

## Supplementary Materials

### An efficient and versatile synthesis of 2, 2'-(alkanediyl)-bis-1*H*-benzimidazoles employing aqueous fluoroboric acid as catalyst: Density Functional Theory calculations and fluorescence studies

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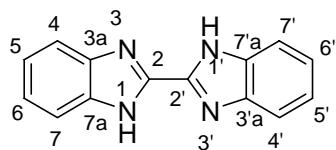
<sup>b</sup>Department of Chemistry, Howard University, Washington DC 20059, USA

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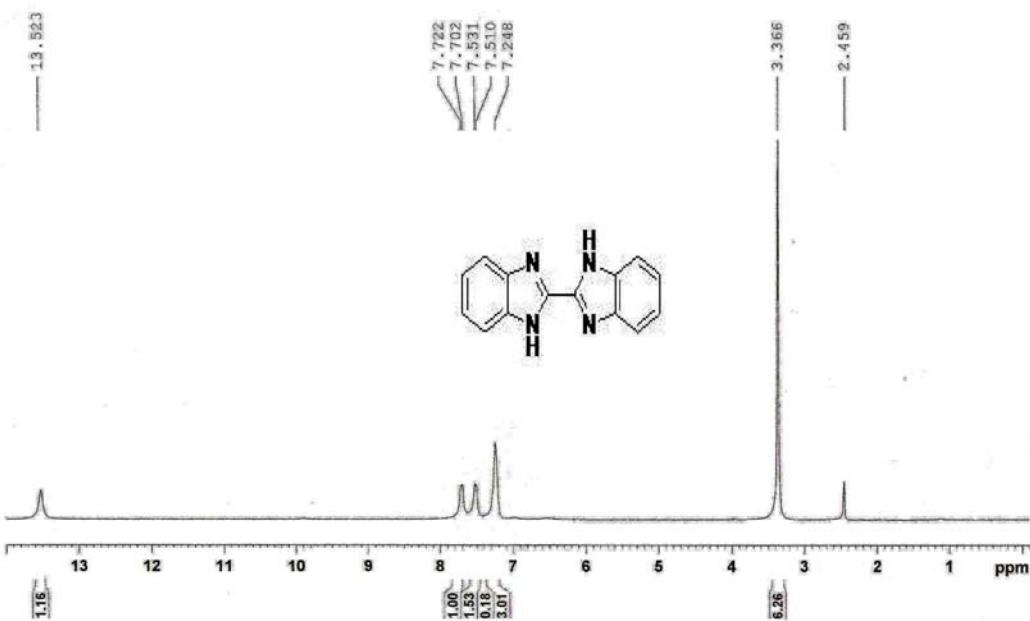
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## 1. Details of $^1\text{H}$ -NMR spectra, $^{13}\text{C}$ -NMR spectra of the crude as well as pure compounds (4a-4q)

$^1\text{H}$ -NMR spectra,  $^{13}\text{C}$ -NMR spectra of the crude as well as pure compounds **4a-4q** ( spectra for compound **4g** is not present since it was insoluble in all possible NMR solvents ) and the **HPLC data** of the crude compounds **4d**, **4i** and **4l**.



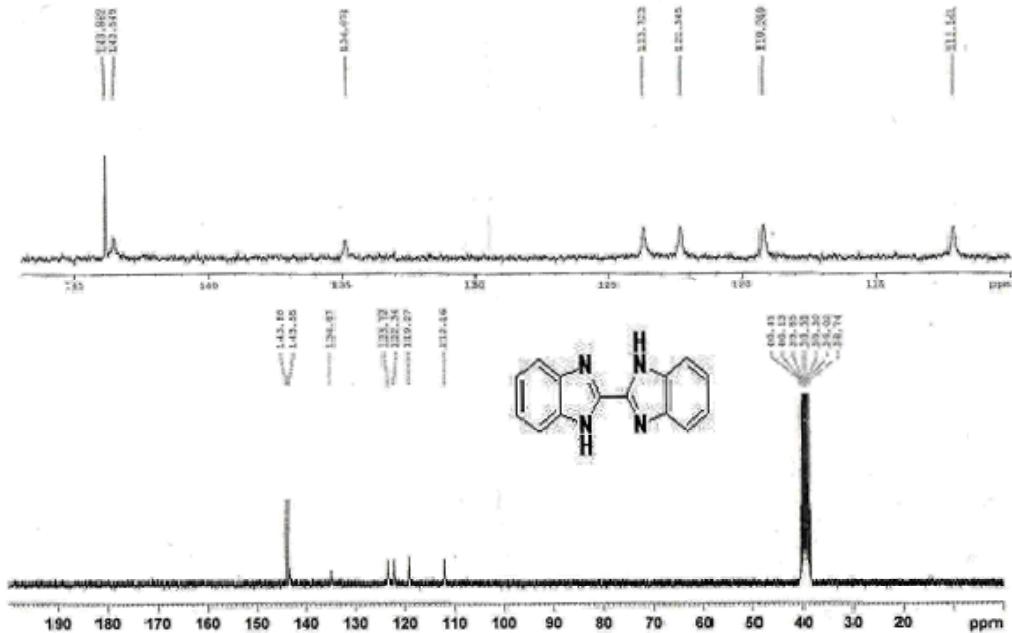
Copy of pure  $^1\text{H}$ -NMR ( $\text{DMSO}-d_6$ ) spectra of compound **4a**:



Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

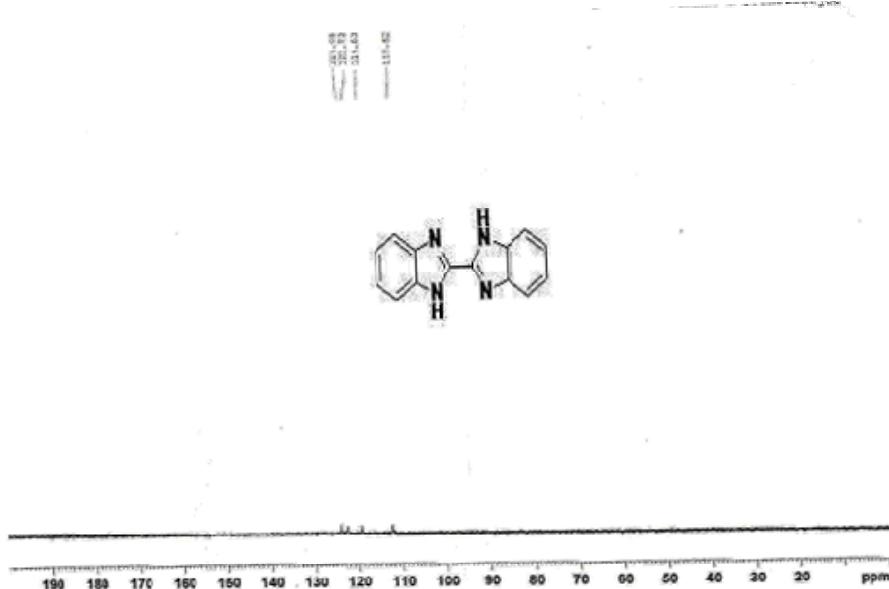
Ratio of the aromatic protons (from left to right): 2: 2: 4 (total 8 protons) indicating the presence of pure simple bis-benzimidazole.

Copy of pure  $^{13}\text{C}$ -NMR (75 MHz,  $\text{DMSO-}d_6$ ) spectra of compound 4a: upper-half of the spectra is the expanded aromatic region.

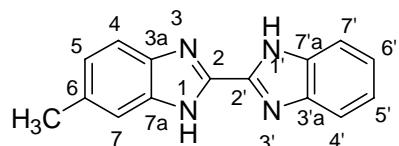


All the seven carbons of one half of the molecule have come separately, the left side three signals disappear in DEPT 135 experiment as they are quaternary carbons while the right side four signals remain in DEPT 135 experiment as they are hydrogen bearing carbons. This convincingly proves the presence of pure simple bis-benzimidazole.

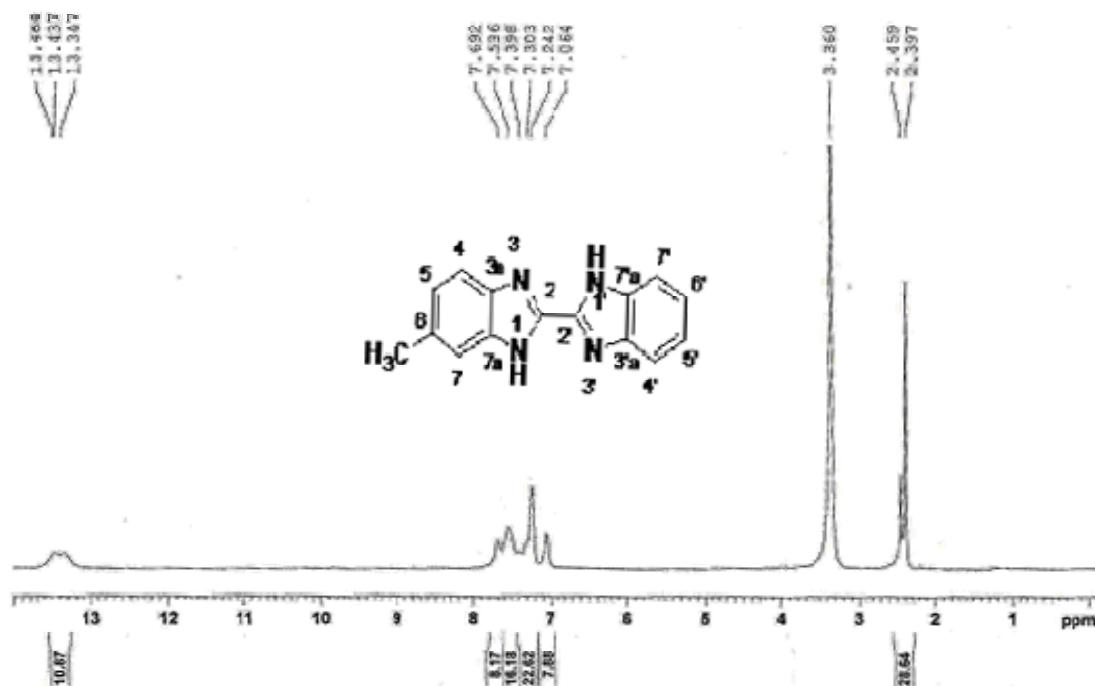
### **Copy of pure DEPT-135 spectra of compound 4a:**



As stated earlier, the left hand side three signals have vanished in the DEPT 135 experiment as they are quaternary carbons while the right hand side four signals remain as they are hydrogen bearing carbons.



**Copy of crude  $^1\text{H-NMR}$  ( $\text{DMSO}-d_6$ ) spectra of compound 4b:**

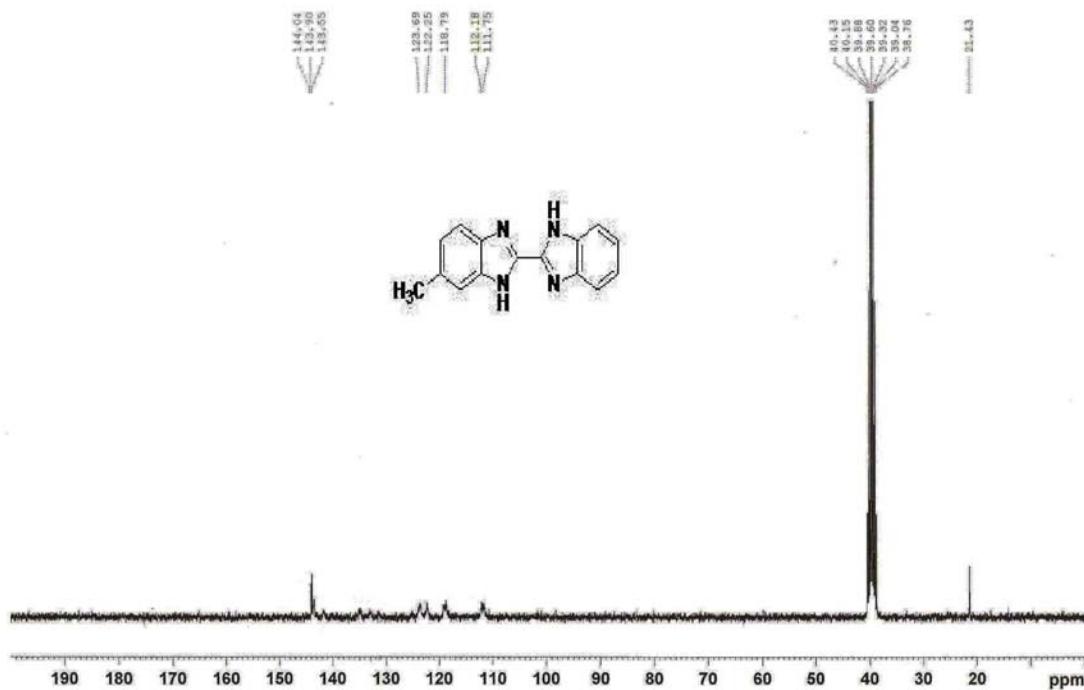


$\delta$  2.40 (br s, 3H, C<sub>6</sub>-CH<sub>3</sub>), 7.06 (s, 1H, C<sub>5</sub>-H), 7.24-7.40 (m, 3H, C<sub>7</sub>-H, C<sub>5</sub>-H and C<sub>6</sub>-H), 7.54 (br s, 2H, C<sub>4</sub>-H and C<sub>7</sub>-H), 7.69 (br s, 1H, C<sub>4</sub>-H) and 13.35-13.46 (m, 2H, N<sub>1</sub>-H and N<sub>1</sub>-H)

Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

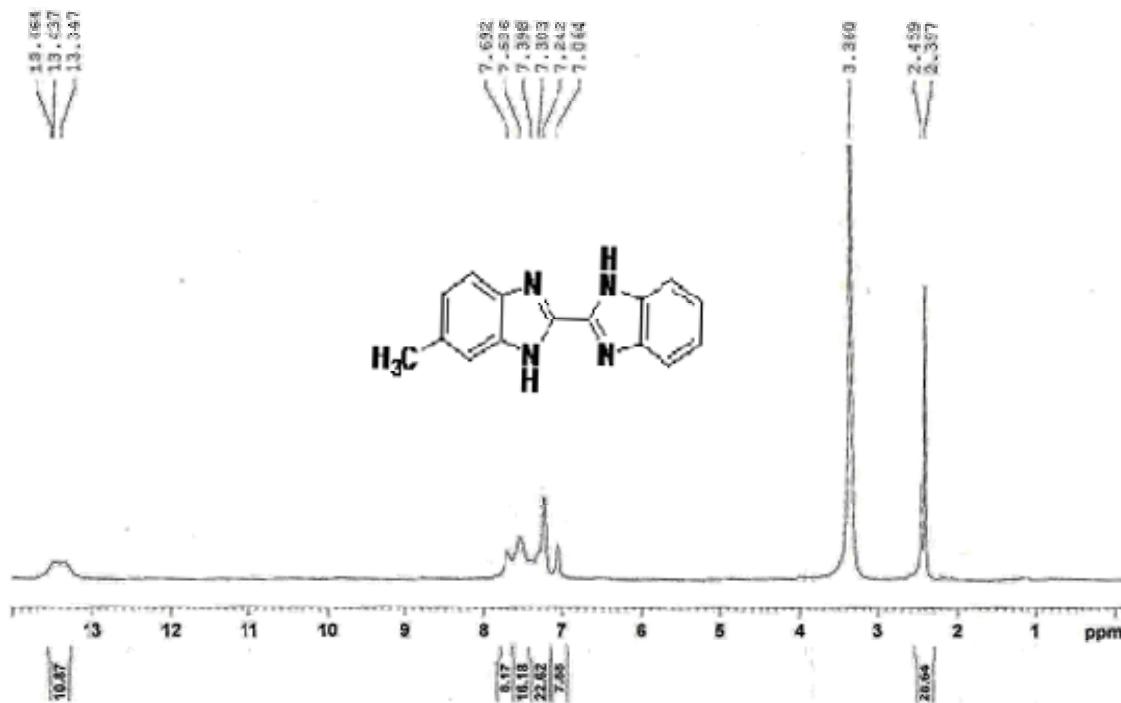
Ratio of the aromatic protons (from left to right): 1: 2: 3: 1 (total 7 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the methyl protons versus the aromatic protons is also satisfactory.

**Copy of crude  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4b:**

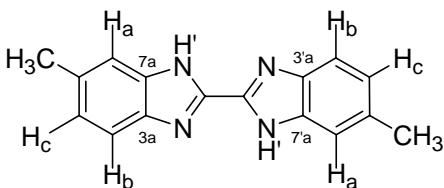
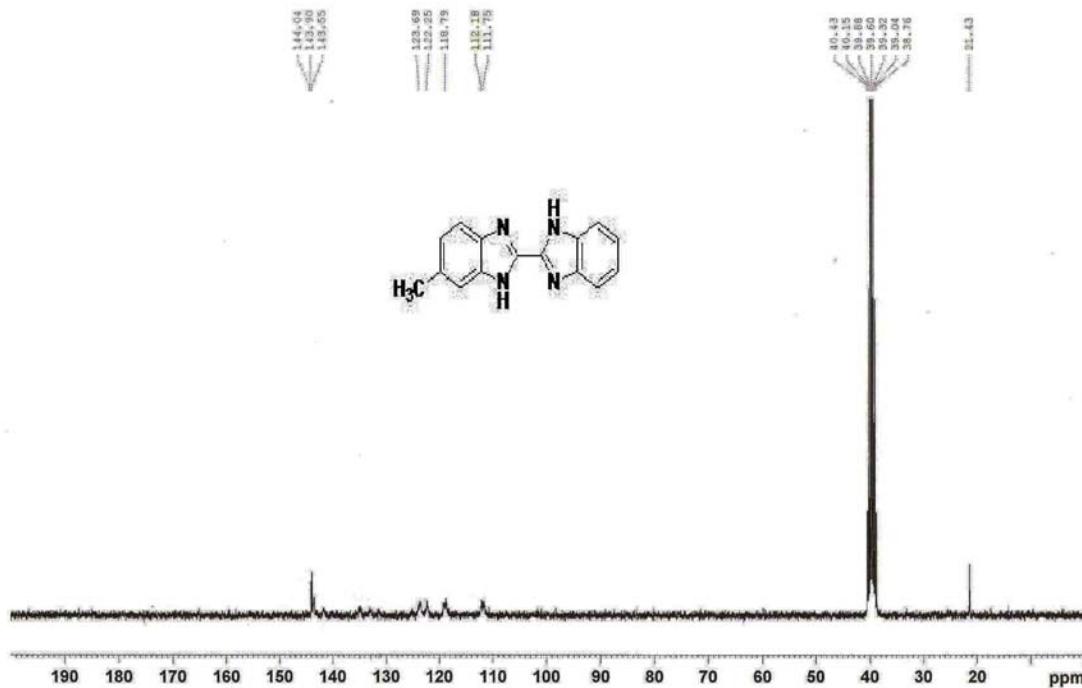


Out of fifteen carbon atoms present, fourteen have come separately.

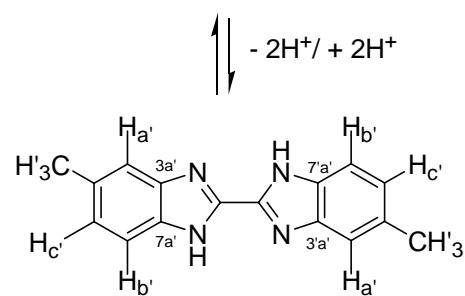
**Copy of pure  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4b:**



**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4b:**



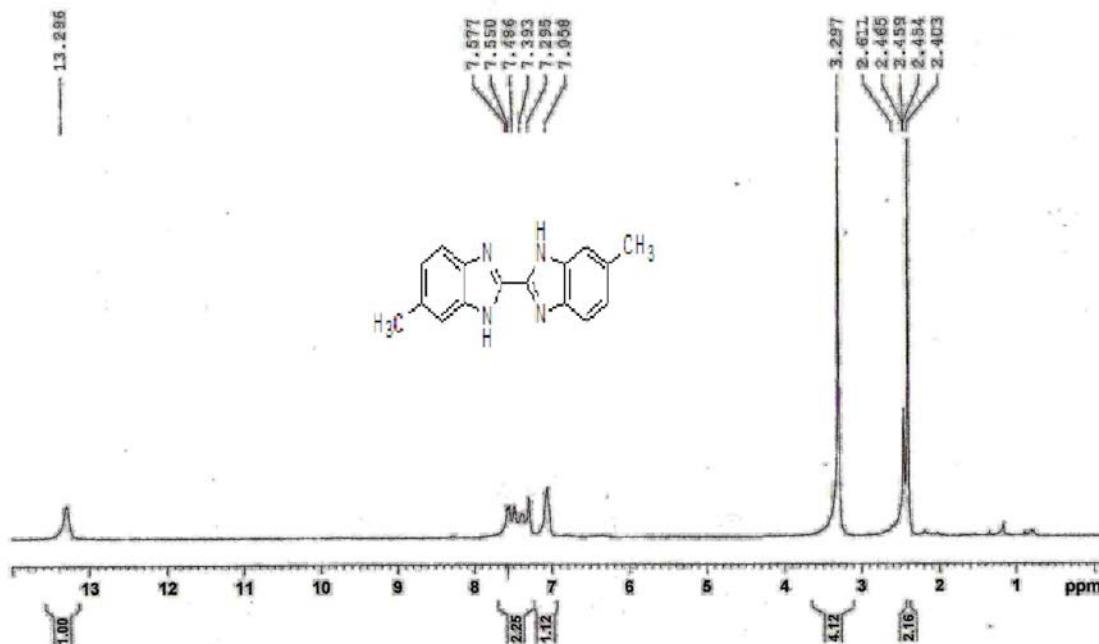
51.6 % of tautomer A



48.4 % of tautomer B

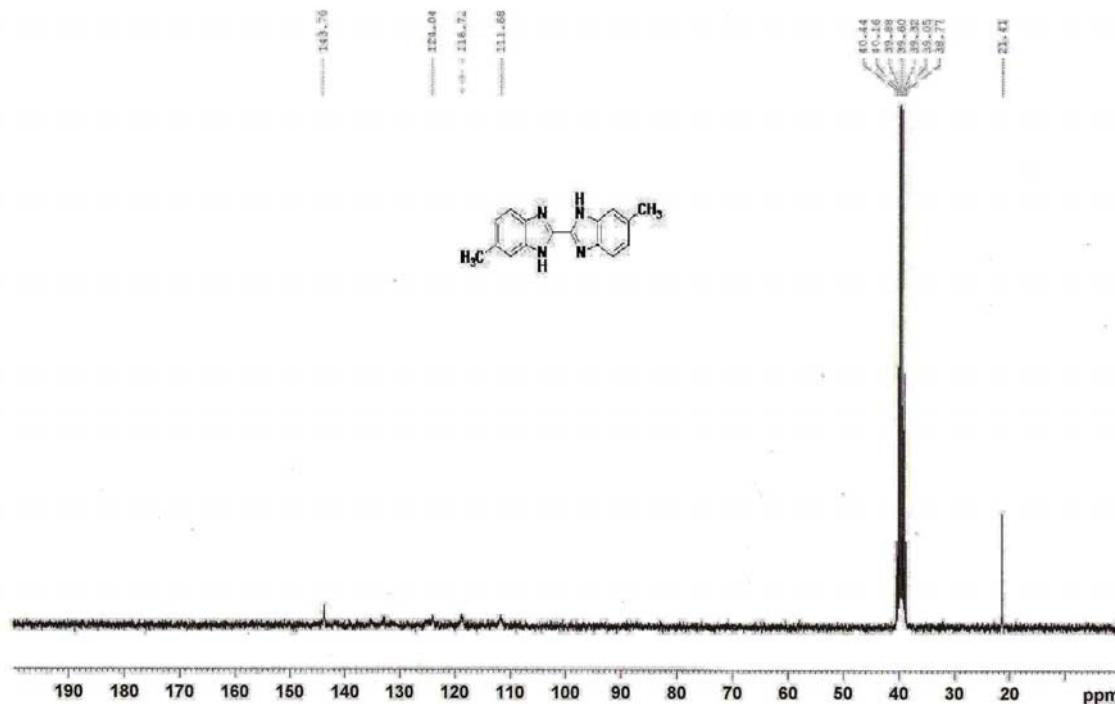
(The percentages of the two tautomers obtained from proton integration ratios of crude  $^1\text{H}$  NMR spectrum).

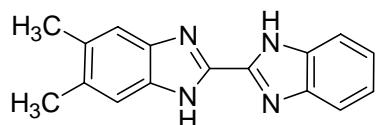
**Copy of pure  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4c:**



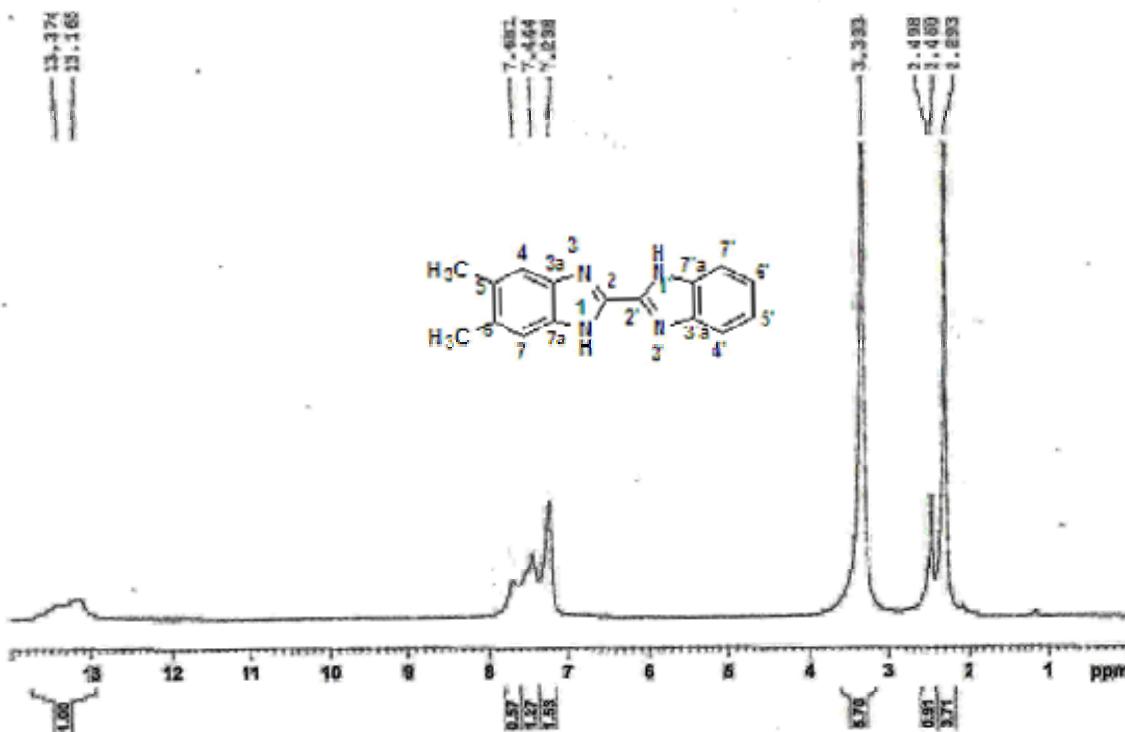
Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4c:**





#### Copy of crude $^1\text{H-NMR}$ ( $\text{DMSO}-d_6$ ) spectra of compound 4d:

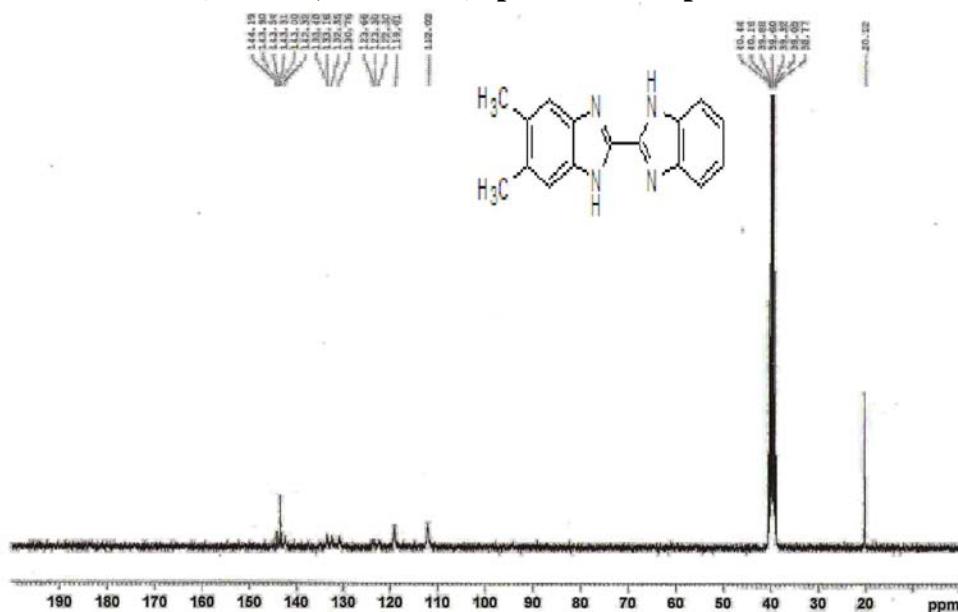


$\delta$  2.29 (s, 6H, C<sub>5</sub>-CH<sub>3</sub> and C<sub>6</sub>-CH<sub>3</sub>), 7.24 (br s, 3H, C<sub>7</sub>-H, C<sub>5'</sub>-H, and C<sub>6'</sub>-H), 7.44-7.68 (m, 3H, C<sub>4</sub>-H, C<sub>4'</sub>-H and C<sub>7</sub>-H) and 13.17-13.37 (m, 2H, N<sub>1</sub>-H and N<sub>1'</sub>-H)

Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

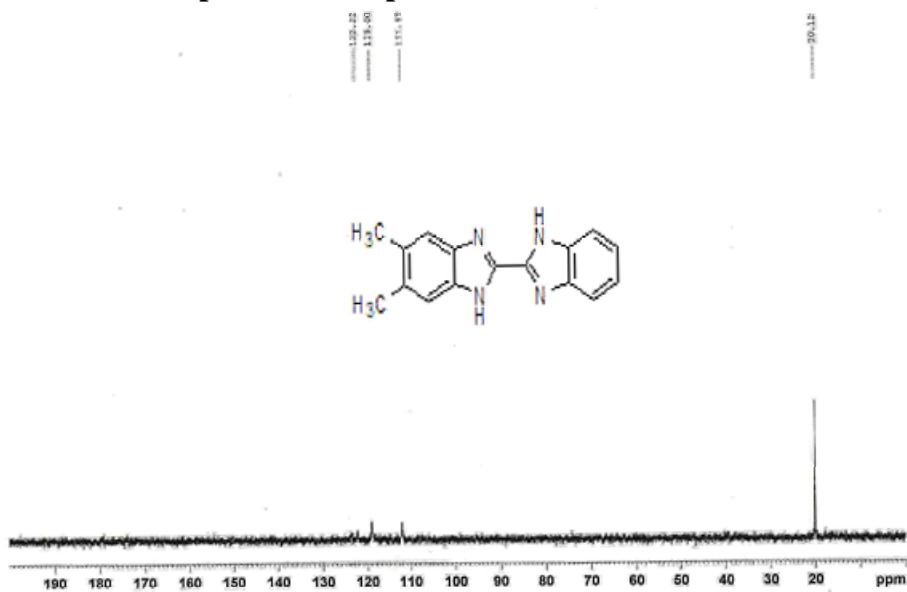
Ratio of the aromatic protons (from left to right): 1: 2: 3 (total 6 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the two methyl group protons versus the aromatic protons is also satisfactory.

**Copy of crude  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4d:**



All the eight quaternary carbons the molecule have come separately, the left side three signals disappear in DEPT 135 experiment as they are the quaternary carbons while the right side five signals remain in DEPT 135 experiment as they are hydrogen bearing carbons. This convincingly proves the presence of pure mixed bis-benzimidazole.

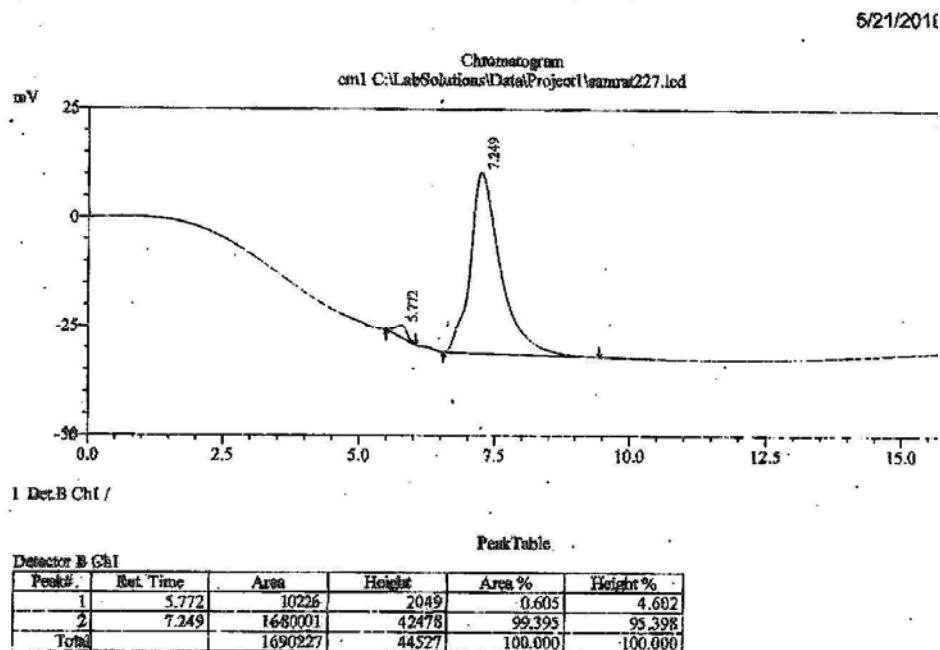
**Copy of crude DEPT-135 spectra of compound 4d:**



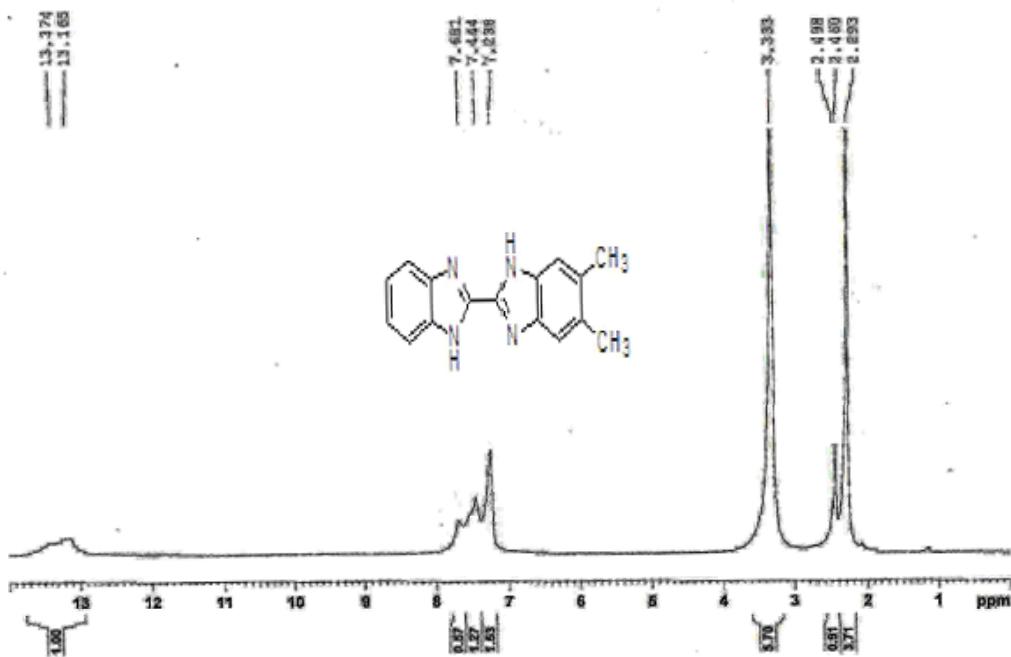
As stated earlier, the left hand side eight signals have vanished in the DEPT 135 experiment as they are quaternary carbons while the right hand side five signals remain as they are hydrogen bearing carbons.

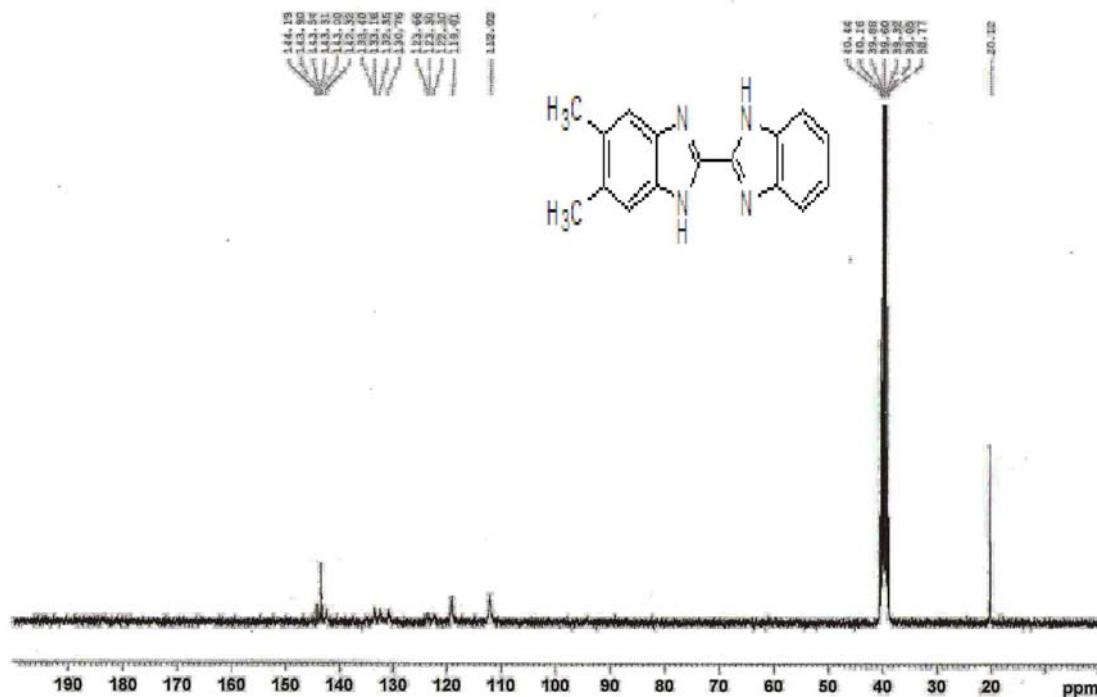
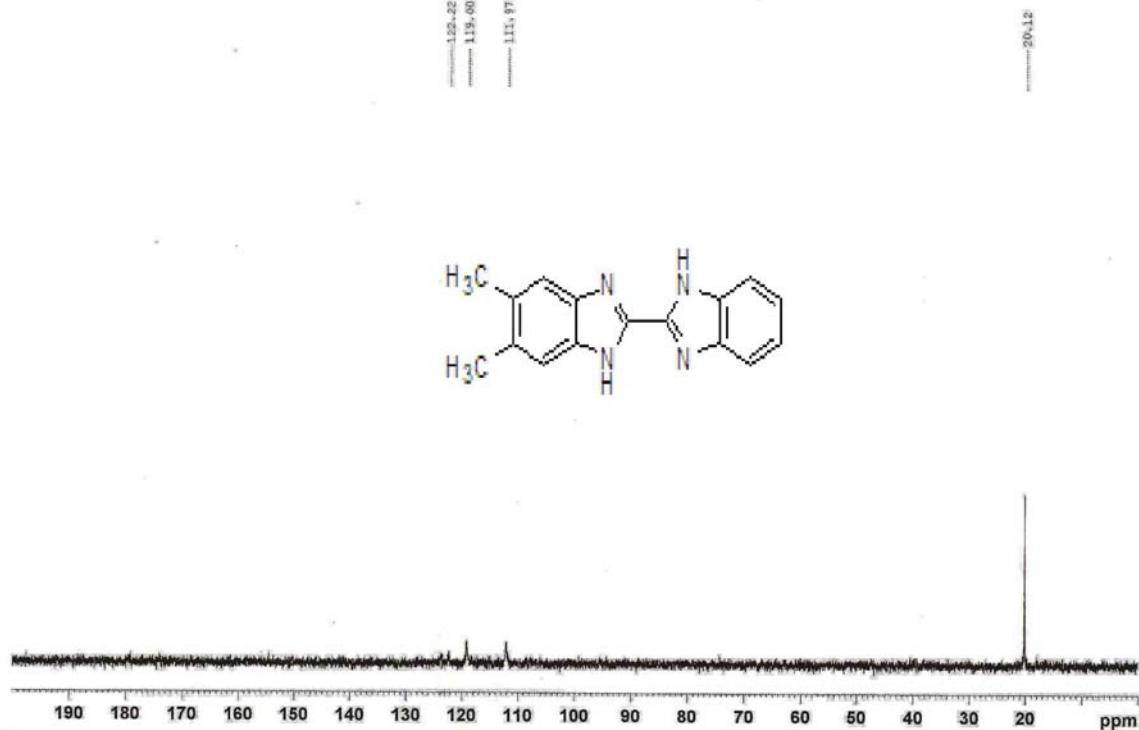
## 2. HPLC data for compound (4d)

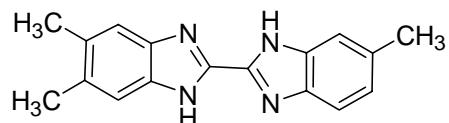
Copy of crude HPLC data of compound 4d (Purity= 99.395%):



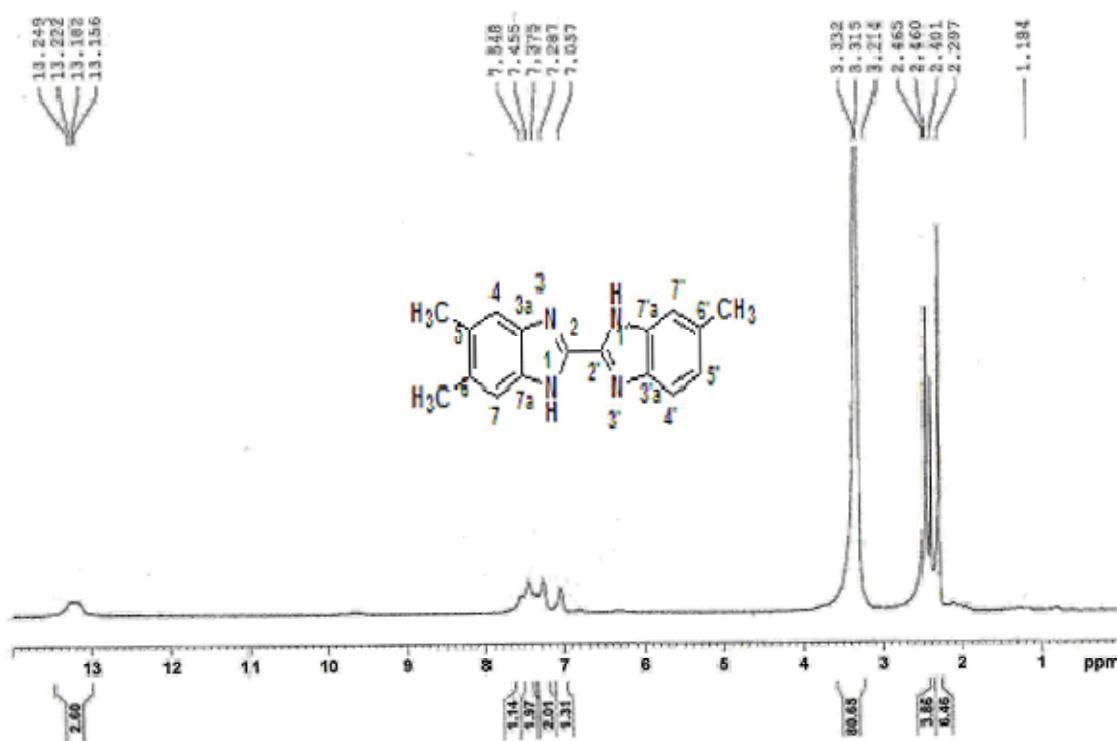
Copy of pure  $^1\text{H-NMR}$  ( $\text{DMSO}-d_6$ ) spectra of compound 4d:



**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz,  $\text{DMSO}-d_6$ ) spectra of compound 4d:****Copy of pure DEPT-135 spectra of compound 4d:**



**Copy of crude  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4e:**

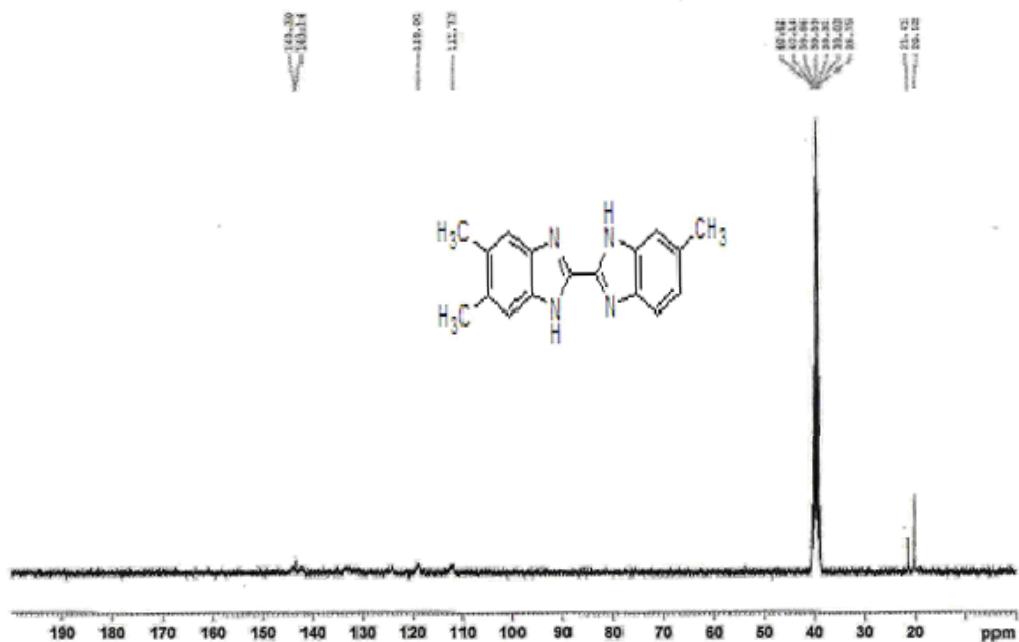


$\delta$  2.30 (s, 6H, C<sub>5</sub>-CH<sub>3</sub> and C<sub>6</sub>-CH<sub>3</sub>), 2.40 (s, 3H, C<sub>6</sub>-CH<sub>3</sub>), 7.06 (br s, 1H, C<sub>5'</sub>-H), 7.29 (br s, C<sub>7</sub>-H and C<sub>7'</sub>-H), 7.46 (br s, 1H, C<sub>4</sub>-H), 7.55 (br s, 1H, C<sub>4'</sub>-H) and 13.16-13.25 (m, 2H, N<sub>1</sub>-H and N<sub>1'</sub>-H)

Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

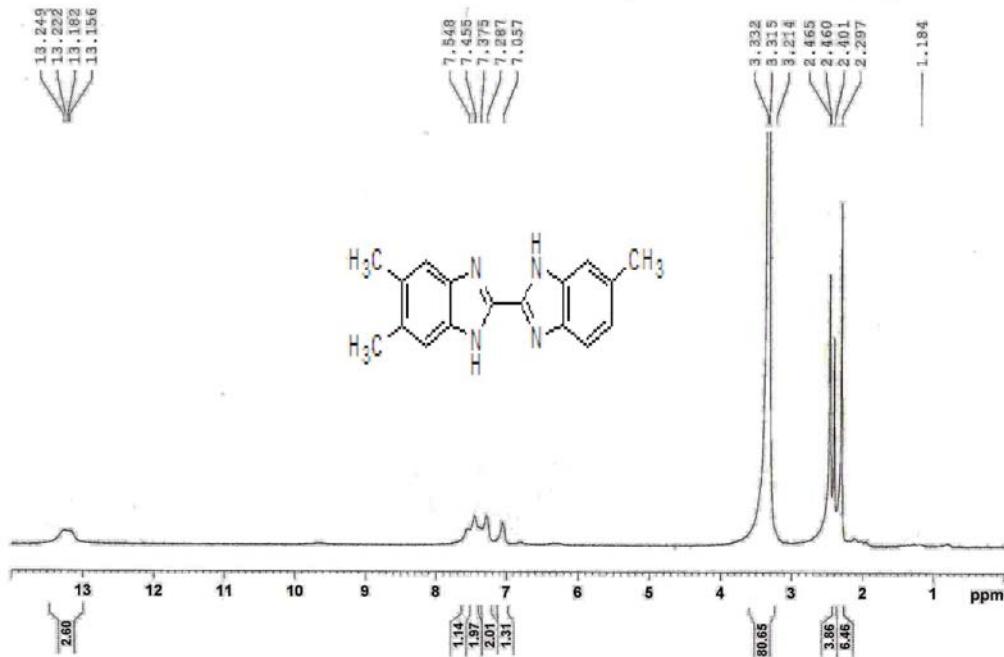
Ratio of the aromatic protons (from left to right): 1: 1: 2: 1 (total 5 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the three methyl group protons versus the aromatic protons is also satisfactory.

Copy of crude  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4e:

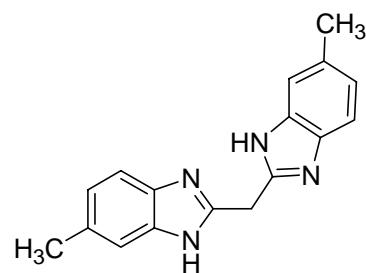
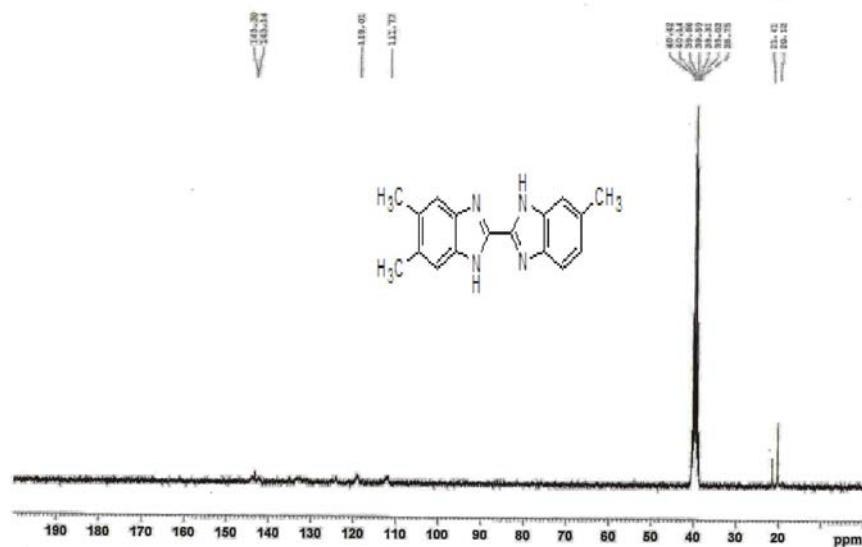


Out of the fifteen types of carbon present, only the carbon atoms of the two types of methyl groups and the two carbon atoms joining the two benzimidazole rings have come separately. Other symmetrical carbons have come in the same place thereby reducing the total number of signals.

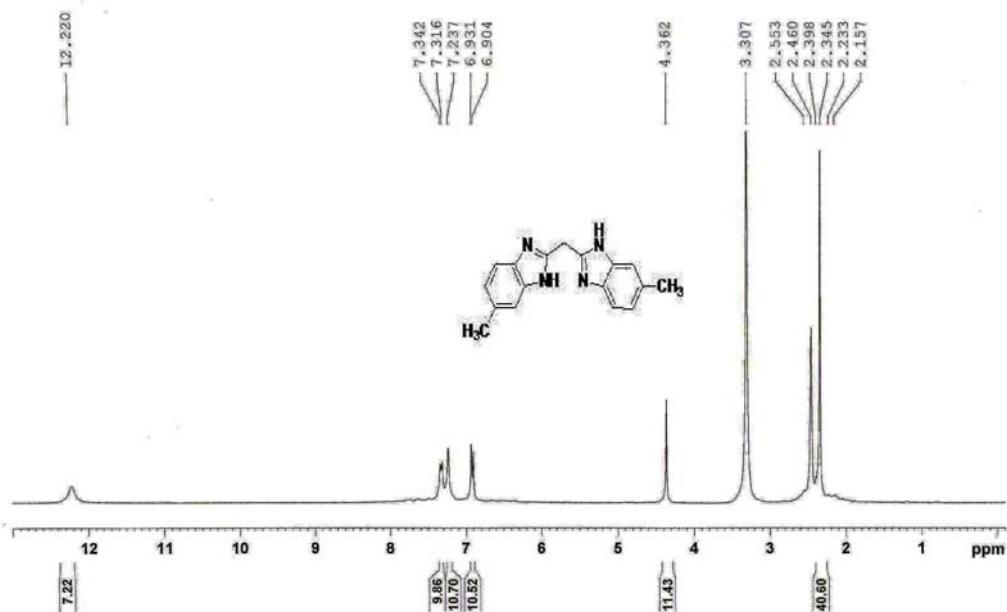
## Copy of pure $^1\text{H-NMR}$ ( $\text{DMSO}-d_6$ ) spectra of compound 4e:



**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4e:**

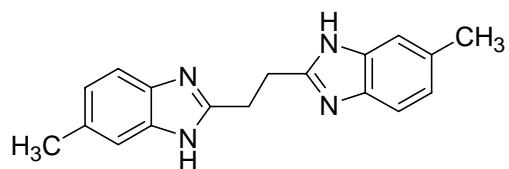


**Copy of pure  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4f:**

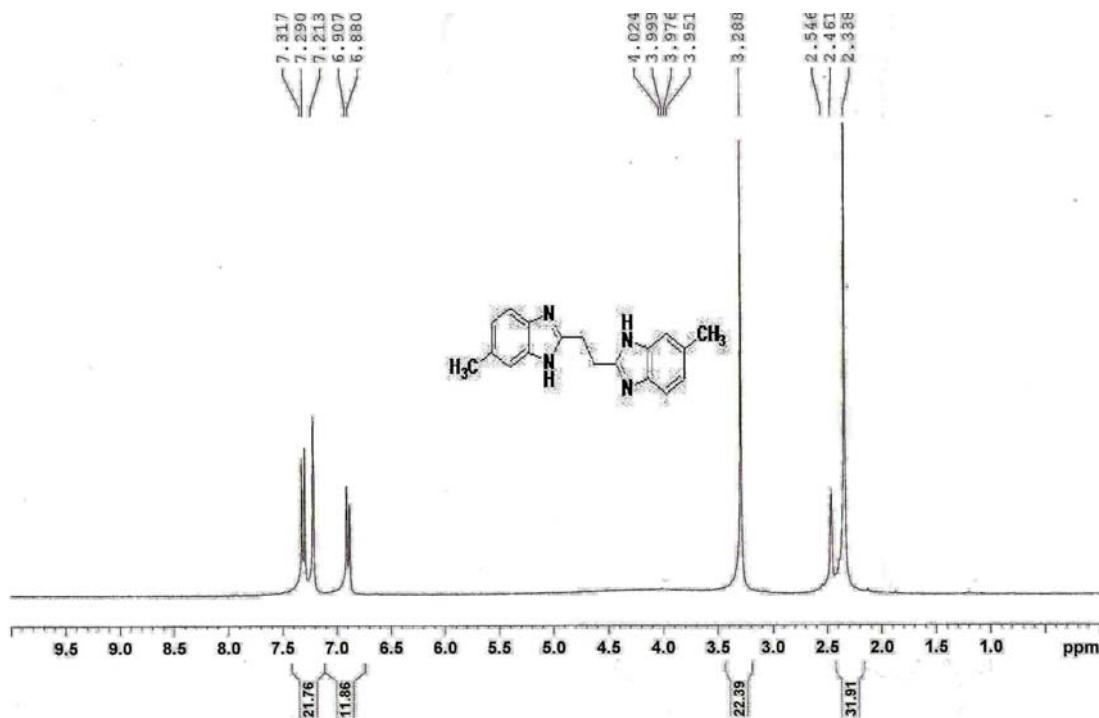


Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure simple bis-benzimidazole. Integration of the two methyl group protons versus the aromatic protons is also satisfactory.



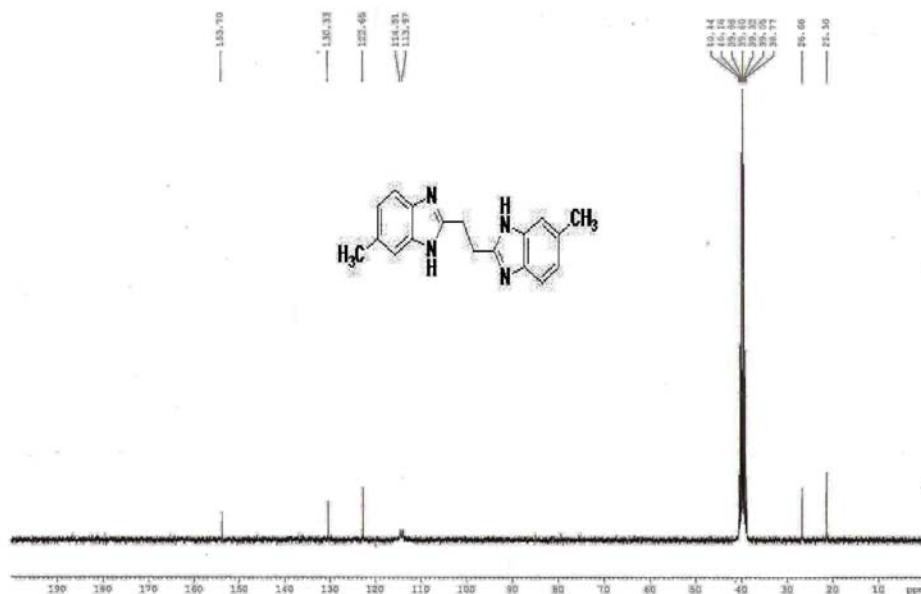
**Copy of pure  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4h:**



Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

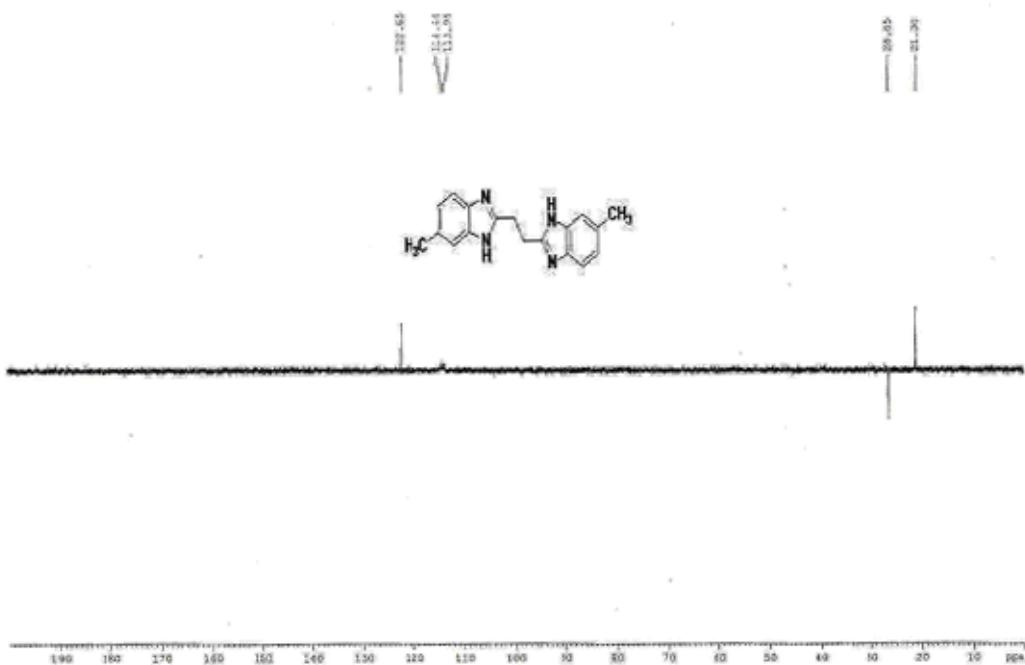
Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure simple bis-benzimidazole. Integration of the two methyl group protons and the two methylene group protons are also satisfactory.

**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4h:**



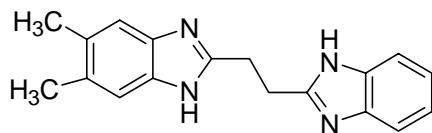
The left side two signals disappear in DEPT 135 experiment as they are quaternary carbons.

**Copy of pure DEPT-135 spectra of compound 4h:**

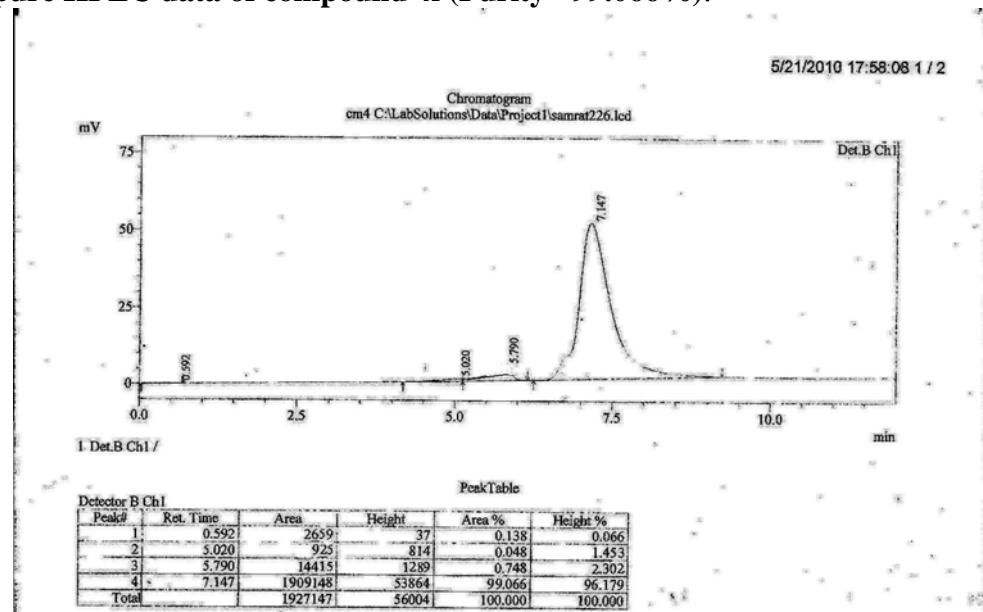


As stated earlier, the left side two signals disappear in DEPT 135 experiment as they are quaternary carbons while the right side five signals remain in DEPT 135 experiment as they are hydrogen bearing carbons. The second signal from the right side is inversed in DEPT-135 experiment showing the presence of the methylene protons. This convincingly proves the presence of pure simple bis-benzimidazole.

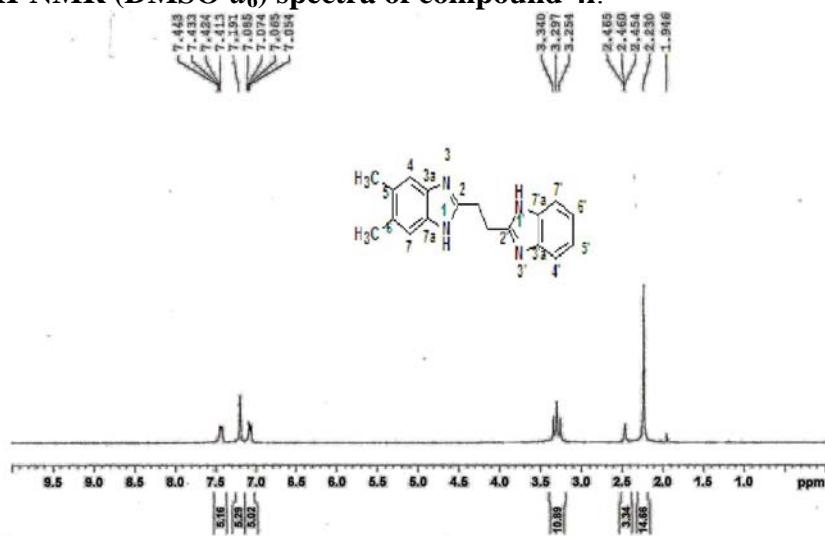
### 3. HPLC data for compound (4i)



Copy of pure HPLC data of compound 4i (Purity= 99.066%):



Copy of pure  $^1\text{H-NMR}$  ( $\text{DMSO}-d_6$ ) spectra of compound 4i:

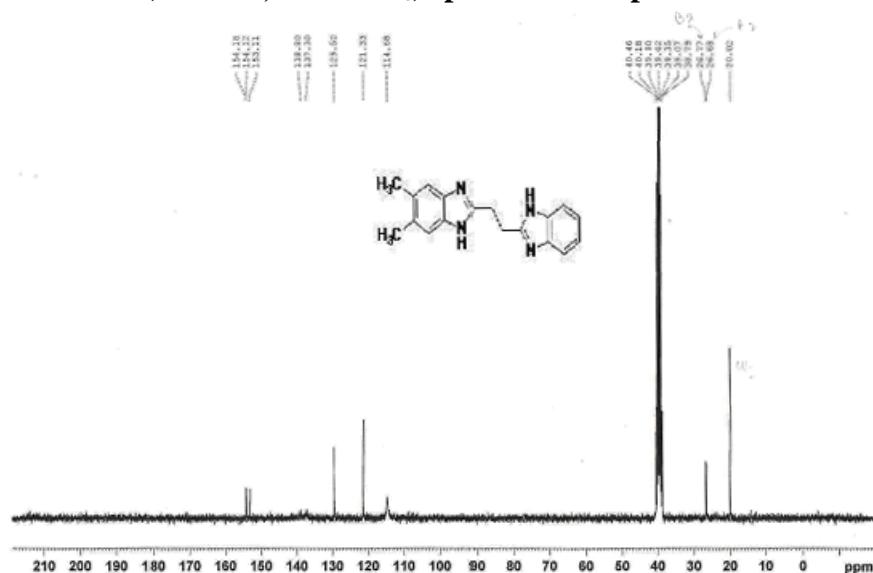


δ 2.23 (s, 6H, C<sub>5</sub>-CH<sub>3</sub> and C<sub>6</sub>-CH<sub>3</sub>), 3.30 (t,  $J=12.9$  Hz, 4H, C<sub>2</sub>-CH<sub>2</sub> and C<sub>2</sub>-CH<sub>2</sub>), 7.07 (dd,  $J=6.0$  Hz, 3.3 Hz, 2H, C<sub>5</sub>-H and C<sub>6</sub>-H), 7.19 (s, 2H, C<sub>4</sub>-H and C<sub>7</sub>-H) and 7.43 (dd,  $J=6.0$  Hz, 3.0 Hz, 2H, C<sub>4</sub>-H and C<sub>7</sub>-H)

Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

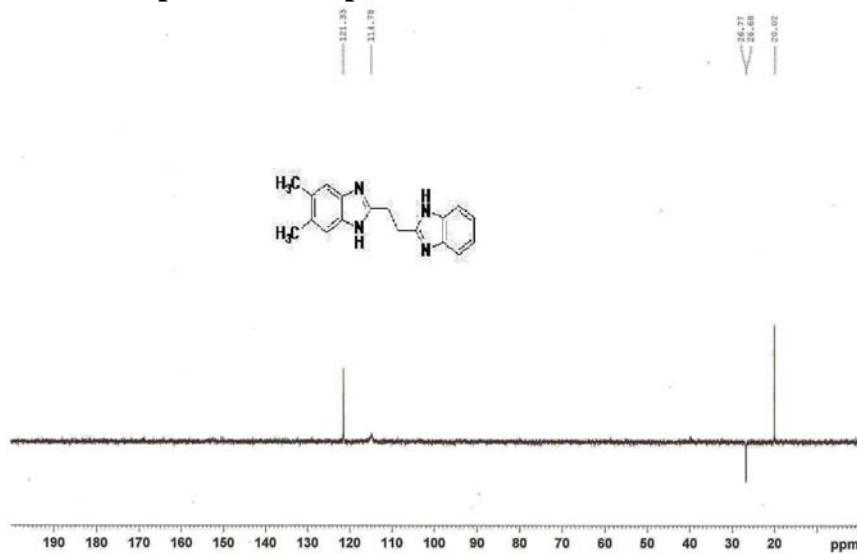
Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the two methyl group protons and the methylene group protons are also satisfactory.

**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4i:**

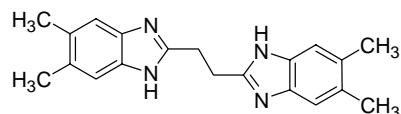


The five signals from the left side are the quarternary carbons and they disappear in DEPT-135 experiment.

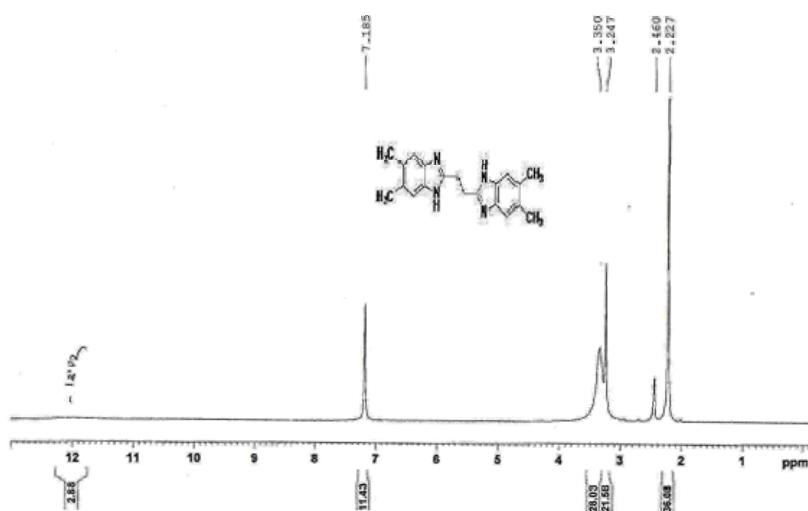
**Copy of pure DEPT-135 spectra of compound 4i:**



As stated earlier, the five signals from the left due to quarternary carbons disappear in DEPT-135 experiment and among the four remaining signals due to hydrogen-bearing carbon atoms, the one that is inverted indicates the presence of the carbon atoms of the methylene groups.

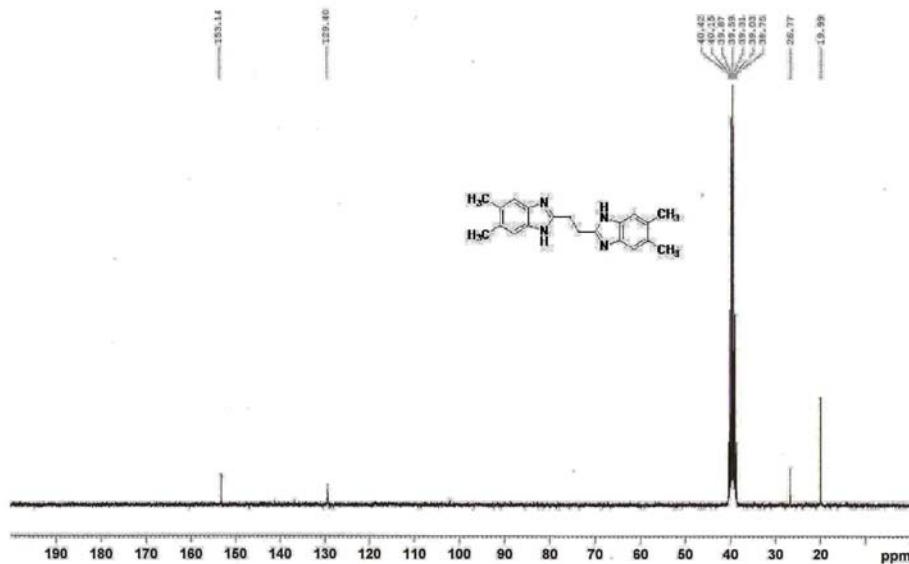


**Copy of pure  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4j:**

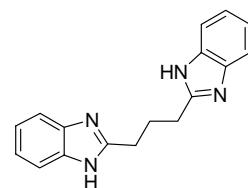
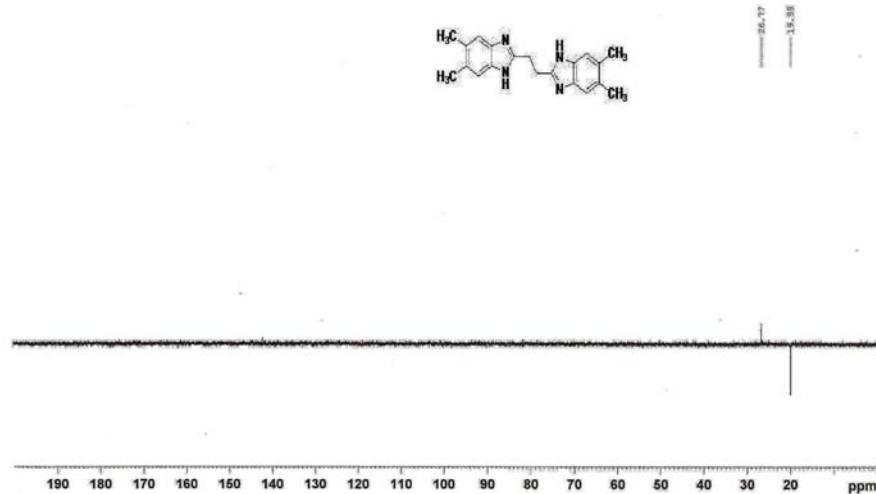


Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

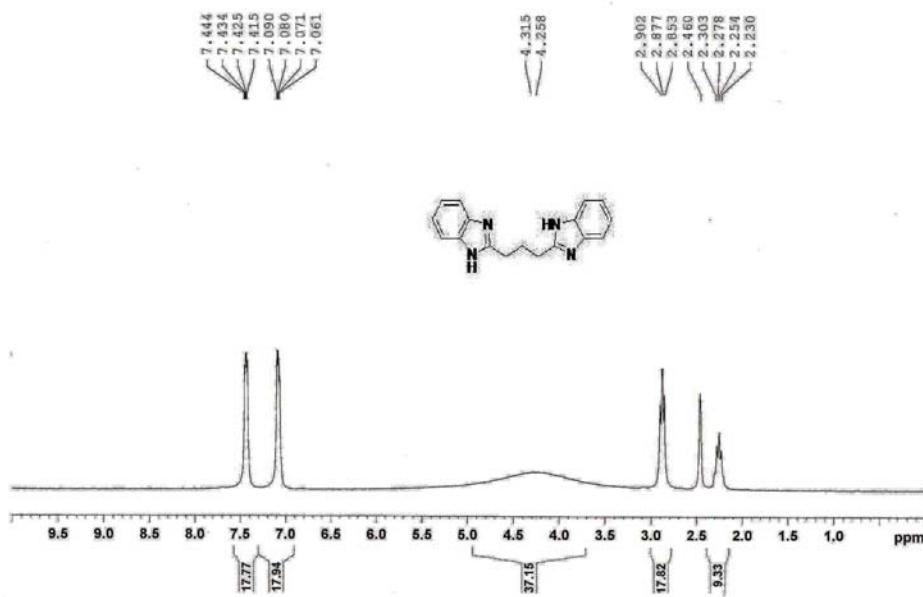
**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4j:**



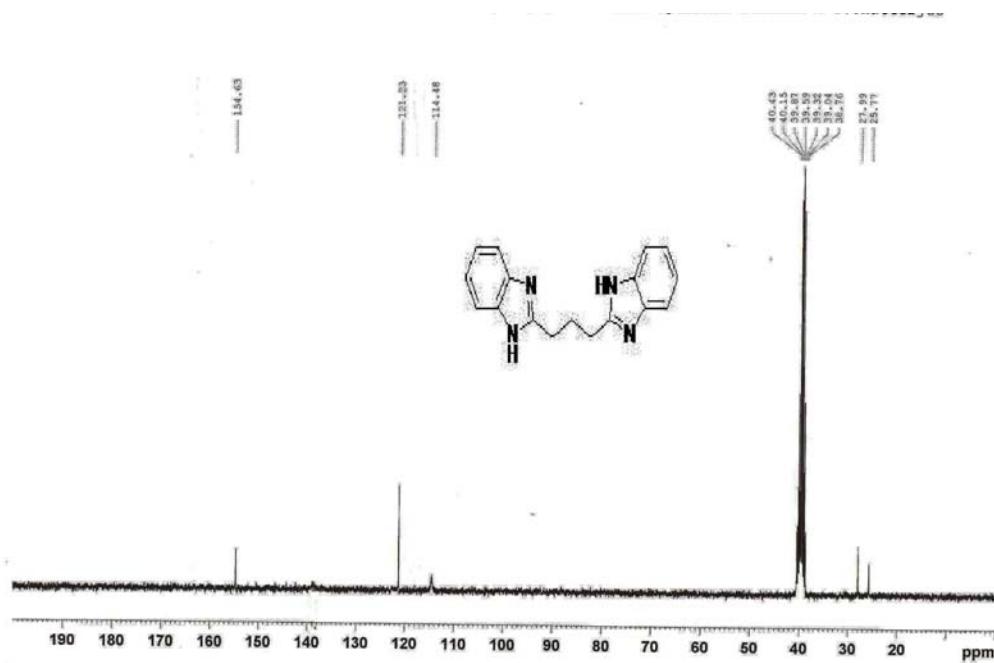
**Copy of pure DEPT-135 spectra of compound 4j:** no remaining signal in the aromatic region due to possible scrambling of the methyl groups; the inversed signal shows the presence of carbon atoms of the methylene groups.



**Copy of pure <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>) spectra of compound 4k:**

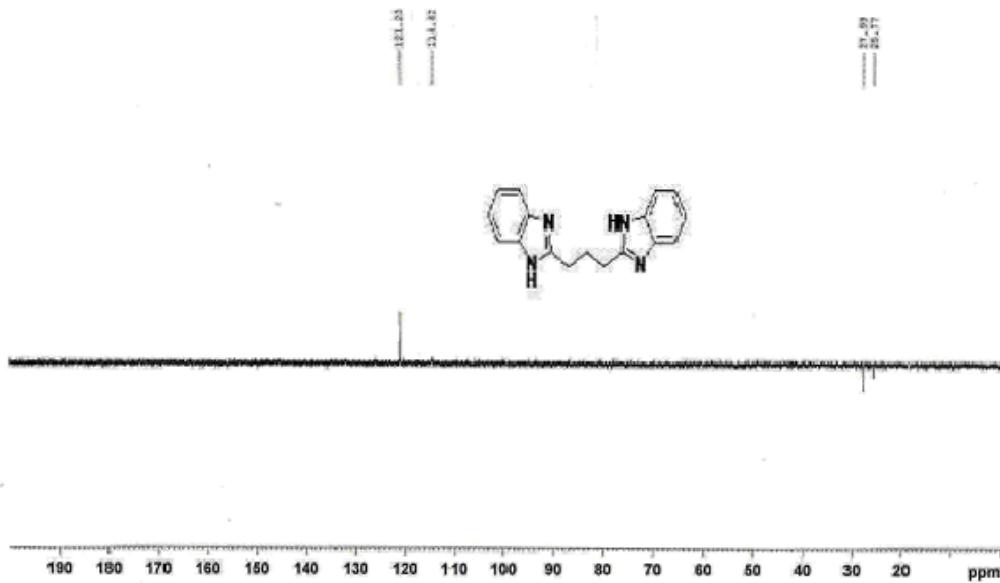


**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz,  $\text{DMSO}-d_6$ ) spectra of compound 4k:**



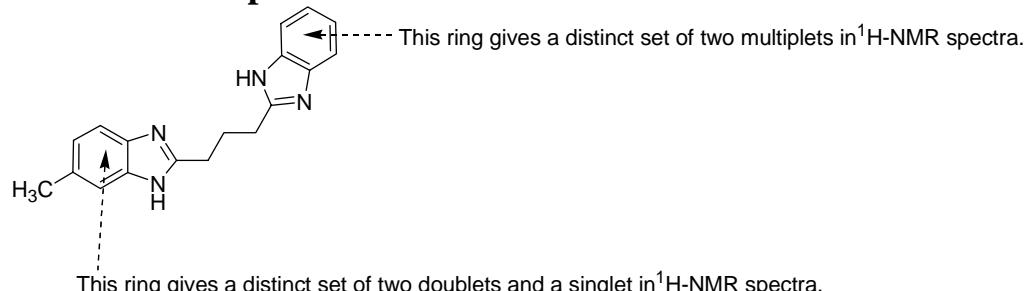
The two signals from left are due to quarternary carbons; the remaining four signals are due to hydrogen bearing carbon atoms.

**Copy of pure DEPT-135 spectra of compound 4k:**

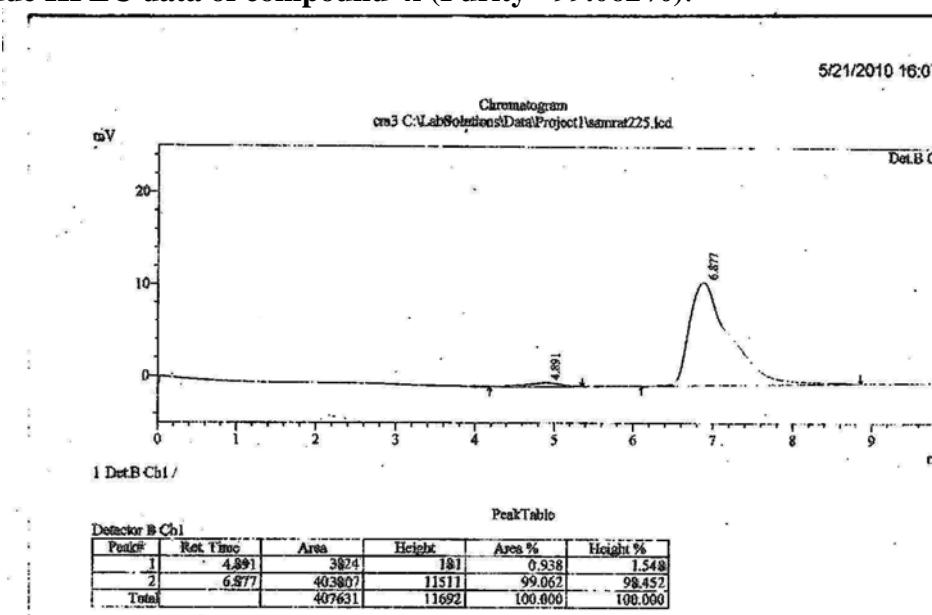


The signals due to quarternary carbon atoms disappear and the two inversed signals are due to the two types of carbon atoms from the three methylene groups present.

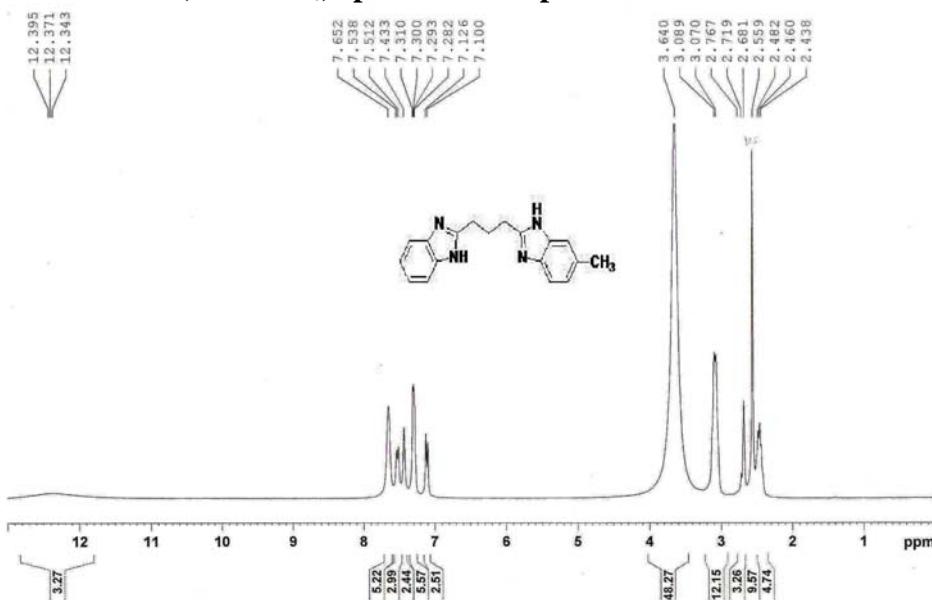
#### 4. HPLC data for compound 4l



**Copy of crude HPLC data of compound 4l (Purity= 99.062%):**



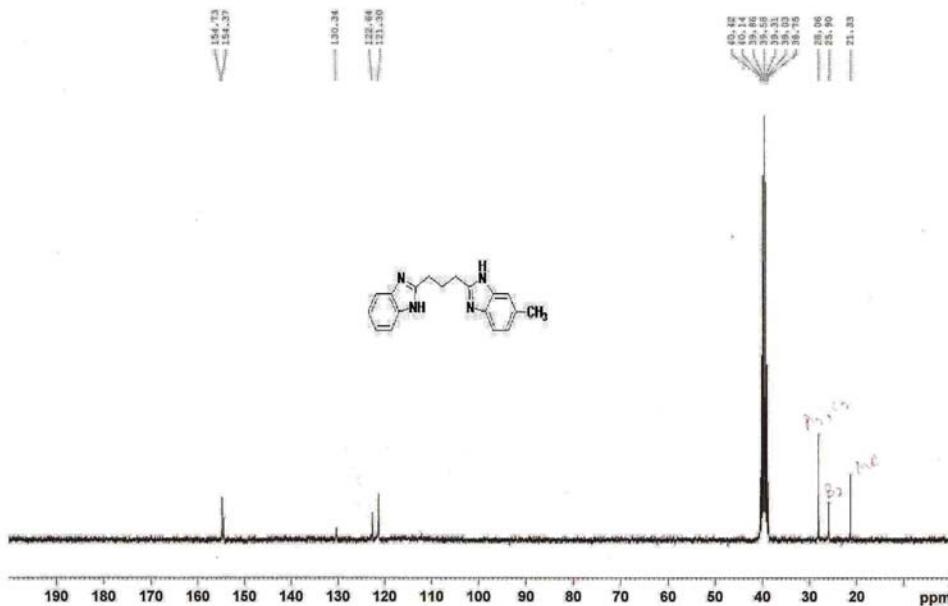
**Copy of crude  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4l:**



Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

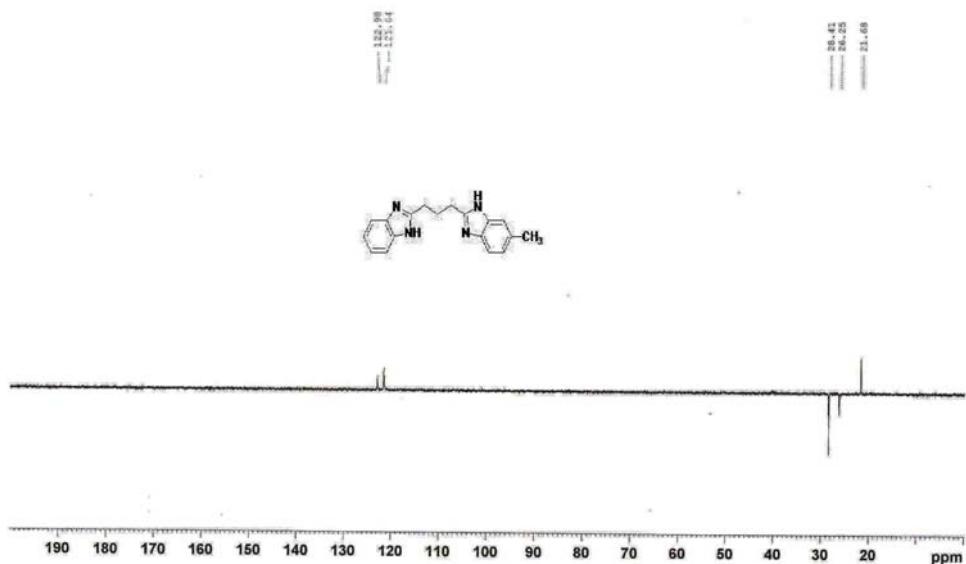
Ratio of the aromatic protons (from left to right): 2: 1: 1: 2: 1 (total 7 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the methyl group protons and the methylene group protons are also satisfactory.

#### Copy of crude $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4l:



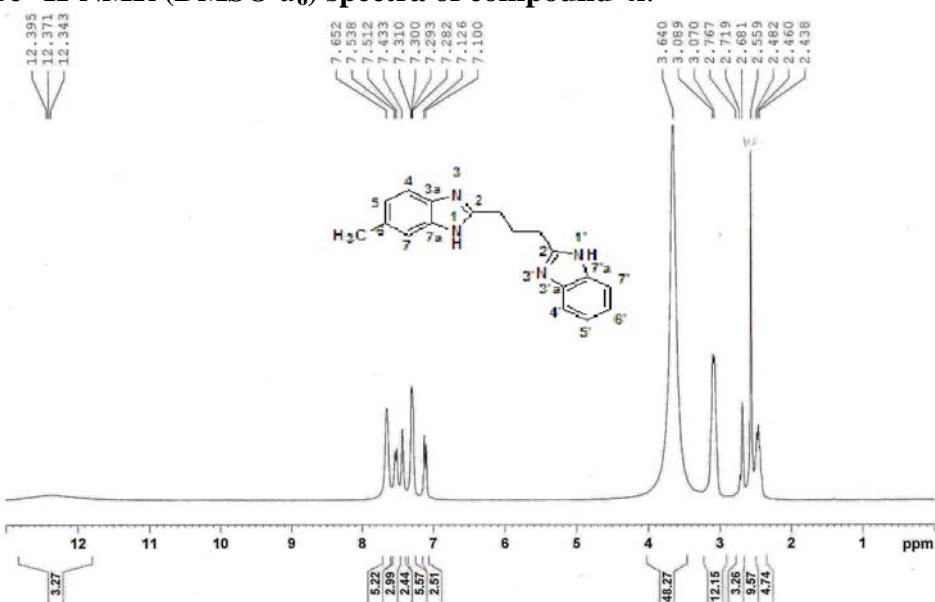
The signals beyond  $\delta$  130.0 are for the quarternary carbon atoms, the remaining five signals are for the hydrogen bearing carbon atoms.

#### Copy of crude DEPT-135 spectra of compound 4l:



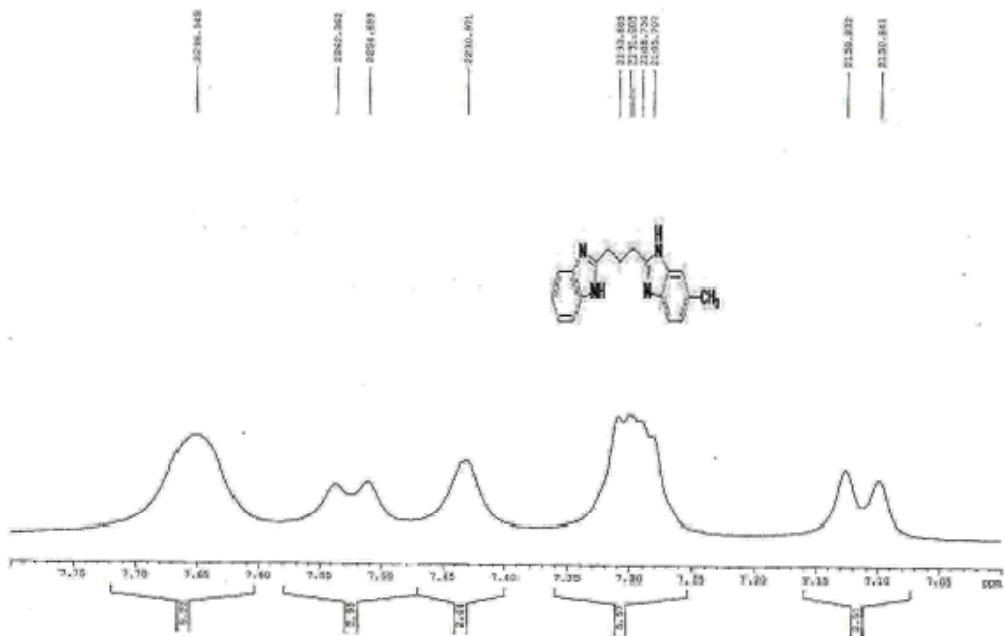
The hydrogen bearing carbon atoms remain in DEPT-135 experiment, the two inverted signals are for the methylene group carbon atoms of two different types.

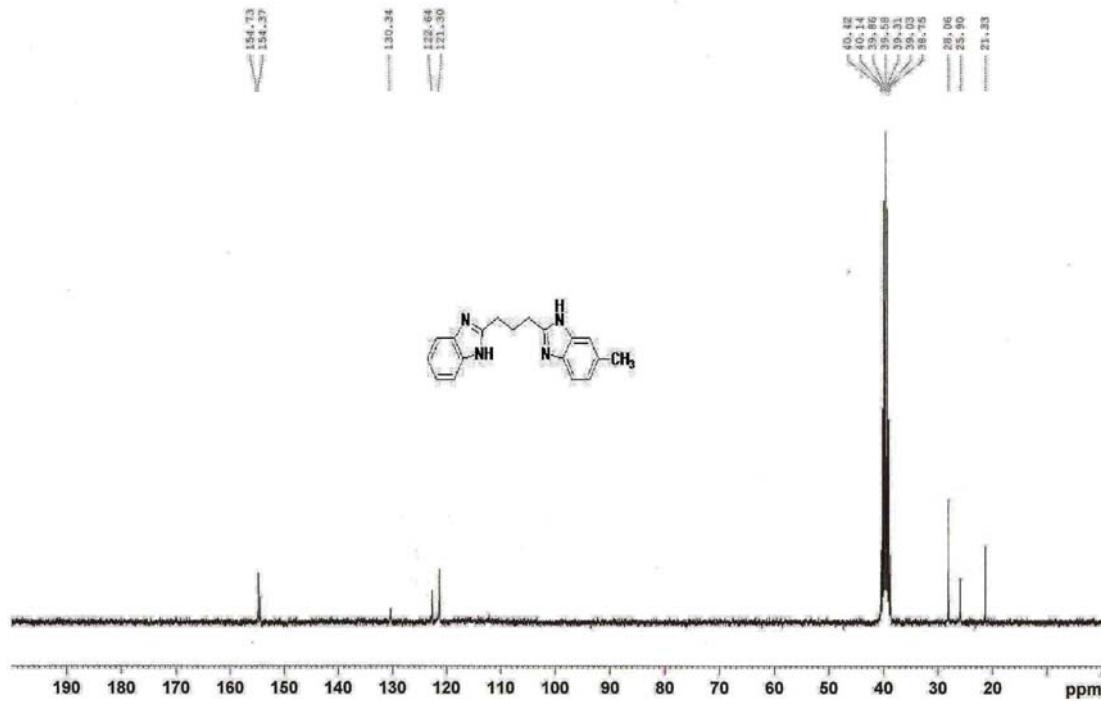
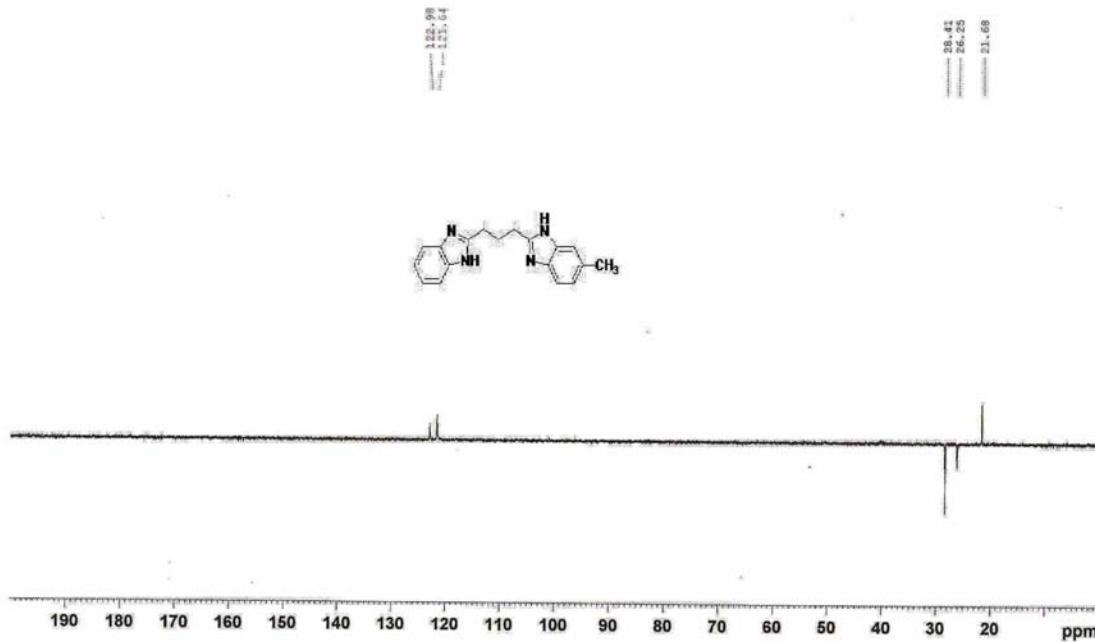
Copy of pure  $^1\text{H-NMR}$  ( $\text{DMSO-}d_6$ ) spectra of compound 4l:

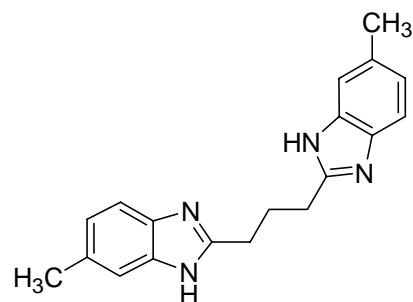


$\delta$  2.44-2.48 (m, 2H, C<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>), 2.56 (s, 3H, C<sub>6</sub>-CH<sub>3</sub>), 3.08 (d,  $J$ =5.7 Hz, 4H, C<sub>2</sub>-CH<sub>2</sub> and C<sub>2</sub>-CH<sub>2</sub>), 7.11(d,  $J$ =7.8 Hz, 1H, C<sub>5</sub>-H), 7.28-7.31 (m, 2H, C<sub>5</sub>-H and C<sub>6</sub>-H), 7.43 (s, 1H, C<sub>7</sub>-H), 7.53 (d,  $J$ =7.8 Hz, 1H, C<sub>4</sub>-H), 7.65 (br s, 2H, C<sub>4</sub>-H and C<sub>7</sub>-H) and 12.37 (br s, 2H, N<sub>1</sub>-H and N<sub>1</sub>-H)

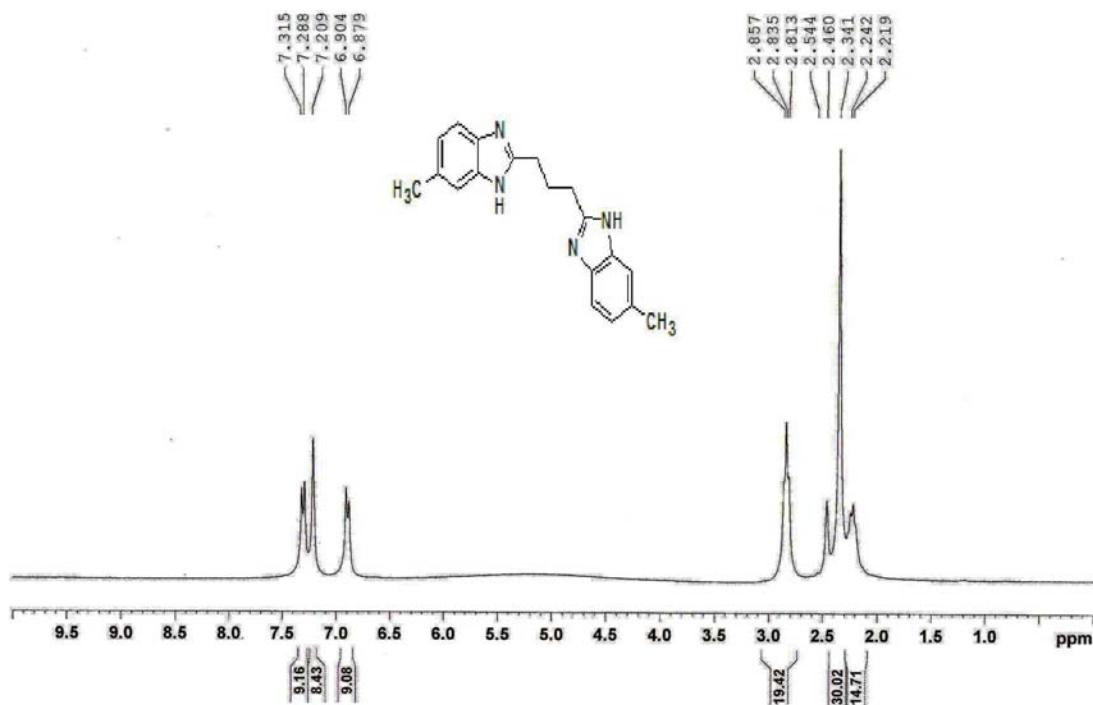
Expanded portion of the aromatic region of pure compound 4l showing the doublet-singlet-doublet(right-hand side ring) and multiplet patterns(left-hand side ring) of the two different halves of the heterodimeric compound.



**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4l:****Copy of pure DEPT-135 spectra of compound 4l:**



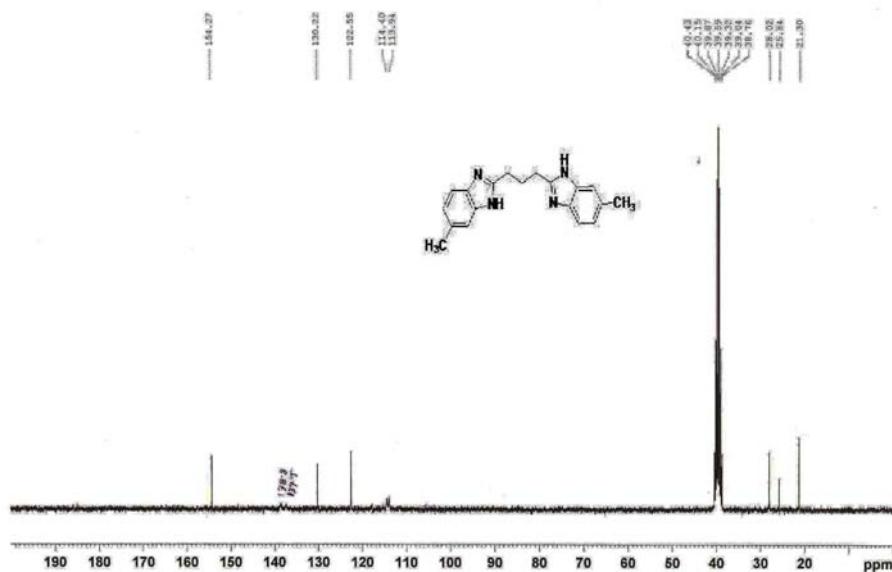
**Copy of pure  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4m:**



Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

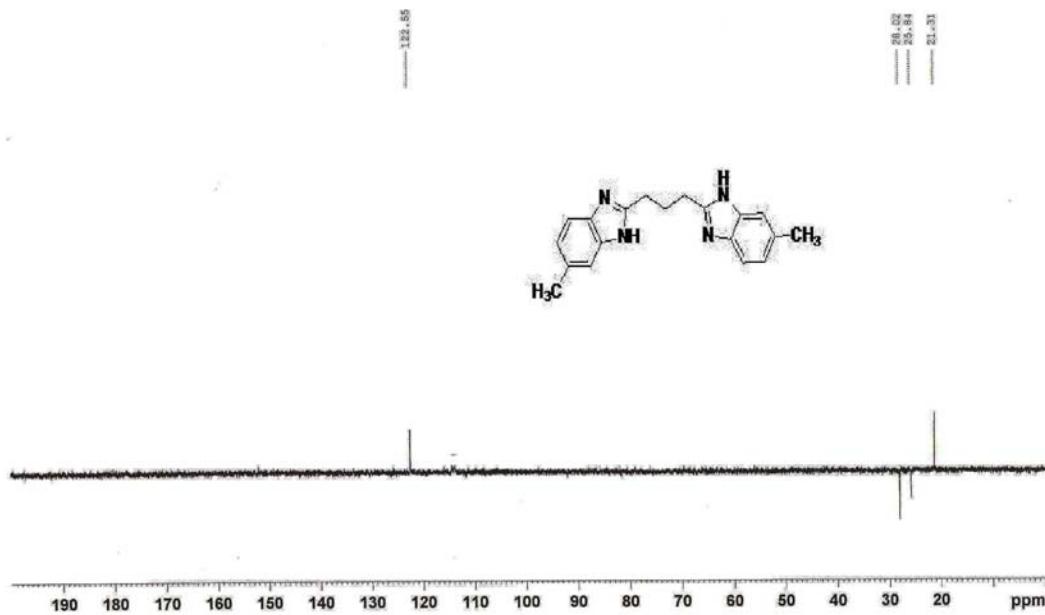
Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure simple bis-benzimidazole. Integration of the two methyl group protons and the methylene group protons are also satisfactory.

**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4m:**

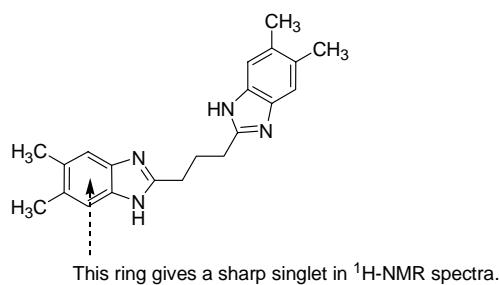


All the seven carbons of one half of the molecule have come separately, the left side four signals disappear in DEPT 135 experiment as they are quaternary carbons while the right side six signals remain in DEPT 135 experiment as they are hydrogen bearing carbons along with the two inversed signals for the two types of carbons of the methylene groups. This convincingly proves the presence of pure simple bis-benzimidazole.

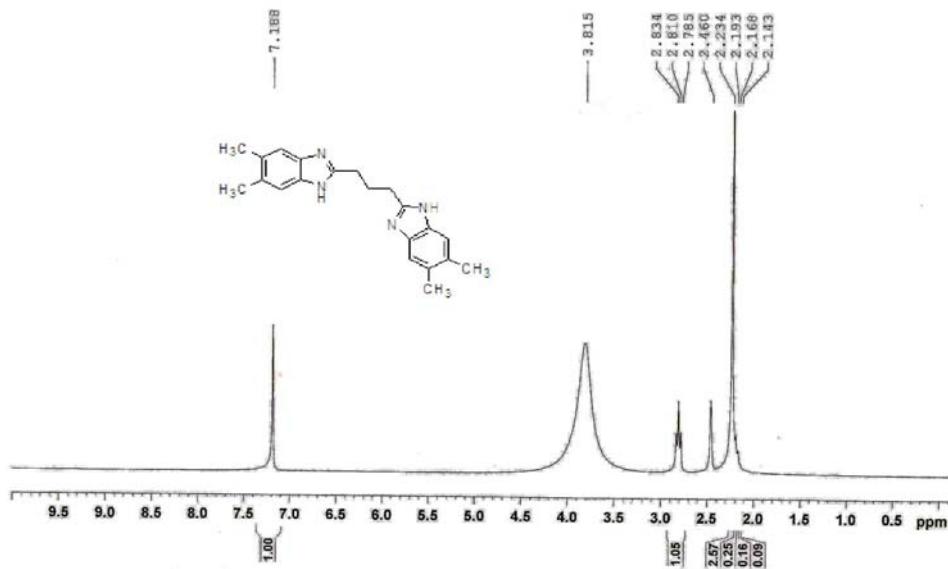
**Copy of pure DEPT-135 spectra of compound 4m:**



As stated earlier, the disappearance and inversion of signals is seen clearly in DEPT-135 experiment.

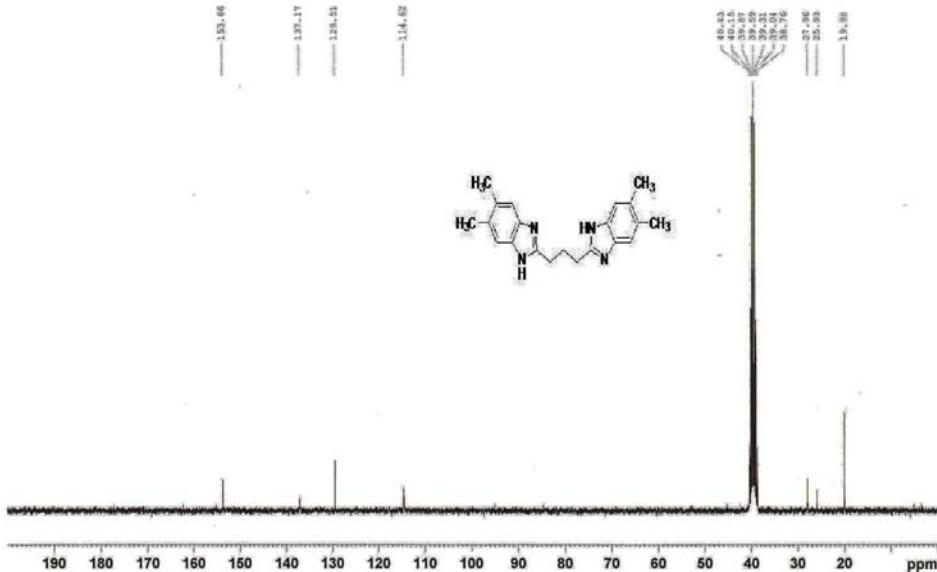


**Copy of pure  $^1\text{H}$ -NMR (DMSO- $d_6$ ) spectra of compound 4n:**



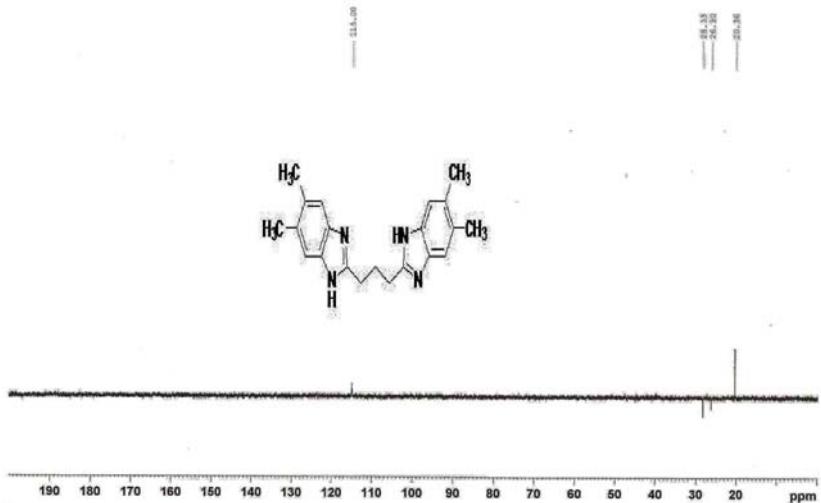
Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4n:**

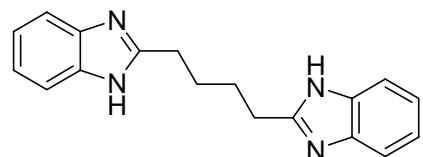


The three signals from left are due to the quarternary carbons.

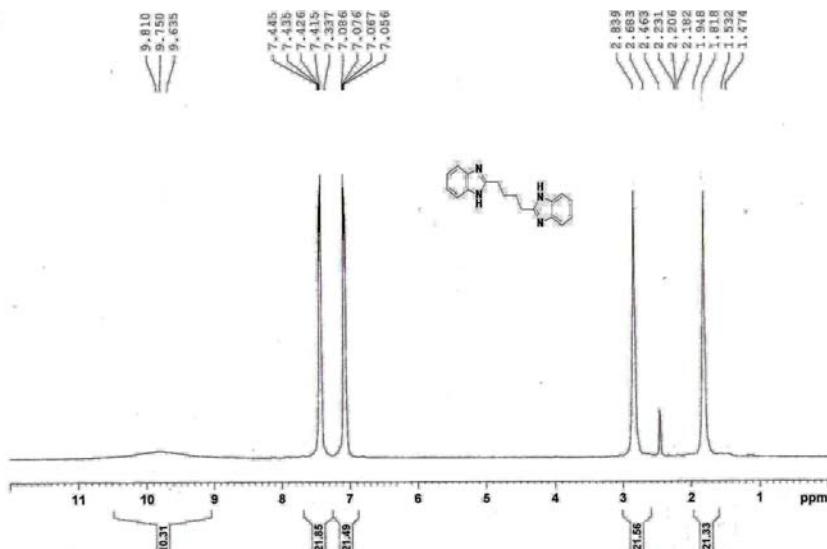
## Copy of pure DEPT-135 spectra of compound 4n:



The signals for the quarternary carbon atoms disappear and the inversed signals are due to the methylene carbon atoms.

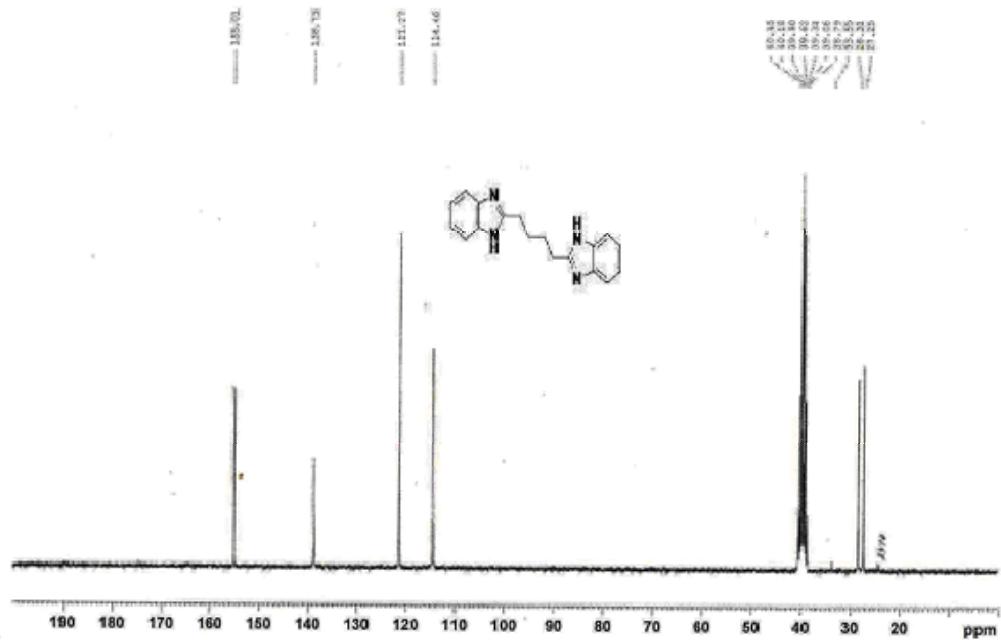


**Copy of pure  $^1\text{H-NMR}$  ( $\text{DMSO-}d_6$ ) spectra of compound 4o:**



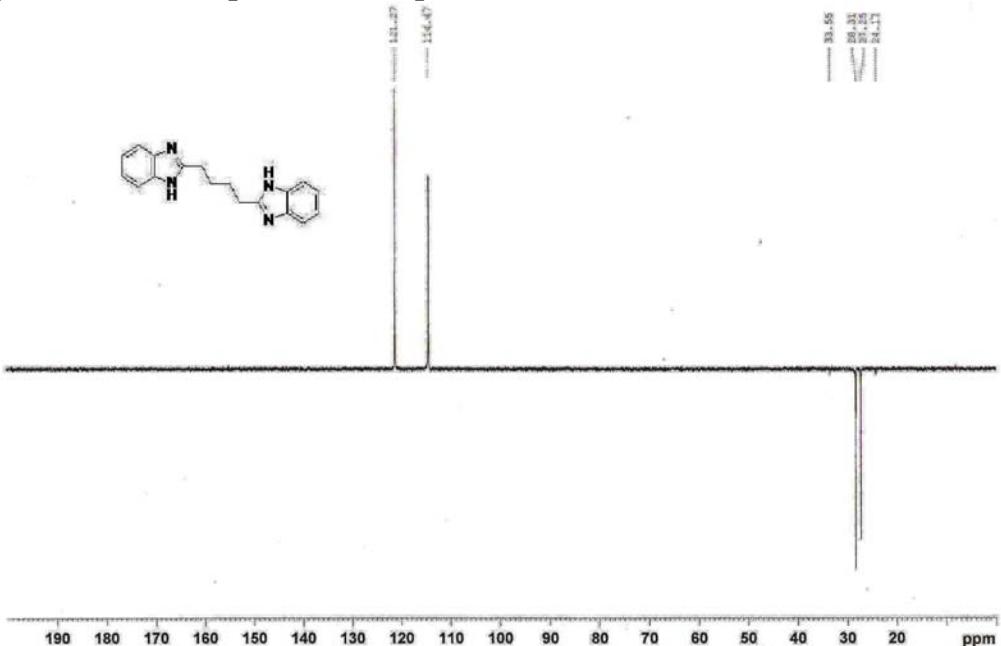
Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d^6$ ) spectra of compound 4o:

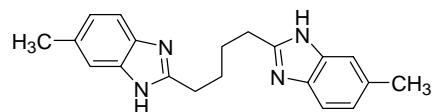


The two signals from the left are the quarternary carbon atoms, the rest are the hydrogen bearing carbon atoms.

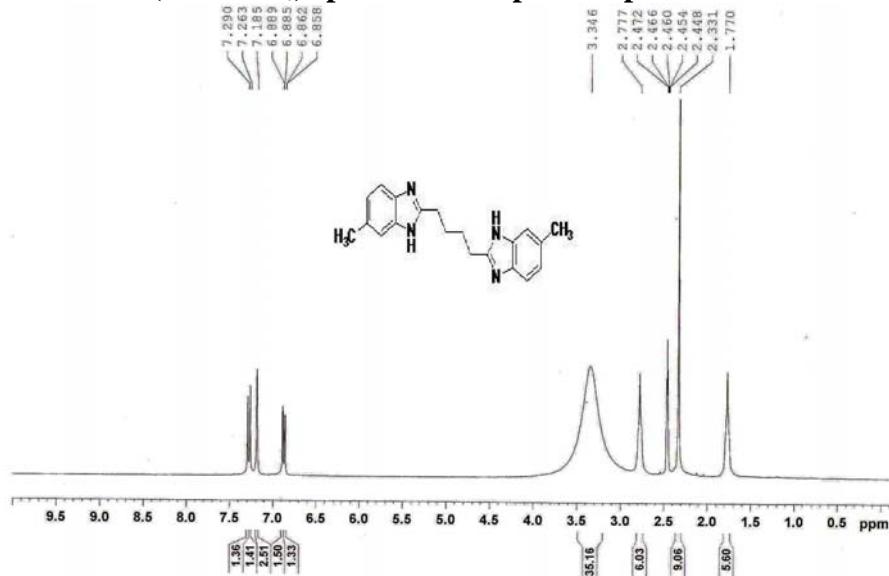
### **Copy of pure DEPT-135 spectra of compound 4o:**



The quarternary carbon signals disappear and the methylene carbon signals are inversed in DEPT-135 experiment.



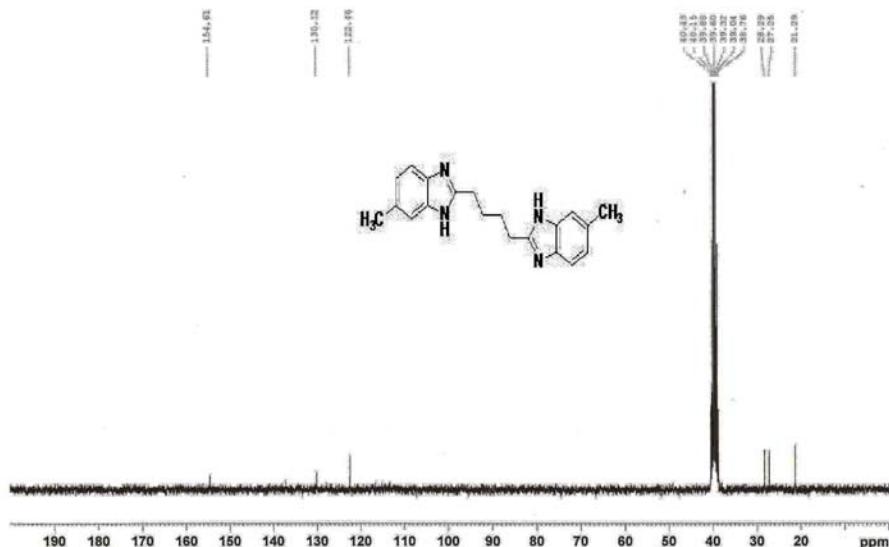
**Copy of pure <sup>1</sup>H-NMR (DMSO-d<sub>6</sub>) spectra of compound 4p:**



Each individual peak has been assigned both in <sup>1</sup>H and in <sup>13</sup>C NMR (please see the details of assignment).

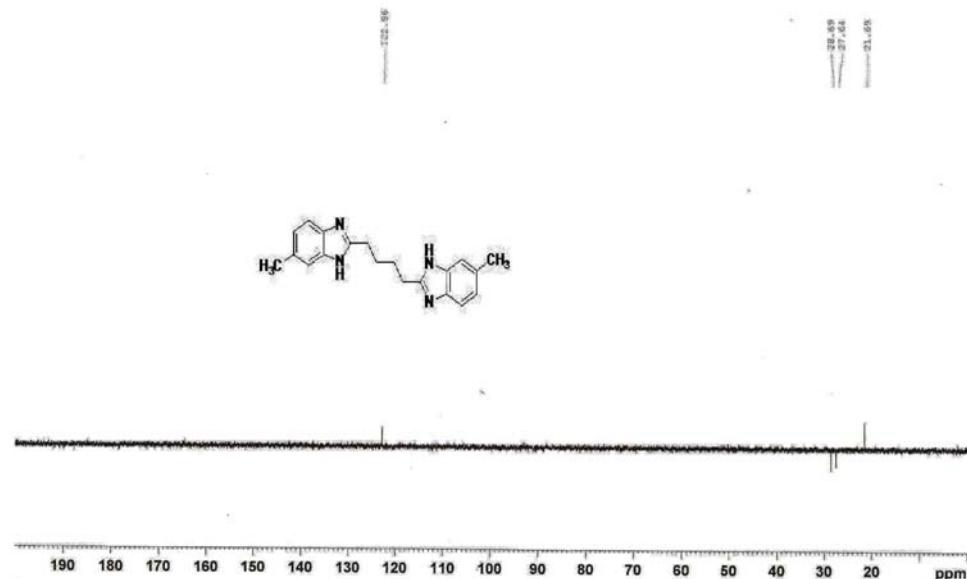
Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the methylene group protons is also satisfactory.

**Copy of pure <sup>13</sup>C-NMR (75 MHz, DMSO-d<sub>6</sub>) spectra of compound 4p:**

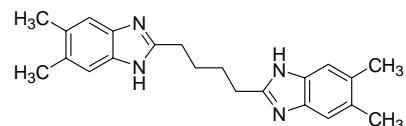


The two signals from left are for the quarternary carbon atoms, the rest are the hydrogen bearing carbon atoms.

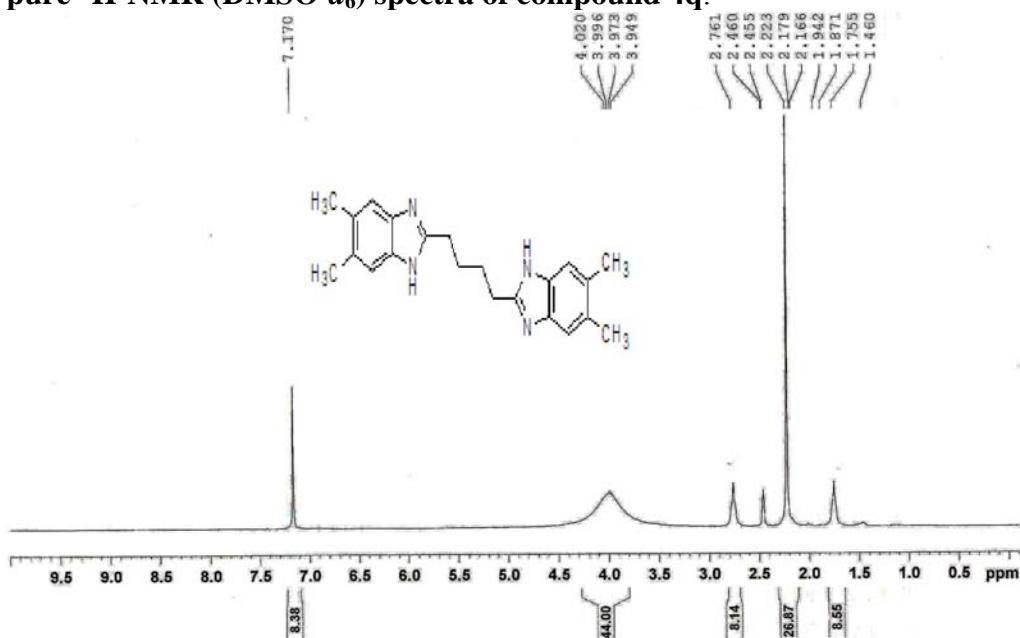
**Copy of pure DEPT-135 spectra of compound 4p:**



The quarternary carbon atom signals disappear and those for the methylene carbon atoms are inverted.

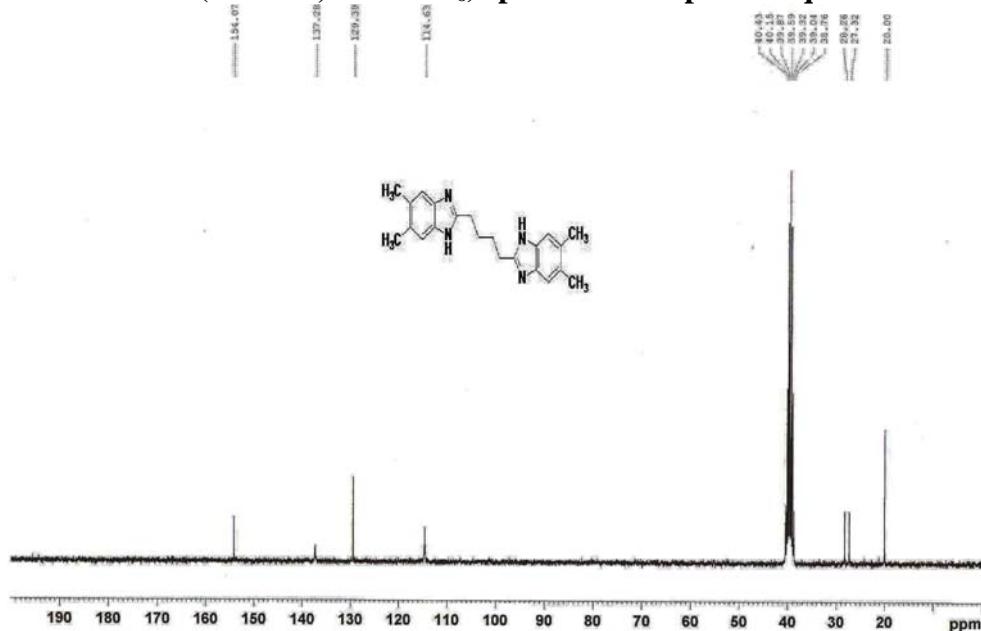


**Copy of pure  $^1\text{H}$ -NMR ( $\text{DMSO}-d_6$ ) spectra of compound 4q:**



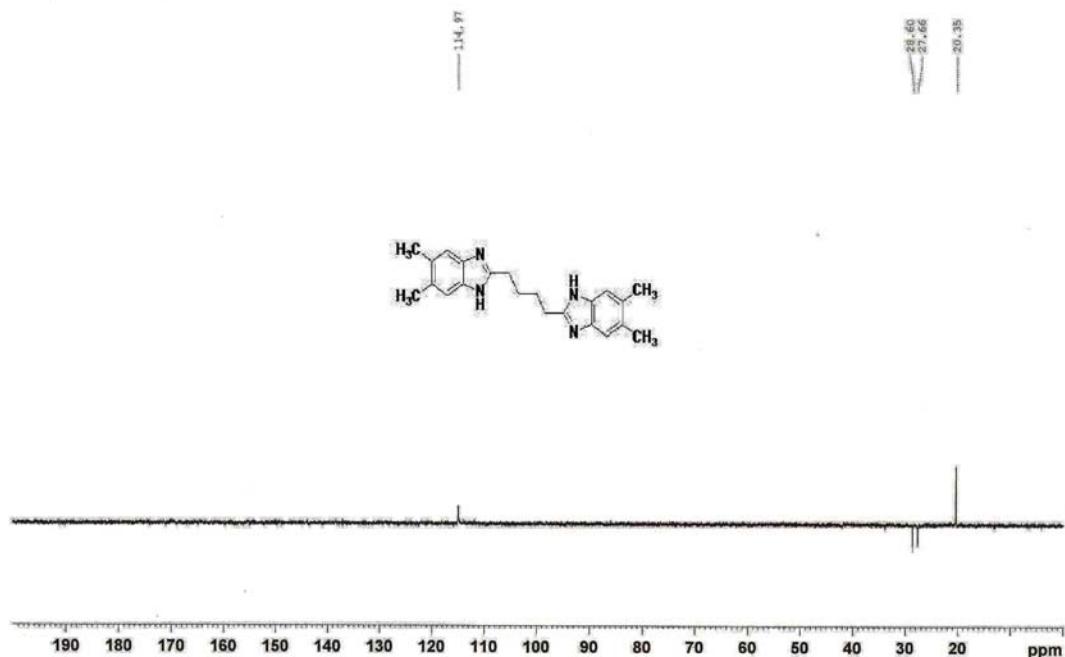
Each individual peak has been assigned both in  $^1\text{H}$  and in  $^{13}\text{C}$  NMR (please see the details of assignment).

**Copy of pure  $^{13}\text{C}$ -NMR (75 MHz, DMSO- $d_6$ ) spectra of compound 4q:**



The three signals from the left are for the quarternary carbon atoms , the rest are for the hydrogen bearing carbon atoms

**Copy of pure DEPT-135 spectra of compound 4q:**



The signals for the quarternary carbon atoms disappear and the methylene carbon atom signals are inversed.

## 5. Computational Details

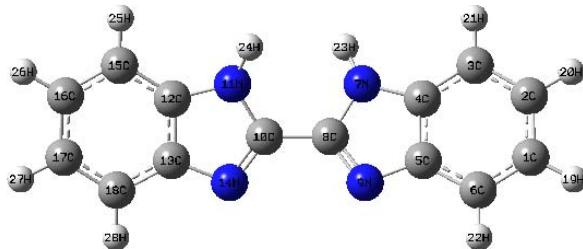
This work is cited as:

Gaussian 03, Revision B.03,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,  
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,  
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,  
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,  
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,  
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,  
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,  
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,  
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,  
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,  
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,  
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,  
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,  
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,  
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,  
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,  
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,  
Gaussian, Inc., Pittsburgh PA, 2003.

B3LYP/6-31G (Gaussian 03: x86-Win32-G03RevB.03 4-May-2003) optimized structures of the most probable isomers of the synthesized bis-1*H*-benzimidazoles (compounds **4a**, **4c**, **4d**, **4e**, **4f**, **4h**, **4l** and **4q**). All optimized energies are given in Hartree-Fock unit.

## Compound 4a : cis-isomer

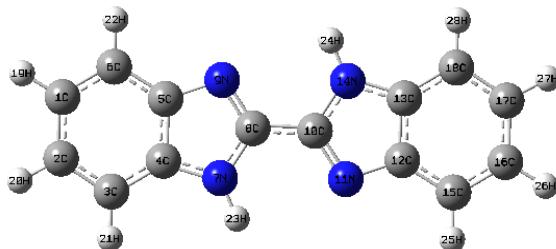


HF=-758.5611264

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.186103	-0.634025	0.189040
2	6	0	5.153207	0.724421	-0.188262
3	6	0	3.950947	1.399625	-0.380540
4	6	0	2.781854	0.662724	-0.184621
5	6	0	2.794856	-0.705347	0.184224
6	6	0	4.017694	-1.361649	0.380633
7	7	0	1.438584	0.988793	-0.266275
8	6	0	0.728907	-0.177057	0.005343
9	7	0	1.504260	-1.194436	0.296722
10	6	0	-0.728881	-0.177095	-0.005864
11	7	0	-1.438471	0.988992	0.265592
12	6	0	-2.781841	0.662747	0.184415
13	6	0	-2.794979	-0.705260	-0.184357
14	7	0	-1.504239	-1.194396	-0.297124
15	6	0	-3.950841	1.399636	0.380720
16	6	0	-5.153197	0.724401	0.188842
17	6	0	-5.186183	-0.634004	-0.188437
18	6	0	-4.017783	-1.361631	-0.380393
19	1	0	6.147674	-1.117823	0.330557
20	1	0	6.088148	1.257853	-0.330536
21	1	0	3.931170	2.446384	-0.668158
22	1	0	4.034191	-2.407424	0.668380
23	1	0	1.059143	1.807521	-0.717285
24	1	0	-1.059210	1.806904	0.718280
25	1	0	-3.930996	2.446409	0.668267
26	1	0	-6.088087	1.257841	0.331416
27	1	0	-6.147772	-1.117855	-0.329666
28	1	0	-4.034372	-2.407405	-0.668123

## Compound 4a : trans-isomer

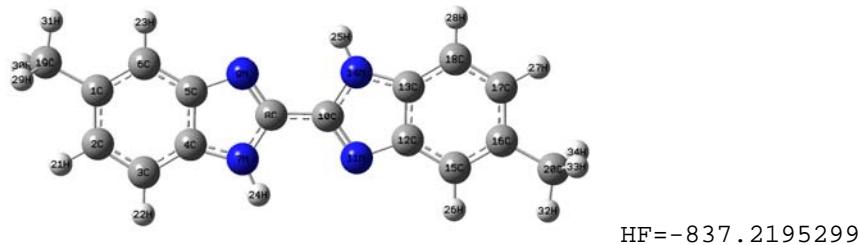


HF=-758.5796288

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.143938	0.744969	0.000023
2	6	0	-5.176178	-0.665208	0.000158
3	6	0	-4.008437	-1.422173	0.000145
4	6	0	-2.803241	-0.716929	0.000046
5	6	0	-2.751389	0.703126	-0.000100
6	6	0	-3.942182	1.442630	-0.000149
7	7	0	-1.481403	-1.114728	-0.000064
8	6	0	-0.722619	0.029936	0.000019
9	7	0	-1.436572	1.137940	-0.000039
10	6	0	0.722622	-0.030058	-0.000109
11	7	0	1.436630	-1.138022	-0.000245
12	6	0	2.751428	-0.703137	-0.000017
13	6	0	2.803203	0.716924	0.000009
14	7	0	1.481348	1.114653	0.000117
15	6	0	3.942252	-1.442587	0.000024
16	6	0	5.143977	-0.744873	0.000014
17	6	0	5.176148	0.665305	0.000059
18	6	0	4.008373	1.422216	0.000089
19	1	0	-6.081075	1.293173	0.000005
20	1	0	-6.135825	-1.173065	0.000249
21	1	0	-4.037763	-2.507200	0.000174
22	1	0	-3.911477	2.527142	-0.000276
23	1	0	-1.094206	-2.046818	-0.000204
24	1	0	1.094057	2.046706	0.000113
25	1	0	3.911589	-2.527101	0.000007
26	1	0	6.081140	-1.293034	0.000015
27	1	0	6.135770	1.173211	0.000089
28	1	0	4.037654	2.507245	0.000188

## Compound 4c: symmetrical trans-isomer

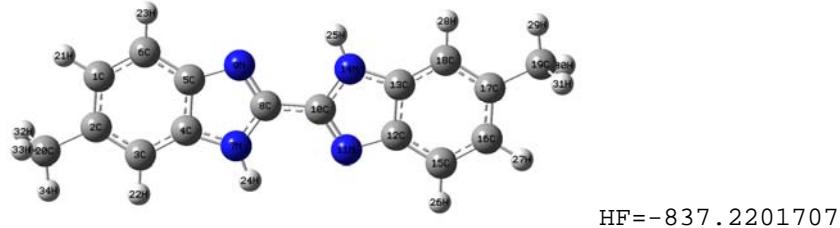


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.207051	0.318836	-0.000370
2	6	0	-5.099806	-1.094666	-0.000090
3	6	0	-3.876182	-1.753331	0.000215
4	6	0	-2.730296	-0.955141	0.000232
5	6	0	-2.802408	0.461331	-0.000051
6	6	0	-4.052496	1.096942	-0.000374
7	7	0	-1.378958	-1.238604	0.000237
8	6	0	-0.722264	-0.032801	0.000164
9	7	0	-1.530799	1.009350	0.000323
10	6	0	0.722262	0.032785	0.000205
11	7	0	1.530806	-1.009362	0.000400
12	6	0	2.802406	-0.461333	0.000082
13	6	0	2.730288	0.955130	0.000271
14	7	0	1.378953	1.238591	0.000557
15	6	0	4.052505	-1.096945	-0.000247
16	6	0	5.207047	-0.318841	-0.000371
17	6	0	5.099797	1.094676	-0.000200
18	6	0	3.876179	1.753331	0.000125
19	6	0	-6.575856	0.960806	-0.000446
20	6	0	6.575869	-0.960770	-0.000510
21	1	0	-6.012391	-1.685129	-0.000134
22	1	0	-3.821172	-2.837474	0.000342
23	1	0	-4.107013	2.181294	-0.000513
24	1	0	-0.912943	-2.133785	0.000432
25	1	0	0.912931	2.133768	0.000757
26	1	0	4.107013	-2.181297	-0.000343
27	1	0	6.012388	1.685127	-0.000308
28	1	0	3.821149	2.837474	0.000259
29	1	0	-7.156723	0.666855	0.881655
30	1	0	-7.157949	0.663993	-0.880759

31	1	0	-6.503251	2.051573	-0.002236
32	1	0	6.503303	-2.051541	-0.002111
33	1	0	7.156830	-0.666651	0.881471
34	1	0	7.157848	-0.664086	-0.880944

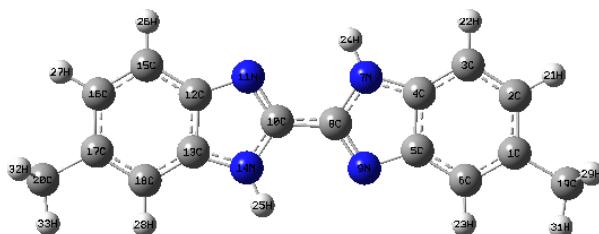
**Compound 4c** : most stable symmetrical trans-isomer



Standard orientation:

Center Number	Atomic Number		Coordinates (Angstroms)		
		Type	X	Y	Z
1	6	0	5.070292	-1.132192	0.000376
2	6	0	5.231330	0.276517	0.000386
3	6	0	4.108051	1.102837	0.000101
4	6	0	2.851596	0.492256	-0.000124
5	6	0	2.687149	-0.916516	-0.000189
6	6	0	3.822884	-1.738947	0.000091
7	7	0	1.565937	0.993863	-0.000360
8	6	0	0.717530	-0.087409	-0.000575
9	7	0	1.342911	-1.248068	-0.000672
10	6	0	-0.717528	0.087365	-0.000529
11	7	0	-1.342892	1.248037	-0.000436
12	6	0	-2.687137	0.916505	-0.000094
13	6	0	-2.851602	-0.492262	0.000015
14	7	0	-1.565949	-0.993888	-0.000230
15	6	0	-3.822862	1.738949	0.000083
16	6	0	-5.070280	1.132211	0.000308
17	6	0	-5.231337	-0.276497	0.000365
18	6	0	-4.108063	-1.102828	0.000190
19	6	0	-6.621750	-0.868071	0.000380
20	6	0	6.621736	0.868116	0.000488
21	1	0	5.961969	-1.753764	0.000596
22	1	0	4.213828	2.183884	0.000180
23	1	0	3.717010	-2.818840	0.000088
24	1	0	1.254221	1.953722	-0.000168
25	1	0	-1.254268	-1.953759	0.000076

26	1	0	-3.716981	2.818841	0.000040
27	1	0	-5.961937	1.753810	0.000448
28	1	0	-4.213857	-2.183875	0.000283
29	1	0	-6.592696	-1.961008	-0.000413
30	1	0	-7.191309	-0.548554	-0.880085
31	1	0	-7.190729	-0.549822	0.881671
32	1	0	7.190846	0.549802	-0.880705
33	1	0	7.191178	0.548703	0.881057
34	1	0	6.592624	1.961053	0.001176

Compound **4c** : unsymmetrical trans-isomer

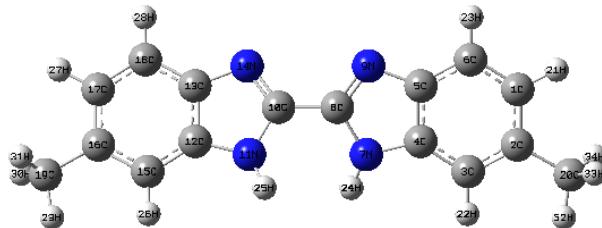
HF=-837.2198856

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.165306	-0.566883	-0.000327
2	6	0	5.177433	0.850631	-0.000046
3	6	0	4.013649	1.610080	0.000281
4	6	0	2.804570	0.911383	0.000178
5	6	0	2.757130	-0.506128	-0.000071
6	6	0	3.949188	-1.244844	-0.000279
7	7	0	1.481833	1.307777	0.000488
8	6	0	0.725901	0.161555	0.000227
9	7	0	1.443859	-0.945030	-0.000066
10	6	0	-0.718966	0.216723	0.000239
11	7	0	-1.439116	1.321081	-0.000225
12	6	0	-2.750888	0.878214	-0.000110
13	6	0	-2.796815	-0.539514	0.000214
14	7	0	-1.473793	-0.931701	0.000616
15	6	0	-3.951517	1.602741	-0.000446
16	6	0	-5.143748	0.893731	-0.000385
17	6	0	-5.186227	-0.523617	0.000003
18	6	0	-3.997798	-1.253050	0.000408
19	6	0	6.474956	-1.322194	-0.000307

20	6	0	-6.522183	-1.229478	-0.000216
21	1	0	6.136438	1.362265	-0.000089
22	1	0	4.050303	2.694998	0.000492
23	1	0	3.912022	-2.329949	-0.000532
24	1	0	1.092646	2.238934	0.000294
25	1	0	-1.082301	-1.861961	0.000240
26	1	0	-3.936315	2.687716	-0.000691
27	1	0	-6.084304	1.438485	-0.000642
28	1	0	-4.012703	-2.339130	0.000778
29	1	0	7.078788	-1.078114	0.881590
30	1	0	7.079805	-1.076191	-0.880950
31	1	0	6.310424	-2.402943	-0.001559
32	1	0	-7.116056	-0.959843	0.880897
33	1	0	-6.401924	-2.316194	-0.000729
34	1	0	-7.116255	-0.959056	-0.880963

## Compound 4c: unstable cis-isomer

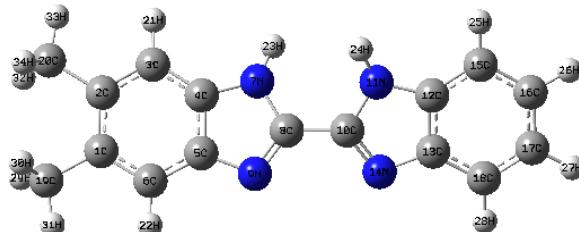


HF=-837.2017569

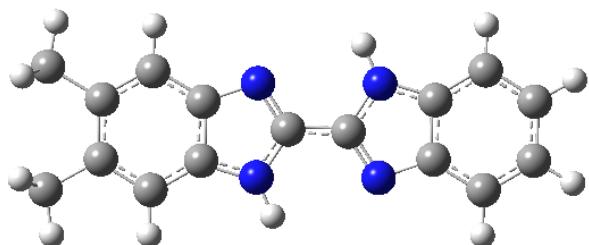
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.180800	0.805814	0.290047
2	6	0	5.171531	-0.560665	-0.086925
3	6	0	3.956715	-1.213954	-0.296478
4	6	0	2.785237	-0.473553	-0.125413
5	6	0	2.790663	0.892844	0.240061
6	6	0	4.015552	1.539642	0.457773
7	7	0	1.444198	-0.799549	-0.234094
8	6	0	0.728285	0.367588	0.020743
9	7	0	1.499397	1.384605	0.325835
10	6	0	-0.728281	0.367579	-0.020908
11	7	0	-1.444135	-0.799723	0.233700
12	6	0	-2.785231	-0.473542	0.125425

13	6	0	-2.790682	0.892817	-0.240065
14	7	0	-1.499400	1.384571	-0.325954
15	6	0	-3.956698	-1.213958	0.296502
16	6	0	-5.171523	-0.560663	0.087088
17	6	0	-5.180816	0.805835	-0.289857
18	6	0	-4.015577	1.539639	-0.457703
19	6	0	-6.480242	-1.296223	0.258604
20	6	0	6.480232	-1.296224	-0.258593
21	1	0	6.140401	1.290238	0.450835
22	1	0	3.933283	-2.261884	-0.582514
23	1	0	4.037123	2.585773	0.744350
24	1	0	1.073874	-1.619382	-0.690515
25	1	0	-1.074030	-1.618621	0.692016
26	1	0	-3.933244	-2.261880	0.582567
27	1	0	-6.140430	1.290270	-0.450535
28	1	0	-4.037143	2.585779	-0.744247
29	1	0	-6.320091	-2.345487	0.521289
30	1	0	-7.076495	-1.269096	-0.660689
31	1	0	-7.090841	-0.844157	1.048953
32	1	0	6.320046	-2.345634	-0.520691
33	1	0	7.076871	-1.268573	0.660420
34	1	0	7.090458	-0.844540	-1.049457

Compound **4d** : cis-isomer

7	7	0	-0.665134	0.990622	-0.202875
8	6	0	0.048065	-0.189130	-0.006239
9	7	0	-0.725619	-1.224742	0.220515
10	6	0	1.505477	-0.183794	-0.017155
11	7	0	2.209988	0.967168	0.323962
12	6	0	3.554936	0.653096	0.224173
13	6	0	3.574568	-0.690586	-0.225245
14	7	0	2.286190	-1.178282	-0.367996
15	6	0	4.720392	1.382520	0.463949
16	6	0	5.926311	0.725806	0.232873
17	6	0	5.965777	-0.607423	-0.224395
18	6	0	4.800620	-1.327941	-0.459355
19	6	0	-5.753307	-1.387387	0.305608
20	6	0	-5.689864	1.488061	-0.302474
21	1	0	-3.165385	2.452257	-0.512472
22	1	0	-3.254980	-2.454509	0.512754
23	1	0	-0.288987	1.834684	-0.607534
24	1	0	1.825814	1.755394	0.822681
25	1	0	4.695416	2.410432	0.812768
26	1	0	6.858547	1.254474	0.407243
27	1	0	6.929621	-1.077579	-0.393876
28	1	0	4.822356	-2.354794	-0.808454
29	1	0	-6.362520	-1.319815	-0.603898
30	1	0	-6.352516	-0.958899	1.118254
31	1	0	-5.604215	-2.447069	0.526778
32	1	0	-6.309064	1.081168	-1.111004
33	1	0	-5.498501	2.540368	-0.528184
34	1	0	-6.299009	1.448180	0.608648

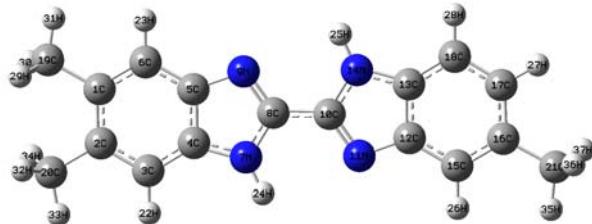
Compound **4d** : stable trans-isomer

HF=-837.2191376

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.389875	0.733642	0.000000
2	6	0	-4.420035	-0.694827	-0.000001
3	6	0	-3.234556	-1.429268	-0.000012
4	6	0	-2.026476	-0.731217	-0.000022
5	6	0	-1.977592	0.683751	-0.000021
6	6	0	-3.174446	1.411955	-0.000010
7	7	0	-0.704493	-1.129308	0.000069
8	6	0	0.052633	0.017076	0.000001
9	7	0	-0.664619	1.123797	-0.000027
10	6	0	1.497560	-0.038210	0.000002
11	7	0	2.217438	-1.142659	-0.000018
12	6	0	3.530083	-0.700991	-0.000008
13	6	0	3.574837	0.719373	0.000019
14	7	0	2.250961	1.110297	-0.000066
15	6	0	4.724715	-1.434043	-0.000020
16	6	0	5.923175	-0.730280	-0.000005
17	6	0	5.948305	0.679805	0.000022
18	6	0	4.776320	1.430610	0.000034
19	6	0	-5.682619	1.516584	0.000012
20	6	0	-5.742918	-1.423765	0.000010
21	1	0	-3.261496	-2.515112	-0.000013
22	1	0	-3.145148	2.497320	-0.000080
23	1	0	-0.316317	-2.060833	-0.000014
24	1	0	1.858242	2.040033	0.000138
25	1	0	4.699656	-2.518730	0.000005
26	1	0	6.863032	-1.273880	-0.000014
27	1	0	6.905271	1.192744	0.000033
28	1	0	4.799975	2.515813	0.000055
29	1	0	-6.297173	1.291289	0.880180
30	1	0	-6.297944	1.290102	-0.879305
31	1	0	-5.487084	2.591810	-0.000788
32	1	0	-6.347303	-1.169733	0.879289
33	1	0	-5.596105	-2.506901	0.000151
34	1	0	-6.347272	-1.169984	-0.879359

## Compound 4e: trans-isomer

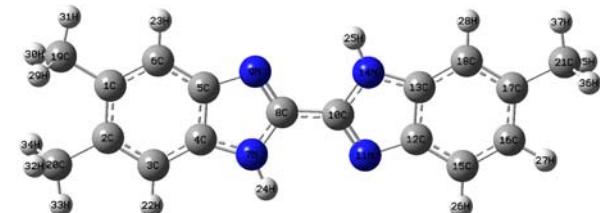


HF=-876.5390786

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.827827	0.632826	0.000057
2	6	0	-4.799253	-0.795634	0.000010
3	6	0	-3.584487	-1.480555	0.000045
4	6	0	-2.406182	-0.733396	0.000127
5	6	0	-2.415324	0.682342	0.000175
6	6	0	-3.641245	1.360549	0.000139
7	7	0	-1.069039	-1.076841	-0.000006
8	6	0	-0.359284	0.099584	0.000182
9	7	0	-1.121410	1.176029	0.000293
10	6	0	1.086562	0.100915	0.000109
11	7	0	1.848184	-0.976146	-0.000084
12	6	0	3.142921	-0.485091	-0.000079
13	6	0	3.133831	0.933235	0.000124
14	7	0	1.796323	1.276365	0.000297
15	6	0	4.363471	-1.175518	-0.000464
16	6	0	5.551637	-0.449539	-0.000572
17	6	0	5.507382	0.967199	-0.000542
18	6	0	4.314056	1.679560	-0.000155
19	6	0	-6.151914	1.361285	-0.000200
20	6	0	-6.090891	-1.578679	-0.000192
21	6	0	6.890310	-1.152225	0.000614
22	1	0	-3.566555	-2.566619	0.000009
23	1	0	-3.656642	2.446220	0.000245
24	1	0	-0.642859	-1.991587	0.000151
25	1	0	1.370199	2.191177	0.000141
26	1	0	4.369716	-2.261232	-0.000832
27	1	0	6.445278	1.516579	-0.000924
28	1	0	4.307324	2.765091	-0.000331

29	1	0	-6.757902	1.108961	0.878627
30	1	0	-6.756302	1.111140	-0.880774
31	1	0	-6.001527	2.443777	0.001260
32	1	0	-6.705253	-1.350371	0.879234
33	1	0	-5.899177	-2.654799	-0.000502
34	1	0	-6.705221	-1.349801	-0.879500
35	1	0	6.768949	-2.238564	-0.015210
36	1	0	7.477257	-0.895741	0.890446
37	1	0	7.491734	-0.871232	-0.871817

Compound **4e**: most stable trans-isomer

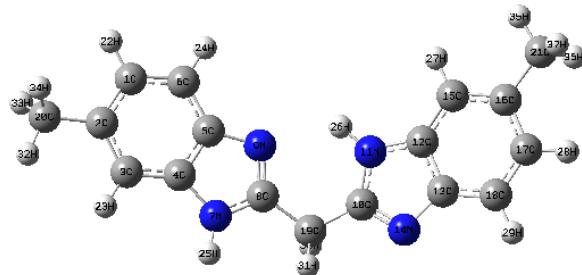
HF=-876.5393751

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.774059	-0.825285	0.000017
2	6	0	4.856816	0.600936	0.000094
3	6	0	3.698983	1.378379	0.000107
4	6	0	2.466102	0.725272	0.000031
5	6	0	2.365021	-0.686825	-0.000034
6	6	0	3.534344	-1.458407	-0.000039
7	7	0	1.159548	1.171826	0.000054
8	6	0	0.360391	0.054108	-0.000022
9	7	0	1.036672	-1.078300	-0.000055
10	6	0	-1.081157	0.163151	-0.000043
11	7	0	-1.760489	1.293200	-0.000098
12	6	0	-3.087698	0.898702	-0.000069
13	6	0	-3.185651	-0.516357	-0.000001
14	7	0	-1.877853	-0.956806	0.000002
15	6	0	-4.260966	1.666569	-0.000145
16	6	0	-5.478607	1.001777	-0.000066
17	6	0	-5.572997	-0.412834	0.000005
18	6	0	-4.411907	-1.185297	0.000008
19	6	0	6.037314	-1.655110	-0.000103

20	6	0	6.205704	1.280592	0.000097
21	6	0	-6.933801	-1.069698	0.000196
22	1	0	3.765839	2.462545	0.000142
23	1	0	3.465273	-2.542003	-0.000101
24	1	0	0.805878	2.116947	0.000050
25	1	0	-1.520516	-1.900661	-0.000016
26	1	0	-4.206070	2.750274	-0.000223
27	1	0	-6.398546	1.580707	-0.000097
28	1	0	-4.466655	-2.270120	0.000043
29	1	0	6.660226	-1.451447	0.879436
30	1	0	6.659789	-1.451854	-0.880052
31	1	0	5.802569	-2.722477	0.000195
32	1	0	6.800365	1.004509	0.879376
33	1	0	6.098889	2.368419	0.000134
34	1	0	6.800367	1.004563	-0.879202
35	1	0	-7.517947	-0.778143	-0.880444
36	1	0	-7.517404	-0.778677	0.881385
37	1	0	-6.852894	-2.160058	-0.000125

Compound **4f**: most stable trans-isomer; cis-form has no existence



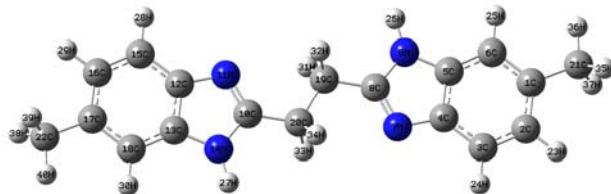
HF=-876.5310818

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.577489	1.805898	-0.119555
2	6	0	-5.310076	0.685525	0.342656
3	6	0	-4.680600	-0.554935	0.453040
4	6	0	-3.333639	-0.632512	0.094692
5	6	0	-2.601021	0.483020	-0.365271
6	6	0	-3.237252	1.725536	-0.473628
7	7	0	-2.420710	-1.675366	0.082996
8	6	0	-1.220264	-1.169927	-0.362272

9	7	0	-1.290910	0.112287	-0.644432
10	6	0	1.304812	-1.382256	-0.276265
11	7	0	1.515461	-0.044226	-0.503326
12	6	0	2.837203	0.209495	-0.190912
13	6	0	3.360393	-1.046893	0.198343
14	7	0	2.374186	-2.023631	0.135288
15	6	0	3.610063	1.373379	-0.207316
16	6	0	4.948378	1.270990	0.172646
17	6	0	5.475421	0.014188	0.559105
18	6	0	4.705426	-1.141301	0.578294
19	6	0	-0.015326	-2.046503	-0.554406
20	6	0	-6.766862	0.845093	0.711713
21	6	0	5.843456	2.489331	0.174349
22	1	0	-5.089000	2.761669	-0.197594
23	1	0	-5.227126	-1.424762	0.806453
24	1	0	-2.691325	2.594687	-0.825812
25	1	0	-2.588000	-2.626120	0.373639
26	1	0	0.755447	0.592412	-0.727416
27	1	0	3.189819	2.329356	-0.507090
28	1	0	6.521473	-0.040673	0.850334
29	1	0	5.124284	-2.096429	0.878763
30	1	0	-0.017272	-2.414765	-1.591793
31	1	0	-0.076741	-2.933107	0.082937
32	1	0	-7.200062	-0.098676	1.053882
33	1	0	-7.358818	1.193601	-0.142447
34	1	0	-6.896859	1.581504	1.513082
35	1	0	5.300584	3.385875	-0.137833
36	1	0	6.694314	2.362089	-0.505394
37	1	0	6.257344	2.681134	1.171333

Compound **4h**: most stable trans-isomer; cis-form has no existence



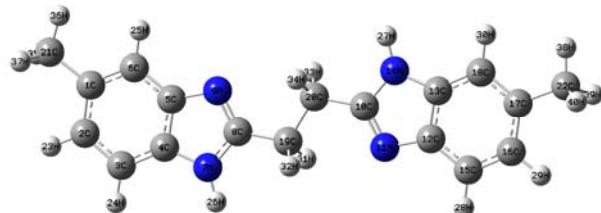
HF=-915.8443704

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.445762	0.160356	0.000385
2	6	0	6.133163	-1.220108	-0.001318
3	6	0	4.824276	-1.686322	-0.002129
4	6	0	3.786809	-0.746465	-0.001250
5	6	0	4.102671	0.630702	0.000405
6	6	0	5.416073	1.103261	0.001212
7	7	0	2.408330	-0.928268	-0.001847
8	6	0	1.900279	0.281438	-0.000619
9	7	0	2.871790	1.265131	0.000756
10	6	0	-1.900284	-0.281468	0.000773
11	7	0	-2.408319	0.928245	-0.000436
12	6	0	-3.786800	0.746465	-0.000467
13	6	0	-4.102686	-0.630704	0.000809
14	7	0	-2.871808	-1.265148	0.001563
15	6	0	-4.824247	1.686334	-0.001607
16	6	0	-6.133146	1.220136	-0.001392
17	6	0	-6.445767	-0.160312	-0.000054
18	6	0	-5.416086	-1.103243	0.001010
19	6	0	0.442010	0.624290	-0.001021
20	6	0	-0.442015	-0.624334	0.001548
21	6	0	7.891831	0.600823	0.001683
22	6	0	-7.891835	-0.600800	0.000594
23	1	0	6.951073	-1.936146	-0.002059
24	1	0	4.601371	-2.748472	-0.003494
25	1	0	5.639035	2.166744	0.002423
26	1	0	2.706510	2.259543	0.002026
27	1	0	-2.706542	-2.259562	0.002524
28	1	0	-4.601325	2.748481	-0.002681
29	1	0	-6.951051	1.936178	-0.002290
30	1	0	-5.639060	-2.166724	0.001977
31	1	0	0.199658	1.242796	-0.873763
32	1	0	0.199910	1.246359	0.869220
33	1	0	-0.199684	-1.246457	-0.868590
34	1	0	-0.199914	-1.242785	0.874397
35	1	0	8.423356	0.226193	0.884295
36	1	0	7.979372	1.690886	-0.000604
37	1	0	8.426206	0.222170	-0.877444

38	1	0	-8.425893	-0.221865	-0.878601
39	1	0	-8.423675	-0.226500	0.883152
40	1	0	-7.979355	-1.690868	-0.002099

Compound **4h**: unstable trans-isomer; cis-form has no existence



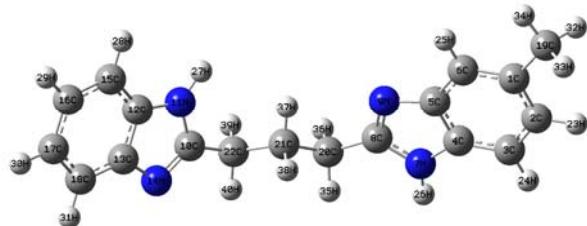
HF=-915.8440751

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.228689	-0.744148	0.000479
2	6	0	-6.428999	0.656696	-0.000485
3	6	0	-5.373021	1.562825	-0.001055
4	6	0	-4.084290	1.028393	-0.000591
5	6	0	-3.849315	-0.364866	0.000292
6	6	0	-4.930774	-1.254147	0.000821
7	7	0	-2.818625	1.592330	-0.001184
8	6	0	-1.906728	0.554960	-0.000356
9	7	0	-2.483360	-0.624347	0.000375
10	6	0	1.855656	-0.225328	-0.000270
11	7	0	2.431982	0.953352	0.000876
12	6	0	3.797801	0.693034	0.000765
13	6	0	4.034474	-0.699977	-0.000474
14	7	0	2.769300	-1.262962	-0.001013
15	6	0	4.887303	1.571984	0.001662
16	6	0	6.167318	1.031505	0.001286
17	6	0	6.400586	-0.364511	0.000027
18	6	0	5.318665	-1.247014	-0.000855
19	6	0	-0.430956	0.812715	-0.000327
20	6	0	0.380163	-0.484284	-0.000645
21	6	0	-7.425438	-1.668941	0.001345
22	6	0	7.819104	-0.886858	-0.000428
23	1	0	-7.447015	1.037932	-0.000845
24	1	0	-5.553288	2.633721	-0.001875
25	1	0	-4.750244	-2.324969	0.001455

26	1	0	-2.596191	2.575469	-0.000987
27	1	0	2.547344	-2.246262	-0.002107
28	1	0	4.725657	2.645157	0.002633
29	1	0	7.024844	1.699624	0.001976
30	1	0	5.480537	-2.321535	-0.001801
31	1	0	-0.153729	1.417985	0.871337
32	1	0	-0.153775	1.418514	-0.871616
33	1	0	0.102898	-1.090156	0.870591
34	1	0	0.103259	-1.089560	-0.872421
35	1	0	-8.056306	-1.508807	0.883617
36	1	0	-7.117077	-2.717886	0.000084
37	1	0	-8.058739	-1.507330	-0.878890
38	1	0	7.844120	-1.980144	-0.000361
39	1	0	8.373037	-0.541219	0.880204
40	1	0	8.372424	-0.541368	-0.881516

Compound **4I**: unstable trans-isomer; cis-form has no existence



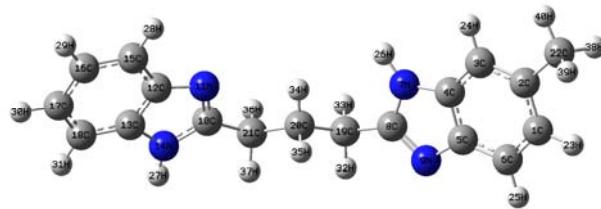
HF=-915.8386045

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.699402	1.463910	0.152706
2	6	0	6.267897	0.255611	0.622735
3	6	0	5.545333	-0.930584	0.698117
4	6	0	4.213658	-0.884146	0.283907
5	6	0	3.614945	0.304861	-0.189987
6	6	0	4.366255	1.485219	-0.254314
7	7	0	3.203626	-1.830232	0.214108
8	6	0	2.081143	-1.196436	-0.279567
9	7	0	2.288085	0.075060	-0.532053
10	6	0	-2.975106	-0.957798	-0.343671
11	7	0	-3.185936	0.303690	-0.870194
12	6	0	-4.399623	0.756697	-0.382346

13	6	0	-4.865396	-0.300562	0.436379
14	7	0	-3.953714	-1.349406	0.437923
15	6	0	-5.118128	1.938726	-0.565234
16	6	0	-6.337070	2.040083	0.101753
17	6	0	-6.817400	0.998612	0.919762
18	6	0	-6.093614	-0.176592	1.096714
19	6	0	6.546299	2.715669	0.100277
20	6	0	0.795534	-1.930473	-0.523690
21	6	0	-0.438878	-1.066918	-0.228288
22	6	0	-1.747399	-1.755589	-0.656117
23	1	0	7.308733	0.256193	0.936204
24	1	0	6.004692	-1.844570	1.062724
25	1	0	3.906466	2.399059	-0.618542
26	1	0	3.264843	-2.798808	0.486150
27	1	0	-2.558175	0.805638	-1.478407
28	1	0	-4.751077	2.743704	-1.194893
29	1	0	-6.929693	2.942856	-0.012130
30	1	0	-7.772979	1.119575	1.421179
31	1	0	-6.458601	-0.981960	1.725771
32	1	0	7.429420	2.576722	-0.534238
33	1	0	6.908345	2.997540	1.096059
34	1	0	5.980437	3.561768	-0.298636
35	1	0	0.771737	-2.846012	0.081211
36	1	0	0.767901	-2.257689	-1.573366
37	1	0	-0.313546	-0.109421	-0.744293
38	1	0	-0.477527	-0.835835	0.841905
39	1	0	-1.709524	-1.968408	-1.734408
40	1	0	-1.863013	-2.715871	-0.145586

Compound 4l: most stable trans-isomer; cis-form has no existence



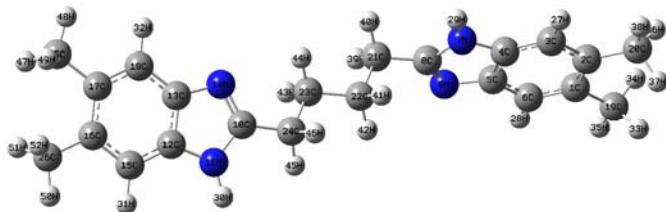
HF=-915.8388506

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.169634	0.189179	0.917628
2	6	0	5.835056	1.312801	0.123889
3	6	0	4.602049	1.356884	-0.528909
4	6	0	3.741384	0.269815	-0.365034
5	6	0	4.071362	-0.853298	0.426863
6	6	0	5.310264	-0.890267	1.078564
7	7	0	2.478224	-0.014586	-0.854582
8	6	0	2.110919	-1.250995	-0.353121
9	7	0	3.035364	-1.779286	0.413671
10	6	0	-2.937987	-0.860770	-0.277812
11	7	0	-2.982209	0.432107	-0.496483
12	6	0	-4.273697	0.817118	-0.158360
13	6	0	-5.022854	-0.301949	0.278747
14	7	0	-4.136584	-1.362733	0.189765
15	6	0	-4.873107	2.081720	-0.194227
16	6	0	-6.201197	2.188574	0.206718
17	6	0	-6.930438	1.063549	0.639200
18	6	0	-6.354437	-0.204058	0.683942
19	6	0	0.791847	-1.882386	-0.674145
20	6	0	-0.419988	-1.039566	-0.237663
21	6	0	-1.751932	-1.743762	-0.532228
22	6	0	6.817271	2.454019	-0.009984
23	1	0	7.135380	0.177243	1.416599
24	1	0	4.329998	2.212192	-1.141464
25	1	0	5.581209	-1.744334	1.690895
26	1	0	1.916792	0.575949	-1.447796
27	1	0	-4.320322	-2.322912	0.435333
28	1	0	-4.306948	2.945319	-0.527552
29	1	0	-6.689706	3.158128	0.187677

30	1	0	-7.965045	1.186447	0.944969
31	1	0	-6.919516	-1.068917	1.018341
32	1	0	0.784976	-2.855144	-0.174277
33	1	0	0.727289	-2.077356	-1.754647
34	1	0	-0.428030	-0.070982	-0.747897
35	1	0	-0.350077	-0.821384	0.833612
36	1	0	-1.769129	-2.065790	-1.583792
37	1	0	-1.836863	-2.659081	0.067479
38	1	0	7.761726	2.119214	-0.454941
39	1	0	7.060735	2.888912	0.966408
40	1	0	6.419088	3.254338	-0.639971

Compound **4q**: only possible stable trans-isomer; cis-form has no existence



HF=-1073.1134303

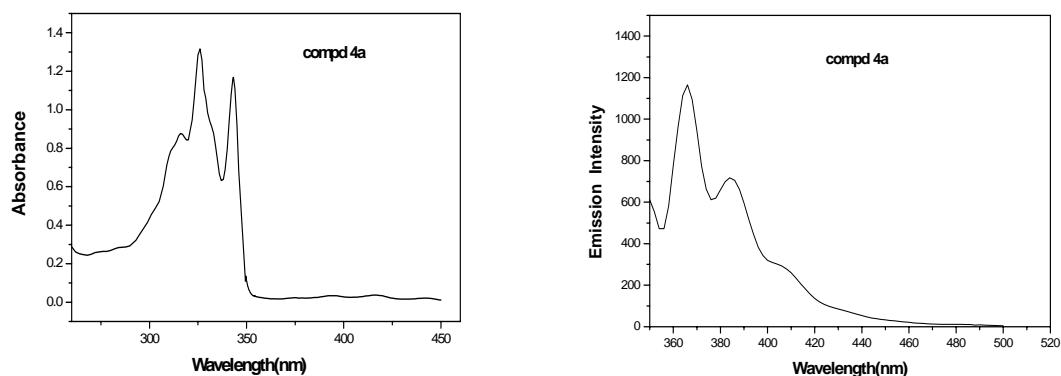
Standard orientation:

Center Number	Atomic Number		Coordinates (Angstroms)		
		Type	X	Y	Z
1	6	0	7.476607	-0.634559	-0.193749
2	6	0	7.419303	0.443870	0.737847
3	6	0	6.227822	1.143057	0.938340
4	6	0	5.105935	0.755613	0.206724
5	6	0	5.143305	-0.307511	-0.720474
6	6	0	6.342300	-1.002153	-0.915802
7	7	0	3.800037	1.213145	0.154044
8	6	0	3.129894	0.436961	-0.775078
9	7	0	3.898687	-0.480669	-1.313781
10	6	0	-3.076428	-0.537330	0.365634
11	7	0	-4.044520	-1.487964	0.631050
12	6	0	-5.276442	-0.893543	0.410931
13	6	0	-4.964549	0.423018	0.012389
14	7	0	-3.587611	0.612798	-0.005298
15	6	0	-6.590743	-1.348108	0.509382
16	6	0	-7.620994	-0.457489	0.201886

17	6	0	-7.325390	0.877783	-0.202004
18	6	0	-6.002883	1.308915	-0.294869
19	6	0	8.772673	-1.384203	-0.402209
20	6	0	8.651258	0.839296	1.518427
21	6	0	1.669998	0.617675	-1.053369
22	6	0	0.770451	-0.195117	-0.099089
23	6	0	-0.720784	0.004259	-0.384511
24	6	0	-1.615290	-0.829466	0.542882
25	6	0	-8.448495	1.834542	-0.531564
26	6	0	-9.055710	-0.920993	0.301622
27	1	0	6.188478	1.964224	1.649123
28	1	0	6.380013	-1.821951	-1.627030
29	1	0	3.410697	1.985412	0.671465
30	1	0	-3.876499	-2.439202	0.918607
31	1	0	-6.820158	-2.365002	0.816455
32	1	0	-5.772044	2.324673	-0.601987
33	1	0	9.138098	-1.837091	0.527725
34	1	0	9.572089	-0.726718	-0.765939
35	1	0	8.646230	-2.186468	-1.133725
36	1	0	9.474559	1.137463	0.857816
37	1	0	9.027508	0.012114	2.132867
38	1	0	8.441689	1.679180	2.186238
39	1	0	1.489176	0.300595	-2.084591
40	1	0	1.405629	1.681541	-0.991233
41	1	0	0.988930	0.089969	0.939262
42	1	0	1.039544	-1.254739	-0.190254
43	1	0	-0.940179	-0.258572	-1.426726
44	1	0	-0.994549	1.059013	-0.274814
45	1	0	-1.434577	-1.900436	0.380418
46	1	0	-1.338430	-0.632353	1.589294
47	1	0	-9.068137	1.469370	-1.359909
48	1	0	-8.055361	2.812957	-0.819285
49	1	0	-9.121828	1.985181	0.321301
50	1	0	-9.111201	-1.964006	0.624561
51	1	0	-9.577577	-0.842958	-0.660066
52	1	0	-9.629285	-0.320478	1.018243

## 6. Details of photophysical studies

For recording absorption and emission spectra of compounds **4d** to **4l** and compound **4a**, dimethyl sulfoxide was used as solvent since compounds **4d** to **4l** were sparingly soluble in other solvents. In fluorescence quantum yield calculations, anthracene was the reference for compounds **4d** and **4e** while the unusual reference BSA (Bovine Serum Albumin, which has an absorption maxima at 280 nm) was the reference for compounds **4q**, **4n** and **4l** whose absorption maxima were also observed around 280 nm range.



**Figure 9.** Absorption and Emission graphs of compound **4a**.

Absorption Spectra plot details of a representative compound: <u>Compound 4d</u>	Emission Spectra plot details of a representative compound: <u>Compound 4d</u>
Coordinates	Coordinates
x y	x y
600 -9.92593E-4	350 56.732
599.5 -0.00104	350.5 63.0599
599 -0.00109	351 70.42405
598.5 -0.0011	351.5 79.05464
598 -0.00108	352 88.33057
597.5 -0.00105	352.5 97.96066
597 -1E-3	353 108.43719
596.5 -9.77778E-4	353.5 119.90809
596 -9.85185E-4	354 132.10585
595.5 -0.001	354.5 144.10242
595 -0.00102	355 156.82072
594.5 -0.00104	355.5 172.36261
594 -0.00105	356 192.46899

<u>593.5</u>	<u>-0.00104</u>	<u>356.5</u>	<u>212.55995</u>
<u>593</u>	<u>-0.00106</u>	<u>357</u>	<u>230.30065</u>
<u>592.5</u>	<u>-0.0011</u>	<u>357.5</u>	<u>245.40754</u>
<u>592</u>	<u>-0.00116</u>	<u>358</u>	<u>262.84187</u>
<u>591.5</u>	<u>-0.00118</u>	<u>358.5</u>	<u>281.99031</u>
<u>591</u>	<u>-0.00117</u>	<u>359</u>	<u>299.425</u>
<u>590.5</u>	<u>-0.00115</u>	<u>359.5</u>	<u>310.97012</u>
<u>590</u>	<u>-0.0011</u>	<u>360</u>	<u>318.61798</u>
<u>589.5</u>	<u>-0.00106</u>	<u>360.5</u>	<u>324.69314</u>
<u>589</u>	<u>-0.00104</u>	<u>361</u>	<u>329.36804</u>
<u>588.5</u>	<u>-0.00107</u>	<u>361.5</u>	<u>331.4458</u>
<u>588</u>	<u>-0.00109</u>	<u>362</u>	<u>331.50869</u>
<u>587.5</u>	<u>-0.0011</u>	<u>362.5</u>	<u>329.8353</u>
<u>587</u>	<u>-0.00115</u>	<u>363</u>	<u>324.00751</u>
<u>586.5</u>	<u>-0.00116</u>	<u>363.5</u>	<u>313.53177</u>
<u>586</u>	<u>-0.00116</u>	<u>364</u>	<u>302.96551</u>
<u>585.5</u>	<u>-0.00116</u>	<u>364.5</u>	<u>296.42502</u>
<u>585</u>	<u>-0.00116</u>	<u>365</u>	<u>291.43769</u>
<u>584.5</u>	<u>-0.00111</u>	<u>365.5</u>	<u>284.2957</u>
<u>584</u>	<u>-0.00106</u>	<u>366</u>	<u>273.58783</u>
<u>583.5</u>	<u>-0.00104</u>	<u>366.5</u>	<u>265.5965</u>
<u>583</u>	<u>-0.00104</u>	<u>367</u>	<u>261.44418</u>
<u>582.5</u>	<u>-0.00104</u>	<u>367.5</u>	<u>260.11529</u>
<u>582</u>	<u>-0.00103</u>	<u>368</u>	<u>257.99791</u>
<u>581.5</u>	<u>-0.00106</u>	<u>368.5</u>	<u>257.00024</u>
<u>581</u>	<u>-0.00107</u>	<u>369</u>	<u>257.32388</u>
<u>580.5</u>	<u>-0.0011</u>	<u>369.5</u>	<u>260.36331</u>
<u>580</u>	<u>-0.0011</u>	<u>370</u>	<u>263.77552</u>
<u>579.5</u>	<u>-0.00106</u>	<u>370.5</u>	<u>269.45459</u>
<u>579</u>	<u>-0.00104</u>	<u>371</u>	<u>277.46403</u>
<u>578.5</u>	<u>-0.00101</u>	<u>371.5</u>	<u>287.99858</u>
<u>578</u>	<u>-9.96296E-4</u>	<u>372</u>	<u>298.04481</u>
<u>577.5</u>	<u>-9.74074E-4</u>	<u>372.5</u>	<u>307.79463</u>
<u>577</u>	<u>-9.66667E-4</u>	<u>373</u>	<u>317.95444</u>
<u>576.5</u>	<u>-9.85185E-4</u>	<u>373.5</u>	<u>329.42222</u>
<u>576</u>	<u>-0.00101</u>	<u>374</u>	<u>341.33704</u>
<u>575.5</u>	<u>-0.00103</u>	<u>374.5</u>	<u>353.98223</u>
<u>575</u>	<u>-0.00103</u>	<u>375</u>	<u>365.47425</u>
<u>574.5</u>	<u>-0.00101</u>	<u>375.5</u>	<u>374.48508</u>
<u>574</u>	<u>-9.7037E-4</u>	<u>376</u>	<u>380.05883</u>

<u>573.5</u>	<u>-9.66667E-4</u>	<u>376.5</u>	<u>384.37895</u>
<u>573</u>	<u>-9.7037E-4</u>	<u>377</u>	<u>387.08607</u>
<u>572.5</u>	<u>-9.88889E-4</u>	<u>377.5</u>	<u>390.64298</u>
<u>572</u>	<u>-9.85185E-4</u>	<u>378</u>	<u>393.7683</u>
<u>571.5</u>	<u>-9.81481E-4</u>	<u>378.5</u>	<u>398.5253</u>
<u>571</u>	<u>-9.88889E-4</u>	<u>379</u>	<u>399.84524</u>
<u>570.5</u>	<u>-9.96296E-4</u>	<u>379.5</u>	<u>399.96662</u>
<u>570</u>	<u>-9.92593E-4</u>	<u>380</u>	<u>399.59687</u>
<u>569.5</u>	<u>-9.77778E-4</u>	<u>380.5</u>	<u>401.50251</u>
<u>569</u>	<u>-9.7037E-4</u>	<u>381</u>	<u>399.39555</u>
<u>568.5</u>	<u>-9.77778E-4</u>	<u>381.5</u>	<u>391.99719</u>
<u>568</u>	<u>-9.85185E-4</u>	<u>382</u>	<u>379.66789</u>
<u>567.5</u>	<u>-9.85185E-4</u>	<u>382.5</u>	<u>369.77296</u>
<u>567</u>	<u>-9.59259E-4</u>	<u>383</u>	<u>363.91895</u>
<u>566.5</u>	<u>-9.51852E-4</u>	<u>383.5</u>	<u>359.15449</u>
<u>566</u>	<u>-9.55556E-4</u>	<u>384</u>	<u>350.94451</u>
<u>565.5</u>	<u>-9.7037E-4</u>	<u>384.5</u>	<u>338.06568</u>
<u>565</u>	<u>-9.7037E-4</u>	<u>385</u>	<u>324.47703</u>
<u>564.5</u>	<u>-9.66667E-4</u>	<u>385.5</u>	<u>310.87694</u>
<u>564</u>	<u>-9.88889E-4</u>	<u>386</u>	<u>299.85627</u>
<u>563.5</u>	<u>-9.88889E-4</u>	<u>386.5</u>	<u>288.99876</u>
<u>563</u>	<u>-0.00101</u>	<u>387</u>	<u>280.33665</u>
<u>562.5</u>	<u>-0.001</u>	<u>387.5</u>	<u>271.65889</u>
<u>562</u>	<u>-0.00101</u>	<u>388</u>	<u>266.03325</u>
<u>561.5</u>	<u>-0.00103</u>	<u>388.5</u>	<u>259.52495</u>
<u>561</u>	<u>-0.00103</u>	<u>389</u>	<u>252.31992</u>
<u>560.5</u>	<u>-0.00103</u>	<u>389.5</u>	<u>243.09077</u>
<u>560</u>	<u>-9.85185E-4</u>	<u>390</u>	<u>236.17598</u>
<u>559.5</u>	<u>-9.55556E-4</u>	<u>390.5</u>	<u>232.4153</u>
<u>559</u>	<u>-9.37037E-4</u>	<u>391</u>	<u>231.94959</u>
<u>558.5</u>	<u>-9.03704E-4</u>	<u>391.5</u>	<u>230.53795</u>
<u>558</u>	<u>-8.81481E-4</u>	<u>392</u>	<u>227.98808</u>
<u>557.5</u>	<u>-8.7037E-4</u>	<u>392.5</u>	<u>225.42935</u>
<u>557</u>	<u>-8.7037E-4</u>	<u>393</u>	<u>225.73312</u>
<u>556.5</u>	<u>-8.62963E-4</u>	<u>393.5</u>	<u>227.40122</u>
<u>556</u>	<u>-8.77778E-4</u>	<u>394</u>	<u>227.16878</u>
<u>555.5</u>	<u>-8.88889E-4</u>	<u>394.5</u>	<u>223.87631</u>
<u>555</u>	<u>-9.03704E-4</u>	<u>395</u>	<u>222.59555</u>
<u>554.5</u>	<u>-8.74074E-4</u>	<u>395.5</u>	<u>224.64543</u>
<u>554</u>	<u>-8.55556E-4</u>	<u>396</u>	<u>227.03924</u>

<u>553.5</u>	<u>-8.66667E-4</u>	<u>396.5</u>	<u>226.67325</u>
<u>553</u>	<u>-8.59259E-4</u>	<u>397</u>	<u>224.55114</u>
<u>552.5</u>	<u>-8.51852E-4</u>	<u>397.5</u>	<u>223.49387</u>
<u>552</u>	<u>-8.44444E-4</u>	<u>398</u>	<u>223.39335</u>
<u>551.5</u>	<u>-8.51852E-4</u>	<u>398.5</u>	<u>223.69774</u>
<u>551</u>	<u>-8.59259E-4</u>	<u>399</u>	<u>223.77448</u>
<u>550.5</u>	<u>-8.55556E-4</u>	<u>399.5</u>	<u>224.31069</u>
<u>550</u>	<u>-8.51852E-4</u>	<u>400</u>	<u>223.38229</u>
<u>549.5</u>	<u>-8.33333E-4</u>	<u>400.5</u>	<u>221.68452</u>
<u>549</u>	<u>-8.03704E-4</u>	<u>401</u>	<u>218.03815</u>
<u>548.5</u>	<u>-8.14815E-4</u>	<u>401.5</u>	<u>215.29076</u>
<u>548</u>	<u>-8.11111E-4</u>	<u>402</u>	<u>211.69316</u>
<u>547.5</u>	<u>-8.03704E-4</u>	<u>402.5</u>	<u>209.03064</u>
<u>547</u>	<u>-8E-4</u>	<u>403</u>	<u>205.77675</u>
<u>546.5</u>	<u>-7.59259E-4</u>	<u>403.5</u>	<u>203.12109</u>
<u>546</u>	<u>-7.59259E-4</u>	<u>404</u>	<u>197.72781</u>
<u>545.5</u>	<u>-7.7037E-4</u>	<u>404.5</u>	<u>191.24793</u>
<u>545</u>	<u>-7.59259E-4</u>	<u>405</u>	<u>184.3698</u>
<u>544.5</u>	<u>-7.74074E-4</u>	<u>405.5</u>	<u>180.57183</u>
<u>544</u>	<u>-8.03704E-4</u>	<u>406</u>	<u>178.34381</u>
<u>543.5</u>	<u>-8.14815E-4</u>	<u>406.5</u>	<u>174.69591</u>
<u>543</u>	<u>-8.33333E-4</u>	<u>407</u>	<u>168.5834</u>
<u>542.5</u>	<u>-8.2963E-4</u>	<u>407.5</u>	<u>162.52889</u>
<u>542</u>	<u>-8.37037E-4</u>	<u>408</u>	<u>157.92507</u>
<u>541.5</u>	<u>-8.25926E-4</u>	<u>408.5</u>	<u>154.70259</u>
<u>541</u>	<u>-7.7037E-4</u>	<u>409</u>	<u>151.00912</u>
<u>540.5</u>	<u>-7.77778E-4</u>	<u>409.5</u>	<u>146.77777</u>
<u>540</u>	<u>-8.03704E-4</u>	<u>410</u>	<u>142.26491</u>
<u>539.5</u>	<u>-8E-4</u>	<u>410.5</u>	<u>137.11597</u>
<u>539</u>	<u>-7.77778E-4</u>	<u>411</u>	<u>132.6325</u>
<u>538.5</u>	<u>-7.74074E-4</u>	<u>411.5</u>	<u>129.59622</u>
<u>538</u>	<u>-7.62963E-4</u>	<u>412</u>	<u>127.14693</u>
<u>537.5</u>	<u>-7.59259E-4</u>	<u>412.5</u>	<u>122.847</u>
<u>537</u>	<u>-7.59259E-4</u>	<u>413</u>	<u>118.23644</u>
<u>536.5</u>	<u>-7.55556E-4</u>	<u>413.5</u>	<u>113.9183</u>
<u>536</u>	<u>-7.77778E-4</u>	<u>414</u>	<u>109.84787</u>
<u>535.5</u>	<u>-8.03704E-4</u>	<u>414.5</u>	<u>107.01937</u>
<u>535</u>	<u>-8.40741E-4</u>	<u>415</u>	<u>106.33624</u>
<u>534.5</u>	<u>-8.74074E-4</u>	<u>415.5</u>	<u>107.76135</u>
<u>534</u>	<u>-8.59259E-4</u>	<u>416</u>	<u>107.3211</u>

<u>533.5</u>	<u>-8.33333E-4</u>	<u>416.5</u>	<u>104.56294</u>
<u>533</u>	<u>-7.85185E-4</u>	<u>417</u>	<u>100.33427</u>
<u>532.5</u>	<u>-7.7037E-4</u>	<u>417.5</u>	<u>97.7481</u>
<u>532</u>	<u>-7.18519E-4</u>	<u>418</u>	<u>96.89148</u>
<u>531.5</u>	<u>-6.88889E-4</u>	<u>418.5</u>	<u>96.51467</u>
<u>531</u>	<u>-6.66667E-4</u>	<u>419</u>	<u>95.25416</u>
<u>530.5</u>	<u>-7.07407E-4</u>	<u>419.5</u>	<u>92.58736</u>
<u>530</u>	<u>-7.55556E-4</u>	<u>420</u>	<u>89.69032</u>
<u>529.5</u>	<u>-7.92593E-4</u>	<u>420.5</u>	<u>89.12612</u>
<u>529</u>	<u>-8.22222E-4</u>	<u>421</u>	<u>89.42852</u>
<u>528.5</u>	<u>-8.25926E-4</u>	<u>421.5</u>	<u>89.41543</u>
<u>528</u>	<u>-8.14815E-4</u>	<u>422</u>	<u>86.74789</u>
<u>527.5</u>	<u>-8.14815E-4</u>	<u>422.5</u>	<u>84.32621</u>
<u>527</u>	<u>-8.2963E-4</u>	<u>423</u>	<u>83.42036</u>
<u>526.5</u>	<u>-8.18519E-4</u>	<u>423.5</u>	<u>84.18528</u>
<u>526</u>	<u>-8E-4</u>	<u>424</u>	<u>82.67125</u>
<u>525.5</u>	<u>-8.14815E-4</u>	<u>424.5</u>	<u>80.3561</u>
<u>525</u>	<u>-8.25926E-4</u>	<u>425</u>	<u>78.87122</u>
<u>524.5</u>	<u>-8.25926E-4</u>	<u>425.5</u>	<u>78.66869</u>
<u>524</u>	<u>-7.85185E-4</u>	<u>426</u>	<u>77.78087</u>
<u>523.5</u>	<u>-7.74074E-4</u>	<u>426.5</u>	<u>75.81255</u>
<u>523</u>	<u>-7.7037E-4</u>	<u>427</u>	<u>74.42726</u>
<u>522.5</u>	<u>-7.7037E-4</u>	<u>427.5</u>	<u>73.63836</u>
<u>522</u>	<u>-7.59259E-4</u>	<u>428</u>	<u>71.65224</u>
<u>521.5</u>	<u>-7.62963E-4</u>	<u>428.5</u>	<u>68.97228</u>
<u>521</u>	<u>-7.85185E-4</u>	<u>429</u>	<u>67.47787</u>
<u>520.5</u>	<u>-8.07407E-4</u>	<u>429.5</u>	<u>66.97458</u>
<u>520</u>	<u>-8.2963E-4</u>	<u>430</u>	<u>65.94436</u>
<u>519.5</u>	<u>-8.14815E-4</u>	<u>430.5</u>	<u>63.18197</u>
<u>519</u>	<u>-8.03704E-4</u>	<u>431</u>	<u>60.53831</u>
<u>518.5</u>	<u>-8.03704E-4</u>	<u>431.5</u>	<u>58.52972</u>
<u>518</u>	<u>-7.85185E-4</u>	<u>432</u>	<u>57.60548</u>
<u>517.5</u>	<u>-7.51852E-4</u>	<u>432.5</u>	<u>55.99556</u>
<u>517</u>	<u>-7.37037E-4</u>	<u>433</u>	<u>53.9396</u>
<u>516.5</u>	<u>-7.51852E-4</u>	<u>433.5</u>	<u>51.23697</u>
<u>516</u>	<u>-7.62963E-4</u>	<u>434</u>	<u>49.64586</u>
<u>515.5</u>	<u>-7.55556E-4</u>	<u>434.5</u>	<u>48.61757</u>
<u>515</u>	<u>-7.48148E-4</u>	<u>435</u>	<u>47.9769</u>
<u>514.5</u>	<u>-7.51852E-4</u>	<u>435.5</u>	<u>46.14402</u>
<u>514</u>	<u>-7.51852E-4</u>	<u>436</u>	<u>43.8556</u>

<u>513.5</u>	<u>-7.66667E-4</u>	<u>436.5</u>	<u>41.2924</u>
<u>513</u>	<u>-7.66667E-4</u>	<u>437</u>	<u>39.82406</u>
<u>512.5</u>	<u>-7.62963E-4</u>	<u>437.5</u>	<u>39.20616</u>
<u>512</u>	<u>-7.37037E-4</u>	<u>438</u>	<u>39.28863</u>
<u>511.5</u>	<u>-7.03704E-4</u>	<u>438.5</u>	<u>38.69508</u>
<u>511</u>	<u>-6.55556E-4</u>	<u>439</u>	<u>37.21497</u>
<u>510.5</u>	<u>-6.37037E-4</u>	<u>439.5</u>	<u>34.72044</u>
<u>510</u>	<u>-6.22222E-4</u>	<u>440</u>	<u>32.61953</u>
<u>509.5</u>	<u>-6.14815E-4</u>	<u>440.5</u>	<u>31.71415</u>
<u>509</u>	<u>-6.51852E-4</u>	<u>441</u>	<u>31.53929</u>
<u>508.5</u>	<u>-6.92593E-4</u>	<u>441.5</u>	<u>31.20987</u>
<u>508</u>	<u>-7.2963E-4</u>	<u>442</u>	<u>29.90887</u>
<u>507.5</u>	<u>-7.48148E-4</u>	<u>442.5</u>	<u>28.25417</u>
<u>507</u>	<u>-7.40741E-4</u>	<u>443</u>	<u>26.63678</u>
<u>506.5</u>	<u>-7.22222E-4</u>	<u>443.5</u>	<u>26.12455</u>
<u>506</u>	<u>-6.96296E-4</u>	<u>444</u>	<u>26.52408</u>
<u>505.5</u>	<u>-7.14815E-4</u>	<u>444.5</u>	<u>26.87881</u>
<u>505</u>	<u>-7.62963E-4</u>	<u>445</u>	<u>26.33856</u>
<u>504.5</u>	<u>-7.74074E-4</u>	<u>445.5</u>	<u>25.24071</u>
<u>504</u>	<u>-7.74074E-4</u>	<u>446</u>	<u>24.20512</u>
<u>503.5</u>	<u>-7.77778E-4</u>	<u>446.5</u>	<u>23.90188</u>
<u>503</u>	<u>-7.48148E-4</u>	<u>447</u>	<u>23.1869</u>
<u>502.5</u>	<u>-6.81481E-4</u>	<u>447.5</u>	<u>22.15887</u>
<u>502</u>	<u>-6.37037E-4</u>	<u>448</u>	<u>20.71938</u>
<u>501.5</u>	<u>-6.25926E-4</u>	<u>448.5</u>	<u>20.2706</u>
<u>501</u>	<u>-6.2963E-4</u>	<u>449</u>	<u>20.4134</u>
<u>500.5</u>	<u>-6.51852E-4</u>	<u>449.5</u>	<u>20.98564</u>
<u>500</u>	<u>-7E-4</u>	<u>450</u>	<u>20.86252</u>
<u>499.5</u>	<u>-7.40741E-4</u>	<u>450.5</u>	<u>20.57603</u>
<u>499</u>	<u>-7.2963E-4</u>	<u>451</u>	<u>19.8599</u>
<u>498.5</u>	<u>-7.14815E-4</u>	<u>451.5</u>	<u>18.99841</u>
<u>498</u>	<u>-7.11111E-4</u>	<u>452</u>	<u>18.59071</u>
<u>497.5</u>	<u>-7.03704E-4</u>	<u>452.5</u>	<u>18.66039</u>
<u>497</u>	<u>-6.96296E-4</u>	<u>453</u>	<u>18.61924</u>
<u>496.5</u>	<u>-6.66667E-4</u>	<u>453.5</u>	<u>18.37427</u>
<u>496</u>	<u>-6.37037E-4</u>	<u>454</u>	<u>17.4845</u>
<u>495.5</u>	<u>-6.44444E-4</u>	<u>454.5</u>	<u>16.62059</u>
<u>495</u>	<u>-6.40741E-4</u>	<u>455</u>	<u>15.67425</u>
<u>494.5</u>	<u>-6.37037E-4</u>	<u>455.5</u>	<u>15.54225</u>
<u>494</u>	<u>-6.33333E-4</u>	<u>456</u>	<u>15.09783</u>

<u>493.5</u>	<u>-6.51852E-4</u>	<u>456.5</u>	<u>14.65507</u>
<u>493</u>	<u>-6.62963E-4</u>	<u>457</u>	<u>13.76489</u>
<u>492.5</u>	<u>-6.44444E-4</u>	<u>457.5</u>	<u>13.71966</u>
<u>492</u>	<u>-6.33333E-4</u>	<u>458</u>	<u>13.61508</u>
<u>491.5</u>	<u>-6.14815E-4</u>	<u>458.5</u>	<u>13.58223</u>
<u>491</u>	<u>-6.03704E-4</u>	<u>459</u>	<u>13.2111</u>
<u>490.5</u>	<u>-5.92593E-4</u>	<u>459.5</u>	<u>12.89035</u>
<u>490</u>	<u>-5.92593E-4</u>	<u>460</u>	<u>12.37737</u>
<u>489.5</u>	<u>-5.96296E-4</u>	<u>460.5</u>	<u>11.6137</u>
<u>489</u>	<u>-5.85185E-4</u>	<u>461</u>	<u>11.11017</u>
<u>488.5</u>	<u>-5.88889E-4</u>	<u>461.5</u>	<u>10.79131</u>
<u>488</u>	<u>-6E-4</u>	<u>462</u>	<u>10.72158</u>
<u>487.5</u>	<u>-5.74074E-4</u>	<u>462.5</u>	<u>10.27871</u>
<u>487</u>	<u>-5.40741E-4</u>	<u>463</u>	<u>9.83643</u>
<u>486.5</u>	<u>-5.18519E-4</u>	<u>463.5</u>	<u>9.50966</u>
<u>486</u>	<u>-5.18519E-4</u>	<u>464</u>	<u>9.58571</u>
<u>485.5</u>	<u>-4.92593E-4</u>	<u>464.5</u>	<u>9.68753</u>
<u>485</u>	<u>-5.07407E-4</u>	<u>465</u>	<u>9.36907</u>
<u>484.5</u>	<u>-5.25926E-4</u>	<u>465.5</u>	<u>8.60097</u>
<u>484</u>	<u>-5.37037E-4</u>	<u>466</u>	<u>7.88788</u>
<u>483.5</u>	<u>-5.37037E-4</u>	<u>466.5</u>	<u>7.80931</u>
<u>483</u>	<u>-5.33333E-4</u>	<u>467</u>	<u>8.02072</u>
<u>482.5</u>	<u>-5.25926E-4</u>	<u>467.5</u>	<u>7.96734</u>
<u>482</u>	<u>-5.18519E-4</u>	<u>468</u>	<u>7.55442</u>
<u>481.5</u>	<u>-4.81481E-4</u>	<u>468.5</u>	<u>7.01551</u>
<u>481</u>	<u>-4.7037E-4</u>	<u>469</u>	<u>6.60723</u>
<u>480.5</u>	<u>-4.62963E-4</u>	<u>469.5</u>	<u>6.54066</u>
<u>480</u>	<u>-4.55556E-4</u>	<u>470</u>	<u>6.88767</u>
<u>479.5</u>	<u>-4.44444E-4</u>	<u>470.5</u>	<u>7.17999</u>
<u>479</u>	<u>-4.33333E-4</u>	<u>471</u>	<u>6.79068</u>
<u>478.5</u>	<u>-4.07407E-4</u>	<u>471.5</u>	<u>5.96495</u>
<u>478</u>	<u>-4.03704E-4</u>	<u>472</u>	<u>5.42279</u>
<u>477.5</u>	<u>-3.92593E-4</u>	<u>472.5</u>	<u>5.68139</u>
<u>477</u>	<u>-3.77778E-4</u>	<u>473</u>	<u>5.90586</u>
<u>476.5</u>	<u>-3.7037E-4</u>	<u>473.5</u>	<u>5.72244</u>
<u>476</u>	<u>-3.51852E-4</u>	<u>474</u>	<u>5.01216</u>
<u>475.5</u>	<u>-3.44444E-4</u>	<u>474.5</u>	<u>4.54177</u>
<u>475</u>	<u>-3.66667E-4</u>	<u>475</u>	<u>4.31646</u>
<u>474.5</u>	<u>-3.59259E-4</u>	<u>475.5</u>	<u>4.24687</u>
<u>474</u>	<u>-3.40741E-4</u>	<u>476</u>	<u>4.08872</u>

<u>473.5</u>	<u>-2.92593E-4</u>	<u>476.5</u>	<u>4.20015</u>
<u>473</u>	<u>-2.51852E-4</u>	<u>477</u>	<u>4.4395</u>
<u>472.5</u>	<u>-2.33333E-4</u>	<u>477.5</u>	<u>4.36335</u>
<u>472</u>	<u>-2.03704E-4</u>	<u>478</u>	<u>3.84737</u>
<u>471.5</u>	<u>-1.44444E-4</u>	<u>478.5</u>	<u>3.14337</u>
<u>471</u>	<u>-1E-4</u>	<u>479</u>	<u>2.93116</u>
<u>470.5</u>	<u>-5.55556E-5</u>	<u>479.5</u>	<u>2.98659</u>
<u>470</u>	<u>-6.66667E-5</u>	<u>480</u>	<u>3.18069</u>
<u>469.5</u>	<u>-5.92593E-5</u>	<u>480.5</u>	<u>3.15301</u>
<u>469</u>	<u>7.40741E-6</u>	<u>481</u>	<u>3.08616</u>
<u>468.5</u>	<u>8.51852E-5</u>	<u>481.5</u>	<u>3.01731</u>
<u>468</u>	<u>1.25926E-4</u>	<u>482</u>	<u>3.12056</u>
<u>467.5</u>	<u>1.92593E-4</u>	<u>482.5</u>	<u>3.19616</u>
<u>467</u>	<u>2.55556E-4</u>	<u>483</u>	<u>3.04592</u>
<u>466.5</u>	<u>3.2963E-4</u>	<u>483.5</u>	<u>2.85976</u>
<u>466</u>	<u>3.85185E-4</u>	<u>484</u>	<u>2.64925</u>
<u>465.5</u>	<u>4.40741E-4</u>	<u>484.5</u>	<u>2.49148</u>
<u>465</u>	<u>5E-4</u>	<u>485</u>	<u>2.0627</u>
<u>464.5</u>	<u>5.62963E-4</u>	<u>485.5</u>	<u>1.52344</u>
<u>464</u>	<u>6.51852E-4</u>	<u>486</u>	<u>1.32128</u>
<u>463.5</u>	<u>7.59259E-4</u>	<u>486.5</u>	<u>1.50564</u>
<u>463</u>	<u>8.2963E-4</u>	<u>487</u>	<u>1.91859</u>
<u>462.5</u>	<u>9.18519E-4</u>	<u>487.5</u>	<u>1.91563</u>
<u>462</u>	<u>0.00101</u>	<u>488</u>	<u>1.72772</u>
<u>461.5</u>	<u>0.00111</u>	<u>488.5</u>	<u>1.43538</u>
<u>461</u>	<u>0.00119</u>	<u>489</u>	<u>1.52733</u>
<u>460.5</u>	<u>0.00127</u>	<u>489.5</u>	<u>1.77486</u>
<u>460</u>	<u>0.00135</u>	<u>490</u>	<u>2.01339</u>
<u>459.5</u>	<u>0.00139</u>	<u>490.5</u>	<u>1.88479</u>
<u>459</u>	<u>0.00144</u>	<u>491</u>	<u>1.57142</u>
<u>458.5</u>	<u>0.00152</u>	<u>491.5</u>	<u>1.55408</u>
<u>458</u>	<u>0.00162</u>	<u>492</u>	<u>1.79216</u>
<u>457.5</u>	<u>0.00168</u>	<u>492.5</u>	<u>1.92789</u>
<u>457</u>	<u>0.00179</u>	<u>493</u>	<u>1.6876</u>
<u>456.5</u>	<u>0.00188</u>	<u>493.5</u>	<u>1.34909</u>
<u>456</u>	<u>0.00198</u>	<u>494</u>	<u>1.02362</u>
<u>455.5</u>	<u>0.00206</u>	<u>494.5</u>	<u>0.74385</u>
<u>455</u>	<u>0.00213</u>	<u>495</u>	<u>0.7308</u>
<u>454.5</u>	<u>0.00216</u>	<u>495.5</u>	<u>0.93597</u>
<u>454</u>	<u>0.00225</u>	<u>496</u>	<u>1.15869</u>

<u>453.5</u>	<u>0.00231</u>	<u>496.5</u>	<u>1.12884</u>
<u>453</u>	<u>0.00237</u>	<u>497</u>	<u>1.25741</u>
<u>452.5</u>	<u>0.0024</u>	<u>497.5</u>	<u>1.40674</u>
<u>452</u>	<u>0.00239</u>	<u>498</u>	<u>1.42926</u>
<u>451.5</u>	<u>0.00243</u>	<u>498.5</u>	<u>1.3148</u>
<u>451</u>	<u>0.00245</u>	<u>499</u>	<u>1.20796</u>
<u>450.5</u>	<u>0.00246</u>	<u>499.5</u>	<u>1.07435</u>
<u>450</u>	<u>0.00247</u>	<u>500</u>	<u>0.83494</u>
<u>449.5</u>	<u>0.00252</u>	<u>500.5</u>	<u>0.77515</u>
<u>449</u>	<u>0.0026</u>	<u>501</u>	<u>0.88478</u>
<u>448.5</u>	<u>0.00266</u>	<u>501.5</u>	<u>1.05715</u>
<u>448</u>	<u>0.00272</u>	<u>502</u>	<u>0.95258</u>
<u>447.5</u>	<u>0.00273</u>	<u>502.5</u>	<u>0.82342</u>
<u>447</u>	<u>0.00275</u>	<u>503</u>	<u>0.69231</u>
<u>446.5</u>	<u>0.00278</u>	<u>503.5</u>	<u>0.51583</u>
<u>446</u>	<u>0.0028</u>	<u>504</u>	<u>0.27618</u>
<u>445.5</u>	<u>0.00285</u>	<u>504.5</u>	<u>0.15936</u>
<u>445</u>	<u>0.00285</u>	<u>505</u>	<u>0.08618</u>
<u>444.5</u>	<u>0.0029</u>	<u>505.5</u>	<u>0.12528</u>
<u>444</u>	<u>0.00296</u>	<u>506</u>	<u>0.11579</u>
<u>443.5</u>	<u>0.00305</u>	<u>506.5</u>	<u>0.2265</u>
<u>443</u>	<u>0.00309</u>	<u>507</u>	<u>0.37222</u>
<u>442.5</u>	<u>0.00317</u>	<u>507.5</u>	<u>0.53241</u>
<u>442</u>	<u>0.00327</u>	<u>508</u>	<u>0.62286</u>
<u>441.5</u>	<u>0.00334</u>	<u>508.5</u>	<u>0.63716</u>
<u>441</u>	<u>0.00343</u>	<u>509</u>	<u>0.66612</u>
<u>440.5</u>	<u>0.00351</u>	<u>509.5</u>	<u>0.65426</u>
<u>440</u>	<u>0.00365</u>	<u>510</u>	<u>0.61558</u>
<u>439.5</u>	<u>0.00383</u>	<u>510.5</u>	<u>0.48888</u>
<u>439</u>	<u>0.00396</u>	<u>511</u>	<u>0.45226</u>
<u>438.5</u>	<u>0.00411</u>	<u>511.5</u>	<u>0.40035</u>
<u>438</u>	<u>0.00424</u>	<u>512</u>	<u>0.40729</u>
<u>437.5</u>	<u>0.00442</u>	<u>512.5</u>	<u>0.45567</u>
<u>437</u>	<u>0.0046</u>	<u>513</u>	<u>0.45204</u>
<u>436.5</u>	<u>0.00481</u>	<u>513.5</u>	<u>0.35841</u>
<u>436</u>	<u>0.00501</u>	<u>514</u>	<u>0.17925</u>
<u>435.5</u>	<u>0.00522</u>	<u>514.5</u>	<u>0.12306</u>
<u>435</u>	<u>0.00547</u>	<u>515</u>	<u>0.12499</u>
<u>434.5</u>	<u>0.00569</u>	<u>515.5</u>	<u>0.12941</u>
<u>434</u>	<u>0.00587</u>	<u>516</u>	<u>0.13165</u>

<u>433.5</u>	<u>0.006</u>	<u>516.5</u>	<u>0.19605</u>
<u>433</u>	<u>0.00612</u>	<u>517</u>	<u>0.26125</u>
<u>432.5</u>	<u>0.00629</u>	<u>517.5</u>	<u>0.29741</u>
<u>432</u>	<u>0.00643</u>	<u>518</u>	<u>0.34714</u>
<u>431.5</u>	<u>0.00654</u>	<u>518.5</u>	<u>0.34225</u>
<u>431</u>	<u>0.00663</u>	<u>519</u>	<u>0.3256</u>
<u>430.5</u>	<u>0.00673</u>	<u>519.5</u>	<u>0.26542</u>
<u>430</u>	<u>0.00677</u>	<u>520</u>	<u>0.27761</u>
<u>429.5</u>	<u>0.00679</u>	<u>520.5</u>	<u>0.2631</u>
<u>429</u>	<u>0.0068</u>	<u>521</u>	<u>0.34464</u>
<u>428.5</u>	<u>0.00674</u>	<u>521.5</u>	<u>0.29716</u>
<u>428</u>	<u>0.00671</u>	<u>522</u>	<u>0.27355</u>
<u>427.5</u>	<u>0.00668</u>	<u>522.5</u>	<u>0.17429</u>
<u>427</u>	<u>0.00664</u>	<u>523</u>	<u>0.20769</u>
<u>426.5</u>	<u>0.0066</u>	<u>523.5</u>	<u>0.19402</u>
<u>426</u>	<u>0.00654</u>	<u>524</u>	<u>0.13366</u>
<u>425.5</u>	<u>0.00649</u>	<u>524.5</u>	<u>0.05014</u>
<u>425</u>	<u>0.00644</u>	<u>525</u>	<u>0.15442</u>
<u>424.5</u>	<u>0.00643</u>	<u>525.5</u>	<u>0.29041</u>
<u>424</u>	<u>0.00639</u>	<u>526</u>	<u>0.24906</u>
<u>423.5</u>	<u>0.00637</u>	<u>526.5</u>	<u>0.0763</u>
<u>423</u>	<u>0.00632</u>	<u>527</u>	<u>-0.08824</u>
<u>422.5</u>	<u>0.0063</u>	<u>527.5</u>	<u>-0.0731</u>
<u>422</u>	<u>0.00628</u>	<u>528</u>	<u>0.16421</u>
<u>421.5</u>	<u>0.00619</u>	<u>528.5</u>	<u>0.35627</u>
<u>421</u>	<u>0.00612</u>	<u>529</u>	<u>0.41158</u>
<u>420.5</u>	<u>0.00604</u>	<u>529.5</u>	<u>0.23635</u>
<u>420</u>	<u>0.00596</u>	<u>530</u>	<u>0.18292</u>
<u>419.5</u>	<u>0.00589</u>	<u>530.5</u>	<u>0.31067</u>
<u>419</u>	<u>0.00581</u>	<u>531</u>	<u>0.53262</u>
<u>418.5</u>	<u>0.00572</u>	<u>531.5</u>	<u>0.54903</u>
<u>418</u>	<u>0.0056</u>	<u>532</u>	<u>0.38362</u>
<u>417.5</u>	<u>0.00555</u>	<u>532.5</u>	<u>0.08553</u>
<u>417</u>	<u>0.00547</u>	<u>533</u>	<u>-0.11019</u>
<u>416.5</u>	<u>0.0054</u>	<u>533.5</u>	<u>-0.05223</u>
<u>416</u>	<u>0.00532</u>	<u>534</u>	<u>0.08308</u>
<u>415.5</u>	<u>0.00527</u>	<u>534.5</u>	<u>0.2219</u>
<u>415</u>	<u>0.00523</u>	<u>535</u>	<u>0.271</u>
<u>414.5</u>	<u>0.00518</u>	<u>535.5</u>	<u>0.34916</u>
<u>414</u>	<u>0.00515</u>	<u>536</u>	<u>0.35468</u>

<u>413.5</u>	<u>0.00515</u>	<u>536.5</u>	<u>0.35887</u>
<u>413</u>	<u>0.00514</u>	<u>537</u>	<u>0.26683</u>
<u>412.5</u>	<u>0.00517</u>	<u>537.5</u>	<u>0.21648</u>
<u>412</u>	<u>0.0052</u>	<u>538</u>	<u>0.09539</u>
<u>411.5</u>	<u>0.00525</u>	<u>538.5</u>	<u>-0.00706</u>
<u>411</u>	<u>0.00527</u>	<u>539</u>	<u>-0.09617</u>
<u>410.5</u>	<u>0.00533</u>	<u>539.5</u>	<u>-0.03891</u>
<u>410</u>	<u>0.00536</u>	<u>540</u>	<u>0.10219</u>
<u>409.5</u>	<u>0.00537</u>	<u>540.5</u>	<u>0.28436</u>
<u>409</u>	<u>0.00543</u>	<u>541</u>	<u>0.25156</u>
<u>408.5</u>	<u>0.00547</u>	<u>541.5</u>	<u>0.13397</u>
<u>408</u>	<u>0.00554</u>	<u>542</u>	<u>0.038</u>
<u>407.5</u>	<u>0.0056</u>	<u>542.5</u>	<u>0.04009</u>
<u>407</u>	<u>0.00563</u>	<u>543</u>	<u>0.01445</u>
<u>406.5</u>	<u>0.00571</u>	<u>543.5</u>	<u>-0.02638</u>
<u>406</u>	<u>0.00574</u>	<u>544</u>	<u>0.07632</u>
<u>405.5</u>	<u>0.00578</u>	<u>544.5</u>	<u>0.32417</u>
<u>405</u>	<u>0.00575</u>	<u>545</u>	<u>0.55742</u>
<u>404.5</u>	<u>0.00569</u>	<u>545.5</u>	<u>0.47724</u>
<u>404</u>	<u>0.00561</u>	<u>546</u>	<u>0.2738</u>
<u>403.5</u>	<u>0.0056</u>	<u>546.5</u>	<u>0.10583</u>
<u>403</u>	<u>0.00561</u>	<u>547</u>	<u>0.12755</u>
<u>402.5</u>	<u>0.0056</u>	<u>547.5</u>	<u>0.15101</u>
<u>402</u>	<u>0.0056</u>	<u>548</u>	<u>0.13059</u>
<u>401.5</u>	<u>0.00562</u>	<u>548.5</u>	<u>0.08831</u>
<u>401</u>	<u>0.00562</u>	<u>549</u>	<u>0.07936</u>
<u>400.5</u>	<u>0.00559</u>	<u>549.5</u>	<u>0.09559</u>
<u>400</u>	<u>0.00555</u>	<u>550</u>	<u>0.11809</u>
<u>399.5</u>	<u>0.0055</u>	<u>550.5</u>	<u>0.15064</u>
<u>399</u>	<u>0.0054</u>	<u>551</u>	<u>0.14475</u>
<u>398.5</u>	<u>0.00536</u>	<u>551.5</u>	<u>0.10848</u>
<u>398</u>	<u>0.00527</u>	<u>552</u>	<u>0.05848</u>
<u>397.5</u>	<u>0.0052</u>	<u>552.5</u>	<u>0.07089</u>
<u>397</u>	<u>0.0051</u>	<u>553</u>	<u>0.11473</u>
<u>396.5</u>	<u>0.005</u>	<u>553.5</u>	<u>0.13352</u>
<u>396</u>	<u>0.00494</u>	<u>554</u>	<u>0.08127</u>
<u>395.5</u>	<u>0.00487</u>	<u>554.5</u>	<u>-0.00914</u>
<u>395</u>	<u>0.00477</u>	<u>555</u>	<u>-0.04716</u>
<u>394.5</u>	<u>0.00473</u>	<u>555.5</u>	<u>-0.02533</u>
<u>394</u>	<u>0.00464</u>	<u>556</u>	<u>0.01473</u>

<u>393.5</u>	<u>0.00457</u>	<u>556.5</u>	<u>0.00582</u>
<u>393</u>	<u>0.00454</u>	<u>557</u>	<u>0.04348</u>
<u>392.5</u>	<u>0.00451</u>	<u>557.5</u>	<u>0.12531</u>
<u>392</u>	<u>0.00442</u>	<u>558</u>	<u>0.18776</u>
<u>391.5</u>	<u>0.0044</u>	<u>558.5</u>	<u>0.14683</u>
<u>391</u>	<u>0.00435</u>	<u>559</u>	<u>0.09495</u>
<u>390.5</u>	<u>0.0043</u>	<u>559.5</u>	<u>0.07995</u>
<u>390</u>	<u>0.00427</u>	<u>560</u>	<u>0.08601</u>
<u>389.5</u>	<u>0.00422</u>	<u>560.5</u>	<u>0.09284</u>
<u>389</u>	<u>0.00419</u>	<u>561</u>	<u>0.05733</u>
<u>388.5</u>	<u>0.00418</u>	<u>561.5</u>	<u>0.0138</u>
<u>388</u>	<u>0.00419</u>	<u>562</u>	<u>-0.00953</u>
<u>387.5</u>	<u>0.00424</u>	<u>562.5</u>	<u>0.08732</u>
<u>387</u>	<u>0.00426</u>	<u>563</u>	<u>0.18815</u>
<u>386.5</u>	<u>0.00429</u>	<u>563.5</u>	<u>0.14896</u>
<u>386</u>	<u>0.00433</u>	<u>564</u>	<u>0.07106</u>
<u>385.5</u>	<u>0.00435</u>	<u>564.5</u>	<u>0.10947</u>
<u>385</u>	<u>0.00435</u>	<u>565</u>	<u>0.3118</u>
<u>384.5</u>	<u>0.00439</u>	<u>565.5</u>	<u>0.40295</u>
<u>384</u>	<u>0.00444</u>	<u>566</u>	<u>0.33377</u>
<u>383.5</u>	<u>0.00446</u>	<u>566.5</u>	<u>0.13071</u>
<u>383</u>	<u>0.00457</u>	<u>567</u>	<u>0.05031</u>
<u>382.5</u>	<u>0.00463</u>	<u>567.5</u>	<u>0.07291</u>
<u>382</u>	<u>0.00465</u>	<u>568</u>	<u>0.13049</u>
<u>381.5</u>	<u>0.00464</u>	<u>568.5</u>	<u>0.09667</u>
<u>381</u>	<u>0.00468</u>	<u>569</u>	<u>0.01138</u>
<u>380.5</u>	<u>0.00474</u>	<u>569.5</u>	<u>-0.01961</u>
<u>380</u>	<u>0.00484</u>	<u>570</u>	<u>0.03773</u>
<u>379.5</u>	<u>0.00494</u>	<u>570.5</u>	<u>0.09792</u>
<u>379</u>	<u>0.0051</u>	<u>571</u>	<u>0.11434</u>
<u>378.5</u>	<u>0.00528</u>	<u>571.5</u>	<u>0.095</u>
<u>378</u>	<u>0.00547</u>	<u>572</u>	<u>0.11263</u>
<u>377.5</u>	<u>0.00562</u>	<u>572.5</u>	<u>0.11638</u>
<u>377</u>	<u>0.0058</u>	<u>573</u>	<u>0.08773</u>
<u>376.5</u>	<u>0.00594</u>	<u>573.5</u>	<u>0.07675</u>
<u>376</u>	<u>0.00617</u>	<u>574</u>	<u>0.13195</u>
<u>375.5</u>	<u>0.0064</u>	<u>574.5</u>	<u>0.17556</u>
<u>375</u>	<u>0.00661</u>	<u>575</u>	<u>0.10798</u>
<u>374.5</u>	<u>0.00684</u>	<u>575.5</u>	<u>-2.04E-4</u>
<u>374</u>	<u>0.00716</u>	<u>576</u>	<u>-0.1071</u>

<u>373.5</u>	<u>0.0075</u>	<u>576.5</u>	<u>-0.10877</u>
<u>373</u>	<u>0.00791</u>	<u>577</u>	<u>-0.01685</u>
<u>372.5</u>	<u>0.0083</u>	<u>577.5</u>	<u>0.11296</u>
<u>372</u>	<u>0.00879</u>	<u>578</u>	<u>0.13959</u>
<u>371.5</u>	<u>0.0093</u>	<u>578.5</u>	<u>0.06082</u>
<u>371</u>	<u>0.00984</u>	<u>579</u>	<u>0.03458</u>
<u>370.5</u>	<u>0.01038</u>	<u>579.5</u>	<u>0.08997</u>
<u>370</u>	<u>0.01105</u>	<u>580</u>	<u>0.1601</u>
<u>369.5</u>	<u>0.01186</u>	<u>580.5</u>	<u>0.15717</u>
<u>369</u>	<u>0.01288</u>	<u>581</u>	<u>0.18058</u>
<u>368.5</u>	<u>0.01416</u>	<u>581.5</u>	<u>0.21687</u>
<u>368</u>	<u>0.01573</u>	<u>582</u>	<u>0.25481</u>
<u>367.5</u>	<u>0.0177</u>	<u>582.5</u>	<u>0.2005</u>
<u>367</u>	<u>0.02017</u>	<u>583</u>	<u>0.11852</u>
<u>366.5</u>	<u>0.02376</u>	<u>583.5</u>	<u>0.1189</u>
<u>366</u>	<u>0.02854</u>	<u>584</u>	<u>0.20274</u>
<u>365.5</u>	<u>0.0347</u>	<u>584.5</u>	<u>0.2676</u>
<u>365</u>	<u>0.04262</u>	<u>585</u>	<u>0.22209</u>
<u>364.5</u>	<u>0.05262</u>	<u>585.5</u>	<u>0.18224</u>
<u>364</u>	<u>0.06514</u>	<u>586</u>	<u>0.19531</u>
<u>363.5</u>	<u>0.08047</u>	<u>586.5</u>	<u>0.19224</u>
<u>363</u>	<u>0.0991</u>	<u>587</u>	<u>0.1066</u>
<u>362.5</u>	<u>0.12143</u>	<u>587.5</u>	<u>0.06558</u>
<u>362</u>	<u>0.14789</u>	<u>588</u>	<u>0.11082</u>
<u>361.5</u>	<u>0.17888</u>	<u>588.5</u>	<u>0.16427</u>
<u>361</u>	<u>0.21477</u>	<u>589</u>	<u>0.18303</u>
<u>360.5</u>	<u>0.25517</u>	<u>589.5</u>	<u>0.15045</u>
<u>360</u>	<u>0.29894</u>	<u>590</u>	<u>0.20437</u>
<u>359.5</u>	<u>0.34704</u>	<u>590.5</u>	<u>0.2412</u>
<u>359</u>	<u>0.39797</u>	<u>591</u>	<u>0.24755</u>
<u>358.5</u>	<u>0.44999</u>	<u>591.5</u>	<u>0.15637</u>
<u>358</u>	<u>0.50053</u>	<u>592</u>	<u>0.13666</u>
<u>357.5</u>	<u>0.54614</u>	<u>592.5</u>	<u>0.11657</u>
<u>357</u>	<u>0.58413</u>	<u>593</u>	<u>0.15832</u>
<u>356.5</u>	<u>0.611</u>	<u>593.5</u>	<u>0.10253</u>
<u>356</u>	<u>0.62839</u>	<u>594</u>	<u>0.12126</u>
<u>355.5</u>	<u>0.63691</u>	<u>594.5</u>	<u>0.16739</u>
<u>355</u>	<u>0.6393</u>	<u>595</u>	<u>0.24704</u>
<u>354.5</u>	<u>0.63784</u>	<u>595.5</u>	<u>0.20944</u>
<u>354</u>	<u>0.63421</u>	<u>596</u>	<u>0.12601</u>

<u>353.5</u>	<u>0.62892</u>	<u>596.5</u>	<u>0.05087</u>
<u>353</u>	<u>0.62497</u>	<u>597</u>	<u>0.12505</u>
<u>352.5</u>	<u>0.62211</u>	<u>597.5</u>	<u>0.30657</u>
<u>352</u>	<u>0.62017</u>	<u>598</u>	<u>0.42781</u>
<u>351.5</u>	<u>0.61892</u>	<u>598.5</u>	<u>0.34014</u>
<u>351</u>	<u>0.61824</u>	<u>599</u>	<u>0.1347</u>
<u>350.5</u>	<u>0.61805</u>	<u>599.5</u>	<u>0.04255</u>
<u>350</u>	<u>0.61819</u>	<u>600</u>	<u>0.08309</u>
<u>349.5</u>	<u>0.61896</u>	<u>600.5</u>	<u>0.11633</u>
<u>349</u>	<u>0.62104</u>	<u>601</u>	<u>0.07378</u>
<u>348.5</u>	<u>0.62487</u>	<u>601.5</u>	<u>0.09056</u>
<u>348</u>	<u>0.63084</u>	<u>602</u>	<u>0.2378</u>
<u>347.5</u>	<u>0.63908</u>	<u>602.5</u>	<u>0.39559</u>
<u>347</u>	<u>0.64956</u>	<u>603</u>	<u>0.39048</u>
<u>346.5</u>	<u>0.66198</u>	<u>603.5</u>	<u>0.26232</u>
<u>346</u>	<u>0.67558</u>	<u>604</u>	<u>0.12085</u>
<u>345.5</u>	<u>0.69007</u>	<u>604.5</u>	<u>0.08105</u>
<u>345</u>	<u>0.70434</u>	<u>605</u>	<u>0.12676</u>
<u>344.5</u>	<u>0.7178</u>	<u>605.5</u>	<u>0.19573</u>
<u>344</u>	<u>0.73043</u>	<u>606</u>	<u>0.2446</u>
<u>343.5</u>	<u>0.74233</u>	<u>606.5</u>	<u>0.24275</u>
<u>343</u>	<u>0.75299</u>	<u>607</u>	<u>0.15124</u>
<u>342.5</u>	<u>0.76455</u>	<u>607.5</u>	<u>0.03142</u>
<u>342</u>	<u>0.77647</u>	<u>608</u>	<u>-0.00645</u>
<u>341.5</u>	<u>0.78937</u>	<u>608.5</u>	<u>0.07436</u>
<u>341</u>	<u>0.80371</u>	<u>609</u>	<u>0.17716</u>
<u>340.5</u>	<u>0.81944</u>	<u>609.5</u>	<u>0.14341</u>
<u>340</u>	<u>0.83617</u>	<u>610</u>	<u>0.03368</u>
<u>339.5</u>	<u>0.85208</u>	<u>610.5</u>	<u>-0.03632</u>
<u>339</u>	<u>0.86587</u>	<u>611</u>	<u>0.03527</u>
<u>338.5</u>	<u>0.87667</u>	<u>611.5</u>	<u>0.1043</u>
<u>338</u>	<u>0.88431</u>	<u>612</u>	<u>0.10942</u>
<u>337.5</u>	<u>0.88793</u>	<u>612.5</u>	<u>0.03482</u>
<u>337</u>	<u>0.88868</u>	<u>613</u>	<u>0.0111</u>
<u>336.5</u>	<u>0.886</u>	<u>613.5</u>	<u>0.0152</u>
<u>336</u>	<u>0.87928</u>	<u>614</u>	<u>0.03306</u>
<u>335.5</u>	<u>0.87198</u>	<u>614.5</u>	<u>0.03843</u>
<u>335</u>	<u>0.86311</u>	<u>615</u>	<u>0.03553</u>
<u>334.5</u>	<u>0.85314</u>	<u>615.5</u>	<u>0.05877</u>
<u>334</u>	<u>0.84338</u>	<u>616</u>	<u>0.10337</u>

<u>333.5</u>	<u>0.83373</u>	<u>616.5</u>	<u>0.13519</u>
<u>333</u>	<u>0.82439</u>	<u>617</u>	<u>0.17602</u>
<u>332.5</u>	<u>0.81507</u>	<u>617.5</u>	<u>0.29861</u>
<u>332</u>	<u>0.80651</u>	<u>618</u>	<u>0.43427</u>
<u>331.5</u>	<u>0.79773</u>	<u>618.5</u>	<u>0.44688</u>
<u>331</u>	<u>0.7896</u>	<u>619</u>	<u>0.22836</u>
<u>330.5</u>	<u>0.78156</u>	<u>619.5</u>	<u>-0.0342</u>
<u>330</u>	<u>0.77471</u>	<u>620</u>	<u>-0.15524</u>
<u>329.5</u>	<u>0.76854</u>	<u>620.5</u>	<u>-0.09105</u>
<u>329</u>	<u>0.76341</u>	<u>621</u>	<u>0.01884</u>
<u>328.5</u>	<u>0.75884</u>	<u>621.5</u>	<u>0.12838</u>
<u>328</u>	<u>0.75468</u>	<u>622</u>	<u>0.15626</u>
<u>327.5</u>	<u>0.75084</u>	<u>622.5</u>	<u>0.1315</u>
<u>327</u>	<u>0.74718</u>	<u>623</u>	<u>0.10736</u>
<u>326.5</u>	<u>0.74334</u>	<u>623.5</u>	<u>0.12272</u>
<u>326</u>	<u>0.73853</u>	<u>624</u>	<u>0.14933</u>
<u>325.5</u>	<u>0.73224</u>	<u>624.5</u>	<u>0.08991</u>
<u>325</u>	<u>0.72522</u>	<u>625</u>	<u>-0.01719</u>
<u>324.5</u>	<u>0.7173</u>	<u>625.5</u>	<u>-0.05124</u>
<u>324</u>	<u>0.70913</u>	<u>626</u>	<u>0.01758</u>
<u>323.5</u>	<u>0.69981</u>	<u>626.5</u>	<u>0.0716</u>
<u>323</u>	<u>0.69053</u>	<u>627</u>	<u>0.06508</u>
<u>322.5</u>	<u>0.68142</u>	<u>627.5</u>	<u>0.04158</u>
<u>322</u>	<u>0.67147</u>	<u>628</u>	<u>0.09116</u>
<u>321.5</u>	<u>0.66109</u>	<u>628.5</u>	<u>0.15761</u>
<u>321</u>	<u>0.65042</u>	<u>629</u>	<u>0.13268</u>
<u>320.5</u>	<u>0.63931</u>	<u>629.5</u>	<u>0.01792</u>
<u>320</u>	<u>0.62805</u>	<u>630</u>	<u>-0.03156</u>
<u>319.5</u>	<u>0.61584</u>	<u>630.5</u>	<u>0.03579</u>
<u>319</u>	<u>0.60319</u>	<u>631</u>	<u>0.14843</u>
<u>318.5</u>	<u>0.5901</u>	<u>631.5</u>	<u>0.12671</u>
<u>318</u>	<u>0.57642</u>	<u>632</u>	<u>0.06903</u>
<u>317.5</u>	<u>0.56265</u>	<u>632.5</u>	<u>0.04965</u>
<u>317</u>	<u>0.54881</u>	<u>633</u>	<u>0.1558</u>
<u>316.5</u>	<u>0.53483</u>	<u>633.5</u>	<u>0.20188</u>
<u>316</u>	<u>0.5214</u>	<u>634</u>	<u>0.14264</u>
<u>315.5</u>	<u>0.50864</u>	<u>634.5</u>	<u>0.0036</u>
<u>315</u>	<u>0.49616</u>	<u>635</u>	<u>0.03397</u>
<u>314.5</u>	<u>0.48394</u>	<u>635.5</u>	<u>0.16462</u>
<u>314</u>	<u>0.47228</u>	<u>636</u>	<u>0.26171</u>

<u>313.5</u>	<u>0.46145</u>	<u>636.5</u>	<u>0.16378</u>
<u>313</u>	<u>0.4514</u>	<u>637</u>	<u>4.18E-4</u>
<u>312.5</u>	<u>0.4418</u>	<u>637.5</u>	<u>-0.08378</u>
<u>312</u>	<u>0.43249</u>	<u>638</u>	<u>0.01668</u>
<u>311.5</u>	<u>0.4233</u>	<u>638.5</u>	<u>0.15773</u>
<u>311</u>	<u>0.41379</u>	<u>639</u>	<u>0.19804</u>
<u>310.5</u>	<u>0.40423</u>	<u>639.5</u>	<u>0.07961</u>
<u>310</u>	<u>0.39434</u>	<u>640</u>	<u>-0.04573</u>
<u>309.5</u>	<u>0.38436</u>	<u>640.5</u>	<u>-0.04475</u>
<u>309</u>	<u>0.37436</u>	<u>641</u>	<u>0.06211</u>
<u>308.5</u>	<u>0.36431</u>	<u>641.5</u>	<u>0.15354</u>
<u>308</u>	<u>0.35461</u>	<u>642</u>	<u>0.17626</u>
<u>307.5</u>	<u>0.34505</u>	<u>642.5</u>	<u>0.16626</u>
<u>307</u>	<u>0.33567</u>	<u>643</u>	<u>0.1735</u>
<u>306.5</u>	<u>0.32658</u>	<u>643.5</u>	<u>0.21116</u>
<u>306</u>	<u>0.31796</u>	<u>644</u>	<u>0.22536</u>
<u>305.5</u>	<u>0.30995</u>	<u>644.5</u>	<u>0.16344</u>
<u>305</u>	<u>0.30248</u>	<u>645</u>	<u>0.10351</u>
<u>304.5</u>	<u>0.2956</u>	<u>645.5</u>	<u>0.04637</u>
<u>304</u>	<u>0.289</u>	<u>646</u>	<u>0.025</u>
<u>303.5</u>	<u>0.28274</u>	<u>646.5</u>	<u>-0.01595</u>
<u>303</u>	<u>0.27677</u>	<u>647</u>	<u>-0.01815</u>
<u>302.5</u>	<u>0.27099</u>	<u>647.5</u>	<u>-0.03817</u>
<u>302</u>	<u>0.2654</u>	<u>648</u>	<u>-0.00492</u>
<u>301.5</u>	<u>0.25984</u>	<u>648.5</u>	<u>0.06212</u>
<u>301</u>	<u>0.25466</u>	<u>649</u>	<u>0.18384</u>
<u>300.5</u>	<u>0.24974</u>	<u>649.5</u>	<u>0.20348</u>
<u>300</u>	<u>0.24519</u>	<u>650</u>	<u>0.05529</u>
<u>299.5</u>	<u>0.24077</u>	<u>650.5</u>	<u>-0.23599</u>
<u>299</u>	<u>0.23661</u>		
<u>298.5</u>	<u>0.23276</u>		
<u>298</u>	<u>0.22928</u>		
<u>297.5</u>	<u>0.22611</u>		
<u>297</u>	<u>0.2231</u>		
<u>296.5</u>	<u>0.22034</u>		
<u>296</u>	<u>0.21794</u>		
<u>295.5</u>	<u>0.21575</u>		
<u>295</u>	<u>0.21379</u>		
<u>294.5</u>	<u>0.21196</u>		
<u>294</u>	<u>0.21049</u>		

<u>293.5</u>	0.20932
<u>293</u>	0.20854
<u>292.5</u>	0.20798
<u>292</u>	0.20771
<u>291.5</u>	0.20758
<u>291</u>	0.20773
<u>290.5</u>	0.208
<u>290</u>	0.20829
<u>289.5</u>	0.20865
<u>289</u>	0.20899
<u>288.5</u>	0.20938
<u>288</u>	0.20963
<u>287.5</u>	0.20981
<u>287</u>	0.20985
<u>286.5</u>	0.20977
<u>286</u>	0.20956
<u>285.5</u>	0.20912
<u>285</u>	0.20866
<u>284.5</u>	0.20816
<u>284</u>	0.20764
<u>283.5</u>	0.2072
<u>283</u>	0.2069
<u>282.5</u>	0.20667
<u>282</u>	0.20649
<u>281.5</u>	0.20648
<u>281</u>	0.20659
<u>280.5</u>	0.20681
<u>280</u>	0.20703
<u>279.5</u>	0.20734
<u>279</u>	0.20759
<u>278.5</u>	0.20778
<u>278</u>	0.20782
<u>277.5</u>	0.20779
<u>277</u>	0.20744
<u>276.5</u>	0.20702
<u>276</u>	0.20651
<u>275.5</u>	0.20574
<u>275</u>	0.20489
<u>274.5</u>	0.20403
<u>274</u>	0.20307

<u>273.5</u>	0.20192
<u>273</u>	0.20076
<u>272.5</u>	0.19981
<u>272</u>	0.19863
<u>271.5</u>	0.19758
<u>271</u>	0.19651
<u>270.5</u>	0.19544
<u>270</u>	0.19425
<u>269.5</u>	0.19325
<u>269</u>	0.19205
<u>268.5</u>	0.191
<u>268</u>	0.18971
<u>267.5</u>	0.18841
<u>267</u>	0.18727
<u>266.5</u>	0.18621
<u>266</u>	0.1851
<u>265.5</u>	0.18443
<u>265</u>	0.18348
<u>264.5</u>	0.18239
<u>264</u>	0.18163
<u>263.5</u>	0.18084
<u>263</u>	0.17982
<u>262.5</u>	0.17876
<u>262</u>	0.17767
<u>261.5</u>	0.1771
<u>261</u>	0.1763
<u>260.5</u>	0.17601
<u>260</u>	0.17595
<u>259.5</u>	0.17581
<u>259</u>	0.17576
<u>258.5</u>	0.17361
<u>258</u>	0.1633
<u>257.5</u>	0.15203
<u>257</u>	0.16097
<u>256.5</u>	0.20383
<u>256</u>	0.2211
<u>255.5</u>	0.09199
<u>255</u>	0.03784
<u>254.5</u>	-0.00498
<u>254</u>	-0.10164

<u>253.5</u>	-0.17424
<u>253</u>	-0.20636
<u>252.5</u>	-0.24557
<u>252</u>	-0.25042
<u>251.5</u>	-0.2662
<u>251</u>	-0.27292
<u>250.5</u>	-0.27568
<u>250</u>	-0.27289
<u>249.5</u>	-0.23096
<u>249</u>	-0.20359
<u>248.5</u>	-0.19535
<u>248</u>	-0.18135
<u>247.5</u>	-0.1388
<u>247</u>	-0.14845
<u>246.5</u>	-0.17415
<u>246</u>	-0.1753
<u>245.5</u>	-0.19524
<u>245</u>	-0.17901
<u>244.5</u>	-0.08499
<u>244</u>	-0.04162
<u>243.5</u>	-0.10041
<u>243</u>	-0.16004
<u>242.5</u>	-0.16855
<u>242</u>	-0.19323
<u>241.5</u>	-0.2075
<u>241</u>	-0.20227
<u>240.5</u>	-0.14929
<u>240</u>	-0.09792
<u>239.5</u>	-0.00498
<u>239</u>	0.16369
<u>238.5</u>	0.18737
<u>238</u>	0.22407
<u>237.5</u>	-0.07234
<u>237</u>	-0.06659
<u>236.5</u>	0.04734
<u>236</u>	2.22222
<u>235.5</u>	2.22222
<u>235</u>	2.22222
<u>234.5</u>	2.22222
<u>234</u>	2.22222

<u>233.5</u>	<u>2.22222</u>
<u>233</u>	<u>2.22222</u>
<u>232.5</u>	<u>-0.0592</u>
<u>232</u>	<u>-0.37272</u>
<u>231.5</u>	<u>2.22222</u>
<u>231</u>	<u>2.22222</u>
<u>230.5</u>	<u>-0.12909</u>
<u>230</u>	<u>-0.49674</u>
<u>229.5</u>	<u>-0.5968</u>
<u>229</u>	<u>-0.64075</u>
<u>228.5</u>	<u>-0.65331</u>
<u>228</u>	<u>-0.63504</u>
<u>227.5</u>	<u>-0.58551</u>
<u>227</u>	<u>-0.47556</u>
<u>226.5</u>	<u>2.22222</u>
<u>226</u>	<u>2.22222</u>
<u>225.5</u>	<u>2.22222</u>
<u>225</u>	<u>-0.40535</u>
<u>224.5</u>	<u>2.22222</u>
<u>224</u>	<u>2.22222</u>
<u>223.5</u>	<u>2.22222</u>
<u>223</u>	<u>-0.19629</u>
<u>222.5</u>	<u>-0.31472</u>
<u>222</u>	<u>-0.37583</u>
<u>221.5</u>	<u>-0.3994</u>
<u>221</u>	<u>-0.39307</u>
<u>220.5</u>	<u>-0.34965</u>
<u>220</u>	<u>-0.25749</u>
<u>219.5</u>	<u>0.18298</u>
<u>219</u>	<u>2.22222</u>
<u>218.5</u>	<u>2.22222</u>
<u>218</u>	<u>-0.10889</u>
<u>217.5</u>	<u>2.22222</u>
<u>217</u>	<u>2.22222</u>
<u>216.5</u>	<u>2.22222</u>
<u>216</u>	<u>0.30682</u>
<u>215.5</u>	<u>2.22222</u>
<u>215</u>	<u>2.22222</u>
<u>214.5</u>	<u>2.22222</u>
<u>214</u>	<u>0.47849</u>

<u>213.5</u>	<u>-0.22689</u>
<u>213</u>	<u>2.22222</u>
<u>212.5</u>	<u>2.22222</u>
<u>212</u>	<u>-0.38947</u>
<u>211.5</u>	<u>-0.46054</u>
<u>211</u>	<u>-0.4168</u>
<u>210.5</u>	<u>-0.24957</u>
<u>210</u>	<u>2.22222</u>
<u>209.5</u>	<u>2.22222</u>
<u>209</u>	<u>2.22222</u>
<u>208.5</u>	<u>2.22222</u>
<u>208</u>	<u>2.22222</u>
<u>207.5</u>	<u>2.22222</u>
<u>207</u>	<u>2.22222</u>
<u>206.5</u>	<u>-2.22222</u>
<u>206</u>	<u>-2.22222</u>
<u>205.5</u>	<u>-2.08105</u>
<u>205</u>	<u>2.22222</u>
<u>204.5</u>	<u>2.22222</u>
<u>204</u>	<u>2.22222</u>
<u>203.5</u>	<u>2.22222</u>
<u>203</u>	<u>2.22222</u>
<u>202.5</u>	<u>2.22222</u>
<u>202</u>	<u>2.22222</u>
<u>201.5</u>	<u>-2.08105</u>
<u>201</u>	<u>-2.22222</u>
<u>200.5</u>	<u>-2.22222</u>
<u>200</u>	<u>2.22222</u>