.564184000
C	3.452425000	1.025661000	1.929305000
C	1.794165000	0.905600000	0.013867000
C	1.030973000	0.715332000	2.530778000



H	0.054803000	-1.235913000	2.414809000
H	1.806558000	-1.316569000	2.251027000
H	0.285678000	-3.539489000	-0.449763000
H	1.472325000	1.428578000	-0.891834000
H	2.290387000	2.364566000	3.149814000
H	2.667179000	0.843353000	3.938102000
H	3.599796000	-0.052604000	1.808953000
H	3.314534000	3.338709000	-1.550811000
H	1.082735000	-1.007095000	3.827975000
C	1.995685000	-0.572968000	-0.398365000
C	2.401831000	-3.390254000	-0.613178000
C	1.143681000	-2.887512000	-0.496470000
C	0.963463000	-1.490273000	-0.403244000
H	4.414654000	1.423023000	2.254999000
C	2.943902000	3.162466000	0.583780000
H	3.921482000	1.441135000	-0.084293000
C	4.242831000	3.797564000	1.087895000
H	1.601989000	3.466006000	-1.126602000
H	2.687053000	4.808893000	-0.800913000
H	2.149800000	3.473375000	1.265735000
C	0.992076000	-0.797796000	2.759506000
H	5.096840000	3.448720000	0.498947000
H	4.193376000	4.883897000	0.995822000
H	4.436221000	3.564302000	2.135227000
C	2.611928000	3.720008000	-0.802948000
H	0.248758000	1.148783000	3.162326000
H	-0.264518000	0.754590000	0.805818000
H	0.551124000	2.240653000	1.110809000
O	-0.339353000	-0.988482000	-0.435520000
C	-1.383623000	-1.557232000	0.178128000
O	-1.350069000	-2.527087000	0.882521000
C	-2.638684000	-0.794897000	-0.107567000
C	-2.635408000	0.357422000	-0.884264000
C	-3.820657000	-1.265932000	0.450050000
C	-3.833323000	1.017680000	-1.086344000
H	-1.724302000	0.737511000	-1.323303000
C	-4.987788000	-0.567597000	0.210417000
H	-3.821573000	-2.159547000	1.058295000
C	-5.031003000	0.581902000	-0.555327000
H	-5.954796000	1.113801000	-0.727474000
H	2.570268000	-4.460050000	-0.627127000
C	3.261214000	-1.106519000	-0.849949000
C	3.486357000	-2.512177000	-0.844386000
C	4.758782000	-3.033232000	-1.190995000
C	5.750307000	-2.216737000	-1.654871000
C	5.475552000	-0.846324000	-1.843633000
C	4.276423000	-0.312276000	-1.454989000
H	4.909602000	-4.104463000	-1.122968000
H	6.713990000	-2.622639000	-1.934410000
H	6.208815000	-0.212371000	-2.326219000
H	4.071228000	0.717635000	-1.700683000
N	-3.834771000	2.245180000	-1.901676000
O	-4.898516000	2.797396000	-2.081405000
O	-2.771644000	2.627060000	-2.340712000
N	-6.245135000	-1.062602000	0.798410000
O	-7.257731000	-0.440129000	0.561327000
O	-6.188277000	-2.061247000	1.482315000

**SCF Done: E(RM062X) = -1606.24076153**

**# of imaginary frequencies = 1 (-33.2438)**

**(M)-3b**

C	0.416024000	-1.647110000	0.562111000
C	0.630870000	-0.467911000	-0.133253000
C	2.772173000	-2.114506000	0.686149000
C	1.486427000	-2.475033000	0.971539000
H	3.594687000	-2.747805000	0.997367000
H	1.294721000	-3.392881000	1.507873000
C	1.974147000	-0.083688000	-0.420488000
C	3.053139000	-0.919010000	-0.008405000
C	4.392260000	-0.544184000	-0.289870000
C	4.674163000	0.617857000	-0.948202000
C	3.613309000	1.460188000	-1.352100000
C	2.312303000	1.123594000	-1.099067000
H	5.189244000	-1.203791000	0.034646000
H	5.698370000	0.898241000	-1.157962000
H	3.833354000	2.386851000	-1.867658000
H	1.535958000	1.803771000	-1.418149000
C	-2.601596000	1.596676000	0.331196000
C	-1.191221000	1.105592000	0.664260000
C	-0.566799000	0.368276000	-0.546814000
C	-1.570500000	-0.473511000	-1.325697000
C	-3.008901000	-0.462849000	-1.057010000
C	-3.535293000	0.426809000	0.041978000
H	-2.571911000	2.257081000	-0.538905000
H	-3.000364000	2.180305000	1.163939000
H	-1.288020000	0.367053000	1.467032000
H	-0.239112000	1.122995000	-1.263110000
H	-1.157895000	-1.363642000	-1.794461000
H	-3.657533000	-0.186755000	0.940642000
H	-4.530637000	0.783856000	-0.240211000
C	-0.265258000	2.225777000	1.180486000
H	0.757312000	1.834319000	1.158029000
C	-3.849909000	-1.657951000	-1.407250000
H	-4.851411000	-1.343061000	-1.709710000
H	-3.396582000	-2.220733000	-2.223279000
H	-3.948585000	-2.313823000	-0.540093000
C	-0.305131000	3.488278000	0.316832000
H	0.491584000	4.173796000	0.612005000
H	-0.182546000	3.273421000	-0.747145000
H	-1.256239000	4.012141000	0.439577000
C	-0.578727000	2.578513000	2.634892000
H	0.104162000	3.348253000	3.000492000
H	-1.595606000	2.965228000	2.737988000
H	-0.481784000	1.703675000	3.281041000
O	-0.879738000	-1.966314000	0.827196000
O	-2.464790000	0.247694000	-2.182343000
C	-1.157190000	-3.172752000	1.518540000
H	-0.707796000	-3.169732000	2.513615000
H	-2.238945000	-3.218374000	1.611885000
H	-0.803950000	-4.039779000	0.956772000

**SCF Done: E(RM062X) = -966.203261640****# of imaginary frequencies = 0****(P)-3b**

C	1.423122000	1.486669000	-0.780992000
C	0.754892000	0.330373000	-0.415024000
C	3.563466000	0.530570000	-0.229579000
C	2.831907000	1.586908000	-0.691161000
H	4.642582000	0.606038000	-0.163578000
H	3.335428000	2.495373000	-0.987796000

C	1.516625000	-0.767422000	0.082716000
C	2.934189000	-0.667671000	0.170940000
C	3.695042000	-1.760852000	0.658930000
C	3.088639000	-2.917672000	1.057020000
C	1.680899000	-3.024253000	0.984950000
C	0.921353000	-1.988243000	0.515852000
H	4.772876000	-1.655121000	0.710218000
H	3.675737000	-3.747504000	1.428969000
H	1.196504000	-3.937662000	1.307658000
H	-0.152435000	-2.105379000	0.482978000
C	-2.934182000	0.052320000	0.725785000
C	-1.453051000	0.417256000	0.847786000
C	-0.756899000	0.282236000	-0.529503000
C	-1.225210000	-0.927544000	-1.329420000
C	-2.364480000	-1.765582000	-0.926234000
C	-3.111886000	-1.411821000	0.337196000
H	-3.409593000	0.685585000	-0.027342000
H	-3.446941000	0.237173000	1.671827000
H	-0.991593000	-0.311492000	1.525509000
H	-1.059367000	1.142079000	-1.129094000
H	-0.469621000	-1.386796000	-1.963272000
H	-2.746847000	-2.059962000	1.141294000
H	-4.170131000	-1.651129000	0.194853000
C	-1.217634000	1.809503000	1.468822000
H	-0.158587000	2.047603000	1.325424000
C	-2.440876000	-3.200270000	-1.368680000
H	-3.481515000	-3.492690000	-1.526282000
H	-1.889578000	-3.344717000	-2.297724000
H	-2.018460000	-3.855015000	-0.603517000
C	-2.037185000	2.916181000	0.803590000
H	-1.731354000	3.890874000	1.189619000
H	-1.902559000	2.931973000	-0.279295000
H	-3.102333000	2.796175000	1.016599000
C	-1.477939000	1.795117000	2.975654000
H	-2.525812000	1.578320000	3.197060000
H	-0.863485000	1.043197000	3.475403000
H	-1.245569000	2.767998000	3.413680000
O	0.661976000	2.523828000	-1.225428000
O	-2.494089000	-0.798529000	-1.976519000
C	1.292561000	3.765422000	-1.491516000
H	0.493885000	4.450248000	-1.763686000
H	1.808170000	4.141729000	-0.605497000
H	1.997367000	3.683361000	-2.321230000

**SCF Done: E(RM062X) = -966.204060191**

**# of imaginary frequencies = 0**

### TS1-3b

C	0.909132000	-3.033024000	1.375586000
C	-0.380192000	-1.750194000	-0.460556000
C	-0.130603000	-2.037018000	0.953971000
C	-0.775886000	-0.314537000	-0.824493000
C	0.413727000	0.646902000	-0.554679000
C	-0.454396000	-0.914110000	1.915879000
C	2.468594000	2.175448000	0.683208000
C	0.231291000	1.975488000	-0.201132000
C	1.241783000	2.720039000	0.460014000
O	-0.939456000	2.591992000	-0.526906000
C	-1.762873000	-0.193816000	1.547707000
C	-2.026874000	0.035465000	0.028429000
C	-3.485476000	-0.739483000	-1.947494000

C	-3.339118000	-0.651208000	-0.428928000
C	-4.523608000	0.132652000	0.144022000
O	-1.290972000	-2.558348000	0.297689000
H	0.604092000	-3.543931000	2.291645000
H	1.852991000	-2.517588000	1.569424000
H	0.128059000	-2.352201000	-1.198669000
H	1.072255000	-3.773537000	0.592030000
H	-1.039752000	-0.263526000	-1.882932000
H	-0.538543000	-1.320932000	2.927699000
H	-2.588221000	-0.786626000	1.947239000
H	0.392312000	-0.221357000	1.928515000
H	-3.336426000	0.240590000	-2.412011000
H	-2.773844000	-1.437871000	-2.391426000
H	-2.221987000	1.089434000	-0.120167000
H	-1.786260000	0.760050000	2.080164000
H	-4.572855000	1.127330000	-0.310096000
H	-4.489259000	-1.081392000	-2.208707000
H	-3.368696000	-1.662839000	-0.023822000
H	-4.441234000	0.263209000	1.224888000
H	-5.466581000	-0.377873000	-0.061842000
H	1.024003000	3.721707000	0.803330000
C	1.779898000	0.189332000	-0.567452000
C	2.789916000	0.918756000	0.120722000
C	4.115748000	0.420836000	0.183343000
C	4.474711000	-0.714685000	-0.486012000
C	3.515028000	-1.370982000	-1.285522000
C	2.217715000	-0.935954000	-1.321177000
H	4.848198000	0.983414000	0.751230000
H	5.492081000	-1.081954000	-0.444645000
H	3.811029000	-2.215180000	-1.895925000
H	1.535257000	-1.415237000	-2.004811000
H	3.226914000	2.725376000	1.227765000
C	-1.418166000	3.635815000	0.312949000
H	-2.470480000	3.760504000	0.067071000
H	-1.318810000	3.364441000	1.365904000
H	-0.892941000	4.572506000	0.121557000

**SCF Done: E(RM062X) = -966.167967251**

**# of imaginary frequencies = 1 (-34.7622)**

### TS2-3b

C	1.287593000	2.711408000	2.067318000
C	1.547012000	1.297200000	-0.087598000
C	1.401174000	1.387765000	1.368165000
C	-1.150758000	1.527181000	-0.880568000
C	-2.439465000	1.904965000	-0.436912000
C	0.905034000	0.080615000	-0.776995000
C	-0.638025000	0.251454000	-0.695747000
C	0.761508000	0.192353000	2.040573000
C	-3.256264000	0.978664000	0.135485000
C	1.244418000	-1.145360000	1.452731000
C	1.474241000	-1.180211000	-0.086973000
C	3.322076000	-1.206373000	-1.887095000
C	2.954775000	-1.497035000	-0.432816000
C	3.220471000	-2.975063000	-0.132549000
O	2.671405000	1.093559000	0.780277000
H	1.785473000	2.672893000	3.039074000
H	0.236087000	2.954255000	2.237517000
H	1.645220000	2.208041000	-0.657659000
H	1.739230000	3.503529000	1.469308000
H	-2.761848000	2.932389000	-0.530474000

H	1.191611000	0.074682000	-1.830222000
H	0.986453000	0.217788000	3.110655000
H	2.187031000	-1.401339000	1.940394000
H	-0.323796000	0.296194000	1.948571000
H	2.623548000	-1.695432000	-2.573656000
H	3.322958000	-0.137350000	-2.106949000
H	0.948464000	-2.040311000	-0.477244000
H	0.527905000	-1.919121000	1.737934000
H	2.655238000	-3.609694000	-0.822121000
H	4.321779000	-1.588827000	-2.103699000
H	3.599686000	-0.896285000	0.207305000
H	2.927147000	-3.243300000	0.884401000
H	4.279655000	-3.212204000	-0.250102000
O	-0.362336000	2.431934000	-1.526029000
C	-1.597152000	-0.767557000	-0.351258000
C	-2.880418000	-0.382978000	0.144963000
C	-3.807220000	-1.361874000	0.585741000
C	-3.539943000	-2.694879000	0.464993000
C	-2.339023000	-3.091419000	-0.159189000
C	-1.409012000	-2.167088000	-0.552340000
H	-4.752381000	-1.021429000	0.993506000
H	-4.256989000	-3.436365000	0.792898000
H	-2.158253000	-4.140582000	-0.358150000
H	-0.558484000	-2.522421000	-1.108308000
H	-4.225618000	1.263380000	0.526873000
C	-0.523888000	3.811036000	-1.221093000
H	0.356964000	4.312377000	-1.615944000
H	-1.413213000	4.223396000	-1.699714000
H	-0.579234000	3.964965000	-0.141180000

**SCF Done: E(RM062X) = -966.167328284**

**# of imaginary frequencies = 1 (-37.7086)**

**(M)-3c bis**

C	-1.531689000	-1.247813000	-0.770474000
C	-2.396583000	-0.564474000	0.041253000
C	-3.208861000	-2.695684000	-1.649787000
C	-1.905618000	-2.305535000	-1.619451000
H	-3.526562000	-3.506134000	-2.294224000
H	-1.151573000	-2.783624000	-2.230929000
C	-3.774193000	-0.967035000	0.006221000
C	-4.171077000	-2.039009000	-0.843033000
C	-5.529655000	-2.438882000	-0.886810000
C	-6.473354000	-1.806644000	-0.127694000
C	-6.090512000	-0.740212000	0.712324000
C	-4.784965000	-0.333662000	0.777782000
H	-5.804094000	-3.258560000	-1.540649000
H	-7.509282000	-2.117745000	-0.168502000
H	-6.837112000	-0.236344000	1.313052000
H	-4.537081000	0.487902000	1.432888000
C	-0.851691000	2.865148000	0.975820000
C	-1.563607000	1.843501000	0.084943000
C	-1.894610000	0.574987000	0.908670000
C	-0.735525000	0.138616000	1.803858000
C	0.431940000	0.998467000	2.087505000
C	0.510348000	2.356133000	1.432608000
H	-1.469103000	3.081949000	1.851198000
H	-0.719911000	3.805154000	0.436336000
H	-0.861494000	1.543833000	-0.702032000
H	-2.681076000	0.843378000	1.614471000
H	-0.613967000	-0.936270000	1.925878000

H	1.186271000	2.282225000	0.573832000
H	0.972588000	3.056182000	2.135251000
C	-2.811046000	2.423859000	-0.612838000
H	-3.394053000	1.580376000	-0.996802000
C	1.737313000	0.420789000	2.568439000
H	2.069647000	0.981306000	3.445302000
H	1.629701000	-0.628376000	2.846892000
H	2.513965000	0.511849000	1.807694000
C	-3.709304000	3.227608000	0.330101000
H	-4.658807000	3.455216000	-0.157649000
H	-3.930657000	2.694992000	1.257352000
H	-3.238035000	4.175839000	0.599377000
C	-2.415391000	3.281231000	-1.815439000
H	-3.302554000	3.673510000	-2.316488000
H	-1.805609000	4.134641000	-1.508678000
H	-1.843827000	2.699747000	-2.541617000
O	-0.198297000	-0.824995000	-0.816033000
C	0.745943000	-1.657410000	-0.350278000
O	0.533106000	-2.733744000	0.131768000
C	4.661716000	0.071091000	-0.536546000
C	4.433199000	-1.183139000	-0.002117000
C	3.180015000	-1.761839000	0.045253000
C	2.103905000	-1.051931000	-0.471389000
C	2.287682000	0.206630000	-1.029123000
C	3.563820000	0.738764000	-1.042640000
H	5.649015000	0.508375000	-0.553981000
H	3.033112000	-2.738393000	0.485383000
H	1.458999000	0.766897000	-1.437915000
O	-0.633867000	0.855710000	3.033293000
N	3.758987000	2.087963000	-1.602474000
O	2.768798000	2.697994000	-1.944651000
O	4.893845000	2.504443000	-1.679012000
N	5.580105000	-1.926178000	0.551328000
O	5.361781000	-3.020240000	1.023414000
O	6.668212000	-1.395638000	0.498673000

**SCF Done: E(RM062X) = -1680.27322377**

**# of imaginary frequencies = 0**

**(M)-3c**

C	-1.526583000	-0.113131000	-1.440817000
C	-2.439469000	-0.345709000	-0.448134000
C	-3.175177000	0.306173000	-3.112927000
C	-1.862570000	0.206591000	-2.769382000
H	-3.462644000	0.550693000	-4.128142000
H	-1.069839000	0.363765000	-3.489485000
C	-3.826576000	-0.237944000	-0.804756000
C	-4.185344000	0.091881000	-2.142662000
C	-5.551565000	0.208448000	-2.499392000
C	-6.538534000	0.015760000	-1.574551000
C	-6.192928000	-0.305405000	-0.245417000
C	-4.881520000	-0.429854000	0.127272000
H	-5.795933000	0.457765000	-3.525469000
H	-7.579774000	0.109281000	-1.855067000
H	-6.973106000	-0.455512000	0.490095000
H	-4.663676000	-0.674799000	1.155978000
C	-0.724853000	0.075451000	3.002327000
C	-1.390491000	0.531320000	1.701810000
C	-1.979893000	-0.689823000	0.956319000
C	-1.041240000	-1.894954000	0.964133000
C	0.144509000	-1.982562000	1.833259000

C	0.482376000	-0.812550000	2.724640000
H	-1.446501000	-0.472930000	3.612956000
H	-0.406963000	0.943300000	3.583638000
H	-0.603950000	0.957681000	1.069724000
H	-2.844153000	-1.028760000	1.527750000
H	-1.050890000	-2.505790000	0.064711000
H	1.268647000	-0.230338000	2.230814000
H	0.909211000	-1.192956000	3.657573000
C	-2.439520000	1.641599000	1.915767000
H	-3.037537000	1.707178000	1.000840000
C	1.280810000	-2.910679000	1.502575000
H	1.586039000	-3.443780000	2.406150000
H	0.988933000	-3.640172000	0.746879000
H	2.145518000	-2.353118000	1.142086000
C	-3.388631000	1.354839000	3.080972000
H	-4.215538000	2.067204000	3.077379000
H	-3.814254000	0.350015000	3.038965000
H	-2.868805000	1.453004000	4.036985000
C	-1.763913000	2.999510000	2.108534000
H	-1.143258000	3.252745000	1.246434000
H	-2.510242000	3.786299000	2.234749000
H	-1.128547000	3.001940000	2.997746000
O	-0.163009000	-0.259946000	-1.151040000
C	0.583533000	0.856719000	-1.132655000
O	0.152333000	1.967519000	-1.262384000
C	4.742237000	0.063380000	-0.471228000
C	4.211438000	1.336733000	-0.390891000
C	2.874128000	1.606383000	-0.604947000
C	2.024757000	0.548079000	-0.902609000
C	2.512772000	-0.749199000	-0.990206000
C	3.863754000	-0.957124000	-0.776635000
H	1.861128000	-1.579205000	-1.224654000
O	-1.072206000	-2.661239000	2.170014000
N	5.117362000	2.452220000	-0.063377000
O	6.287354000	2.190207000	0.112825000
O	4.634946000	3.561232000	0.009708000
N	4.390821000	-2.330047000	-0.868870000
O	5.580977000	-2.486980000	-0.703945000
O	3.597783000	-3.217474000	-1.099082000
H	2.492123000	2.615703000	-0.540769000
H	5.792249000	-0.124568000	-0.303292000

**SCF Done: E(RM062X) = -1680.27149182**

**# of imaginary frequencies = 0**

**(P)-3c**

C	-1.083222000	-1.719345000	0.326473000
C	-2.019019000	-0.758319000	0.052896000
C	-2.688088000	-3.471887000	0.545264000
C	-1.386730000	-3.070567000	0.570954000
H	-2.949563000	-4.506919000	0.728294000
H	-0.577964000	-3.759367000	0.777464000
C	-3.391694000	-1.172443000	0.042788000
C	-3.719016000	-2.535713000	0.285032000
C	-5.075348000	-2.947412000	0.267091000
C	-6.078015000	-2.051643000	0.024978000
C	-5.762472000	-0.695731000	-0.207537000
C	-4.462283000	-0.269232000	-0.198817000
H	-5.299279000	-3.991726000	0.451359000
H	-7.110978000	-2.374891000	0.013506000
H	-6.557494000	0.015629000	-0.392651000

H	-4.256342000	0.776853000	-0.373704000
C	-1.816025000	3.070101000	0.555633000
C	-1.896143000	1.604211000	0.987300000
C	-1.599210000	0.673191000	-0.215190000
C	-2.159261000	1.172034000	-1.542308000
C	-2.782037000	2.494375000	-1.700398000
C	-2.870379000	3.400258000	-0.495453000
H	-0.824860000	3.282638000	0.148190000
H	-1.954346000	3.720574000	1.421411000
H	-2.926005000	1.412175000	1.310233000
H	-0.516891000	0.682412000	-0.360778000
H	-2.448138000	0.393342000	-2.244983000
H	-3.873931000	3.302059000	-0.067537000
H	-2.770942000	4.436819000	-0.830798000
C	-0.982266000	1.273655000	2.186452000
H	-0.938336000	0.182448000	2.267334000
C	-3.791897000	2.726084000	-2.789054000
H	-3.717029000	3.750025000	-3.161645000
H	-3.628559000	2.036318000	-3.616853000
H	-4.802998000	2.579919000	-2.403223000
C	0.447850000	1.789385000	2.013351000
H	1.094286000	1.381579000	2.793712000
H	0.876862000	1.514829000	1.046496000
H	0.481672000	2.878517000	2.092926000
C	-1.573488000	1.797850000	3.495141000
H	-1.649946000	2.887702000	3.487199000
H	-2.570672000	1.388447000	3.668567000
H	-0.940360000	1.519138000	4.339786000
O	0.266551000	-1.361656000	0.447045000
C	1.006117000	-1.347962000	-0.673509000
O	0.594653000	-1.628575000	-1.763493000
C	5.028463000	-0.042134000	0.028420000
C	4.569182000	-0.372507000	-1.232324000
C	3.278052000	-0.801077000	-1.472076000
C	2.405993000	-0.909089000	-0.396692000
C	2.826131000	-0.593276000	0.889331000
C	4.127910000	-0.164015000	1.068175000
H	6.040765000	0.296399000	0.191877000
H	2.948764000	-1.044834000	-2.472486000
H	2.157383000	-0.674333000	1.733946000
O	-1.444242000	2.245530000	-2.153295000
N	4.573548000	0.189915000	2.427226000
O	3.758802000	0.110735000	3.321092000
O	5.725053000	0.541244000	2.566183000
N	5.500441000	-0.254499000	-2.368255000
O	5.082264000	-0.546590000	-3.467329000
O	6.626712000	0.126010000	-2.132199000

**SCF Done: E(RM062X) = -1680.27217783**

**# of imaginary frequencies = 0**

**(P)-3c bis**

C	-1.021473000	-1.385140000	-0.970004000
C	-2.045267000	-0.605318000	-0.501774000
C	-2.455531000	-3.183916000	-1.609199000
C	-1.200026000	-2.664712000	-1.531387000
H	-2.619009000	-4.165042000	-2.037998000
H	-0.336913000	-3.209214000	-1.890875000
C	-3.369224000	-1.152290000	-0.575640000
C	-3.567612000	-2.446161000	-1.131148000
C	-4.875245000	-2.986457000	-1.206943000



C	-5.953619000	-2.282040000	-0.750216000
C	-5.765200000	-0.999033000	-0.194250000
C	-4.513790000	-0.450856000	-0.109544000
H	-5.001511000	-3.973744000	-1.635904000
H	-6.949021000	-2.702874000	-0.811208000
H	-6.618888000	-0.442181000	0.171101000
H	-4.404378000	0.532087000	0.325958000
C	-1.909852000	2.240609000	2.115830000
C	-1.883007000	0.794115000	1.617948000
C	-1.764093000	0.768569000	0.073188000
C	-2.592995000	1.843324000	-0.621374000
C	-3.273007000	2.924834000	0.107185000
C	-3.146794000	2.976423000	1.610886000
H	-1.013123000	2.765062000	1.776530000
H	-1.900955000	2.260601000	3.207250000
H	-2.841899000	0.335996000	1.887119000
H	-0.731090000	1.018758000	-0.176543000
H	-2.994274000	1.565730000	-1.593622000
H	-4.049793000	2.532474000	2.043531000
H	-3.129520000	4.024759000	1.923221000
C	-0.784146000	-0.059891000	2.281124000
H	-0.726620000	-0.998814000	1.720984000
C	-4.484464000	3.587539000	-0.486443000
H	-5.394997000	3.112918000	-0.114921000
H	-4.468012000	3.513443000	-1.573647000
H	-4.513933000	4.642336000	-0.204470000
C	0.596466000	0.599023000	2.247918000
H	1.364538000	-0.116612000	2.551169000
H	0.860960000	0.975003000	1.256280000
H	0.640643000	1.443566000	2.939720000
C	-1.153104000	-0.426206000	3.718887000
H	-2.112036000	-0.946737000	3.758577000
H	-0.393980000	-1.080240000	4.152543000
H	-1.221277000	0.462201000	4.351010000
O	0.276637000	-0.859244000	-0.959611000
C	1.210961000	-1.479246000	-0.221639000
O	1.016009000	-2.446554000	0.458873000
C	5.047921000	0.421302000	-0.450454000
C	3.972760000	0.903826000	-1.170217000
C	2.719523000	0.320611000	-1.134483000
C	2.537536000	-0.802027000	-0.336813000
C	3.591616000	-1.322073000	0.403087000
C	4.821409000	-0.698190000	0.327117000
H	6.017263000	0.895076000	-0.493371000
H	1.907387000	0.737361000	-1.712578000
H	3.446850000	-2.193883000	1.025744000
O	-2.045451000	3.161725000	-0.594908000
N	5.944012000	-1.244178000	1.110308000
O	5.727193000	-2.221735000	1.792648000
O	7.013914000	-0.681484000	1.023243000
N	4.174249000	2.096791000	-2.011852000
O	3.224130000	2.501275000	-2.645976000
O	5.277230000	2.599010000	-2.017348000

**SCF Done: E(RM062X) = -1680.27285261**

**# of imaginary frequencies = 0**

### TS1-3c

C	-4.959778000	2.371021000	0.680271000
C	-2.831407000	1.811178000	-0.678642000
C	-3.484160000	2.116338000	0.597055000

C	-1.640840000	0.845516000	-0.645127000
C	-2.102252000	-0.584354000	-0.259503000
C	-2.792868000	1.563424000	1.825404000
C	-3.089673000	-2.921321000	1.066900000
C	-1.288742000	-1.499057000	0.372108000
C	-1.761453000	-2.639152000	1.056084000
O	0.098689000	-1.364587000	0.475116000
C	-1.268697000	1.737444000	1.744667000
C	-0.613943000	1.442360000	0.360053000
C	0.578732000	2.534501000	-1.644224000
C	0.171675000	2.666478000	-0.176866000
C	1.431116000	2.854223000	0.674398000
O	-2.696843000	3.103889000	-0.077048000
H	-5.178562000	3.107929000	1.456114000
H	-5.477900000	1.443241000	0.934175000
H	-3.414449000	1.880069000	-1.584034000
H	-5.342380000	2.733632000	-0.274154000
H	-1.185377000	0.788615000	-1.635809000
H	-3.167952000	2.078192000	2.714135000
H	-1.040098000	2.770948000	2.010948000
H	-3.071550000	0.511074000	1.935466000
H	1.084505000	1.580046000	-1.827852000
H	-0.275415000	2.599043000	-2.320205000
H	0.160532000	0.709210000	0.540267000
H	-0.810366000	1.110990000	2.512829000
H	2.134504000	2.033798000	0.495843000
H	1.273256000	3.332904000	-1.912982000
H	-0.451489000	3.554469000	-0.071574000
H	1.205935000	2.875335000	1.742380000
H	1.937930000	3.786238000	0.417923000
H	-1.039884000	-3.246319000	1.586732000
C	2.257979000	-0.953884000	-0.332435000
C	3.119646000	-0.728850000	-1.398889000
C	2.719880000	-0.885548000	0.976456000
C	4.441671000	-0.435763000	-1.127707000
H	2.757036000	-0.775404000	-2.416434000
C	4.054262000	-0.590729000	1.186717000
H	2.059345000	-1.049521000	1.815618000
C	4.944488000	-0.357685000	0.157033000
H	5.981470000	-0.123515000	0.346492000
C	0.821253000	-1.215948000	-0.646436000
O	0.383053000	-1.251742000	-1.760885000
N	4.551107000	-0.510352000	2.572110000
O	5.727523000	-0.267602000	2.731940000
O	3.751562000	-0.691075000	3.464525000
N	5.359244000	-0.187080000	-2.254095000
O	6.511993000	0.076601000	-1.989170000
O	4.903028000	-0.261393000	-3.374057000
C	-3.456609000	-1.046108000	-0.474186000
C	-3.963382000	-2.158767000	0.254577000
C	-5.318519000	-2.547940000	0.110084000
C	-6.135348000	-1.932723000	-0.795525000
C	-5.602477000	-0.928050000	-1.628310000
C	-4.311700000	-0.500220000	-1.469772000
H	-5.681695000	-3.372130000	0.713022000
H	-7.165554000	-2.244524000	-0.909416000
H	-6.211198000	-0.503440000	-2.416649000
H	-3.919865000	0.210135000	-2.178293000
H	-3.478401000	-3.760027000	1.630881000

**SCF Done: E(RM062X) = -1680.23899719**

# of imaginary frequencies = 1 (-20.0296)

TS1<sup>o</sup>-3c

C	4.919130000	1.898805000	-1.638315000
C	2.964224000	1.939186000	0.057417000
C	3.462720000	1.758279000	-1.309069000
C	1.770952000	1.076218000	0.484465000
C	2.168717000	-0.426162000	0.561422000
C	2.624732000	0.854394000	-2.189619000
C	2.920862000	-3.147535000	0.089198000
C	1.261097000	-1.450757000	0.411012000
C	1.612347000	-2.796153000	0.165881000
O	-0.105583000	-1.209262000	0.591524000
C	1.120744000	1.113999000	-2.007632000
C	0.639343000	1.353823000	-0.544750000
C	-0.279473000	3.142597000	1.064780000
C	-0.057568000	2.730950000	-0.389805000
C	-1.410677000	2.674299000	-1.106127000
O	2.769121000	2.953035000	-0.935367000
H	5.046398000	2.320572000	-2.637711000
H	5.396443000	0.916302000	-1.618418000
H	3.647357000	2.289715000	0.815556000
H	5.417596000	2.542866000	-0.913346000
H	1.433684000	1.381666000	1.476980000
H	2.894626000	1.020478000	-3.236089000
H	0.866377000	1.999020000	-2.593550000
H	2.881940000	-0.184948000	-1.964653000
H	-0.782540000	2.347455000	1.625650000
H	0.654946000	3.380136000	1.576038000
H	-0.164777000	0.663937000	-0.335636000
H	0.573129000	0.279623000	-2.449583000
H	-2.093099000	2.000498000	-0.576782000
H	-0.914209000	4.029846000	1.109571000
H	0.555953000	3.490852000	-0.872919000
H	-1.316564000	2.314843000	-2.132733000
H	-1.876261000	3.661076000	-1.136011000
H	0.821498000	-3.518577000	0.017102000
C	-2.349059000	-1.047274000	-0.059490000
C	-3.343237000	-1.231919000	-1.011834000
C	-2.636481000	-0.434860000	1.154301000
C	-4.620841000	-0.794004000	-0.722965000
H	-3.115785000	-1.700764000	-1.959011000
C	-3.932198000	-0.011697000	1.385359000
H	-1.871001000	-0.280958000	1.901071000
C	-4.950869000	-0.174235000	0.467345000
H	-5.955080000	0.168020000	0.668529000
C	-0.959658000	-1.463976000	-0.413740000
O	-0.651949000	-1.917050000	-1.479293000
N	-4.240566000	0.655775000	2.662603000
O	-5.385771000	1.004540000	2.850323000
O	-3.328361000	0.816259000	3.444050000
N	-5.681341000	-0.984635000	-1.728725000
O	-6.791190000	-0.581916000	-1.455383000
O	-5.376817000	-1.532303000	-2.765684000
C	3.536934000	-0.863399000	0.748067000
C	3.915546000	-2.196178000	0.421905000
C	5.271601000	-2.597267000	0.513953000
C	6.224468000	-1.751968000	1.007333000
C	5.834878000	-0.481766000	1.476421000
C	4.539865000	-0.055497000	1.349355000

H	5.527841000	-3.607132000	0.215213000
H	7.256316000	-2.069210000	1.085922000
H	6.560065000	0.158804000	1.962351000
H	4.271993000	0.886631000	1.795276000
H	3.212297000	-4.162572000	-0.150514000

**SCF Done: E(RM062X) = -1680.23672562**

**# of imaginary frequencies = 1 (-31.1701)**

**TS2-3c**

C	0.748540000	-0.005682000	3.540821000
C	0.699794000	0.925099000	1.127285000
C	1.407929000	0.697295000	2.390468000
C	1.094372000	-1.592176000	-0.150601000
C	1.427566000	-2.947511000	0.022130000
C	1.544924000	0.889629000	-0.158863000
C	1.994441000	-0.580191000	-0.395717000
C	2.915676000	0.610412000	2.288069000
C	2.726682000	-3.329083000	-0.089625000
C	3.503112000	1.648215000	1.314776000
C	2.676528000	1.926453000	0.025509000
C	1.109314000	3.654270000	-1.077252000
C	2.211151000	3.406857000	-0.048263000
C	3.423358000	4.279580000	-0.385285000
O	0.895252000	1.991520000	2.060793000
H	1.105593000	0.398566000	4.490577000
H	0.990459000	-1.070328000	3.513480000
H	-0.342656000	0.650047000	1.069291000
H	-0.334670000	0.109449000	3.492402000
H	0.639083000	-3.643351000	0.276611000
H	0.930339000	1.182471000	-1.012741000
H	3.352529000	0.758367000	3.279401000
H	3.609614000	2.589937000	1.856424000
H	3.175084000	-0.408701000	1.985722000
H	1.393813000	3.263935000	-2.059614000
H	0.162886000	3.193200000	-0.788087000
H	3.342683000	1.846634000	-0.821262000
H	4.512542000	1.328552000	1.046691000
H	3.771336000	4.070377000	-1.401494000
H	0.933757000	4.726499000	-1.185204000
H	1.836686000	3.705400000	0.929688000
H	4.256458000	4.099242000	0.297158000
H	3.166835000	5.339161000	-0.329555000
O	-0.268936000	-1.330748000	0.036534000
C	-0.984095000	-0.917122000	-1.022648000
O	-0.548910000	-0.758324000	-2.127398000
C	-2.406220000	-0.657467000	-0.646034000
C	-2.866452000	-0.858215000	0.649382000
C	-3.261710000	-0.188266000	-1.635028000
C	-4.191945000	-0.578530000	0.926578000
H	-2.213333000	-1.225276000	1.427899000
C	-4.575864000	0.072129000	-1.300219000
H	-2.901673000	-0.030485000	-2.642019000
C	-5.076185000	-0.111316000	-0.025135000
H	-6.107243000	0.101430000	0.215005000
N	-4.685556000	-0.783048000	2.300060000
O	-5.852292000	-0.538840000	2.518200000
O	-3.893178000	-1.181344000	3.125995000
N	-5.488839000	0.572528000	-2.343388000
O	-6.637210000	0.791973000	-2.024057000
O	-5.034114000	0.733533000	-3.454826000

C	3.316753000	-1.033696000	-0.773287000
C	3.689729000	-2.391323000	-0.531054000
C	5.010571000	-2.832450000	-0.798296000
C	5.928448000	-2.005978000	-1.378520000
C	5.529281000	-0.710246000	-1.761210000
C	4.274900000	-0.244735000	-1.471295000
H	5.262471000	-3.859089000	-0.559222000
H	6.931371000	-2.353961000	-1.589387000
H	6.212267000	-0.078432000	-2.315005000
H	3.999562000	0.715526000	-1.869045000
H	3.026470000	-4.353402000	0.093538000

**SCF Done: E(RM062X) = -1680.23412635**

**# of imaginary frequencies = 1 (-43.3138)**

### TS2'-3c

C	0.154171000	-0.517413000	3.171096000
C	0.651029000	0.847598000	1.010226000
C	1.077637000	0.277076000	2.294901000
C	1.070286000	-1.369289000	-0.776550000
C	1.256739000	-2.751888000	-0.976285000
C	1.718135000	0.972200000	-0.090915000
C	2.082057000	-0.450459000	-0.608840000
C	2.562314000	0.001605000	2.414159000
C	2.518496000	-3.250302000	-0.996520000
C	3.423419000	1.129449000	1.817024000
C	2.881475000	1.790507000	0.516593000
C	1.699940000	3.906859000	-0.370339000
C	2.579303000	3.301104000	0.721933000
C	3.909939000	4.056730000	0.779286000
O	0.772907000	1.668118000	2.175826000
H	0.352354000	-0.288279000	4.220754000
H	0.311872000	-1.585407000	3.014894000
H	-0.383322000	0.767938000	0.709731000
H	-0.887588000	-0.284173000	2.947442000
H	0.391677000	-3.391820000	-1.076704000
H	1.297134000	1.521794000	-0.935363000
H	2.820286000	-0.130168000	3.468371000
H	3.526260000	1.909072000	2.574266000
H	2.767372000	-0.954775000	1.923689000
H	2.113571000	3.707699000	-1.364103000
H	0.679871000	3.518740000	-0.341241000
H	3.685132000	1.810334000	-0.203314000
H	4.426094000	0.733065000	1.641691000
H	4.406952000	4.027431000	-0.195237000
H	1.644032000	4.990244000	-0.246289000
H	2.072860000	3.431488000	1.676746000
H	4.590755000	3.623358000	1.515009000
H	3.751427000	5.103828000	1.044171000
O	-0.248092000	-0.904271000	-0.832885000
C	-1.178095000	-1.443451000	-0.026746000
O	-0.971990000	-2.296275000	0.788557000
C	-2.515657000	-0.816317000	-0.246160000
C	-2.706538000	0.192501000	-1.182367000
C	-3.571643000	-1.260319000	0.540230000
C	-3.970882000	0.737339000	-1.311103000
H	-1.893727000	0.550553000	-1.797567000
C	-4.812516000	-0.680381000	0.365738000
H	-3.419865000	-2.041869000	1.271556000
C	-5.048646000	0.324213000	-0.553386000
H	-6.027013000	0.765593000	-0.671694000

N	-4.180784000	1.811812000	-2.297836000
O	-5.297516000	2.272054000	-2.396055000
O	-3.223032000	2.168394000	-2.949003000
N	-5.937607000	-1.147611000	1.195255000
O	-7.017777000	-0.627411000	1.018160000
O	-5.711980000	-2.022575000	2.002463000
C	3.411186000	-0.954091000	-0.898161000
C	3.621378000	-2.363548000	-0.986863000
C	4.926375000	-2.889625000	-1.158725000
C	6.001455000	-2.069007000	-1.341882000
C	5.785992000	-0.679665000	-1.417932000
C	4.542148000	-0.146007000	-1.208800000
H	5.042765000	-3.967051000	-1.175226000
H	6.993644000	-2.478056000	-1.481905000
H	6.606955000	-0.020482000	-1.670683000
H	4.427365000	0.909487000	-1.375750000
H	2.694748000	-4.314740000	-1.089366000

**SCF Done: E(RM062X) = -1680.23348118**

**# of imaginary frequencies = 1 (-40.5406)**

**Cartesian coordinates of updated calculated minima and located transition states in DMSO or THF at the IEFPCM/M06-2X-D3/6-311+G(2d,p) level of theory.**

**(M)-1a**

C	-3.821235000	-2.247097000	-1.595992000
C	-1.673389000	-1.095357000	-1.127449000
C	-2.996753000	-1.136281000	-1.012913000
C	-0.783237000	-0.019793000	-0.537943000
C	0.496707000	-0.609537000	0.034834000
C	-3.751517000	-0.074371000	-0.255510000
C	2.823052000	-1.781698000	1.158641000
C	0.428280000	-1.593931000	0.999375000
C	1.585661000	-2.183991000	1.557131000
O	-0.797107000	-2.009859000	1.431215000
C	-2.922121000	1.189781000	-0.060216000
C	-1.531993000	0.860442000	0.486554000
C	-1.178338000	2.663834000	2.229715000
C	-0.720922000	2.112209000	0.879058000
C	-0.764150000	3.219671000	-0.176328000
H	-4.540571000	-1.857945000	-2.322081000
H	-4.401756000	-2.742287000	-0.811572000
H	-0.506566000	0.626392000	-1.373303000
H	-4.678354000	0.158338000	-0.789329000
H	-2.818547000	1.695500000	-1.025925000
H	-4.057781000	-0.483244000	0.715808000
H	-2.225447000	2.975411000	2.193536000
H	-1.075907000	1.913014000	3.015792000
H	-1.665121000	0.256992000	1.390433000
H	-3.442291000	1.881125000	0.607564000
H	-1.752449000	3.684689000	-0.211948000
H	-0.585252000	3.535831000	2.513367000
H	0.322282000	1.798418000	0.993267000
H	-0.535173000	2.852196000	-1.178942000
H	-0.039371000	3.999570000	0.064905000
H	-3.199415000	-2.994648000	-2.088671000
H	-0.687242000	-2.697881000	2.096393000
C	1.796970000	-0.171619000	-0.378492000
C	2.963640000	-0.763786000	0.187099000
C	4.251301000	-0.330473000	-0.214299000
C	4.404990000	0.662691000	-1.139381000
C	3.258827000	1.263653000	-1.701320000
C	2.002196000	0.861649000	-1.336423000
H	5.116062000	-0.805417000	0.235454000
H	5.392328000	0.989912000	-1.438871000
H	3.372914000	2.055087000	-2.431783000
H	1.158375000	1.356420000	-1.793454000
H	3.711577000	-2.232200000	1.584852000
H	1.470067000	-2.960071000	2.306183000
H	-1.163316000	-1.882314000	-1.678238000

**SCF Done: E(RM062X) = -851.697865060**

**# of imaginary frequencies = 0**

**(P)-1a**

C	2.213873000	3.428986000	-1.551840000
C	1.111479000	1.215076000	-1.328613000
C	2.040897000	2.076339000	-0.924597000
C	0.869574000	-0.149960000	-0.717584000
C	-0.610320000	-0.491506000	-0.642016000

C	2.963806000	1.749634000	0.221538000
C	-3.336974000	-1.259975000	-0.562265000
C	-1.056209000	-1.663071000	-1.214046000
C	-2.416734000	-2.048373000	-1.181945000
O	-0.148659000	-2.485448000	-1.822115000
C	3.005102000	0.254382000	0.518071000
C	1.594559000	-0.326548000	0.635873000
C	1.849848000	-1.876368000	2.623361000
C	1.574427000	-1.789883000	1.121762000
C	2.539959000	-2.696571000	0.356651000
H	3.215793000	3.534066000	-1.977169000
H	2.107897000	4.214575000	-0.797367000
H	1.480721000	3.604931000	-2.338935000
H	1.308330000	-0.875131000	-1.408002000
H	3.967573000	2.119280000	-0.009794000
H	3.533004000	-0.250985000	-0.297013000
H	2.637740000	2.306288000	1.110126000
H	2.852395000	-1.513809000	2.864149000
H	1.129797000	-1.283295000	3.191109000
H	1.054828000	0.263365000	1.386097000
H	3.574622000	0.068952000	1.431796000
H	3.578353000	-2.442208000	0.583280000
H	1.783820000	-2.910320000	2.968371000
H	0.559818000	-2.167077000	0.954963000
H	2.396365000	-2.629255000	-0.723063000
H	2.385239000	-3.737714000	0.647202000
H	-0.601636000	-3.255716000	-2.181236000
H	-2.712698000	-2.978882000	-1.654121000
H	-4.380158000	-1.551789000	-0.533669000
C	-1.572432000	0.337659000	0.018817000
C	-2.941709000	-0.050603000	0.057408000
C	-3.894981000	0.766564000	0.713751000
C	-3.522978000	1.931910000	1.322293000
C	-2.167859000	2.325380000	1.293435000
C	-1.224863000	1.557885000	0.664258000
H	-4.930000000	0.443637000	0.723487000
H	-4.256998000	2.550271000	1.822973000
H	-1.869116000	3.248590000	1.774759000
H	-0.198887000	1.893808000	0.650739000
H	0.461677000	1.486256000	-2.157634000

**SCF Done: E(RM062X) = -851.700609108**

**# of imaginary frequencies = 0**

### TS1-1a

C	-1.253750000	3.478261000	-0.846386000
C	-0.784968000	1.444055000	0.487261000
C	-1.194094000	1.989992000	-0.655300000
C	-0.747173000	-0.056463000	0.741537000
C	0.604850000	-0.726115000	0.373869000
C	-1.707732000	1.168580000	-1.807904000
C	2.971185000	-1.897489000	-0.725999000
C	0.689580000	-2.066823000	0.041483000
C	1.850625000	-2.638603000	-0.535518000
C	-1.741960000	-0.338192000	-1.526768000
C	-1.971432000	-0.628107000	-0.037863000
C	-3.447625000	-0.151617000	1.991767000
C	-3.327191000	-0.082484000	0.468781000
C	-4.478017000	-0.867856000	-0.165820000
H	-0.895731000	4.012017000	0.034063000
H	-2.278337000	3.799184000	-1.057040000



H	-0.540838000	2.114909000	1.301852000
H	-0.645451000	3.779657000	-1.703828000
H	-0.902927000	-0.226803000	1.810606000
H	-2.717622000	1.534689000	-2.032612000
H	-2.509731000	-0.810924000	-2.140583000
H	-1.117862000	1.380953000	-2.705155000
H	-3.212290000	-1.157902000	2.352564000
H	-2.778648000	0.552671000	2.488703000
H	-2.021219000	-1.701704000	0.102972000
H	-0.792915000	-0.789046000	-1.825056000
H	-4.417257000	-1.925275000	0.108361000
H	-4.466437000	0.086351000	2.304096000
H	-3.434443000	0.964936000	0.175005000
H	-4.473374000	-0.800791000	-1.254377000
H	-5.439573000	-0.487114000	0.184153000
H	1.816649000	-3.678814000	-0.842192000
O	-0.368257000	-2.905582000	0.252513000
H	3.846724000	-2.324213000	-1.200303000
H	-0.145264000	-3.786902000	-0.065648000
C	1.855944000	-0.006409000	0.363979000
C	3.016711000	-0.570880000	-0.240713000
C	4.227742000	0.161600000	-0.305882000
C	4.341718000	1.392029000	0.275233000
C	3.238634000	1.913565000	0.980876000
C	2.045769000	1.242331000	1.020725000
H	5.073916000	-0.294532000	-0.807443000
H	5.273007000	1.941909000	0.230987000
H	3.337383000	2.850541000	1.515193000
H	1.255401000	1.654617000	1.621437000

**SCF Done: E(RM062X) = -851.675039999**

**# of imaginary frequencies = 1 (-50.223)**

### TS2-1a

C	3.057469000	2.559607000	1.437725000
C	1.638483000	1.418348000	-0.242024000
C	2.203786000	1.417733000	0.963338000
C	0.787345000	0.273916000	-0.794060000
C	-0.725835000	0.581450000	-0.606341000
C	2.103174000	0.251953000	1.910218000
C	-3.306228000	1.514039000	0.185222000
C	-1.150934000	1.882258000	-0.816127000
C	-2.416376000	2.356746000	-0.399065000
O	-0.321805000	2.760546000	-1.450110000
C	1.197203000	-0.862082000	1.389583000
C	1.340889000	-1.014900000	-0.130507000
C	2.911705000	-1.461686000	-2.087191000
C	2.791119000	-1.336858000	-0.566742000
C	3.265801000	-2.636798000	0.087808000
H	4.069852000	2.213249000	1.667021000
H	2.653798000	2.985905000	2.360501000
H	1.806455000	2.270489000	-0.884624000
H	3.122432000	3.350928000	0.690986000
H	0.962937000	0.222926000	-1.872157000
H	3.121044000	-0.127927000	2.070443000
H	1.417015000	-1.800300000	1.900588000
H	1.764155000	0.600170000	2.890817000
H	2.162271000	-2.157356000	-2.478045000
H	2.783298000	-0.505034000	-2.594238000
H	0.779635000	-1.887593000	-0.441933000
H	0.156581000	-0.623233000	1.619821000

H	2.590712000	-3.462261000	-0.158943000
H	3.896818000	-1.845160000	-2.359714000
H	3.457735000	-0.534080000	-0.243340000
H	3.318394000	-2.557053000	1.174140000
H	4.261652000	-2.901967000	-0.271914000
H	-2.647760000	3.408576000	-0.528585000
H	-0.721881000	3.636650000	-1.457911000
H	-4.258403000	1.876842000	0.553001000
C	-1.757824000	-0.350994000	-0.221266000
C	-3.016547000	0.132283000	0.250971000
C	-4.005131000	-0.765609000	0.724628000
C	-3.823025000	-2.117355000	0.665011000
C	-2.645744000	-2.613425000	0.070590000
C	-1.658372000	-1.766060000	-0.356364000
H	-4.928205000	-0.348195000	1.111125000
H	-4.586847000	-2.796949000	1.020142000
H	-2.526628000	-3.679826000	-0.076971000
H	-0.826376000	-2.198560000	-0.881771000

**SCF Done: E(RM062X) = -851.672791349**

**# of imaginary frequencies = 1 (-50.857)**

**(M)-1b**

C	-3.826146000	-1.446749000	-2.197958000
C	-1.633939000	-0.558391000	-1.445025000
C	-2.960691000	-0.539851000	-1.371711000
C	-0.705366000	0.310309000	-0.619796000
C	0.527995000	-0.458860000	-0.168017000
C	-3.680051000	0.380707000	-0.419650000
C	2.760655000	-1.963883000	0.698753000
C	0.379938000	-1.630168000	0.560021000
C	1.495884000	-2.386052000	0.988986000
O	-0.889711000	-2.018449000	0.850181000
C	-2.788083000	1.519954000	0.060542000
C	-1.438323000	0.996137000	0.554226000
C	-1.041917000	2.354337000	2.654792000
C	-0.573749000	2.083355000	1.224713000
C	-0.525802000	3.394002000	0.435997000
H	-4.496494000	-0.867657000	-2.839408000
H	-4.461254000	-2.060276000	-1.551440000
H	-0.371529000	1.103125000	-1.291899000
H	-4.573799000	0.779331000	-0.910114000
H	-2.623234000	2.212246000	-0.771750000
H	-4.041762000	-0.205861000	0.434662000
H	-2.070462000	2.724225000	2.669058000
H	-1.000626000	1.446503000	3.260035000
H	-1.636248000	0.223492000	1.303831000
H	-3.291543000	2.084371000	0.849539000
H	-1.485464000	3.914331000	0.487334000
H	-0.413916000	3.109640000	3.132059000
H	0.447218000	1.691572000	1.286470000
H	-0.289767000	3.239649000	-0.619062000
H	0.234030000	4.058114000	0.852424000
H	-3.230867000	-2.109867000	-2.825841000
C	1.852752000	-0.009314000	-0.458518000
C	2.976261000	-0.771577000	-0.022277000
C	4.294457000	-0.329960000	-0.303610000
C	4.518527000	0.830299000	-0.986085000
C	3.415427000	1.600202000	-1.417535000
C	2.133170000	1.197268000	-1.165342000
H	5.123358000	-0.937492000	0.042138000

H	5.527350000	1.162549000	-1.194711000
H	3.586154000	2.524555000	-1.955544000
H	1.327118000	1.825042000	-1.513963000
H	3.615890000	-2.542469000	1.027994000
H	1.354050000	-3.298588000	1.549176000
H	-1.150043000	-1.240405000	-2.140556000
C	-1.091318000	-3.242774000	1.531395000
H	-0.677567000	-4.082520000	0.968769000
H	-0.652413000	-3.218789000	2.531398000
H	-2.168570000	-3.361158000	1.614547000

**SCF Done: E(RM062X) = -890.984572209**

**# of imaginary frequencies = 0**

**(P)-1b**

C	-2.503329000	-3.132232000	-2.038034000
C	-1.215607000	-1.095150000	-1.438842000
C	-2.230213000	-1.920160000	-1.195777000
C	-0.874719000	0.127384000	-0.612037000
C	0.626150000	0.326143000	-0.460241000
C	-3.153991000	-1.699637000	-0.025103000
C	3.396471000	0.826218000	-0.212807000
C	1.177516000	1.550012000	-0.802955000
C	2.565265000	1.799574000	-0.686360000
O	0.321410000	2.511182000	-1.251658000
C	-3.071237000	-0.275028000	0.512671000
C	-1.618986000	0.148412000	0.742421000
C	-1.794813000	1.374754000	2.952494000
C	-1.486111000	1.506693000	1.460725000
C	-2.347505000	2.608409000	0.840822000
H	-3.498261000	-3.076037000	-2.488364000
H	-2.487434000	-4.035986000	-1.421046000
H	-1.766602000	-3.244452000	-2.833437000
H	-1.234130000	0.987181000	-1.182000000
H	-4.179471000	-1.932471000	-0.328295000
H	-3.529776000	0.402434000	-0.214834000
H	-2.904737000	-2.420815000	0.764578000
H	-2.830978000	1.068988000	3.117689000
H	-1.144273000	0.636405000	3.425967000
H	-1.153310000	-0.601333000	1.393227000
H	-3.647429000	-0.189500000	1.437018000
H	-3.409868000	2.419146000	1.014027000
H	-1.650055000	2.329749000	3.461970000
H	-0.438665000	1.813396000	1.371626000
H	-2.184255000	2.698836000	-0.234422000
H	-2.106571000	3.571839000	1.295255000
H	2.974284000	2.758223000	-0.969821000
H	4.459715000	1.016280000	-0.123212000
C	1.493500000	-0.685967000	0.050689000
C	2.889874000	-0.432782000	0.172745000
C	3.754611000	-1.434875000	0.682737000
C	3.269782000	-2.649855000	1.072363000
C	1.884780000	-2.909905000	0.964781000
C	1.026863000	-1.965693000	0.472010000
H	4.812785000	-1.210715000	0.758791000
H	3.935195000	-3.409465000	1.462372000
H	1.496652000	-3.871885000	1.276640000
H	-0.023865000	-2.201152000	0.394991000
H	-0.567618000	-1.288648000	-2.290821000
C	0.828011000	3.808087000	-1.508588000
H	1.547124000	3.799252000	-2.330480000

H -0.031413000 4.411279000 -1.789527000  
H 1.293802000 4.233584000 -0.616914000  
**SCF Done: E(RM062X) = -890.987319393**  
**# of imaginary frequencies = 0**

**TS1-1b**

C -0.982898000 -3.674319000 1.027474000  
C -0.644767000 -1.702817000 -0.433637000  
C -1.017981000 -2.200224000 0.742912000  
C -0.698957000 -0.221121000 -0.779876000  
C 0.615025000 0.540207000 -0.453001000  
C -1.580494000 -1.342788000 1.845579000  
C 2.887612000 1.868699000 0.644891000  
C 0.621413000 1.898469000 -0.175884000  
C 1.736443000 2.551232000 0.405321000  
C -1.709258000 0.139242000 1.473515000  
C -1.956241000 0.320817000 -0.029610000  
C -3.401167000 -0.375201000 -2.017894000  
C -3.276770000 -0.337485000 -0.494213000  
C -4.471898000 0.418670000 0.092186000  
H -0.593011000 -4.238668000 0.180288000  
H -1.984673000 -4.045650000 1.263485000  
H -0.356296000 -2.406958000 -1.204319000  
H -0.355213000 -3.882012000 1.898666000  
H -0.867236000 -0.125148000 -1.856071000  
H -2.565367000 -1.756085000 2.097666000  
H -2.505548000 0.599405000 2.060236000  
H -0.977306000 -1.462620000 2.751038000  
H -3.225512000 0.617565000 -2.444225000  
H -2.691771000 -1.069739000 -2.470477000  
H -2.073910000 1.377723000 -0.241142000  
H -0.790097000 0.664998000 1.741825000  
H -4.474033000 1.457352000 -0.252104000  
H -4.404201000 -0.692586000 -2.309945000  
H -3.321715000 -1.367751000 -0.131875000  
H -4.462758000 0.424759000 1.182783000  
H -5.409447000 -0.040439000 -0.227493000  
H 1.660733000 3.598226000 0.664384000  
O -0.472715000 2.645463000 -0.500534000  
H 3.732144000 2.355245000 1.118359000  
C 1.898228000 -0.113560000 -0.402200000  
C 3.014165000 0.532707000 0.204607000  
C 4.260389000 -0.134135000 0.316065000  
C 4.447917000 -1.374862000 -0.221241000  
C 3.387168000 -1.978662000 -0.928157000  
C 2.162547000 -1.373256000 -1.011393000  
H 5.072411000 0.381023000 0.816910000  
H 5.405587000 -1.873304000 -0.142727000  
H 3.546241000 -2.926058000 -1.428399000  
H 1.404780000 -1.843789000 -1.612395000  
C -0.821460000 3.734111000 0.343565000  
H -0.219788000 4.617913000 0.125411000  
H -1.866247000 3.956674000 0.134979000  
H -0.710140000 3.461875000 1.395373000

**SCF Done: E(RM062X) = -890.960990352**  
**# of imaginary frequencies = 1 (-47.2872)**

**TS2-1b**

C 2.947726000 2.280479000 1.724641000  
C 1.609029000 1.244809000 -0.083460000

C	2.142402000	1.158317000	1.133378000
C	0.797718000	0.130578000	-0.746331000
C	-0.724734000	0.386436000	-0.547763000
C	2.056170000	-0.088236000	1.973033000
C	-3.309880000	1.222837000	0.312286000
C	-1.165440000	1.696113000	-0.660064000
C	-2.434225000	2.124180000	-0.207168000
O	-0.342207000	2.600275000	-1.265616000
C	1.205271000	-1.185144000	1.333758000
C	1.380893000	-1.194975000	-0.190990000
C	3.005282000	-1.398947000	-2.144642000
C	2.849843000	-1.427511000	-0.622620000
C	3.354623000	-2.769322000	-0.085972000
H	3.964731000	1.947299000	1.952744000
H	2.506771000	2.615655000	2.667815000
H	1.783307000	2.146348000	-0.653670000
H	3.004979000	3.133554000	1.048088000
H	0.985460000	0.179482000	-1.821778000
H	3.082963000	-0.445040000	2.129173000
H	1.453614000	-2.156044000	1.764305000
H	1.679737000	0.160854000	2.969994000
H	2.288675000	-2.077369000	-2.618502000
H	2.853152000	-0.401941000	-2.559024000
H	0.856229000	-2.052280000	-0.597029000
H	0.152848000	-1.008206000	1.564088000
H	2.713857000	-3.587907000	-0.428482000
H	4.008518000	-1.721216000	-2.429944000
H	3.482157000	-0.639161000	-0.207353000
H	3.381176000	-2.794688000	1.003926000
H	4.366489000	-2.965941000	-0.445053000
H	-2.694049000	3.172308000	-0.265288000
H	-4.269575000	1.541334000	0.701547000
C	-1.737449000	-0.589092000	-0.227674000
C	-3.001930000	-0.155175000	0.276538000
C	-3.977718000	-1.098321000	0.687324000
C	-3.773568000	-2.439700000	0.541009000
C	-2.584111000	-2.879956000	-0.074270000
C	-1.610182000	-1.991896000	-0.443683000
H	-4.908048000	-0.721919000	1.097742000
H	-4.527710000	-3.152725000	0.848266000
H	-2.445009000	-3.933839000	-0.281765000
H	-0.763782000	-2.378686000	-0.981231000
C	-0.278516000	3.908044000	-0.712664000
H	0.629930000	4.361584000	-1.104490000
H	-1.134211000	4.513936000	-1.014422000
H	-0.221788000	3.861301000	0.377265000

**SCF Done: E(RM062X) = -890.959611538**

**# of imaginary frequencies = 1 (-49.8429)**

**(M)-1c**

C	-0.572629000	0.048216000	1.726623000
C	-1.791895000	0.552750000	0.979260000
C	-1.482537000	1.857760000	0.211286000
C	-0.722476000	2.802056000	1.145071000
C	0.622790000	2.214498000	1.555237000
C	0.517002000	0.771438000	1.975158000
H	-2.536765000	0.794388000	1.739862000
H	-0.812520000	1.592062000	-0.615106000
H	-0.575258000	3.774386000	0.669842000
H	-1.323460000	2.973574000	2.043669000

H	1.342624000	2.300411000	0.730890000
H	1.054280000	2.790760000	2.379745000
H	-0.613904000	-0.983433000	2.068589000
C	-2.739673000	2.501282000	-0.407434000
H	-3.352240000	1.692606000	-0.819551000
C	-2.365207000	3.421492000	-1.569690000
H	-1.832559000	2.873101000	-2.349220000
H	-1.724147000	4.240435000	-1.233672000
H	-3.258466000	3.863691000	-2.015321000
C	-3.590766000	3.264749000	0.609689000
H	-4.549523000	3.540550000	0.167021000
H	-3.091404000	4.185417000	0.920975000
H	-3.795929000	2.680108000	1.508716000
C	-3.384014000	-2.530303000	-1.669358000
C	-2.384036000	-0.523062000	0.078850000
C	-1.604110000	-1.175828000	-0.839953000
C	-2.071830000	-2.172743000	-1.714089000
H	-3.771393000	-3.294517000	-2.332002000
H	-1.375944000	-2.632134000	-2.404018000
C	-4.262717000	-1.900583000	-0.754492000
C	-3.771286000	-0.893190000	0.124621000
C	-4.704544000	-0.289070000	1.009853000
C	-6.022077000	-0.659646000	1.020704000
C	-6.497600000	-1.660783000	0.148765000
C	-5.631491000	-2.265109000	-0.717225000
H	-4.386043000	0.480663000	1.696153000
H	-6.706041000	-0.178564000	1.708481000
H	-7.541847000	-1.945012000	0.169180000
H	-5.976755000	-3.036247000	-1.396112000
O	-0.261172000	-0.800909000	-0.970083000
C	0.659375000	-1.622464000	-0.441794000
O	0.429033000	-2.702663000	0.022419000
C	1.710649000	0.206985000	2.690545000
H	2.622054000	0.384969000	2.108511000
H	1.855230000	0.704318000	3.653496000
H	1.611523000	-0.865554000	2.862522000
C	2.022897000	-1.015279000	-0.482959000
C	3.084810000	-1.768074000	0.000648000
C	2.223672000	0.284344000	-0.928417000
C	4.342388000	-1.195386000	0.024805000
H	2.924507000	-2.775586000	0.358928000
C	3.501771000	0.809162000	-0.872699000
H	1.403494000	0.881267000	-1.300367000
C	4.587480000	0.095702000	-0.402598000
H	5.576955000	0.526903000	-0.366668000
N	5.474093000	-1.986855000	0.541893000
O	6.565384000	-1.460216000	0.553648000
O	5.239985000	-3.112923000	0.921969000
N	3.714261000	2.198080000	-1.318264000
O	2.735087000	2.834189000	-1.645050000
O	4.850605000	2.617445000	-1.323202000

**SCF Done: E(RM062X) = -1605.05920541**

**# of imaginary frequencies = 0**

**(P)-1c**

C	-2.600060000	2.033571000	-0.607118000
C	-1.822224000	0.919761000	0.063797000
C	-1.947290000	0.950552000	1.604701000
C	-1.829715000	2.400488000	2.077470000
C	-2.954377000	3.260709000	1.512192000

C	-3.110197000	3.087670000	0.023124000
H	-0.770141000	1.101728000	-0.172108000
H	-2.948892000	0.593589000	1.869891000
H	-0.871201000	2.810016000	1.742696000
H	-1.834043000	2.447100000	3.168776000
H	-2.772541000	4.316784000	1.732878000
H	-3.906636000	3.013066000	1.999335000
H	-2.733595000	1.940235000	-1.682247000
C	-0.940254000	0.003042000	2.286354000
H	-0.947392000	-0.935652000	1.722923000
C	0.491912000	0.543115000	2.286354000
H	0.798977000	0.918242000	1.306445000
H	0.598270000	1.365932000	2.997400000
H	1.192711000	-0.241928000	2.580250000
C	-1.370576000	-0.331995000	3.714473000
H	-1.396603000	0.562884000	4.341075000
H	-0.670202000	-1.033815000	4.171661000
H	-2.363203000	-0.786328000	3.728852000
C	-2.639090000	-3.003807000	-1.654588000
C	-2.156082000	-0.442417000	-0.523937000
C	-1.158754000	-1.246296000	-1.009540000
C	-1.372175000	-2.514584000	-1.583718000
H	-2.830163000	-3.977322000	-2.089360000
H	-0.524038000	-3.075452000	-1.953703000
C	-3.727159000	-2.245089000	-1.155233000
C	-3.494322000	-0.960108000	-0.591020000
C	-4.619484000	-0.243200000	-0.101487000
C	-5.881186000	-0.770135000	-0.168867000
C	-6.102928000	-2.044078000	-0.732164000
C	-5.045099000	-2.761360000	-1.215010000
H	-4.482428000	0.739469000	0.323549000
H	-6.718987000	-0.200744000	0.213799000
H	-7.106440000	-2.447308000	-0.779661000
H	-5.195190000	-3.742189000	-1.651205000
O	0.158859000	-0.765125000	-1.000656000
C	1.063058000	-1.411264000	-0.248451000
O	0.831070000	-2.366918000	0.435950000
C	-3.893879000	4.149816000	-0.690766000
H	-4.891755000	4.244457000	-0.251984000
H	-3.409305000	5.124244000	-0.585200000
H	-4.002111000	3.926872000	-1.752019000
C	2.413617000	-0.779208000	-0.353489000
C	3.440379000	-1.326880000	0.405033000
C	2.643105000	0.329883000	-1.157925000
C	4.691111000	-0.744637000	0.340138000
H	3.258062000	-2.187743000	1.033378000
C	3.915439000	0.871377000	-1.182032000
H	1.852608000	0.768168000	-1.750038000
C	4.964554000	0.360022000	-0.443857000
H	5.949517000	0.801506000	-0.477323000
N	5.785295000	-1.319677000	1.144276000
O	6.871913000	-0.788586000	1.069966000
O	5.527531000	-2.286034000	1.827689000
N	4.167014000	2.051324000	-2.030004000
O	3.239932000	2.477139000	-2.683597000
O	5.284272000	2.519896000	-2.018672000

**SCF Done: E(RM062X) = -1605.05499687**

**# of imaginary frequencies = 0**

**TS1-1c**

C	-4.157204000	3.788597000	-0.013740000
C	-2.855174000	1.824483000	-0.772795000
C	-3.103926000	2.733813000	0.166859000
C	-1.767706000	0.761244000	-0.668251000
C	-2.266488000	-0.588422000	-0.089136000
C	-2.301560000	2.832658000	1.435434000
C	-3.255716000	-2.844577000	1.377482000
C	-1.459512000	-1.461811000	0.604705000
C	-1.928493000	-2.558930000	1.354888000
C	-1.183602000	1.792417000	1.531859000
C	-0.625116000	1.440379000	0.146618000
C	0.341430000	2.336081000	-2.038241000
C	0.007444000	2.650845000	-0.579425000
C	1.285377000	3.080125000	0.146229000
H	-4.679917000	3.678258000	-0.963678000
H	-3.711675000	4.786861000	0.026768000
H	-3.410983000	1.903869000	-1.697727000
H	-4.892534000	3.737105000	0.793868000
H	-1.404114000	0.540127000	-1.675783000
H	-1.881109000	3.845557000	1.469179000
H	-0.392867000	2.154683000	2.189781000
H	-2.967041000	2.766304000	2.301445000
H	0.913936000	1.404488000	-2.111404000
H	-0.552968000	2.231799000	-2.653872000
H	0.207142000	0.765019000	0.297947000
H	-1.568675000	0.879654000	1.992272000
H	2.026278000	2.273235000	0.122731000
H	0.947526000	3.134687000	-2.469767000
H	-0.689928000	3.491987000	-0.567259000
H	1.104202000	3.342116000	1.189205000
H	1.728625000	3.949733000	-0.341984000
H	-1.205581000	-3.136077000	1.916341000
O	-0.070248000	-1.313619000	0.697156000
H	-3.642523000	-3.657935000	1.978848000
C	-3.633210000	-1.034312000	-0.239801000
C	-4.133306000	-2.114427000	0.542320000
C	-5.492305000	-2.504044000	0.437835000
C	-6.326103000	-1.916659000	-0.469458000
C	-5.809854000	-0.933593000	-1.337681000
C	-4.514459000	-0.506976000	-1.222902000
H	-5.845335000	-3.305022000	1.077077000
H	-7.359272000	-2.228678000	-0.552279000
H	-6.438248000	-0.521824000	-2.117452000
H	-4.145864000	0.197943000	-1.946526000
C	0.646082000	-1.355522000	-0.437403000
O	0.201378000	-1.573999000	-1.527535000
C	2.086457000	-1.045602000	-0.182498000
C	2.943498000	-1.020756000	-1.275792000
C	2.553515000	-0.734429000	1.088787000
C	4.266622000	-0.682751000	-1.068825000
H	2.575738000	-1.253041000	-2.265796000
C	3.888141000	-0.404039000	1.235664000
H	1.895841000	-0.738160000	1.946222000
C	4.774133000	-0.366280000	0.176956000
H	5.811511000	-0.099709000	0.315029000
N	4.388968000	-0.063609000	2.580340000
O	3.596170000	-0.096460000	3.495996000
O	5.560235000	0.228311000	2.683103000
N	5.180409000	-0.646979000	-2.225949000
O	6.334008000	-0.340645000	-2.017336000



O 4.718257000 -0.925329000 -3.310391000  
**SCF Done: E(RM062X) = -1605.03052027**  
**# of imaginary frequencies = 1 (-40.4416)**

**TS2-1c**

C	0.068658000	2.728514000	2.510040000
C	0.671061000	1.299490000	0.579296000
C	1.050555000	2.143841000	1.535574000
C	1.624673000	0.701057000	-0.454791000
C	2.119489000	-0.704895000	-0.003644000
C	2.464011000	2.646430000	1.662182000
C	2.832631000	-3.149965000	1.316660000
C	1.214292000	-1.553253000	0.595691000
C	1.536962000	-2.747014000	1.263562000
O	-0.152669000	-1.253505000	0.650087000
C	3.417587000	2.064793000	0.615124000
C	2.685908000	1.803675000	-0.707821000
C	1.184242000	2.797215000	-2.521354000
C	2.077173000	3.092771000	-1.315337000
C	3.195102000	4.052113000	-1.731156000
H	0.053617000	3.819502000	2.431604000
H	0.358129000	2.489031000	3.536826000
H	-0.384149000	1.069927000	0.508763000
H	-0.941150000	2.353727000	2.341149000
H	1.068799000	0.534151000	-1.381014000
H	2.422966000	3.739417000	1.573237000
H	4.266553000	2.733664000	0.470140000
H	2.835926000	2.451826000	2.672564000
H	1.706124000	2.163478000	-3.245311000
H	0.258356000	2.295333000	-2.235917000
H	3.399978000	1.484347000	-1.457783000
H	3.830758000	1.123323000	0.981488000
H	3.843167000	3.587566000	-2.480415000
H	0.910921000	3.725649000	-3.026010000
H	1.465047000	3.597394000	-0.564837000
H	3.816154000	4.353389000	-0.886927000
H	2.774152000	4.958055000	-2.170795000
H	0.739102000	-3.299445000	1.742030000
H	3.120253000	-4.040929000	1.860792000
C	3.455128000	-1.249761000	-0.127728000
C	3.811515000	-2.429387000	0.595935000
C	5.138933000	-2.927072000	0.555356000
C	6.090183000	-2.345312000	-0.230037000
C	5.723403000	-1.254821000	-1.042882000
C	4.459915000	-0.731538000	-0.992713000
H	5.371138000	-3.803884000	1.148732000
H	7.098516000	-2.737369000	-0.261668000
H	6.442560000	-0.832778000	-1.733687000
H	4.223895000	0.052588000	-1.686314000
C	-0.856956000	-1.307328000	-0.488425000
O	-0.416097000	-1.609054000	-1.561005000
C	-2.283821000	-0.921493000	-0.262085000
C	-3.147307000	-0.971217000	-1.349266000
C	-2.737951000	-0.501658000	0.982230000
C	-4.464156000	-0.598729000	-1.162953000
H	-2.790924000	-1.294086000	-2.317618000
C	-4.065286000	-0.134468000	1.107898000
H	-2.076563000	-0.458078000	1.835913000
C	-4.958222000	-0.172352000	0.055275000
H	-5.991016000	0.118716000	0.177282000

N	-5.387301000	-0.651935000	-2.311812000
O	-6.537132000	-0.320928000	-2.120471000
O	-4.936665000	-1.023293000	-3.373052000
N	-4.551305000	0.324247000	2.422366000
O	-3.748013000	0.374023000	3.328131000
O	-5.721723000	0.624194000	2.512074000

**SCF Done: E(RM062X) = -1605.02617999**

**# of imaginary frequencies = 1 (-52.6247)**

**(M)-1'a**

C	-0.827897000	-0.190183000	0.348493000
C	-1.280684000	-0.971488000	-0.724221000
C	-2.631995000	-1.096573000	-1.018984000
C	-3.587427000	-0.444744000	-0.249247000
C	-3.150739000	0.332344000	0.815236000
C	-1.795191000	0.466754000	1.120964000
H	-2.936977000	-1.709973000	-1.862062000
H	-3.881279000	0.851498000	1.425815000
C	2.919251000	0.545792000	-0.251341000
C	1.413241000	0.715325000	-0.457207000
C	0.659304000	-0.066729000	0.640314000
C	1.280366000	-1.422215000	0.908009000
C	2.464999000	-1.822264000	0.457319000
C	3.330202000	-0.916523000	-0.380397000
H	3.189120000	0.899405000	0.749253000
H	3.474971000	1.157309000	-0.966796000
H	1.156481000	0.253267000	-1.415701000
H	0.755055000	0.507908000	1.566529000
H	3.270720000	-1.238235000	-1.427957000
H	4.376500000	-1.044664000	-0.085276000
O	-0.347350000	-1.614478000	-1.487624000
C	-5.051447000	-0.592155000	-0.567302000
H	-5.656564000	0.056826000	0.064748000
H	-5.252291000	-0.340022000	-1.609996000
H	-5.381079000	-1.621415000	-0.411030000
C	-1.408678000	1.340306000	2.290006000
H	-0.780703000	2.176032000	1.973122000
H	-2.298943000	1.750359000	2.764614000
H	-0.851286000	0.781820000	3.044787000
C	0.971628000	2.191689000	-0.520032000
H	-0.116436000	2.206268000	-0.389753000
C	1.592033000	3.056698000	0.579978000
H	1.492869000	2.607351000	1.570761000
H	2.657023000	3.216268000	0.394101000
H	1.111125000	4.036613000	0.608110000
C	1.270207000	2.799913000	-1.890546000
H	2.342790000	2.787380000	-2.101085000
H	0.763330000	2.247166000	-2.684050000
H	0.938384000	3.839467000	-1.935024000
H	0.683894000	-2.105275000	1.508851000
C	3.006614000	-3.196875000	0.723471000
H	3.215538000	-3.712416000	-0.218936000
H	3.952652000	-3.143598000	1.269669000
H	2.305805000	-3.801668000	1.299095000
H	-0.794616000	-2.116285000	-2.177882000

**SCF Done: E(RM062X) = -776.692344539**

**# of imaginary frequencies = 0**

**(P)-1'a**

C	0.816418000	-0.252188000	-0.321151000
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C	1.751047000	0.550436000	-0.990925000
C	3.114954000	0.450533000	-0.754891000
C	3.601404000	-0.462187000	0.172780000
C	2.686257000	-1.258610000	0.846668000
C	1.311117000	-1.172622000	0.614744000
H	3.799674000	1.096254000	-1.296838000
H	3.047208000	-1.971579000	1.580187000
C	-2.900566000	0.657901000	0.237011000
C	-1.390174000	0.757569000	0.458808000
C	-0.663023000	-0.066082000	-0.629013000
C	-1.351622000	-1.382643000	-0.912889000
C	-2.558044000	-1.726905000	-0.473219000
C	-3.380922000	-0.783287000	0.365618000
H	-3.139725000	1.019407000	-0.768323000
H	-3.435778000	1.296993000	0.943322000
H	-1.169166000	0.296029000	1.428341000
H	-0.710558000	0.514047000	-1.554985000
H	-3.339740000	-1.107630000	1.413917000
H	-4.431480000	-0.862364000	0.069047000
O	1.273484000	1.460879000	-1.895307000
C	5.081063000	-0.578866000	0.423896000
H	5.283572000	-1.227646000	1.275348000
H	5.590352000	-0.995450000	-0.447799000
H	5.522611000	0.398879000	0.623580000
C	0.418817000	-2.115165000	1.388930000
H	-0.502690000	-1.644824000	1.725417000
H	0.128775000	-2.969220000	0.773190000
H	0.951971000	-2.494286000	2.260584000
C	-0.880201000	2.210916000	0.536438000
H	0.211757000	2.171062000	0.471178000
C	-1.384027000	3.090998000	-0.608269000
H	-1.190372000	2.642766000	-1.584002000
H	-2.458077000	3.272338000	-0.518483000
H	-0.883035000	4.060997000	-0.583738000
C	-1.230864000	2.848013000	1.881738000
H	-2.312922000	2.920925000	2.016894000
H	-0.824549000	2.266104000	2.711776000
H	-0.824115000	3.859424000	1.946549000
H	-0.789031000	-2.088759000	-1.519953000
C	-3.163520000	-3.071991000	-0.750460000
H	-2.490681000	-3.705383000	-1.328924000
H	-3.398427000	-3.583286000	0.188426000
H	-4.104919000	-2.971101000	-1.297749000
H	2.012793000	1.944353000	-2.279383000

**SCF Done: E(RM062X) = -776.692423773**

**# of imaginary frequencies = 0**

### TS1-1'a

C	-2.228051000	3.236335000	-0.655987000
C	-1.113894000	1.403945000	0.584242000
C	-1.676140000	1.844463000	-0.538642000
C	1.848466000	0.983044000	0.647725000
C	3.193984000	0.877265000	0.290948000
C	-0.561421000	-0.001775000	0.758390000
C	0.959528000	-0.100604000	0.458774000
C	-1.868047000	0.966337000	-1.747308000
C	3.739944000	-0.286170000	-0.228893000
C	1.564702000	-1.303678000	0.046378000
C	2.905385000	-1.385050000	-0.318418000
C	-1.331439000	-0.456061000	-1.561358000

C	-1.477033000	-0.917230000	-0.105931000
C	-3.063625000	-1.226307000	1.867238000
C	-2.948176000	-0.930704000	0.370771000
C	-3.745861000	-1.974204000	-0.415638000
H	-2.082406000	3.805858000	0.262281000
H	-3.298040000	3.210307000	-0.883385000
H	-1.088342000	2.073797000	1.434524000
H	-1.744450000	3.773821000	-1.476870000
H	3.838055000	1.736165000	0.443750000
H	-0.679210000	-0.284967000	1.808850000
H	-2.945304000	0.940281000	-1.957675000
H	-1.838301000	-1.138169000	-2.245230000
H	-1.413881000	1.440253000	-2.623342000
H	-2.496946000	-2.125872000	2.127704000
H	-2.692564000	-0.402803000	2.479061000
H	-1.141836000	-1.944948000	-0.029969000
H	-0.271805000	-0.486738000	-1.827196000
H	-3.313716000	-2.970282000	-0.280163000
H	-4.106487000	-1.395514000	2.143001000
H	-3.405105000	0.045477000	0.189732000
H	-3.766653000	-1.757897000	-1.484471000
H	-4.779612000	-2.008448000	-0.065971000
C	5.178093000	-0.358867000	-0.663533000
H	5.788481000	0.360897000	-0.118160000
H	5.589475000	-1.355709000	-0.502687000
H	5.269121000	-0.131503000	-1.728325000
H	3.295595000	-2.339402000	-0.660517000
O	0.834291000	-2.461672000	0.021857000
C	1.467065000	2.288409000	1.312799000
H	0.886099000	2.938025000	0.659145000
H	0.883062000	2.119580000	2.217430000
H	2.374388000	2.818835000	1.599190000
H	1.405183000	-3.182548000	-0.264917000

**SCF Done: E(RM062X) = -776.671380618**

**# of imaginary frequencies = 1 (-50.5621)**

### TS2-1'a

C	2.174409000	3.306987000	0.531920000
C	1.062257000	1.417925000	-0.623311000
C	1.655379000	1.898519000	0.466724000
C	-1.828359000	0.934193000	-0.688984000
C	-3.171330000	0.924376000	-0.327732000
C	0.552718000	-0.012783000	-0.755505000
C	-0.963206000	-0.152145000	-0.449389000
C	1.919502000	1.056439000	1.687641000
C	-3.749384000	-0.202067000	0.230038000
C	-1.594294000	-1.332357000	0.004902000
C	-2.948448000	-1.326586000	0.350055000
C	1.367443000	-0.364379000	1.567746000
C	1.493122000	-0.875921000	0.127807000
C	3.039668000	-1.366434000	-1.834128000
C	2.954210000	-0.898048000	-0.379872000
C	3.807499000	-1.814858000	0.500274000
H	1.982570000	3.848836000	-0.394272000
H	3.252214000	3.313158000	0.721804000
H	0.955411000	2.068895000	-1.480042000
H	1.706331000	3.853704000	1.355641000
H	-3.770413000	1.811616000	-0.511548000
H	0.677488000	-0.313280000	-1.800440000
H	3.007085000	1.028333000	1.837459000

H	1.874629000	-1.028128000	2.269499000
H	1.516280000	1.554668000	2.574924000
H	2.502023000	-2.310945000	-1.967387000
H	2.621212000	-0.637691000	-2.529044000
H	1.189642000	-1.914686000	0.099971000
H	0.309519000	-0.370360000	1.844367000
H	3.391135000	-2.826949000	0.520959000
H	4.080105000	-1.531430000	-2.120832000
H	3.376779000	0.107977000	-0.327198000
H	3.873086000	-1.455636000	1.527954000
H	4.824320000	-1.880968000	0.108625000
C	-5.188722000	-0.207279000	0.666695000
H	-5.799071000	0.427048000	0.023250000
H	-5.599416000	-1.216741000	0.649446000
H	-5.281288000	0.171667000	1.687278000
H	-3.391495000	-2.248286000	0.710903000
C	-0.932175000	-2.691642000	0.098878000
H	-0.331147000	-2.802066000	1.003333000
H	-0.296996000	-2.897358000	-0.762314000
H	-1.705884000	-3.457621000	0.127729000
O	-1.350528000	2.033262000	-1.346790000
H	-2.061625000	2.676512000	-1.438297000

**SCF Done: E(RM062X) = -776.670417725**

**# of imaginary frequencies = 1 (-48.5440)**

**(M)-1'b**

C	0.781786000	0.076705000	-0.499406000
C	1.296166000	-0.889771000	0.388310000
C	2.661506000	-1.008848000	0.618457000
C	3.561005000	-0.165055000	-0.030914000
C	3.063568000	0.787617000	-0.903341000
C	1.691810000	0.918105000	-1.144360000
H	3.043063000	-1.754362000	1.302985000
H	3.752545000	1.451695000	-1.413686000
C	-2.980542000	0.516435000	0.292513000
C	-1.478066000	0.705736000	0.508391000
C	-0.717681000	0.187733000	-0.732473000
C	-1.292823000	-1.111928000	-1.257401000
C	-2.452366000	-1.641693000	-0.881923000
C	-3.331901000	-0.958372000	0.133220000
H	-3.285645000	1.049547000	-0.614052000
H	-3.544419000	0.949745000	1.122615000
H	-1.184109000	0.075462000	1.353192000
H	-0.859396000	0.929650000	-1.524147000
H	-3.235299000	-1.479169000	1.094522000
H	-4.379310000	-1.069270000	-0.165051000
O	0.380527000	-1.687974000	1.000568000
C	0.849655000	-2.692171000	1.878435000
H	-0.034251000	-3.214890000	2.234907000
H	1.504046000	-3.396536000	1.359399000
H	1.382985000	-2.258286000	2.727768000
C	5.038673000	-0.304962000	0.222013000
H	5.603548000	0.446966000	-0.327903000
H	5.264839000	-0.193896000	1.284241000
H	5.394222000	-1.290629000	-0.085242000
C	1.236634000	1.990312000	-2.105373000
H	0.586765000	2.717806000	-1.614029000
H	2.096150000	2.525648000	-2.506262000
H	0.679764000	1.570884000	-2.945708000
C	-1.093924000	2.158280000	0.856350000

H	-0.010915000	2.246149000	0.713860000
C	-1.775144000	3.196272000	-0.039019000
H	-1.683821000	2.956011000	-1.100764000
H	-2.840463000	3.269886000	0.193182000
H	-1.333415000	4.182209000	0.119636000
C	-1.382523000	2.468875000	2.325264000
H	-2.448122000	2.366724000	2.546794000
H	-0.833967000	1.792911000	2.984301000
H	-1.092182000	3.492744000	2.570617000
H	-0.683870000	-1.636077000	-1.990870000
C	-2.948822000	-2.955480000	-1.412458000
H	-3.119424000	-3.658008000	-0.590807000
H	-3.907220000	-2.831862000	-1.924710000
H	-2.238384000	-3.404008000	-2.107046000

**SCF Done: E(RM062X) = -815.980035946**

**# of imaginary frequencies = 0**

**(P)-1'b**

C	0.664493000	-0.444737000	-0.214277000
C	1.721343000	0.353345000	-0.699246000
C	3.048359000	0.060859000	-0.414780000
C	3.367642000	-1.044281000	0.372575000
C	2.336790000	-1.828585000	0.858657000
C	0.993894000	-1.548284000	0.578487000
H	3.846760000	0.683986000	-0.794592000
H	2.571259000	-2.686258000	1.480102000
C	-2.952326000	0.826078000	0.301174000
C	-1.459633000	0.697321000	0.611267000
C	-0.765639000	-0.045817000	-0.553787000
C	-1.581333000	-1.215819000	-1.056642000
C	-2.848151000	-1.460546000	-0.736373000
C	-3.610821000	-0.544371000	0.185843000
H	-3.075363000	1.356688000	-0.648581000
H	-3.454998000	1.420548000	1.067761000
H	-1.361831000	0.073900000	1.508159000
H	-0.696948000	0.659876000	-1.385650000
H	-3.687501000	-1.015539000	1.174736000
H	-4.638320000	-0.443280000	-0.177464000
O	1.358561000	1.430113000	-1.453175000
C	2.368360000	2.332606000	-1.859235000
H	1.858221000	3.135381000	-2.385704000
H	2.899088000	2.741470000	-0.995855000
H	3.082719000	1.853313000	-2.532695000
C	4.807850000	-1.356261000	0.681223000
H	4.891240000	-2.240965000	1.311473000
H	5.372382000	-1.536066000	-0.235905000
H	5.284922000	-0.521607000	1.198757000
C	-0.040510000	-2.488380000	1.153874000
H	-0.928542000	-1.971415000	1.511010000
H	-0.375373000	-3.207336000	0.403120000
H	0.391926000	-3.046587000	1.984150000
C	-0.786627000	2.046322000	0.936447000
H	0.294358000	1.874803000	0.929380000
C	-1.091490000	3.139076000	-0.089364000
H	-0.885166000	2.810432000	-1.109095000
H	-2.137799000	3.449716000	-0.030904000
H	-0.475179000	4.019315000	0.106654000
C	-1.158962000	2.525629000	2.340247000
H	-2.230904000	2.721756000	2.422751000
H	-0.891864000	1.782381000	3.094545000

H	-0.637019000	3.454232000	2.581014000
H	-1.065352000	-1.897865000	-1.729167000
C	-3.587736000	-2.666745000	-1.237337000
H	-2.955343000	-3.295136000	-1.864855000
H	-3.947445000	-3.268230000	-0.396514000
H	-4.469438000	-2.372870000	-1.813731000

**SCF Done: E(RM062X) = -815.980286713**

**# of imaginary frequencies = 0**

**TS1-1'b**

C	-2.516957000	3.213461000	-0.811082000
C	-1.309153000	1.519133000	0.533426000
C	-1.867639000	1.872485000	-0.621479000
C	1.658804000	1.334252000	0.656478000
C	3.012277000	1.335769000	0.297566000
C	-0.657730000	0.166436000	0.775160000
C	0.872243000	0.177863000	0.495803000
C	-1.957716000	0.936318000	-1.798338000
C	3.650237000	0.213112000	-0.191330000
C	1.579923000	-0.993911000	0.125739000
C	2.920190000	-0.967421000	-0.244615000
C	-1.351620000	-0.446294000	-1.532972000
C	-1.500220000	-0.844048000	-0.059674000
C	-3.115812000	-1.100347000	1.900645000
C	-2.979000000	-0.923271000	0.387698000
C	-3.678582000	-2.084554000	-0.323497000
H	-2.437834000	3.829021000	0.085383000
H	-3.575752000	3.098941000	-1.062372000
H	-1.359721000	2.220666000	1.356601000
H	-2.052255000	3.751797000	-1.642306000
H	3.578305000	2.252391000	0.421482000
H	-0.769719000	-0.082488000	1.834921000
H	-3.021781000	0.840724000	-2.050657000
H	-1.811382000	-1.184991000	-2.191046000
H	-1.494073000	1.400195000	-2.674834000
H	-2.497163000	-1.933332000	2.249480000
H	-2.817938000	-0.204267000	2.447238000
H	-1.106932000	-1.844444000	0.075285000
H	-0.287242000	-0.435754000	-1.780387000
H	-3.192565000	-3.033544000	-0.077550000
H	-4.152196000	-1.318387000	2.166524000
H	-3.499186000	-0.001878000	0.114184000
H	-3.667141000	-1.971056000	-1.408249000
H	-4.722163000	-2.153030000	-0.009789000
C	5.090383000	0.243742000	-0.625833000
H	5.582255000	1.155493000	-0.287928000
H	5.639275000	-0.612158000	-0.230066000
H	5.165532000	0.205117000	-1.715037000
H	3.416811000	-1.874299000	-0.559220000
C	1.565199000	-3.360764000	-0.228900000
H	1.889673000	-3.296988000	-1.270066000
H	2.424902000	-3.576585000	0.409621000
H	0.831414000	-4.156601000	-0.127267000
O	0.907327000	-2.177209000	0.177521000
C	1.169756000	2.621082000	1.287290000
H	0.561458000	3.217451000	0.607902000
H	0.578145000	2.428684000	2.181992000
H	2.031162000	3.218733000	1.583476000

**SCF Done: E(RM062X) = -815.957921337**

**# of imaginary frequencies = 1 (-44.6101)**

**TS2-1'b**

C	1.972121000	3.251707000	0.957421000
C	1.030137000	1.414484000	-0.413088000
C	1.589585000	1.817194000	0.725414000
C	-1.807120000	0.643698000	-0.498110000
C	-3.119985000	0.453737000	-0.083461000
C	0.660813000	-0.034208000	-0.716304000
C	-0.824267000	-0.373917000	-0.410789000
C	1.954303000	0.865265000	1.834538000
C	-3.546087000	-0.792113000	0.359762000
C	-1.307619000	-1.656560000	-0.092151000
C	-2.639955000	-1.833042000	0.304662000
C	1.554174000	-0.581222000	1.541013000
C	1.702864000	-0.895800000	0.047529000
C	3.251100000	-0.959020000	-1.973287000
C	3.148898000	-0.704259000	-0.467973000
C	4.104006000	-1.643854000	0.272593000
H	1.717172000	3.878560000	0.102631000
H	3.046719000	3.340026000	1.145143000
H	0.855708000	2.149258000	-1.187202000
H	1.464491000	3.649581000	1.840964000
H	-3.830502000	1.267277000	-0.129601000
H	0.793674000	-0.190199000	-1.791335000
H	3.040525000	0.935110000	1.980547000
H	2.144187000	-1.267442000	2.150323000
H	1.511983000	1.205347000	2.776283000
H	2.802527000	-1.923577000	-2.232803000
H	2.752424000	-0.185480000	-2.558215000
H	1.506665000	-1.949214000	-0.105814000
H	0.509336000	-0.736085000	1.823227000
H	3.789790000	-2.685591000	0.153712000
H	4.296934000	-0.982434000	-2.285777000
H	3.473082000	0.321911000	-0.279905000
H	4.152113000	-1.425521000	1.340049000
H	5.115398000	-1.553318000	-0.128159000
C	-4.955901000	-0.992814000	0.845430000
H	-5.672155000	-0.490728000	0.193357000
H	-5.209624000	-2.051768000	0.886748000
H	-5.080325000	-0.578233000	1.848551000
H	-2.970162000	-2.832277000	0.566848000
C	-2.302372000	2.924024000	-1.013595000
H	-2.589908000	3.149239000	0.016031000
H	-1.748984000	3.763628000	-1.427514000
H	-3.198831000	2.751990000	-1.613891000
C	-0.514136000	-2.943123000	-0.197084000
H	0.112772000	-3.121453000	0.678717000
H	0.119690000	-2.962583000	-1.083035000
H	-1.210398000	-3.777496000	-0.272351000
O	-1.424707000	1.817551000	-1.067831000

**SCF Done: E(RM062X) = -815.957351706****# of imaginary frequencies = 1 (-47.3146)****(M)-1'c**

C	2.090887000	-2.882092000	1.285240000
C	2.353529000	-1.375405000	1.271892000
C	1.958480000	-0.809065000	-0.106850000
C	2.367969000	-1.704395000	-1.256813000
C	2.806269000	-2.952250000	-1.125064000
C	2.930942000	-3.596931000	0.232187000



H	2.294498000	-3.297391000	2.274904000
H	1.032781000	-3.064600000	1.071679000
H	3.431413000	-1.228006000	1.400316000
H	0.865833000	-0.789451000	-0.123778000
H	2.282091000	-1.265909000	-2.248161000
H	2.633251000	-4.647141000	0.158467000
H	3.988284000	-3.604413000	0.527063000
C	3.223844000	-3.787161000	-2.299927000
H	2.607717000	-4.687469000	-2.373091000
H	4.258370000	-4.122457000	-2.179330000
H	3.145992000	-3.233943000	-3.235550000
C	1.649308000	-0.618960000	2.417702000
H	1.704301000	0.448290000	2.176805000
C	0.171600000	-0.988666000	2.565909000
H	-0.326400000	-0.300323000	3.252040000
H	0.059664000	-1.997446000	2.970312000
H	-0.362013000	-0.951486000	1.613559000
C	2.375756000	-0.821767000	3.746817000
H	1.890688000	-0.252810000	4.542344000
H	3.415163000	-0.494051000	3.680842000
H	2.369586000	-1.873311000	4.043763000
C	3.169873000	3.338952000	-0.728801000
C	1.837833000	2.988721000	-0.543601000
C	1.508782000	1.665336000	-0.342493000
C	2.433546000	0.621984000	-0.313310000
C	3.781251000	0.984691000	-0.472343000
C	4.114405000	2.323542000	-0.682892000
H	1.050997000	3.733489000	-0.548111000
H	5.161696000	2.577567000	-0.810407000
C	3.560517000	4.769802000	-0.980108000
H	3.285138000	5.071694000	-1.992857000
H	3.050911000	5.441449000	-0.288205000
H	4.635131000	4.908038000	-0.867996000
C	4.919458000	-0.003754000	-0.381775000
H	4.633218000	-1.003176000	-0.698648000
H	5.753001000	0.331610000	-0.998730000
H	5.281930000	-0.068851000	0.647435000
O	0.155602000	1.398698000	-0.074719000
C	-0.589961000	0.923711000	-1.083592000
O	-0.193891000	0.736958000	-2.197928000
C	-4.593062000	-0.013262000	0.133090000
C	-4.155873000	-0.190385000	-1.165568000
C	-2.871441000	0.113028000	-1.571744000
C	-1.983619000	0.625248000	-0.634701000
C	-2.382580000	0.825594000	0.680920000
C	-3.677511000	0.495131000	1.032620000
H	-5.600388000	-0.263381000	0.430143000
H	-2.557723000	-0.045601000	-2.593902000
H	-1.703366000	1.224491000	1.420077000
N	-5.104781000	-0.733480000	-2.155028000
O	-4.705136000	-0.878913000	-3.288390000
O	-6.221765000	-0.998224000	-1.769324000
N	-4.099530000	0.686549000	2.432097000
O	-3.267527000	1.089508000	3.215030000
O	-5.248882000	0.426125000	2.708925000

**SCF Done: E(RM062X) = -1530.02574172**

**# of imaginary frequencies = 0**

**(P)-1'c**

C	-1.102675000	2.880242000	0.961759000
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C	-1.877512000	1.815136000	0.182922000
C	-2.108386000	0.596631000	1.104471000
C	-0.842185000	0.221370000	1.848615000
C	0.236720000	0.993330000	1.953593000
C	0.278621000	2.380027000	1.366211000
H	-1.010323000	3.795099000	0.372111000
H	-1.663946000	3.137779000	1.865400000
H	-1.243418000	1.475780000	-0.644925000
H	-2.846455000	0.894299000	1.855688000
H	-0.832676000	-0.765789000	2.305080000
H	0.730100000	3.058786000	2.096783000
H	0.954623000	2.389849000	0.501680000
C	1.480242000	0.544614000	2.666149000
H	1.651306000	1.145834000	3.563257000
H	2.357446000	0.685237000	2.024624000
H	1.425574000	-0.505897000	2.954334000
C	-3.185357000	2.353842000	-0.430651000
H	-3.797370000	1.487125000	-0.703158000
C	-3.992094000	3.220947000	0.539347000
H	-4.988359000	3.412533000	0.136337000
H	-3.505404000	4.187088000	0.692005000
H	-4.111416000	2.753222000	1.519180000
C	-2.906732000	3.131178000	-1.717146000
H	-3.835473000	3.504489000	-2.153070000
H	-2.413300000	2.499490000	-2.458260000
H	-2.262753000	3.993022000	-1.524630000
C	-3.721550000	-2.810152000	-1.092883000
C	-2.405611000	-2.405265000	-1.263040000
C	-1.927164000	-1.328357000	-0.542834000
C	-2.691190000	-0.596918000	0.360988000
C	-4.024043000	-1.010893000	0.530047000
C	-4.507811000	-2.097743000	-0.193542000
H	-1.742443000	-2.916621000	-1.950582000
H	-5.540562000	-2.397849000	-0.051357000
C	-4.267501000	-3.998299000	-1.837091000
H	-3.816465000	-4.083419000	-2.825680000
H	-4.052788000	-4.921960000	-1.294893000
H	-5.348384000	-3.924655000	-1.953430000
C	-4.957870000	-0.300371000	1.477763000
H	-5.107716000	0.740738000	1.185461000
H	-5.930345000	-0.789784000	1.485223000
H	-4.572284000	-0.301954000	2.499028000
O	-0.605377000	-0.924073000	-0.777909000
C	0.364742000	-1.631518000	-0.176800000
O	0.197522000	-2.644277000	0.439127000
C	4.224025000	0.200943000	-0.530957000
C	4.046391000	-1.039158000	0.051627000
C	2.810768000	-1.647750000	0.156537000
C	1.700935000	-0.989098000	-0.355551000
C	1.833566000	0.256216000	-0.954056000
C	3.092340000	0.824089000	-1.019166000
H	5.197740000	0.662969000	-0.594253000
H	2.703187000	-2.611208000	0.634718000
H	0.977128000	0.781193000	-1.351403000
N	3.232648000	2.160736000	-1.623036000
O	2.213120000	2.750965000	-1.910797000
O	4.353521000	2.585717000	-1.787762000
N	5.229078000	-1.732400000	0.594545000
O	5.054015000	-2.815951000	1.105125000
O	6.298282000	-1.172630000	0.494249000

SCF Done: E(RM062X) = -1530.03361853

# of imaginary frequencies = 0

TS1-1'c

C	4.589915000	-3.592806000	-0.364695000
C	3.206473000	-1.660587000	-1.059317000
C	3.495854000	-2.586928000	-0.149791000
C	3.891883000	1.199149000	-0.492658000
C	4.311696000	2.371354000	0.134514000
C	2.093351000	-0.638241000	-0.895833000
C	2.583142000	0.701171000	-0.284197000
C	2.712124000	-2.745624000	1.126406000
C	3.492359000	3.133420000	0.954121000
C	1.758875000	1.553535000	0.459794000
C	2.180179000	2.715071000	1.080572000
C	1.546418000	-1.759364000	1.261357000
C	0.975921000	-1.383465000	-0.111102000
C	0.109230000	-2.282013000	-2.340187000
C	0.389236000	-2.597211000	-0.870846000
C	-0.913046000	-3.042663000	-0.199274000
H	5.102653000	-3.432976000	-1.313196000
H	4.186686000	-4.609578000	-0.353167000
H	3.764982000	-1.664062000	-1.986501000
H	5.326643000	-3.536412000	0.441552000
H	5.326617000	2.710041000	-0.043818000
H	1.713543000	-0.381334000	-1.889500000
H	2.339634000	-3.777108000	1.148813000
H	0.774255000	-2.182626000	1.905549000
H	3.385733000	-2.663764000	1.984833000
H	-0.480072000	-1.362924000	-2.430848000
H	1.027311000	-2.154877000	-2.915499000
H	0.121104000	-0.740652000	0.046484000
H	1.889800000	-0.847003000	1.754656000
H	-1.676786000	-2.264692000	-0.304115000
H	-0.461017000	-3.091114000	-2.800134000
H	1.095920000	-3.429794000	-0.833761000
H	-0.786175000	-3.248714000	0.864472000
H	-1.298528000	-3.948267000	-0.670630000
C	3.997999000	4.364432000	1.653383000
H	3.194300000	5.082258000	1.816231000
H	4.416014000	4.106714000	2.629193000
H	4.784445000	4.847978000	1.074132000
H	1.455101000	3.284373000	1.649461000
O	0.395111000	1.284105000	0.660305000
C	4.891756000	0.581521000	-1.444809000
H	5.352828000	-0.318356000	-1.039356000
H	4.426607000	0.319391000	-2.394815000
H	5.679890000	1.304428000	-1.650436000
C	-0.421482000	1.467444000	-0.387483000
O	-0.087242000	1.898568000	-1.453366000
C	-1.813831000	1.019271000	-0.077012000
C	-2.109890000	0.331148000	1.093294000
C	-2.797573000	1.246580000	-1.030421000
C	-3.402253000	-0.120586000	1.281303000
H	-1.350705000	0.131996000	1.836434000
C	-4.075360000	0.785548000	-0.781755000
H	-2.561703000	1.767093000	-1.947986000
C	-4.413197000	0.094529000	0.366158000
H	-5.416377000	-0.267156000	0.534663000
N	-5.126540000	1.026815000	-1.787602000

O	-6.235604000	0.604530000	-1.546910000
O	-4.811650000	1.631405000	-2.787897000
N	-3.711368000	-0.887663000	2.501537000
O	-4.868305000	-1.186994000	2.694319000
O	-2.785563000	-1.173492000	3.228626000

**SCF Done: E(RM062X) = -1530.00709290**

**# of imaginary frequencies = 1 (-32.0219)**

**TS2-1'c**

C	-0.294836000	-2.589423000	2.346591000
C	-0.993491000	-1.179330000	0.435249000
C	-1.328047000	-1.985695000	1.438801000
C	-3.689743000	1.461227000	-0.351205000
C	-3.931006000	2.759510000	0.107070000
C	-1.991082000	-0.570823000	-0.546290000
C	-2.414569000	0.873074000	-0.164588000
C	-2.747478000	-2.423725000	1.683292000
C	-2.971918000	3.555787000	0.712085000
C	-1.453439000	1.742384000	0.366686000
C	-1.696716000	3.027120000	0.808252000
O	-0.115257000	1.343997000	0.506329000
C	-3.748454000	-1.781457000	0.721810000
C	-3.135495000	-1.604320000	-0.674792000
C	-1.983667000	-2.727487000	-2.649857000
C	-2.674535000	-2.941307000	-1.301782000
C	-3.870516000	-3.878803000	-1.483476000
C	0.636693000	1.311612000	-0.600432000
O	0.263242000	1.613432000	-1.698038000
C	-4.856988000	0.834013000	-1.086630000
C	-3.292700000	4.931771000	1.225686000
H	-0.321246000	-3.681398000	2.287885000
H	-0.495943000	-2.323784000	3.387979000
H	0.062023000	-1.008160000	0.270795000
H	0.711905000	-2.251988000	2.096950000
H	-4.924179000	3.170667000	-0.035624000
H	-1.491514000	-0.473646000	-1.514831000
H	-2.768678000	-3.516694000	1.583131000
H	-4.665613000	-2.370804000	0.681281000
H	-3.026016000	-2.220727000	2.721620000
H	-2.603501000	-2.111048000	-3.308450000
H	-1.013209000	-2.241006000	-2.545012000
H	-3.891428000	-1.235740000	-1.359365000
H	-4.027819000	-0.798451000	1.108384000
H	-4.635000000	-3.411337000	-2.111468000
H	-1.817007000	-3.684625000	-3.147226000
H	-1.960614000	-3.431171000	-0.635422000
H	-4.331988000	-4.147605000	-0.532661000
H	-3.558467000	-4.803827000	-1.971346000
H	-4.567500000	0.492295000	-2.080157000
H	-5.299227000	-0.005962000	-0.551509000
H	-5.634728000	1.584358000	-1.216051000
H	-2.446375000	5.606137000	1.094549000
H	-4.155195000	5.351606000	0.708869000
H	-3.526512000	4.898357000	2.292218000
H	-0.872165000	3.599556000	1.215636000
C	2.017740000	0.821930000	-0.302177000
C	2.354514000	0.316744000	0.947722000
C	2.952173000	0.846296000	-1.328995000
C	3.636722000	-0.162160000	1.139264000
H	1.634730000	0.286340000	1.753578000

C	4.223144000	0.369752000	-1.074966000
H	2.685072000	1.228693000	-2.304070000
C	4.600325000	-0.144058000	0.150782000
H	5.597540000	-0.519441000	0.324629000
N	3.990542000	-0.726792000	2.454232000
O	5.141211000	-1.059592000	2.627607000
O	3.104477000	-0.824480000	3.275069000
N	5.223204000	0.398642000	-2.158401000
O	6.330280000	-0.022272000	-1.906341000
O	4.871879000	0.841501000	-3.228841000

**SCF Done: E(RM062X) = -1530.00573409**

**# of imaginary frequencies = 1 (-28.6132)**

**(M)-2'a**

C	-2.882543000	0.857294000	-0.184819000
C	-3.556890000	-0.431494000	0.290787000
C	-2.825623000	-1.681480000	-0.203218000
C	-1.351595000	-1.621592000	0.206766000
C	-0.675700000	-0.318313000	-0.258891000
C	-1.419250000	0.928378000	0.276555000
H	-3.571658000	-0.446534000	1.390762000
H	-4.601901000	-0.457875000	-0.039217000
H	-2.930998000	0.906068000	-1.281583000
H	-3.436610000	1.721047000	0.196293000
H	-1.281413000	-1.710738000	1.299446000
H	-0.812586000	-2.481340000	-0.210862000
H	-0.856966000	-0.263704000	-1.341851000
H	-1.446781000	0.880083000	1.372296000
H	-2.865269000	-1.680110000	-1.303525000
C	0.833847000	-0.344235000	-0.052204000
C	1.667105000	-0.625097000	-1.152382000
C	1.468008000	-0.137088000	1.191770000
C	3.057008000	-0.648956000	-1.045157000
C	2.861259000	-0.175193000	1.283900000
C	3.674708000	-0.415334000	0.176659000
H	3.636944000	-0.867552000	-1.936982000
H	3.324009000	-0.012278000	2.254363000
C	-0.706602000	2.244168000	-0.099785000
H	0.291971000	2.197612000	0.355482000
C	-0.506742000	2.419187000	-1.608261000
H	0.010724000	3.361678000	-1.811517000
H	0.092490000	1.612726000	-2.042673000
H	-1.466835000	2.452582000	-2.134663000
C	-1.419269000	3.463208000	0.489858000
H	-1.629620000	3.323781000	1.555883000
H	-0.800501000	4.358717000	0.380878000
H	-2.369011000	3.656987000	-0.018988000
C	-3.489397000	-2.958206000	0.304882000
H	-4.534326000	-3.013953000	-0.014888000
H	-2.972079000	-3.848962000	-0.064306000
H	-3.471065000	-2.987992000	1.400193000
C	0.707231000	0.161718000	2.464546000
H	0.374503000	1.205255000	2.493309000
H	-0.176526000	-0.466852000	2.586614000
H	1.354666000	0.001717000	3.329135000
C	5.176853000	-0.410109000	0.298066000
H	5.492344000	-0.705719000	1.301344000
H	5.634898000	-1.090224000	-0.423897000
H	5.577985000	0.590821000	0.107815000
O	1.187848000	-0.870175000	-2.411963000

H 0.256388000 -1.114979000 -2.377585000  
**SCF Done: E(RM062X) = -777.707675605**  
**# of imaginary frequencies = 0**

**(P)-2'a**

C	2.887716000	0.831953000	0.230557000
C	3.550386000	-0.445596000	-0.291431000
C	2.791022000	-1.709051000	0.119925000
C	1.320244000	-1.599726000	-0.291482000
C	0.667535000	-0.311587000	0.246650000
C	1.434119000	0.941493000	-0.253663000
H	3.590941000	-0.404486000	-1.390170000
H	4.587104000	-0.506050000	0.059062000
H	2.914098000	0.835229000	1.328791000
H	3.461574000	1.701172000	-0.105335000
H	1.251929000	-1.633589000	-1.391029000
H	0.762870000	-2.470293000	0.075194000
H	0.839269000	-0.321403000	1.329124000
H	1.504127000	0.932686000	-1.353189000
H	2.817630000	-1.774588000	1.218459000
C	-0.842803000	-0.325207000	0.056140000
C	-1.450245000	-0.047105000	-1.178154000
C	-1.689803000	-0.688381000	1.124326000
C	-2.835850000	-0.050080000	-1.334850000
C	-3.074936000	-0.696441000	0.953222000
C	-3.667451000	-0.363712000	-0.265984000
H	-3.242542000	0.184047000	-2.314440000
H	-3.707584000	-0.975988000	1.792059000
C	0.737126000	2.267652000	0.111947000
H	-0.230830000	2.257365000	-0.406677000
C	0.456666000	2.412520000	1.609153000
H	0.010811000	3.389930000	1.816866000
H	-0.241648000	1.649445000	1.963845000
H	1.377969000	2.338786000	2.197168000
C	1.517963000	3.478848000	-0.403858000
H	1.806163000	3.352556000	-1.452870000
H	0.910183000	4.384887000	-0.326072000
H	2.429463000	3.644437000	0.179359000
C	3.437947000	-2.964346000	-0.458339000
H	4.479218000	-3.056097000	-0.135090000
H	2.903273000	-3.866450000	-0.145993000
H	3.427991000	-2.929047000	-1.553599000
C	-1.128788000	-1.101160000	2.466716000
H	-0.413341000	-1.923854000	2.367967000
H	-0.606101000	-0.280045000	2.968764000
H	-1.933170000	-1.432820000	3.125674000
C	-5.166605000	-0.337074000	-0.419534000
H	-5.645655000	-1.040265000	0.265722000
H	-5.561811000	0.659836000	-0.198252000
H	-5.464823000	-0.589553000	-1.439801000
O	-0.735593000	0.260158000	-2.303590000
H	0.192178000	0.034883000	-2.174861000

**SCF Done: E(RM062X) = -777.709208926**  
**# of imaginary frequencies = 0**

**TS1-2'a**

C	0.434442000	2.930328000	-1.143835000
C	1.860123000	0.571085000	0.944496000
C	3.164585000	0.236952000	0.579076000
C	-0.710611000	0.272892000	0.704061000

C	0.753527000	-0.163117000	0.455714000
C	-1.599101000	1.557148000	-1.750533000
C	3.456175000	-0.858238000	-0.220862000
C	1.094551000	-1.378672000	-0.176038000
C	2.399213000	-1.686316000	-0.554433000
O	0.137922000	-2.339751000	-0.376147000
C	-2.581383000	0.603520000	-1.080914000
C	-1.784470000	-0.401407000	-0.232310000
C	-3.457927000	-2.308499000	-0.369689000
C	-2.666558000	-1.386231000	0.556906000
C	-3.609247000	-0.693225000	1.542943000
H	1.124329000	2.085918000	-1.209207000
H	0.380557000	3.396120000	-2.131352000
H	0.855102000	3.664051000	-0.452644000
H	3.979201000	0.844444000	0.958984000
H	-0.938675000	-0.045283000	1.729425000
H	-2.075718000	2.154182000	-2.531443000
H	-0.819521000	0.960056000	-2.240286000
H	-3.312555000	1.170972000	-0.498137000
H	-3.144229000	0.047890000	-1.834046000
H	-1.261859000	-0.987673000	-0.979049000
H	-3.978469000	-3.078621000	0.203989000
H	-4.212214000	-1.753347000	-0.932595000
H	-2.796001000	-2.803762000	-1.084067000
H	-1.978072000	-2.014464000	1.131755000
H	-4.115908000	-1.431184000	2.168583000
H	-3.079541000	-0.004772000	2.205547000
H	-4.379445000	-0.125673000	1.015106000
C	1.753878000	1.684749000	1.965383000
H	1.611133000	2.664919000	1.509259000
H	0.941344000	1.513953000	2.670510000
H	2.683208000	1.723936000	2.532931000
C	4.859738000	-1.160419000	-0.668636000
H	5.053725000	-0.716079000	-1.647817000
H	5.589837000	-0.751940000	0.030137000
H	5.024019000	-2.234702000	-0.756187000
H	2.581588000	-2.613988000	-1.089261000
C	-0.953480000	2.472737000	-0.701071000
H	-1.578213000	3.368387000	-0.611630000
C	-0.986402000	1.797087000	0.680751000
H	-0.368773000	2.357037000	1.370835000
H	-2.002630000	1.897013000	1.071322000
H	0.552079000	-3.111642000	-0.777539000

**SCF Done: E(RM062X) = -777.881463891**

**# of imaginary frequencies = 1 (-34.3513)**

**TS2-2'a**

C	1.787548000	0.513889000	1.002699000
C	3.124849000	0.288124000	0.708761000
C	-0.724501000	0.220372000	0.689913000
C	0.732859000	-0.240862000	0.441528000
C	-1.352809000	1.399980000	-1.835800000
C	3.502395000	-0.772243000	-0.100172000
C	1.144323000	-1.415466000	-0.229996000
C	2.498937000	-1.631248000	-0.513662000
C	-2.455599000	0.542288000	-1.225506000
C	-1.827116000	-0.435162000	-0.213136000
C	-3.801951000	-2.026955000	-0.258341000
C	-2.864900000	-1.204613000	0.626506000
C	-3.678836000	-0.316225000	1.569743000

H	3.875956000	0.943612000	1.140076000
H	-0.943457000	-0.063502000	1.726501000
H	-1.701816000	1.948169000	-2.713952000
H	-0.545134000	0.738090000	-2.174439000
H	-3.214190000	1.187065000	-0.771706000
H	-2.961256000	-0.038882000	-1.999206000
H	-1.357074000	-1.163811000	-0.857064000
H	-4.428672000	-2.683254000	0.348798000
H	-4.464940000	-1.378593000	-0.835992000
H	-3.239149000	-2.646853000	-0.961279000
H	-2.299043000	-1.906635000	1.251786000
H	-4.355381000	-0.928061000	2.170159000
H	-3.044968000	0.246840000	2.257165000
H	-4.289648000	0.396592000	1.010647000
C	4.943141000	-0.996514000	-0.469011000
H	5.237694000	-0.334936000	-1.287024000
H	5.602923000	-0.787890000	0.374075000
H	5.108768000	-2.023338000	-0.794215000
H	2.770920000	-2.530999000	-1.055109000
C	-0.807064000	2.369843000	-0.780054000
C	-0.959417000	1.752494000	0.620734000
H	-0.354638000	2.298697000	1.333444000
H	-1.997326000	1.889842000	0.934793000
O	1.485829000	1.495844000	1.906436000
H	2.304632000	1.902700000	2.210858000
C	0.256150000	-2.593305000	-0.598505000
H	0.864877000	-3.496798000	-0.576051000
H	-0.562678000	-2.734714000	0.104005000
H	-0.162834000	-2.516167000	-1.603842000
H	-1.442767000	3.262596000	-0.790406000
C	0.613362000	2.820134000	-1.114921000
H	0.998385000	3.512531000	-0.362881000
H	1.293894000	1.968042000	-1.171202000
H	0.632054000	3.325717000	-2.084097000

**SCF Done: E(RM062X) = -777.882136789**

**# of imaginary frequencies = 1 (-45.5810)**

**(M)-2<sup>b</sup>**

C	3.017043000	0.666937000	0.436139000
C	3.651870000	-0.497954000	-0.325832000
C	2.808592000	-1.771528000	-0.237064000
C	1.379780000	-1.487381000	-0.708390000
C	0.748087000	-0.307378000	0.053143000
C	1.603810000	0.972121000	-0.082224000
H	3.757667000	-0.221508000	-1.385771000
H	4.662956000	-0.693614000	0.050969000
H	2.973524000	0.415764000	1.505003000
H	3.652674000	1.554091000	0.343751000
H	1.397777000	-1.283567000	-1.788473000
H	0.757202000	-2.379683000	-0.567819000
H	0.806520000	-0.582978000	1.111091000
H	1.719807000	1.213880000	-1.146868000
H	2.756047000	-2.064172000	0.822920000
C	-0.735255000	-0.165971000	-0.262310000
C	-1.663544000	-0.662101000	0.683949000
C	-1.253231000	0.378690000	-1.447321000
C	-3.037878000	-0.601926000	0.469887000
C	-2.639588000	0.428574000	-1.650822000
C	-3.540567000	-0.050822000	-0.710769000
H	-3.732447000	-0.984529000	1.209089000



H	-3.016306000	0.855223000	-2.577360000
C	0.945663000	2.196799000	0.585423000
H	-0.023016000	2.338208000	0.086377000
C	0.658179000	1.994088000	2.075556000
H	0.164401000	2.879295000	2.488521000
H	0.007171000	1.132239000	2.252628000
H	1.585054000	1.842806000	2.640044000
C	1.761486000	3.472130000	0.365005000
H	2.026723000	3.597628000	-0.690727000
H	1.191396000	4.352343000	0.677230000
H	2.689411000	3.460300000	0.946187000
C	3.437060000	-2.916208000	-1.026366000
H	4.444105000	-3.142520000	-0.662380000
H	2.835389000	-3.827366000	-0.952319000
H	3.515439000	-2.651239000	-2.087073000
C	-0.380744000	0.958802000	-2.537875000
H	-0.001213000	1.948220000	-2.258627000
H	0.482706000	0.331065000	-2.765139000
H	-0.960842000	1.077246000	-3.455669000
C	-5.028426000	0.003404000	-0.945838000
H	-5.260747000	0.510054000	-1.884903000
H	-5.455719000	-1.003322000	-0.989023000
H	-5.535389000	0.536398000	-0.135963000
O	-1.130261000	-1.203707000	1.820166000
C	-2.016561000	-1.653136000	2.825631000
H	-1.390226000	-2.008619000	3.643137000
H	-2.657102000	-0.839510000	3.183981000
H	-2.645527000	-2.475309000	2.466323000

**SCF Done: E(RM062X) = -816.989064783**

**# of imaginary frequencies = 0**

**(P)-2'b**

C	-2.974811000	0.722957000	-0.400900000
C	-3.590957000	-0.439441000	0.381985000
C	-2.837498000	-1.753700000	0.163101000
C	-1.346576000	-1.563367000	0.453115000
C	-0.748558000	-0.402479000	-0.361495000
C	-1.496263000	0.912365000	-0.032787000
H	-3.566649000	-0.198962000	1.455355000
H	-4.646229000	-0.566927000	0.111866000
H	-3.074313000	0.528753000	-1.478375000
H	-3.537099000	1.638925000	-0.190504000
H	-1.199794000	-1.357944000	1.523047000
H	-0.804142000	-2.490839000	0.228284000
H	-0.981065000	-0.613095000	-1.413142000
H	-1.461324000	1.058301000	1.053289000
H	-2.934696000	-2.021526000	-0.900900000
C	0.767302000	-0.386300000	-0.252273000
C	1.425879000	0.097984000	0.897021000
C	1.559319000	-0.938378000	-1.269945000
C	2.814877000	0.087822000	1.002158000
C	2.955141000	-0.949575000	-1.151230000
C	3.595545000	-0.434278000	-0.032411000
H	3.305914000	0.474345000	1.888208000
H	3.548699000	-1.379647000	-1.954295000
C	-0.838291000	2.155760000	-0.661388000
H	0.168382000	2.218532000	-0.225900000
C	-0.677339000	2.060415000	-2.180021000
H	-0.239536000	2.982049000	-2.576227000
H	-0.019015000	1.234150000	-2.463599000

H	-1.644563000	1.916231000	-2.674404000
C	-1.577824000	3.442050000	-0.285857000
H	-1.772801000	3.489055000	0.790874000
H	-0.986499000	4.320177000	-0.562527000
H	-2.538444000	3.517844000	-0.805932000
C	-3.428931000	-2.882018000	1.003049000
H	-4.488663000	-3.033163000	0.774791000
H	-2.904804000	-3.826367000	0.826353000
H	-3.345848000	-2.646429000	2.070228000
C	0.942257000	-1.563865000	-2.501072000
H	0.234543000	-2.356317000	-2.236925000
H	0.395161000	-0.834659000	-3.107781000
H	1.718434000	-2.003373000	-3.130505000
C	5.098714000	-0.431178000	0.080793000
H	5.555635000	-1.012779000	-0.722747000
H	5.493870000	0.588196000	0.024634000
H	5.423583000	-0.853037000	1.036276000
O	0.619677000	0.566324000	1.893252000
C	1.230133000	1.096118000	3.053107000
H	0.416196000	1.416489000	3.702679000
H	1.830851000	0.339209000	3.569744000
H	1.864094000	1.956870000	2.812406000

**SCF Done: E(RM062X) = -816.990531217**

**# of imaginary frequencies = 0**

### TS1-2'b

C	-0.407176000	-2.965151000	-1.369028000
C	-1.812005000	-0.873697000	0.966371000
C	-3.123813000	-0.547817000	0.604603000
C	0.745787000	-0.522957000	0.726363000
C	-0.727293000	-0.083911000	0.538235000
C	1.676317000	-1.611106000	-1.833387000
C	-3.427617000	0.584077000	-0.128159000
C	-1.088019000	1.181441000	0.003273000
C	-2.392378000	1.475833000	-0.383300000
O	-0.121344000	2.141373000	-0.049783000
C	2.628761000	-0.700143000	-1.068403000
C	1.799362000	0.232847000	-0.170996000
C	3.376366000	2.225810000	-0.197228000
C	2.655888000	1.196198000	0.672090000
C	3.656165000	0.470728000	1.574335000
H	-1.062169000	-2.091569000	-1.395498000
H	-0.348702000	-3.371062000	-2.382415000
H	-0.871896000	-3.721995000	-0.733003000
H	-3.926432000	-1.202024000	0.928752000
H	0.995306000	-0.292605000	1.770242000
H	2.186459000	-2.157885000	-2.629759000
H	0.917620000	-0.983770000	-2.317524000
H	3.350959000	-1.300322000	-0.508230000
H	3.205138000	-0.086276000	-1.764230000
H	1.256619000	0.841874000	-0.886661000
H	3.879262000	2.972115000	0.421975000
H	4.136803000	1.754326000	-0.824382000
H	2.671319000	2.744121000	-0.851607000
H	1.957233000	1.743008000	1.312613000
H	4.129084000	1.173474000	2.263649000
H	3.178216000	-0.310093000	2.171181000
H	4.448891000	0.004256000	0.984653000
C	-1.691500000	-2.048989000	1.914961000
H	-1.578127000	-3.002795000	1.397853000

H	-0.858932000	-1.932366000	2.607136000
H	-2.606558000	-2.108864000	2.504169000
C	-4.829176000	0.880294000	-0.587695000
H	-5.557613000	0.296027000	-0.025761000
H	-5.067769000	1.938282000	-0.471157000
H	-4.947005000	0.632993000	-1.645458000
H	-2.620900000	2.421650000	-0.853799000
C	0.987210000	-2.590713000	-0.870734000
H	1.581515000	-3.510770000	-0.847626000
C	1.018018000	-2.039293000	0.564969000
H	0.392685000	-2.656989000	1.195876000
H	2.031020000	-2.182438000	0.950370000
C	-0.442903000	3.408887000	-0.589713000
H	-0.750981000	3.329979000	-1.634900000
H	-1.231281000	3.897438000	-0.012803000
H	0.469013000	3.997258000	-0.524731000

**SCF Done: E(RM062X) = -817.168113380**

**# of imaginary frequencies = 1 (-44.0785)**

### TS2-2'b

C	2.012622000	1.334596000	1.754463000
C	1.073220000	1.637630000	-0.585809000
C	1.904532000	-0.580522000	0.098651000
C	1.753211000	-0.158888000	1.567983000
C	0.792568000	0.114970000	-0.744696000
C	1.096072000	2.180418000	0.858033000
H	-0.950067000	2.927413000	0.864088000
H	-0.765506000	1.375656000	1.683203000
H	-3.873865000	0.780906000	-0.266924000
H	0.967643000	-0.120811000	-1.799638000
H	3.059234000	1.549589000	1.519686000
H	1.865894000	1.617578000	2.800777000
H	0.735861000	-0.401905000	1.892397000
H	3.049299000	-1.779896000	-2.073485000
H	-0.189654000	2.852066000	2.457914000
C	-0.645037000	-0.392237000	-0.444391000
C	-3.289326000	-1.179683000	0.339617000
C	-3.049466000	0.087845000	-0.177197000
C	-1.777113000	0.450813000	-0.603161000
H	2.420831000	-0.742221000	2.204562000
C	3.337760000	-0.363903000	-0.451202000
H	1.787946000	-1.653876000	0.056572000
C	4.346179000	-1.169210000	0.373139000
H	2.900348000	-0.092888000	-2.581729000
H	4.488663000	-0.769146000	-2.242737000
H	3.628605000	0.685444000	-0.374811000
C	-0.285890000	2.338439000	1.498276000
H	4.066811000	-2.227216000	0.397573000
H	5.342468000	-1.096068000	-0.067010000
H	4.413657000	-0.813934000	1.401859000
C	3.444874000	-0.770279000	-1.922772000
H	1.526429000	3.185723000	0.795125000
H	0.407162000	2.241243000	-1.188522000
H	2.071214000	1.792843000	-1.003181000
C	-0.948079000	-1.722596000	-0.087751000
C	-2.240602000	-2.076731000	0.324262000
O	-1.584252000	1.637513000	-1.240703000
C	-2.659082000	2.551685000	-1.332169000
H	-2.255267000	3.436368000	-1.818790000
H	-3.475744000	2.146955000	-1.934122000

H	-3.035762000	2.821510000	-0.342307000
C	-0.002031000	-2.903950000	-0.198929000
H	-0.595968000	-3.806102000	-0.342335000
H	0.669089000	-2.813974000	-1.052049000
H	0.599180000	-3.054154000	0.699815000
C	-4.654273000	-1.558656000	0.845786000
H	-4.834184000	-1.122143000	1.831073000
H	-5.436967000	-1.192886000	0.179593000
H	-4.752905000	-2.640189000	0.935707000
H	-2.421270000	-3.104433000	0.620526000

**SCF Done: E(RM062X) = -817.172027096**

**# of imaginary frequencies = 1 (-51.3152)**

**(M)-2'c**

C	-1.765007000	1.570090000	-0.538700000
C	-2.490173000	0.578709000	0.123080000
C	-3.660179000	2.992146000	-0.844618000
C	-2.305797000	2.745789000	-1.020834000
H	-1.662572000	3.453605000	-1.529883000
C	-3.864555000	0.832735000	0.291049000
C	-4.411500000	2.021780000	-0.189856000
O	-0.402551000	1.352070000	-0.807326000
C	-1.349792000	-3.111677000	0.637111000
C	-2.339117000	-2.022158000	0.201848000
C	-1.762405000	-0.655152000	0.631490000
C	-1.539556000	-0.607462000	2.153805000
C	-0.576847000	-1.706138000	2.604638000
C	-1.091011000	-3.069200000	2.143256000
H	-0.399605000	-2.980179000	0.107005000
H	-1.734353000	-4.096060000	0.363077000
H	-3.262213000	-2.206083000	0.760715000
H	-0.762933000	-0.629838000	0.188160000
H	-2.025623000	-3.286702000	2.675730000
H	-0.377864000	-3.849042000	2.424733000
H	-1.146290000	0.372561000	2.435612000
C	-2.701833000	-2.073528000	-1.294978000
H	-3.454169000	-1.294402000	-1.461658000
C	-0.365466000	-1.669228000	4.113631000
H	0.341043000	-2.439142000	4.430822000
H	0.020256000	-0.699328000	4.434809000
H	-1.310968000	-1.845032000	4.634270000
C	-1.522660000	-1.765416000	-2.220187000
H	-1.840528000	-1.820647000	-3.263354000
H	-0.711770000	-2.485610000	-2.085055000
H	-1.123907000	-0.763392000	-2.050409000
C	-3.342259000	-3.408518000	-1.675946000
H	-2.607468000	-4.216532000	-1.677848000
H	-3.771243000	-3.352795000	-2.678207000
H	-4.140301000	-3.678144000	-0.979415000
H	-2.490728000	-0.734514000	2.681691000
H	0.388501000	-1.524551000	2.112329000
C	0.470113000	1.606211000	0.177238000
O	0.204981000	2.179268000	1.196499000
C	4.369491000	0.000288000	-0.599343000
C	4.111471000	0.821195000	0.482210000
C	2.863281000	1.353844000	0.738762000
C	1.824721000	1.058990000	-0.135202000
C	2.038159000	0.238404000	-1.235521000
C	3.307078000	-0.272469000	-1.437852000
H	5.352235000	-0.410083000	-0.777604000

H	2.692702000	1.983839000	1.600547000
H	1.237181000	-0.005571000	-1.918472000
N	5.218974000	1.131339000	1.403695000
O	4.975980000	1.849208000	2.349142000
O	6.303578000	0.648997000	1.158765000
N	3.537027000	-1.154990000	-2.595430000
O	4.661695000	-1.572503000	-2.767388000
O	2.586204000	-1.409621000	-3.302550000
C	-4.804728000	-0.152397000	0.941673000
H	-5.034615000	-0.977460000	0.262726000
H	-4.394542000	-0.582600000	1.852986000
H	-5.743334000	0.340126000	1.192076000
C	-4.284793000	4.275002000	-1.321261000
H	-5.338032000	4.131646000	-1.561480000
H	-4.222198000	5.042585000	-0.546463000
H	-3.773837000	4.655268000	-2.205684000
H	-5.473751000	2.193230000	-0.049693000

**SCF Done: E(RM062X) = -1531.27128360**

**# of imaginary frequencies = 0**

**(P)-2'c**

C	2.002863000	-1.091576000	-0.870897000
C	2.810394000	-0.157216000	-0.230112000
C	3.842808000	-2.498450000	-1.467617000
C	2.480235000	-2.238257000	-1.478367000
H	1.784014000	-2.914790000	-1.958334000
C	4.194764000	-0.408049000	-0.257151000
C	4.678174000	-1.564805000	-0.861703000
O	0.634359000	-0.803830000	-0.971485000
C	0.765890000	2.295278000	2.009240000
C	1.068674000	0.933824000	1.373473000
C	2.256105000	1.108664000	0.398730000
C	1.904933000	2.140300000	-0.687694000
C	1.505000000	3.493399000	-0.098820000
C	0.394498000	3.318918000	0.936588000
H	1.640122000	2.652414000	2.564397000
H	-0.052617000	2.201559000	2.726132000
H	0.179693000	0.686952000	0.786904000
H	3.064323000	1.545328000	0.990965000
H	-0.516409000	2.986341000	0.420243000
H	0.162495000	4.284692000	1.393667000
H	2.759110000	2.268617000	-1.359914000
C	1.264656000	-0.211685000	2.383081000
H	1.487120000	-1.112328000	1.801537000
C	1.088861000	4.464777000	-1.197675000
H	1.886092000	4.598713000	-1.931686000
H	0.839159000	5.443675000	-0.783370000
H	0.206434000	4.085777000	-1.720988000
C	2.437820000	0.014758000	3.335487000
H	2.553165000	-0.841608000	4.002602000
H	3.378034000	0.141158000	2.795675000
H	2.278387000	0.899492000	3.956224000
C	-0.016830000	-0.495569000	3.167176000
H	-0.244662000	0.309450000	3.869088000
H	0.085697000	-1.416547000	3.744120000
H	-0.874598000	-0.611355000	2.498512000
H	1.081306000	1.751833000	-1.299176000
H	2.383123000	3.901785000	0.417888000
C	-0.249254000	-1.610488000	-0.365605000
O	0.016232000	-2.637174000	0.191723000

C	-4.230721000	-0.016025000	-0.438718000
C	-3.948421000	-1.274329000	0.057046000
C	-2.673730000	-1.805525000	0.074774000
C	-1.631675000	-1.045478000	-0.439902000
C	-1.871801000	0.222795000	-0.953636000
C	-3.164659000	0.708706000	-0.932790000
H	-5.233861000	0.382770000	-0.433365000
H	-2.485659000	-2.787877000	0.484593000
H	-1.072646000	0.828520000	-1.355314000
N	-5.059414000	-2.076534000	0.600255000
O	-4.794382000	-3.175936000	1.032784000
O	-6.165981000	-1.584855000	0.578940000
N	-3.414600000	2.065327000	-1.450489000
O	-2.452456000	2.716567000	-1.797880000
O	-4.562833000	2.445109000	-1.493168000
H	5.749102000	-1.738370000	-0.871010000
C	5.183240000	0.572727000	0.325114000
H	5.058208000	1.566921000	-0.108711000
H	5.070645000	0.675132000	1.406216000
H	6.201303000	0.242592000	0.125906000
C	4.396696000	-3.754144000	-2.084460000
H	5.398424000	-3.586551000	-2.479686000
H	4.463700000	-4.550231000	-1.339405000
H	3.758260000	-4.109962000	-2.892753000

**SCF Done: E(RM062X) = -1531.25463795**

**# of imaginary frequencies = 0**

#### TS1-2'c

C	-2.995736000	3.361105000	-0.054681000
C	-2.896426000	1.454943000	-1.704493000
C	-1.012841000	1.780167000	-0.100915000
C	-1.993497000	2.570847000	0.777433000
C	-1.803803000	0.686647000	-0.906658000
C	-3.823428000	2.422219000	-0.938443000
H	-5.565153000	1.124744000	-0.755684000
H	-4.569200000	1.163166000	0.695521000
H	-0.845099000	-2.113744000	2.686695000
H	-1.134133000	0.262159000	-1.660660000
H	-2.460909000	4.080637000	-0.682118000
H	-3.659744000	3.940577000	0.592248000
H	-2.524419000	1.863980000	1.424014000
H	1.737904000	1.614605000	-0.868607000
H	-5.586309000	2.547272000	0.291111000
C	-2.205771000	-0.500901000	0.000106000
C	-2.912334000	-2.265610000	2.148892000
C	-1.629572000	-1.847430000	1.990467000
C	-1.299632000	-1.012101000	0.905746000
H	-1.441097000	3.232610000	1.446093000
C	-0.137973000	2.681190000	-1.007623000
H	-0.307693000	1.309166000	0.578218000
C	0.454895000	3.853057000	-0.220130000
H	0.694286000	0.993819000	-2.157987000
H	1.545742000	2.520022000	-2.364237000
H	-0.740902000	3.102144000	-1.814986000
C	-4.946274000	1.768620000	-0.130567000
H	0.978281000	3.487660000	0.669284000
H	1.178417000	4.391318000	-0.835412000
H	-0.303739000	4.566265000	0.102622000
C	1.016290000	1.898808000	-1.639403000
H	-4.311239000	3.028068000	-1.709031000

H	-3.490705000	0.809880000	-2.339651000
H	-2.334568000	2.068891000	-2.411898000
O	0.070583000	-0.712262000	0.861589000
C	0.789598000	-1.204554000	-0.157219000
O	0.341268000	-1.804299000	-1.093426000
C	2.244172000	-0.906747000	0.012491000
C	2.726131000	-0.226946000	1.124055000
C	3.106143000	-1.306395000	-1.000224000
C	4.080471000	0.042859000	1.192026000
H	2.065980000	0.094479000	1.916625000
C	4.449684000	-1.010322000	-0.877478000
H	2.728033000	-1.830718000	-1.866679000
C	4.972779000	-0.333202000	0.207436000
H	6.026341000	-0.108688000	0.281502000
H	-3.205698000	-2.865680000	3.001226000
C	-3.479061000	-1.190778000	0.008018000
C	-3.851596000	-1.995222000	1.126316000
C	-5.131764000	-2.602253000	1.176557000
C	-5.987679000	-2.533081000	0.114868000
C	-5.565667000	-1.877510000	-1.058565000
C	-4.363345000	-1.224859000	-1.104459000
H	-5.396546000	-3.162861000	2.065626000
H	-6.955245000	-3.016850000	0.152838000
H	-6.192910000	-1.896563000	-1.941077000
H	-4.065379000	-0.786829000	-2.039129000
N	4.598740000	0.771484000	2.363642000
O	5.790005000	0.990270000	2.405699000
O	3.800952000	1.107651000	3.211652000
N	5.369853000	-1.427470000	-1.950574000
O	6.544042000	-1.157869000	-1.818134000
O	4.894772000	-2.013856000	-2.898536000

**SCF Done: E(RM062X) = -1606.24378457**

**# of imaginary frequencies = 1 (-38.7279)**

### TS2-2'c

C	-2.750855000	-1.556969000	2.598872000
C	-1.041305000	-1.286077000	0.746445000
C	-3.425777000	-1.528107000	0.157487000
C	-3.789570000	-1.089480000	1.583500000
C	-2.110327000	-0.813200000	-0.280073000
C	-1.351661000	-1.038660000	2.238456000
H	-0.198193000	0.801134000	2.451889000
H	-1.929029000	1.074193000	2.259083000
H	-0.529968000	3.618807000	-0.078480000
H	-1.806163000	-1.212215000	-1.253118000
H	-2.744275000	-2.650232000	2.632560000
H	-3.019270000	-1.216965000	3.602661000
H	-3.860430000	0.003228000	1.600386000
H	-3.681240000	-2.954745000	-2.165415000
H	-1.300722000	0.460421000	3.787226000
C	-2.274753000	0.707904000	-0.510000000
C	-2.601994000	3.564666000	-0.684011000
C	-1.390210000	3.004752000	-0.316216000
C	-1.247445000	1.630840000	-0.272040000
H	-4.779737000	-1.459290000	1.853521000
C	-3.382661000	-3.067482000	-0.016234000
H	-4.241235000	-1.226345000	-0.484799000
C	-4.734471000	-3.679696000	0.360697000
H	-1.994602000	-3.223921000	-1.706918000
H	-3.155301000	-4.539078000	-1.589727000

H	-2.635611000	-3.510580000	0.645195000
C	-1.184758000	0.410740000	2.702439000
H	-5.541905000	-3.213395000	-0.212219000
H	-4.741593000	-4.748671000	0.140929000
H	-4.958923000	-3.559763000	1.420844000
C	-3.027057000	-3.464122000	-1.450950000
H	-0.618970000	-1.630950000	2.796113000
H	-0.041349000	-0.927776000	0.532571000
H	-0.974648000	-2.367630000	0.609454000
O	0.065663000	1.230297000	0.024984000
C	0.768565000	0.680687000	-0.975281000
O	0.342327000	0.448739000	-2.070733000
C	2.166752000	0.364411000	-0.552168000
C	2.629149000	0.656051000	0.724556000
C	2.998892000	-0.246354000	-1.481576000
C	3.932042000	0.322727000	1.043821000
H	1.996454000	1.135071000	1.456973000
C	4.291475000	-0.554570000	-1.107580000
H	2.636633000	-0.473647000	-2.474047000
C	4.792283000	-0.284100000	0.151171000
H	5.806260000	-0.535246000	0.423110000
C	-3.439559000	1.294351000	-1.066107000
C	-3.585596000	2.682156000	-1.101768000
N	4.428094000	0.625846000	2.398144000
O	5.572669000	0.324640000	2.654658000
O	3.659002000	1.156203000	3.168894000
N	5.180240000	-1.201260000	-2.089559000
O	6.307128000	-1.466605000	-1.733721000
O	4.727021000	-1.425687000	-3.189750000
C	-2.816272000	5.052351000	-0.682312000
H	-3.562118000	5.341435000	-1.422420000
H	-3.171277000	5.386783000	0.295195000
H	-1.888533000	5.583320000	-0.895534000
C	-4.543422000	0.533946000	-1.775563000
H	-4.169459000	-0.360944000	-2.270659000
H	-5.359409000	0.246864000	-1.110146000
H	-4.966102000	1.181860000	-2.542630000
H	-4.506881000	3.084881000	-1.509769000

**SCF Done: E(RM062X) = -1531.22058429**

**# of imaginary frequencies = 1 (-35.9157)**

**(M)-3'b**

C	1.351617000	-0.921179000	0.360253000
C	0.897026000	0.120850000	-0.470601000
C	3.650582000	-0.294101000	-0.008727000
C	2.705589000	-1.125969000	0.591635000
H	3.043118000	-1.928260000	1.234003000
C	1.848954000	0.941714000	-1.077473000
C	3.210138000	0.725384000	-0.836882000
C	-2.792112000	0.681655000	0.536286000
C	-1.275546000	0.872573000	0.605945000
C	-0.593887000	0.317560000	-0.670103000
C	-1.239734000	-0.959988000	-1.190205000
C	-2.473047000	-1.522119000	-0.637116000
C	-3.155317000	-0.798578000	0.497392000
H	-3.190909000	1.174115000	-0.354032000
H	-3.268563000	1.147568000	1.401685000
H	-0.913555000	0.270497000	1.445625000
H	-0.735129000	1.050897000	-1.467938000



H	-0.560093000	-1.648691000	-1.686818000
H	-2.855707000	-1.282731000	1.432703000
H	-4.237326000	-0.931839000	0.399825000
C	-0.860109000	2.332158000	0.878605000
H	0.216306000	2.398261000	0.685037000
C	-2.745352000	-2.995858000	-0.746920000
H	-3.817320000	-3.178355000	-0.853214000
H	-2.229252000	-3.418381000	-1.609050000
H	-2.402027000	-3.508215000	0.153997000
C	-1.570818000	3.340778000	-0.026575000
H	-1.116972000	4.328521000	0.076777000
H	-1.524742000	3.060856000	-1.081537000
H	-2.625019000	3.430228000	0.246855000
C	-1.072906000	2.706699000	2.345739000
H	-0.738742000	3.729029000	2.534832000
H	-2.129297000	2.650400000	2.619609000
H	-0.515554000	2.039543000	3.006484000
O	0.380731000	-1.705238000	0.905626000
O	-2.485132000	-0.807196000	-1.883907000
C	0.778846000	-2.774409000	1.744506000
H	1.322350000	-2.407587000	2.618044000
H	-0.138586000	-3.260595000	2.065928000
H	1.400528000	-3.489819000	1.201626000
C	5.117130000	-0.518325000	0.248424000
H	5.725995000	0.196573000	-0.303764000
H	5.345686000	-0.413561000	1.310903000
H	5.415109000	-1.525261000	-0.050067000
C	1.449695000	2.065725000	-2.002728000
H	0.817647000	2.799670000	-1.498618000
H	2.334410000	2.581718000	-2.372759000
H	0.891111000	1.694349000	-2.864508000
H	3.937257000	1.373138000	-1.314126000

**SCF Done: E(RM062X) = -891.198181981**

**# of imaginary frequencies = 0**

**(P)-3'b**

C	1.872657000	0.324361000	-0.672127000
C	0.771600000	-0.410676000	-0.188154000
C	3.427638000	-1.192756000	0.376047000
C	3.178404000	-0.057933000	-0.395950000
H	4.014728000	0.516540000	-0.770828000
C	1.029072000	-1.545435000	0.585344000
C	2.351028000	-1.918167000	0.855664000
C	-2.764738000	0.982505000	0.524302000
C	-1.251541000	0.838853000	0.703073000
C	-0.631550000	0.080520000	-0.498721000
C	-1.509850000	-1.041473000	-1.029841000
C	-2.874266000	-1.294243000	-0.549229000
C	-3.447895000	-0.381444000	0.508097000
H	-2.980558000	1.504344000	-0.411077000
H	-3.183652000	1.584181000	1.333325000
H	-1.088545000	0.225329000	1.597369000
H	-0.553995000	0.788035000	-1.326137000
H	-0.972677000	-1.878515000	-1.469583000
H	-3.334420000	-0.870817000	1.481475000
H	-4.522664000	-0.275844000	0.330988000
C	-0.536096000	2.180573000	0.963175000
H	0.539102000	1.984922000	0.902202000
C	-3.463828000	-2.673868000	-0.634625000
H	-4.538599000	-2.616679000	-0.821737000

H	-2.995968000	-3.242188000	-1.438684000
H	-3.311971000	-3.206119000	0.306732000
C	-0.872537000	3.257203000	-0.069038000
H	-0.240876000	4.134594000	0.086018000
H	-0.7111402000	2.910100000	-1.090864000
H	-1.912851000	3.578448000	0.026045000
C	-0.821245000	2.697487000	2.374034000
H	-1.877900000	2.943258000	2.503649000
H	-0.550697000	1.955782000	3.128711000
H	-0.247899000	3.605631000	2.571518000
O	1.572714000	1.426486000	-1.414782000
O	-2.644656000	-0.648059000	-1.809267000
C	2.636749000	2.267138000	-1.821355000
H	2.175602000	3.103130000	-2.340806000
H	3.195453000	2.635970000	-0.957961000
H	3.315851000	1.746859000	-2.500349000
H	2.531733000	-2.798674000	1.462922000
C	-0.068728000	-2.423698000	1.142105000
H	-0.954390000	-1.862460000	1.434337000
H	-0.385782000	-3.167313000	0.406501000
H	0.295066000	-2.963202000	2.016081000
C	4.846127000	-1.599412000	0.674830000
H	5.396301000	-1.796724000	-0.247304000
H	5.374957000	-0.804761000	1.204749000
H	4.875590000	-2.498442000	1.289320000

**SCF Done: E(RM062X) = -891.196942131**

**# of imaginary frequencies = 0**

### TS1-3'b

C	0.789091000	3.537438000	1.028768000
C	1.178236000	1.565014000	-0.610882000
C	1.103119000	2.095490000	0.754607000
C	0.748656000	0.111021000	-0.820996000
C	-0.789738000	-0.026087000	-0.633167000
C	0.737765000	1.089185000	1.825140000
C	-3.547483000	-0.168002000	0.108503000
C	-1.394014000	-1.229209000	-0.185018000
C	-2.722361000	-1.279438000	0.226233000
O	-0.646970000	-2.367476000	-0.223218000
C	1.441591000	-0.264447000	1.624321000
C	1.598061000	-0.750471000	0.153373000
C	3.325627000	-1.010330000	-1.744500000
C	3.092204000	-0.901099000	-0.238587000
C	3.650433000	-2.150753000	0.448780000
O	2.368999000	1.835460000	0.143068000
H	1.350770000	3.888466000	1.897455000
H	-0.274977000	3.655178000	1.246499000
H	1.088084000	2.252055000	-1.438687000
H	1.043889000	4.159068000	0.169542000
H	0.981743000	-0.189556000	-1.845636000
H	1.001530000	1.494078000	2.806372000
H	2.438072000	-0.189933000	2.064880000
H	-0.349708000	0.972238000	1.816991000
H	2.704484000	-1.798946000	-2.181261000
H	3.104260000	-0.076263000	-2.264238000
H	1.214482000	-1.759066000	0.098757000
H	0.903173000	-1.015048000	2.208143000
H	3.182000000	-3.050466000	0.037896000
H	4.369557000	-1.260821000	-1.945555000
H	3.644698000	-0.036211000	0.127264000

H	3.463595000	-2.139291000	1.524692000
H	4.728581000	-2.233059000	0.295979000
H	-3.136158000	-2.198066000	0.617308000
C	-1.682289000	1.029401000	-0.903115000
C	-3.023042000	0.950818000	-0.510173000
C	-1.183773000	-3.563161000	0.312288000
H	-0.394843000	-4.305877000	0.224564000
H	-1.452299000	-3.439507000	1.363690000
H	-2.057641000	-3.893666000	-0.253093000
H	-3.671375000	1.795882000	-0.714950000
C	-1.330461000	2.267377000	-1.704276000
H	-0.894495000	3.061588000	-1.098197000
H	-0.642610000	2.038666000	-2.517534000
H	-2.242671000	2.661833000	-2.150274000
C	-4.969929000	-0.212856000	0.595862000
H	-5.446781000	-1.158127000	0.333200000
H	-5.005877000	-0.119852000	1.683816000
H	-5.555882000	0.601488000	0.170615000

**SCF Done: E(RM062X) = -891.163023834**

**# of imaginary frequencies = 1 (-37.6208)**

### TS2-3'b

C	0.149933000	3.127427000	1.458722000
C	0.892724000	1.483456000	-0.393929000
C	0.777040000	1.835935000	1.021981000
C	-1.752847000	0.376869000	-0.723212000
C	-3.052027000	0.094639000	-0.323939000
C	0.778517000	-0.005330000	-0.748378000
C	-0.671788000	-0.515002000	-0.508961000
C	0.715937000	0.669180000	1.985575000
C	-3.360740000	-1.141335000	0.232323000
C	1.698151000	-0.452468000	1.603486000
C	1.850896000	-0.747616000	0.081691000
C	3.459306000	-0.492579000	-1.914551000
C	3.312817000	-0.535663000	-0.394180000
C	4.175931000	-1.672928000	0.160345000
O	2.037197000	1.934435000	0.350191000
H	0.648332000	3.514680000	2.350625000
H	-0.901953000	2.963988000	1.704287000
H	0.594774000	2.208032000	-1.134708000
H	0.211840000	3.872586000	0.665133000
H	-3.839303000	0.821652000	-0.468099000
H	0.997312000	-0.134918000	-1.811114000
H	0.946454000	1.021567000	2.995229000
H	2.680145000	-0.179057000	1.994397000
H	-0.313716000	0.301623000	2.009371000
H	2.987508000	-1.365373000	-2.377770000
H	3.013118000	0.404437000	-2.347358000
H	1.701040000	-1.806174000	-0.070398000
H	1.400329000	-1.360085000	2.134578000
H	3.887629000	-2.624393000	-0.297568000
H	4.516112000	-0.501840000	-2.189883000
H	3.682330000	0.405691000	0.011525000
H	4.067854000	-1.776863000	1.241854000
H	5.232359000	-1.502844000	-0.056714000
O	-1.467675000	1.524736000	-1.397018000
C	-1.030869000	-1.811931000	-0.094084000
C	-2.352688000	-2.083829000	0.289126000
C	-2.435339000	2.557735000	-1.432428000
H	-1.944014000	3.410798000	-1.894271000

H	-3.301098000	2.270714000	-2.032919000
H	-2.760959000	2.824637000	-0.424561000
C	-4.756037000	-1.441608000	0.707705000
H	-4.890531000	-2.509029000	0.879984000
H	-4.963481000	-0.919867000	1.644765000
H	-5.498648000	-1.111449000	-0.020214000
C	-0.128558000	-3.032644000	-0.089121000
H	0.500232000	-3.097054000	0.800355000
H	-0.754630000	-3.923814000	-0.104918000
H	0.513135000	-3.070310000	-0.968627000
H	-2.590504000	-3.084550000	0.632609000

**SCF Done: E(RM062X) = -891.164455342**

**# of imaginary frequencies = 1 (-37.2570)**

**(M)-3'c**

C	-1.839002000	-1.413548000	-0.518802000
C	-2.696285000	-0.663775000	0.275432000
C	-3.530138000	-2.991138000	-1.120158000
C	-2.219788000	-2.546652000	-1.214515000
H	-1.490506000	-3.069034000	-1.822215000
C	-4.024473000	-1.118342000	0.369422000
C	-4.410435000	-2.261522000	-0.323945000
C	-1.249694000	2.905749000	0.742579000
C	-1.945735000	1.760761000	0.001761000
C	-2.212431000	0.590199000	0.979196000
C	-1.016179000	0.304612000	1.884654000
C	0.129448000	1.227791000	2.026152000
C	0.140962000	2.502023000	1.217200000
H	-1.852857000	3.205690000	1.603179000
H	-1.166163000	3.778024000	0.091060000
H	-1.253114000	1.392756000	-0.764368000
H	-3.003114000	0.912996000	1.660753000
H	-0.850916000	-0.743461000	2.128383000
H	0.798811000	2.354154000	0.354168000
H	0.592212000	3.294691000	1.821910000
C	-3.229982000	2.213999000	-0.722414000
H	-3.795601000	1.311308000	-0.977658000
C	1.468088000	0.750398000	2.525395000
H	1.808262000	1.419443000	3.319287000
H	1.404771000	-0.261892000	2.926853000
H	2.217212000	0.774815000	1.732559000
C	-4.122692000	3.107267000	0.142754000
H	-5.098101000	3.237027000	-0.330033000
H	-4.286329000	2.695002000	1.141005000
H	-3.677967000	4.097874000	0.263518000
C	-2.897825000	2.921332000	-2.036507000
H	-2.300424000	3.819534000	-1.861030000
H	-2.335445000	2.265623000	-2.704321000
H	-3.810981000	3.228217000	-2.550416000
O	-0.523034000	-0.953559000	-0.671427000
O	-0.901172000	1.165026000	3.017988000
H	-5.439792000	-2.594676000	-0.244238000
C	-5.050309000	-0.389772000	1.200017000
H	-4.741792000	-0.315359000	2.244515000
H	-5.212169000	0.625636000	0.832991000
H	-6.003249000	-0.915092000	1.166472000
C	-3.981011000	-4.236673000	-1.833308000
H	-3.351941000	-4.444014000	-2.698433000
H	-3.926600000	-5.099881000	-1.166088000
H	-5.014282000	-4.142736000	-2.167333000

C	0.466880000	-1.673464000	-0.123744000
O	0.319718000	-2.686708000	0.499353000
C	1.792502000	-1.027029000	-0.353669000
C	2.914105000	-1.627503000	0.203464000
C	1.902500000	0.169672000	-1.049548000
C	4.136939000	-1.002503000	0.055648000
H	2.824628000	-2.555169000	0.751472000
C	3.151036000	0.753619000	-1.159154000
H	1.037442000	0.644070000	-1.490252000
C	4.292034000	0.195038000	-0.617309000
H	5.256437000	0.671735000	-0.711841000
N	3.267424000	2.040454000	-1.867893000
O	4.378963000	2.494538000	-2.027562000
O	2.240398000	2.566078000	-2.240616000
N	5.331372000	-1.628575000	0.651490000
O	6.389577000	-1.053179000	0.519318000
O	5.179164000	-2.678904000	1.235610000

**SCF Done: E(RM062X) = -1605.26772357**

**# of imaginary frequencies = 0**

**(P)-3'c**

C	1.338948000	1.801495000	-0.208333000
C	2.316505000	0.809244000	-0.238255000
C	2.916899000	3.575612000	-0.486451000
C	1.602567000	3.149760000	-0.327668000
H	0.781276000	3.855582000	-0.288446000
C	3.642882000	1.242158000	-0.400783000
C	3.911724000	2.606881000	-0.517677000
C	2.265068000	-2.694184000	1.385961000
C	2.224077000	-1.164729000	1.355547000
C	1.934504000	-0.650865000	-0.078407000
C	2.551051000	-1.498009000	-1.181426000
C	3.269367000	-2.752421000	-0.922455000
C	3.382629000	-3.238603000	0.502698000
H	1.309813000	-3.098221000	1.043358000
H	2.413241000	-3.041386000	2.410343000
H	3.219932000	-0.805944000	1.639467000
H	0.857696000	-0.742706000	-0.238232000
H	2.791818000	-0.957804000	-2.094284000
H	4.359070000	-2.933307000	0.893615000
H	3.372883000	-4.332669000	0.498500000
C	1.234532000	-0.564129000	2.376795000
H	1.120440000	0.496374000	2.129769000
C	4.322312000	-3.231975000	-1.880795000
H	4.322981000	-4.323252000	-1.927406000
H	4.141331000	-2.836260000	-2.880232000
H	5.309656000	-2.906804000	-1.546468000
C	-0.150471000	-1.211821000	2.324693000
H	-0.856995000	-0.645460000	2.935835000
H	-0.551171000	-1.262244000	1.309187000
H	-0.118440000	-2.230521000	2.718298000
C	1.791625000	-0.635683000	3.798768000
H	1.931063000	-1.670866000	4.119052000
H	2.753981000	-0.124986000	3.870819000
H	1.103558000	-0.164033000	4.503173000
O	0.000792000	1.442502000	0.021171000
O	1.928055000	-2.759082000	-1.432397000
H	4.943435000	2.920694000	-0.636380000
C	4.809630000	0.286259000	-0.484426000
H	4.701332000	-0.571375000	0.176785000

H	4.924404000	-0.099445000	-1.500356000
H	5.732207000	0.802803000	-0.222925000
C	3.236063000	5.040250000	-0.612132000
H	2.711322000	5.479096000	-1.462454000
H	2.921535000	5.582855000	0.281159000
H	4.304886000	5.197417000	-0.749933000
C	-0.720241000	1.037829000	-1.033883000
O	-0.308783000	0.971644000	-2.158125000
C	-2.104865000	0.648848000	-0.630753000
C	-2.956598000	0.163422000	-1.614205000
C	-2.529349000	0.743147000	0.688766000
C	-4.231852000	-0.222873000	-1.249335000
H	-2.623708000	0.087744000	-2.639915000
C	-3.814143000	0.336531000	0.996277000
H	-1.875950000	1.120122000	1.462114000
C	-4.694313000	-0.151815000	0.050805000
H	-5.693521000	-0.464742000	0.314790000
N	-4.263647000	0.417488000	2.396910000
O	-5.405215000	0.090848000	2.639518000
O	-3.461649000	0.802535000	3.220244000
N	-5.141187000	-0.740835000	-2.286646000
O	-6.250227000	-1.084494000	-1.938721000
O	-4.723664000	-0.790604000	-3.423069000

**SCF Done: E(RM062X) = -1605.26497870**

**# of imaginary frequencies = 0**

### TS1-3'c

C	5.134823000	-2.340509000	0.899566000
C	3.160771000	-1.822096000	-0.705204000
C	3.676893000	-2.069067000	0.648436000
C	3.738236000	1.060897000	-0.874137000
C	4.191329000	2.310990000	-0.441034000
C	1.976658000	-0.853072000	-0.830857000
C	2.444859000	0.595639000	-0.518812000
C	2.868920000	-1.449374000	1.773733000
C	3.411452000	3.188366000	0.305089000
C	1.642885000	1.567814000	0.106025000
C	2.095962000	2.807438000	0.533705000
O	0.275764000	1.373364000	0.360922000
C	1.355365000	-1.615137000	1.547813000
C	0.854432000	-1.414627000	0.085661000
C	-0.112942000	-2.612302000	-1.973710000
C	0.142089000	-2.678831000	-0.466679000
C	-1.200277000	-2.838966000	0.257561000
C	4.683895000	0.324549000	-1.802444000
C	3.949808000	4.501410000	0.805688000
O	2.960108000	-3.083259000	-0.059791000
H	5.256440000	-3.044551000	1.728253000
H	5.648896000	-1.411872000	1.166000000
H	3.831419000	-1.919581000	-1.549348000
H	5.607436000	-2.761205000	0.008443000
H	5.196821000	2.614748000	-0.722114000
H	1.616598000	-0.845929000	-1.866173000
H	3.146805000	-1.918542000	2.724402000
H	1.081637000	-2.626640000	1.864036000
H	3.147032000	-0.392091000	1.853655000
H	-0.599444000	-1.665639000	-2.245147000
H	0.808750000	-2.698436000	-2.556024000
H	0.047544000	-0.695022000	0.126749000
H	0.830743000	-0.927023000	2.219169000

H	-1.889707000	-2.037105000	-0.038285000
H	-0.776099000	-3.425821000	-2.282604000
H	0.759938000	-3.554531000	-0.254386000
H	-1.090991000	-2.799018000	1.345794000
H	-1.672136000	-3.791825000	0.001018000
H	5.303147000	-0.411165000	-1.282550000
H	4.148779000	-0.183320000	-2.607845000
H	5.357789000	1.048151000	-2.264566000
H	4.345362000	4.393371000	1.820649000
H	4.761964000	4.861440000	0.170432000
H	3.167450000	5.263087000	0.836252000
H	1.390741000	3.466994000	1.029650000
C	-1.941229000	0.967820000	-0.288488000
C	-2.889588000	0.801470000	-1.295694000
C	-2.279354000	0.764613000	1.048670000
C	-4.175181000	0.429984000	-0.935624000
H	-2.620898000	0.949496000	-2.334774000
C	-3.581906000	0.392473000	1.346404000
H	-1.548208000	0.879898000	1.839185000
C	-4.557766000	0.214342000	0.379071000
H	-5.566231000	-0.081477000	0.636483000
C	-0.542437000	1.296375000	-0.702936000
O	-0.198100000	1.421254000	-1.850529000
N	-3.945874000	0.162903000	2.754062000
O	-5.094299000	-0.158342000	2.991851000
O	-3.074444000	0.307710000	3.589641000
N	-5.181455000	0.245029000	-1.993880000
O	-6.301642000	-0.082434000	-1.652194000
O	-4.828192000	0.431317000	-3.142204000

**SCF Done: E(RM062X) = -1605.21221228**

**# of imaginary frequencies = 1 (-21.3543)**

### TS2-3'c

C	-0.708732000	-0.438719000	3.244805000
C	-0.981750000	-1.042643000	0.745072000
C	-1.540318000	-0.925188000	2.094359000
C	-1.341683000	1.697178000	-0.168488000
C	-1.565719000	3.054696000	-0.058800000
C	-1.936340000	-0.769800000	-0.426600000
C	-2.311094000	0.737250000	-0.488167000
C	-3.038345000	-0.705866000	2.153739000
C	-2.827744000	3.563047000	-0.312345000
C	-3.562072000	1.284202000	-0.868592000
C	-3.784398000	2.658996000	-0.745967000
C	-3.781940000	-1.601391000	1.147573000
C	-3.132291000	-1.733922000	-0.262541000
C	-1.921768000	-3.378201000	-1.831344000
C	-2.817844000	-3.214256000	-0.604357000
C	-4.139000000	-3.949856000	-0.846065000
C	-3.134523000	5.025495000	-0.150719000
O	-1.192076000	-2.202918000	1.555060000
H	-1.024503000	-0.915049000	4.175411000
H	-0.825407000	0.641140000	3.359696000
H	0.074617000	-0.867121000	0.609553000
H	0.345494000	-0.662817000	3.077062000
H	-0.736634000	3.695874000	0.214949000
H	-1.426143000	-0.994153000	-1.366605000
H	-3.397000000	-0.924148000	3.163268000
H	-3.845223000	-2.599475000	1.584323000
H	-3.240235000	0.353133000	1.971681000

H	-2.317500000	-2.815274000	-2.682801000
H	-0.900083000	-3.042158000	-1.646552000
H	-3.867032000	-1.464520000	-1.007980000
H	-4.809153000	-1.240177000	1.061514000
H	-4.624829000	-3.567711000	-1.749136000
H	-1.874073000	-4.429461000	-2.122152000
H	-2.318709000	-3.672615000	0.248778000
H	-4.834438000	-3.825209000	-0.013988000
H	-3.969025000	-5.019231000	-0.983795000
H	-3.423203000	5.243740000	0.879931000
H	-2.263543000	5.637133000	-0.385740000
H	-3.957970000	5.326711000	-0.797536000
H	-4.760787000	3.039761000	-1.024193000
C	-4.717600000	0.529422000	-1.498221000
H	-4.385514000	-0.107413000	-2.317449000
H	-5.268633000	-0.083819000	-0.785507000
H	-5.418935000	1.250916000	-1.913248000
O	-0.011009000	1.327599000	0.083001000
C	0.747357000	1.008056000	-0.976473000
O	0.371230000	1.004950000	-2.113702000
C	2.128882000	0.625873000	-0.555832000
C	2.498928000	0.599687000	0.782918000
C	3.034480000	0.267968000	-1.545987000
C	3.783763000	0.204337000	1.102330000
H	1.806539000	0.879713000	1.563621000
C	4.307586000	-0.109637000	-1.168336000
H	2.743837000	0.284280000	-2.586800000
C	4.716907000	-0.154273000	0.150564000
H	5.716419000	-0.457683000	0.423071000
N	4.175327000	0.159539000	2.522333000
O	5.318952000	-0.144505000	2.777520000
O	3.326532000	0.428120000	3.344375000
N	5.276010000	-0.486923000	-2.213755000
O	6.386851000	-0.810142000	-1.855700000
O	4.898753000	-0.449030000	-3.363627000

**SCF Done: E(RM062X) = -1605.21020143**

**# of imaginary frequencies = 1 (-34.1805)**