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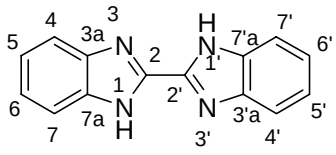
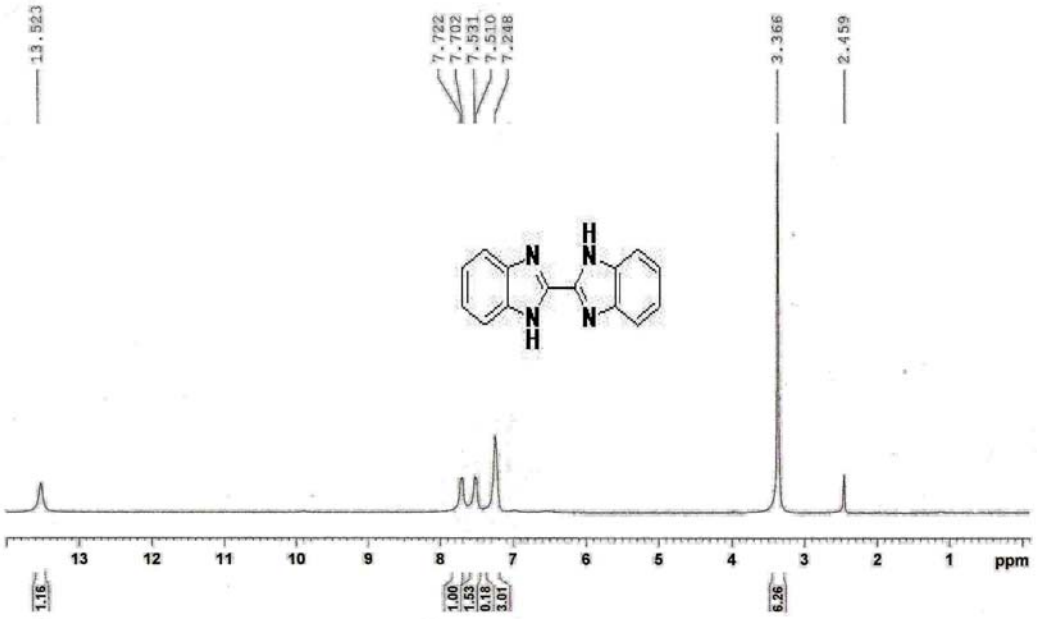
1. Details of ^{1}H-NMR spectra, ^{13}C-NMR spectra of the crude as well as pure compounds (4a-4q)

^{1}H-NMR spectra, ^{13}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**.



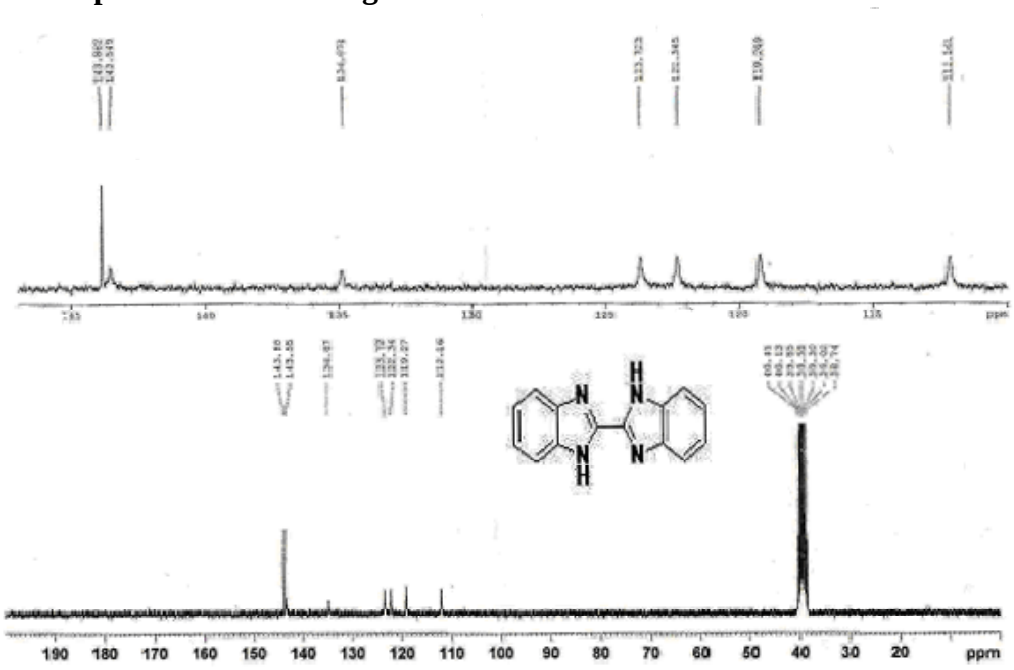
Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4a:



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

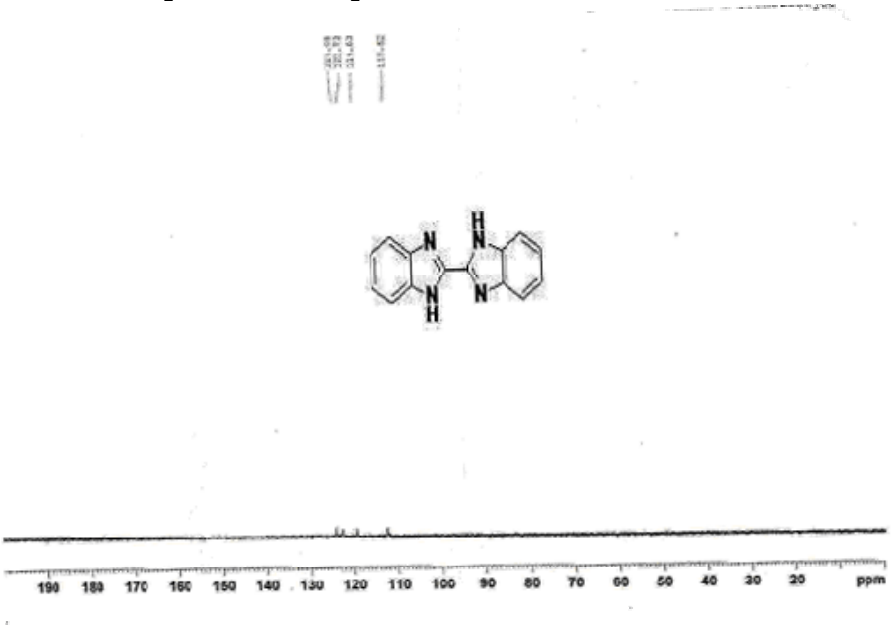
Ratio of the aromatic protons (from left to right): 2: 2: 4 (total 8 protons) indicating the presence of pure simple bis-benzimidazole.

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

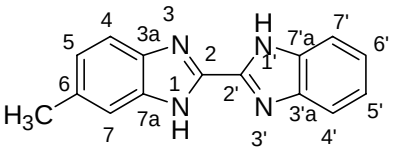


All the seven carbons of one half of the molecule have come separately, the left side three signals disappear in DEPT 135 experiment as they are quaternary carbons while the right side four signals remain in DEPT 135 experiment as they are hydrogen bearing carbons. This convincingly proves the presence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

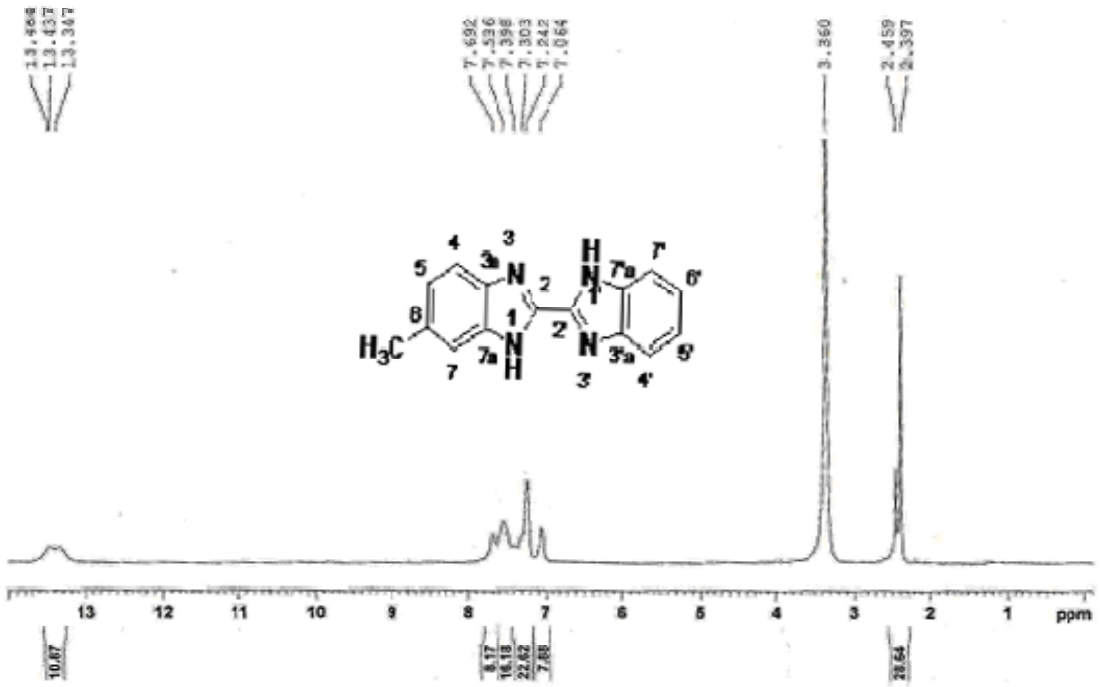
Copy of pure DEPT-135 spectra of compound 4a:



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}H-NMR (DMSO-d_6) spectra of compound 4b:

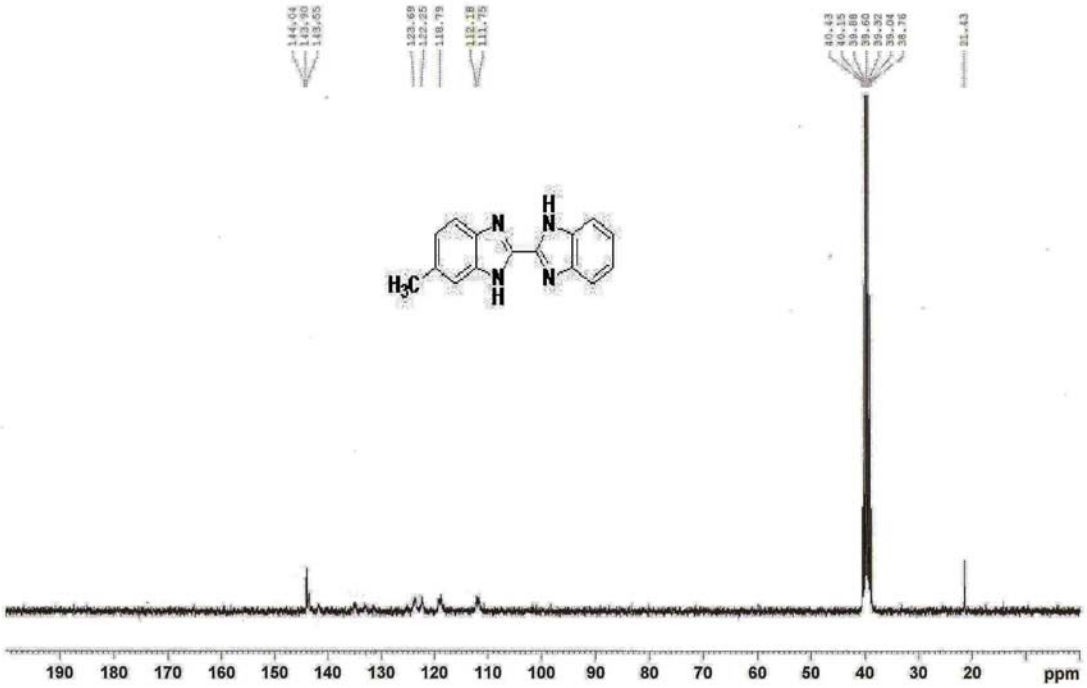


δ 2.40 (br s, 3H, C_6-C<u>H</u>$_3$), 7.06 (s, 1H, C_5-H), 7.24-7.40 (m, 3H, C_7-H, $C_{5'}$-H and $C_{6'}$-H), 7.54 (br s, 2H, $C_{4'}$-H and $C_{7'}$-H), 7.69 (br s, 1H, C_4-H) and 13.35-13.46 (m, 2H, N_1-H and $N_{1'}$-H)

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

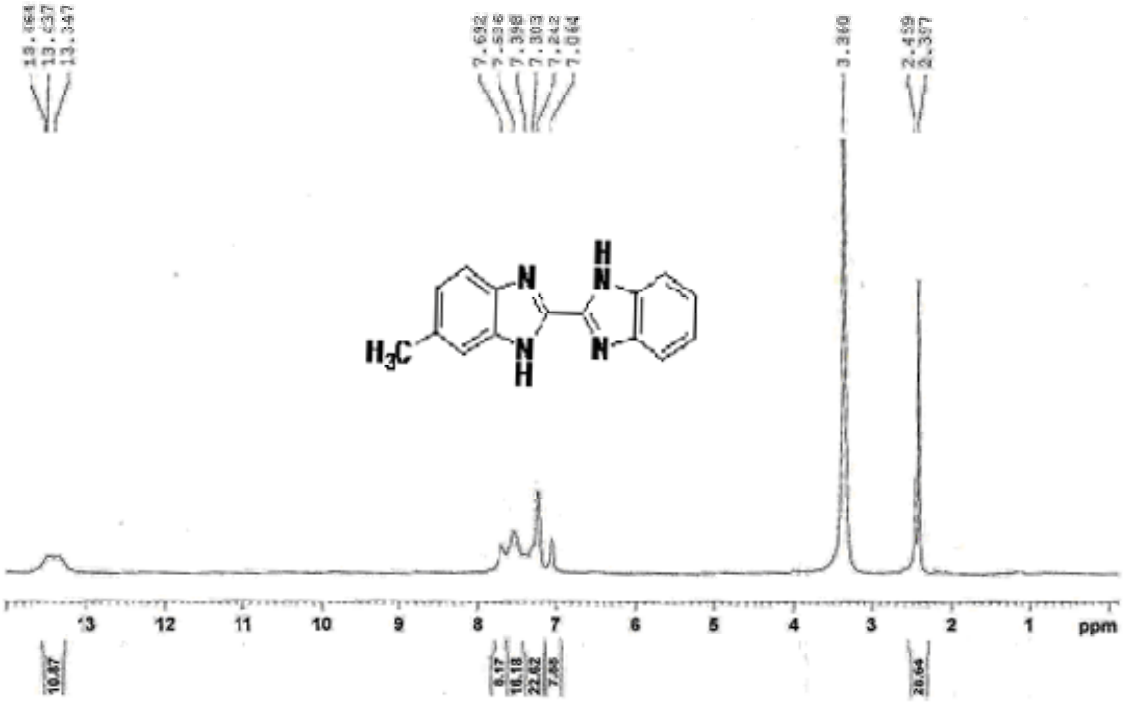
Ratio of the aromatic protons (from left to right): 1: 2: 3: 1 (total 7 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the methyl protons versus the aromatic protons is also satisfactory.

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

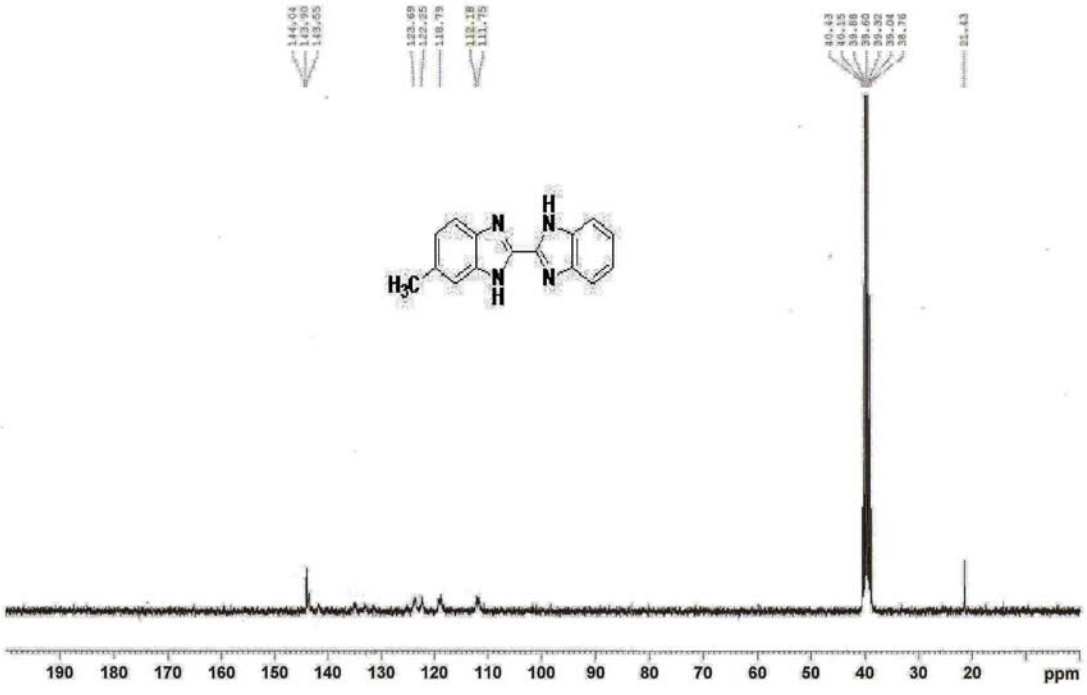


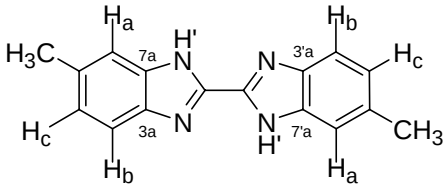
Out of fifteen carbon atoms present, fourteen have come separately.

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

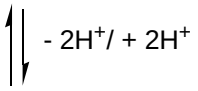


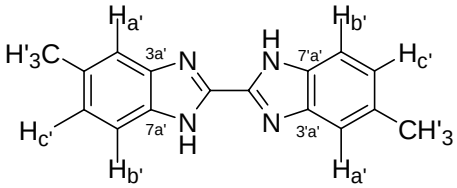
Copy of pure ^{13}C-NMR (75 MHz, DMSO-d_6) spectra of compound 4b:





51.6 % of tautomer A

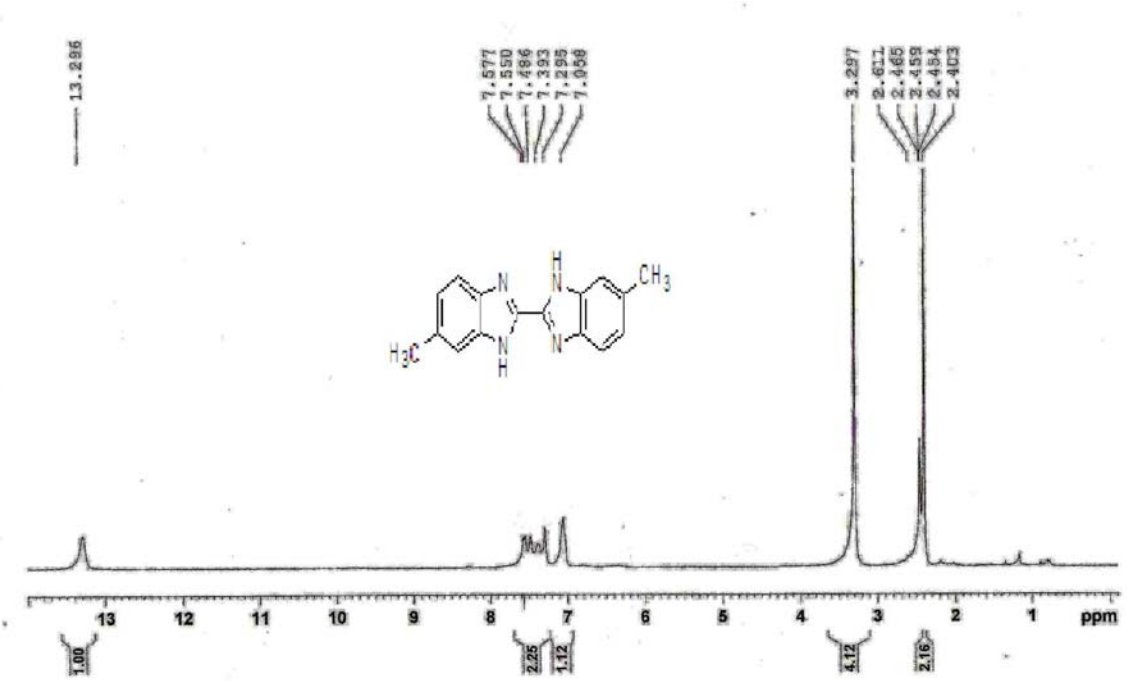




48.4 % of tautomer B

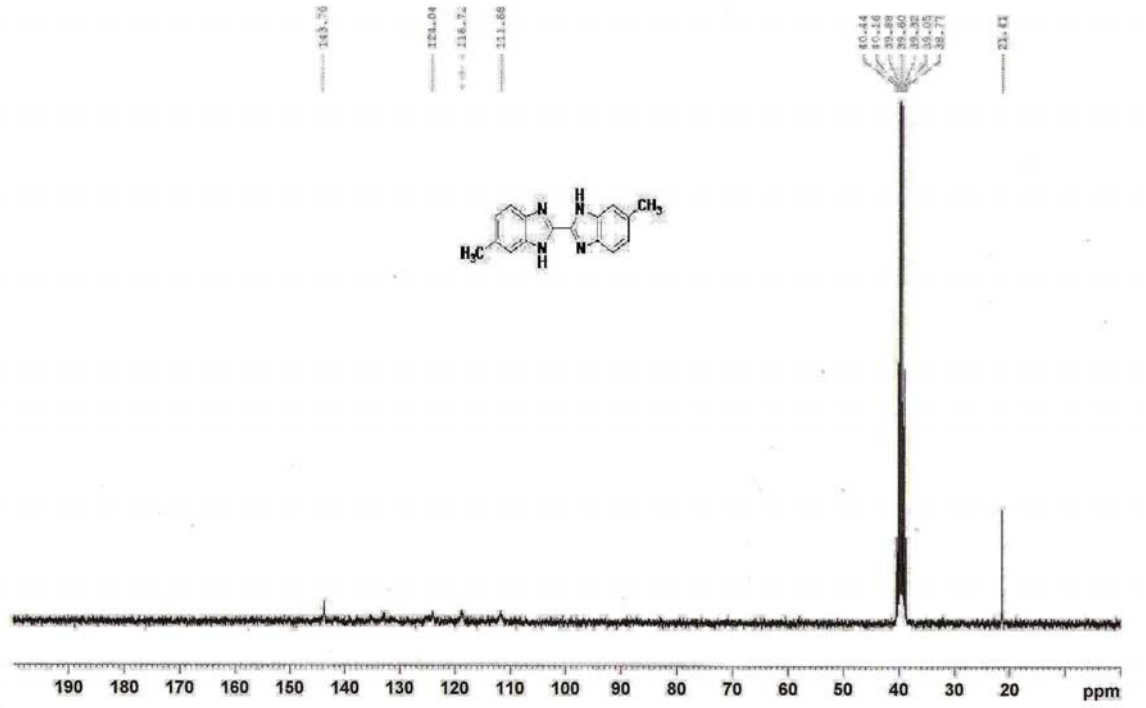
(The percentages of the two tautomers obtained from proton integration ratios of crude ^{1}H NMR spectrum).

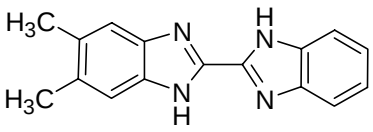
Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4c:



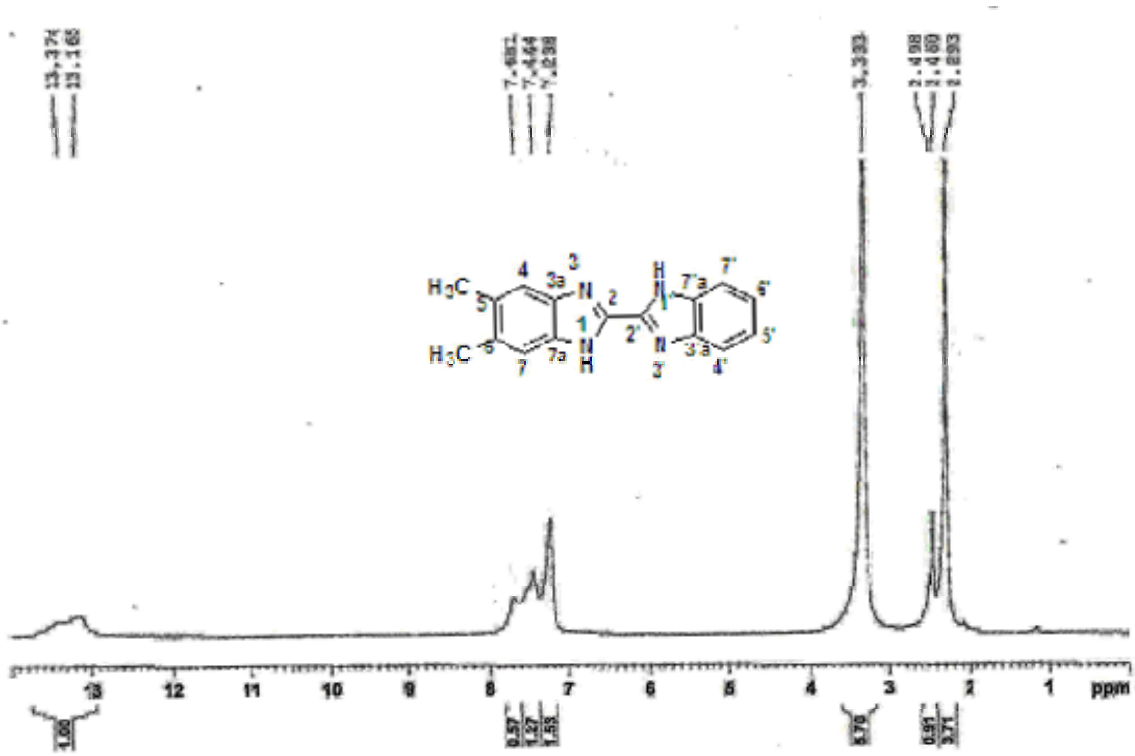
Each individual peak has been assigned both in ^{1}H and in ^{13}C NMR (please see the details of assignment).

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





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

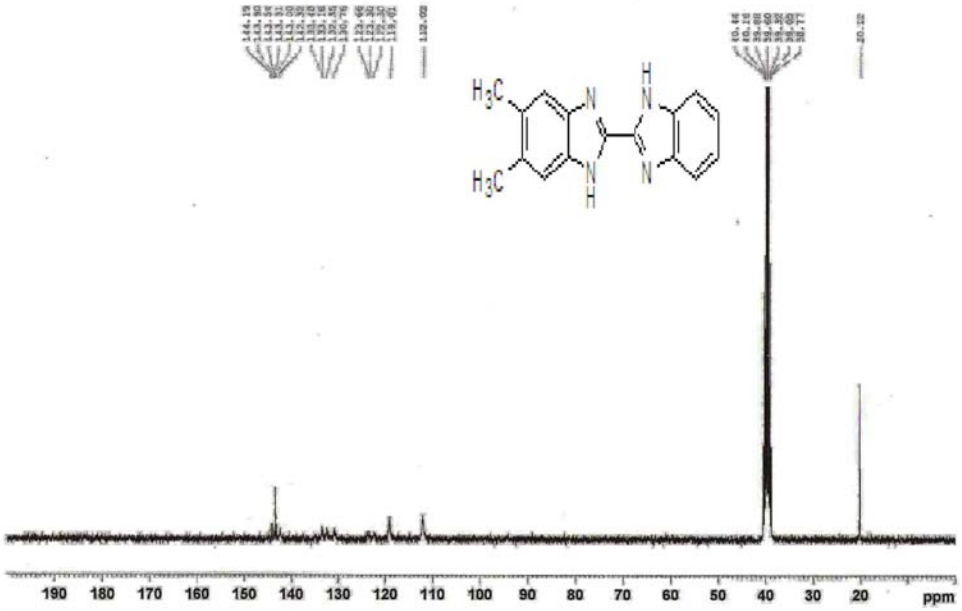


δ 2.29 (s, 6H, C_5-C<u>H</u>$_3$ and C_6-C<u>H</u>$_3$), 7.24 (br s, 3H, C_7-H, $C_{5'}$-H, and $C_{6'}$-H), 7.44-7.68 (m, 3H, C_4-H, $C_{4'}$-H and $C_{7'}$-H) and 13.17-13.37 (m, 2H, N_1-H and $N_{1'}$-H)

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

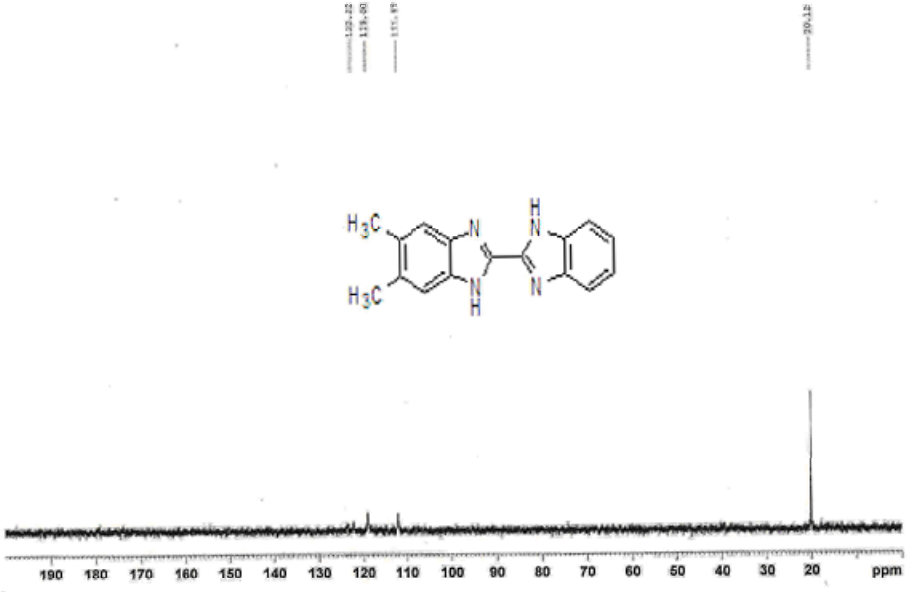
Ratio of the aromatic protons (from left to right): 1: 2: 3 (total 6 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the two methyl group protons versus the aromatic protons is also satisfactory.

Copy of crude ^{13}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.

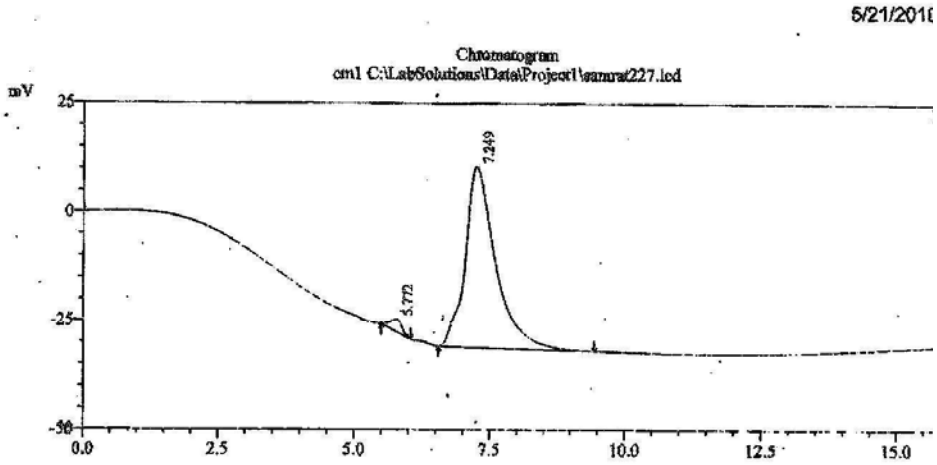
Copy of crude DEPT-135 spectra of compound 4d:



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%):

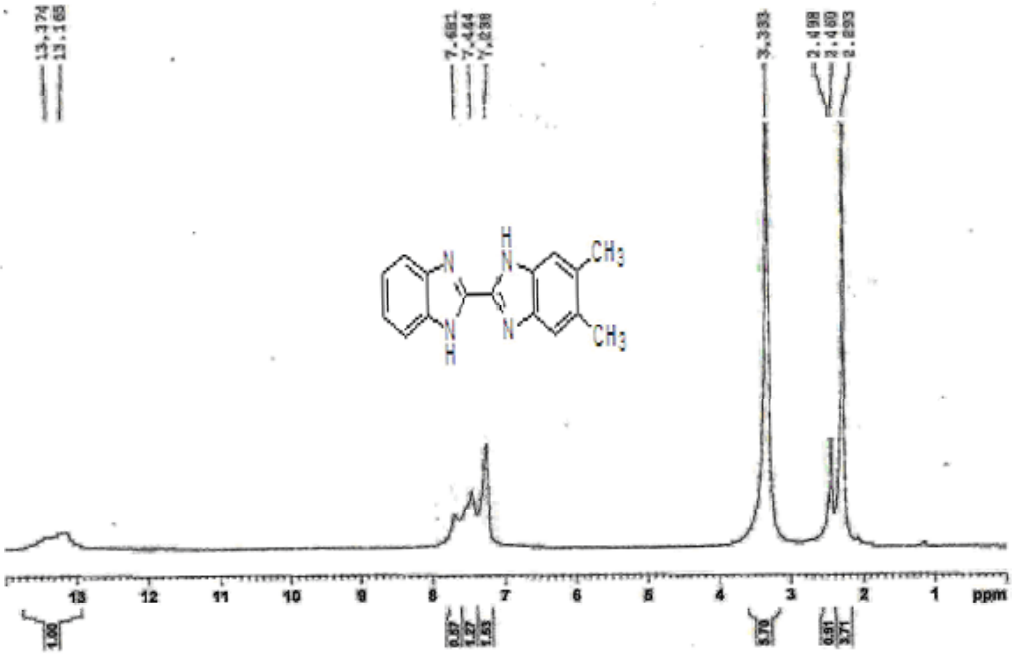


PeakTable

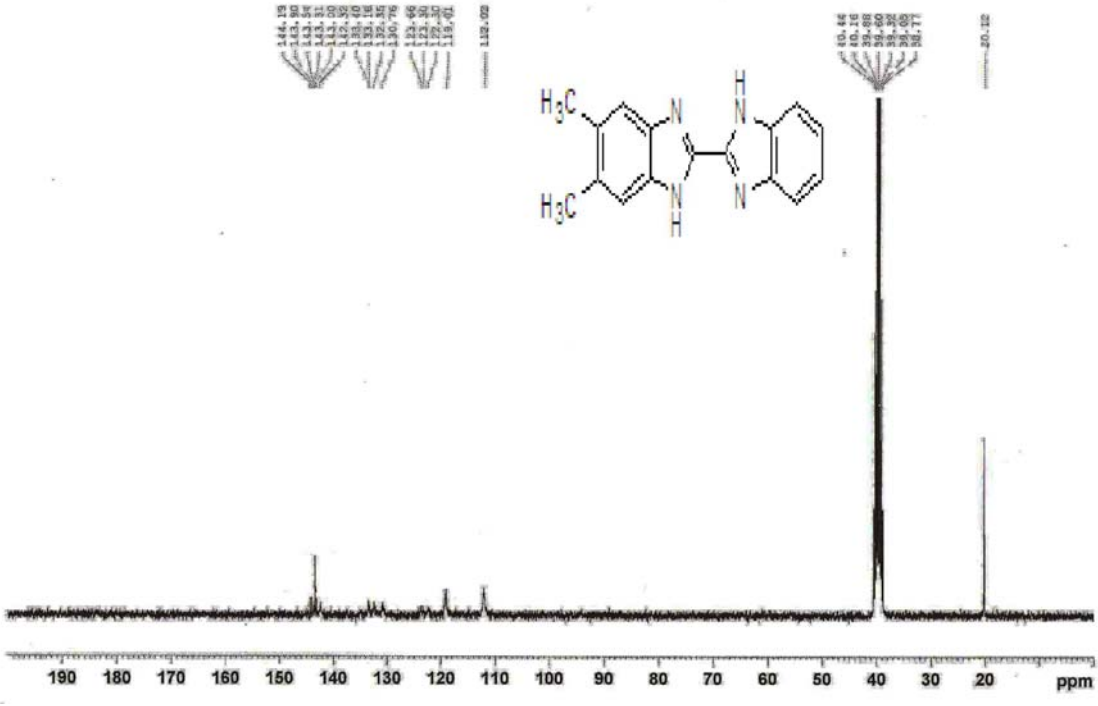
Detector B Ch1

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.772	10226	2049	0.605	4.602
2	7.249	1680001	42478	99.395	95.398
Total		1690227	44527	100.000	100.000

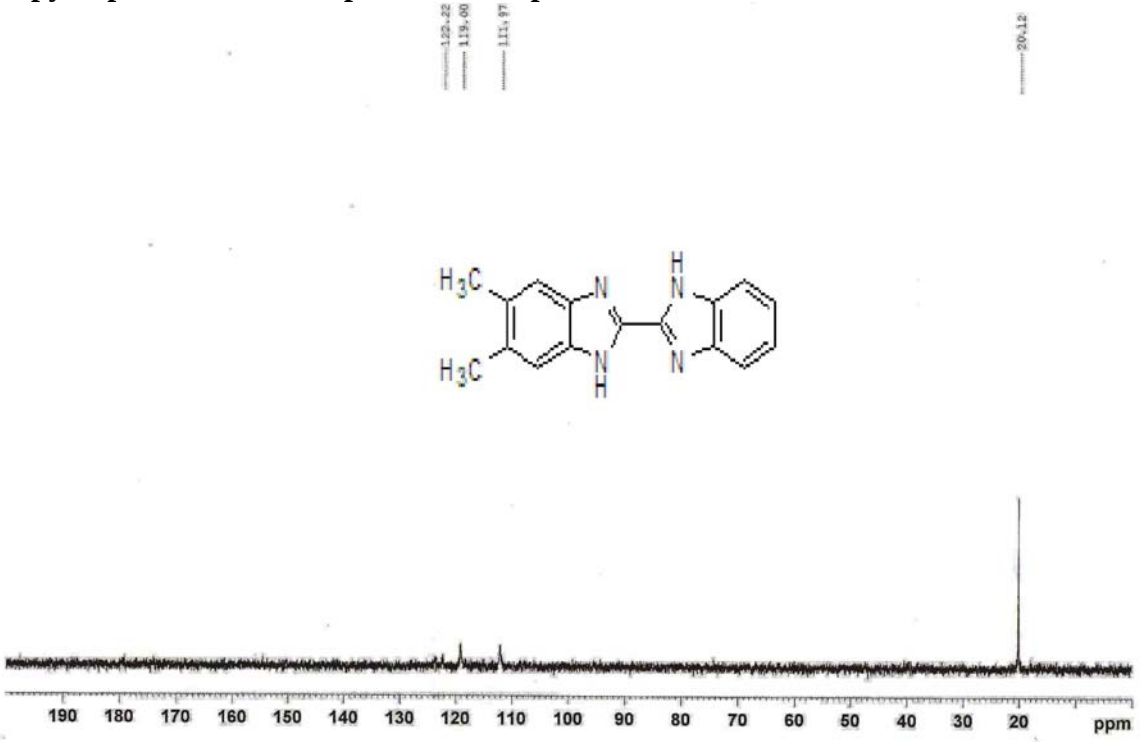
Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4d:

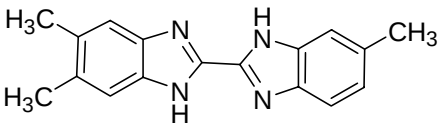


Copy of pure ^{13}C-NMR (75 MHz, DMSO-d_6) spectra of compound 4d:

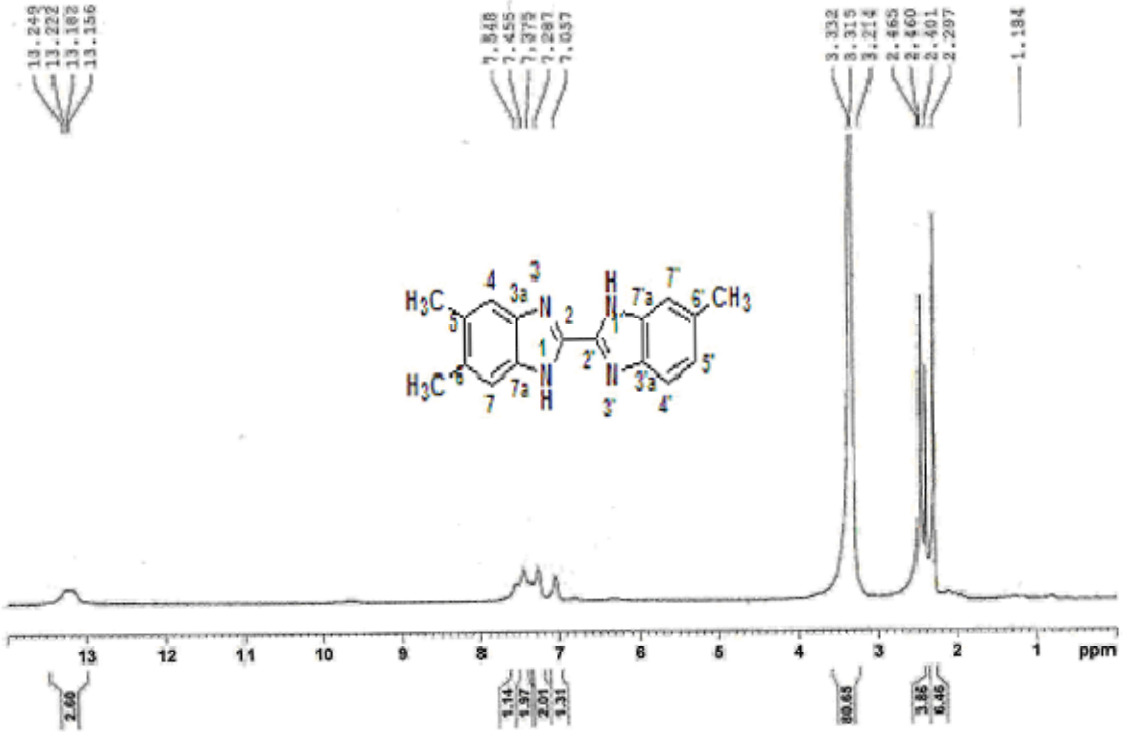


Copy of pure DEPT-135 spectra of compound 4d:





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

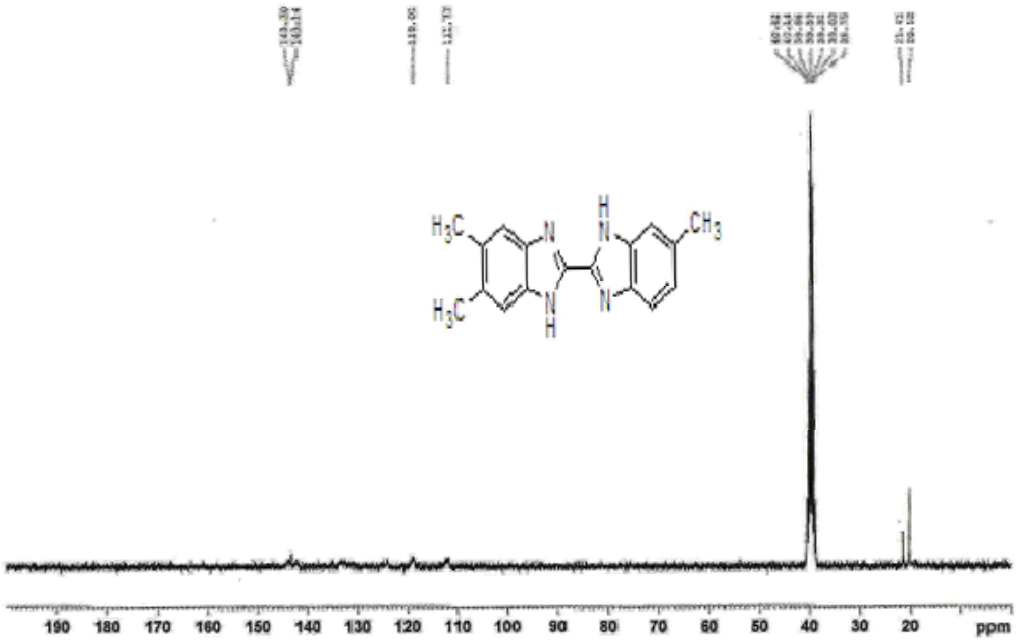


δ 2.30 (s, 6H, C_5-C<u>H</u>$_3$ and C_6-C<u>H</u>$_3$), 2.40 (s, 3H, $C_{6'}$-C<u>H</u>$_3$), 7.06 (br s, 1H, $C_{5'}$-H), 7.29 (br s, C_7-H and $C_{7'}$-H), 7.46 (br s, 1H, C_4-H), 7.55 (br s, 1H, $C_{4'}$-H) and 13.16-13.25 (m, 2H, N_1-H and $N_{1'}$-H)

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

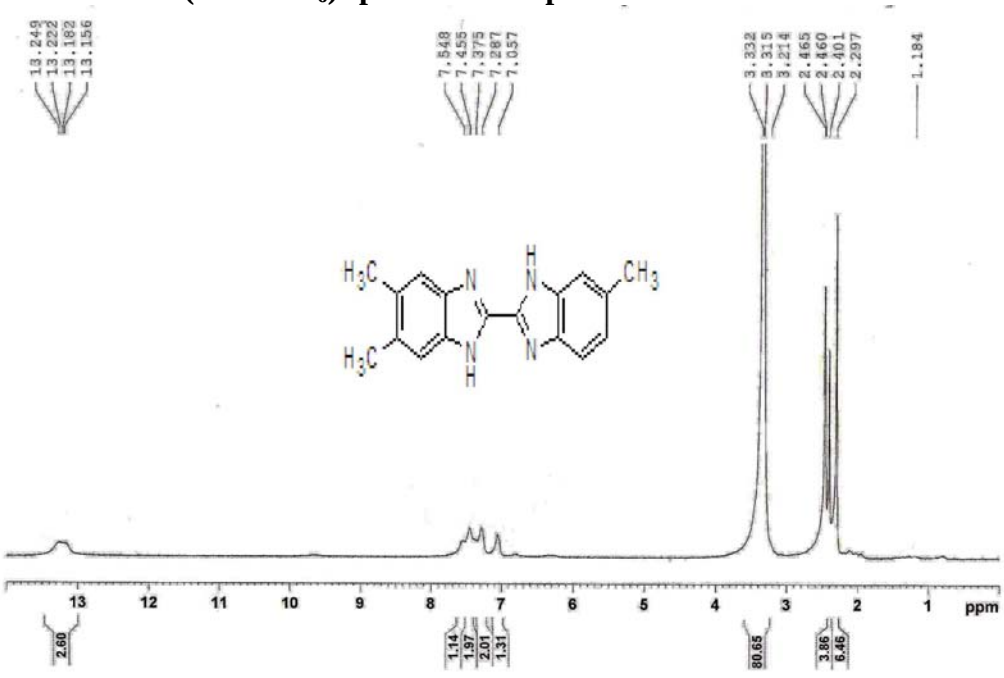
Ratio of the aromatic protons (from left to right): 1: 1: 2: 1 (total 5 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the three methyl group protons versus the aromatic protons is also satisfactory.

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

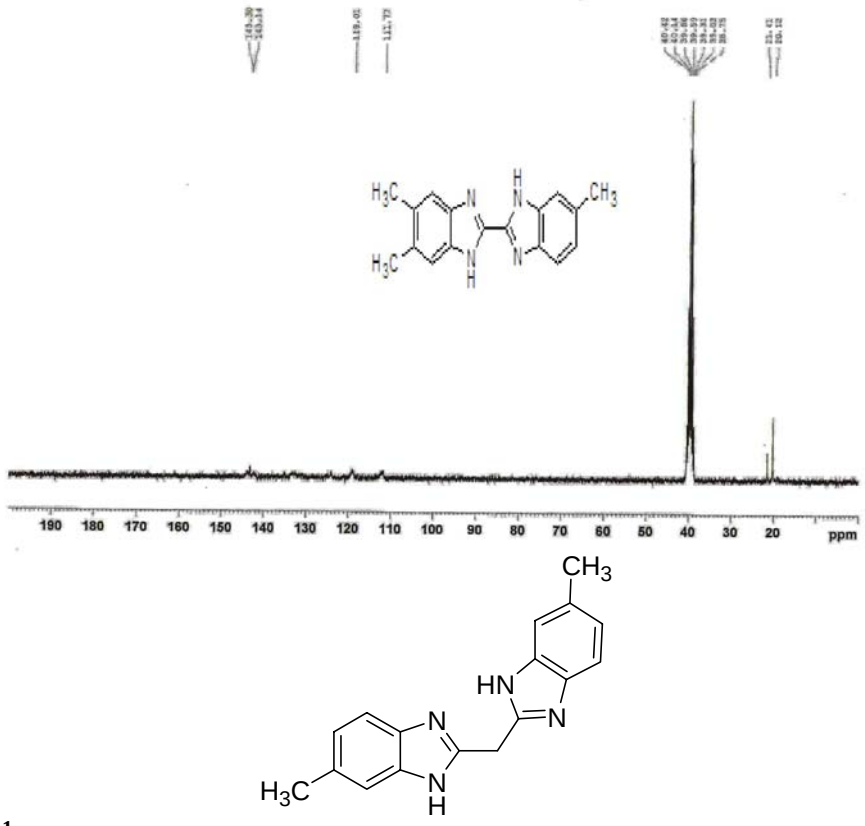


Out of the fifteen types of carbon present, only the carbon atoms of the two types of methyl groups and the two carbon atoms joining the two benzimidazole rings have come separately. Other symmetrical carbons have come in the same place thereby reducing the total number of signals.

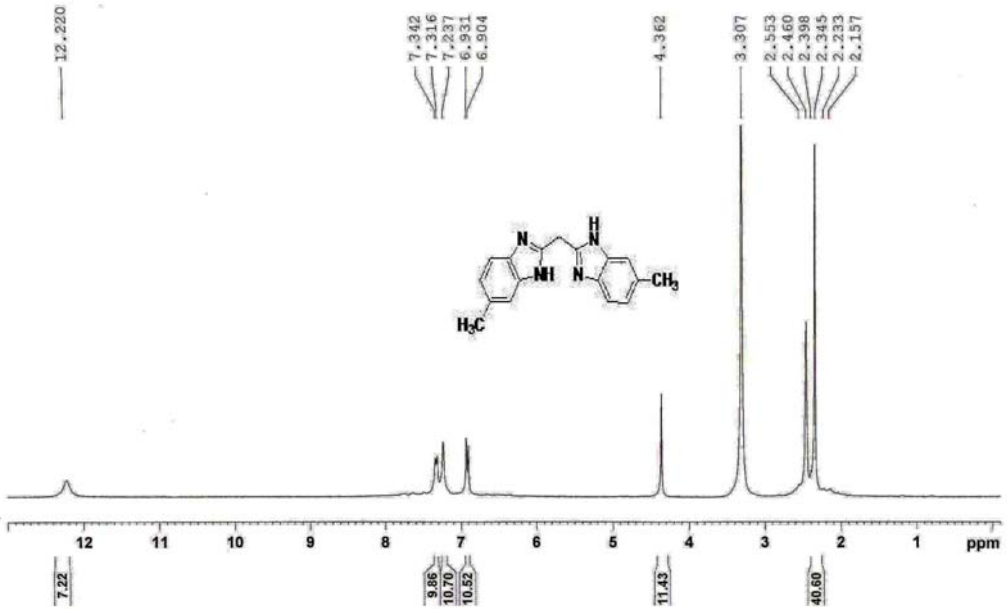
Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4e:



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

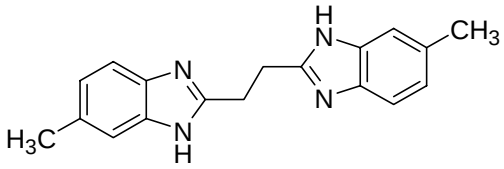


Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4f:

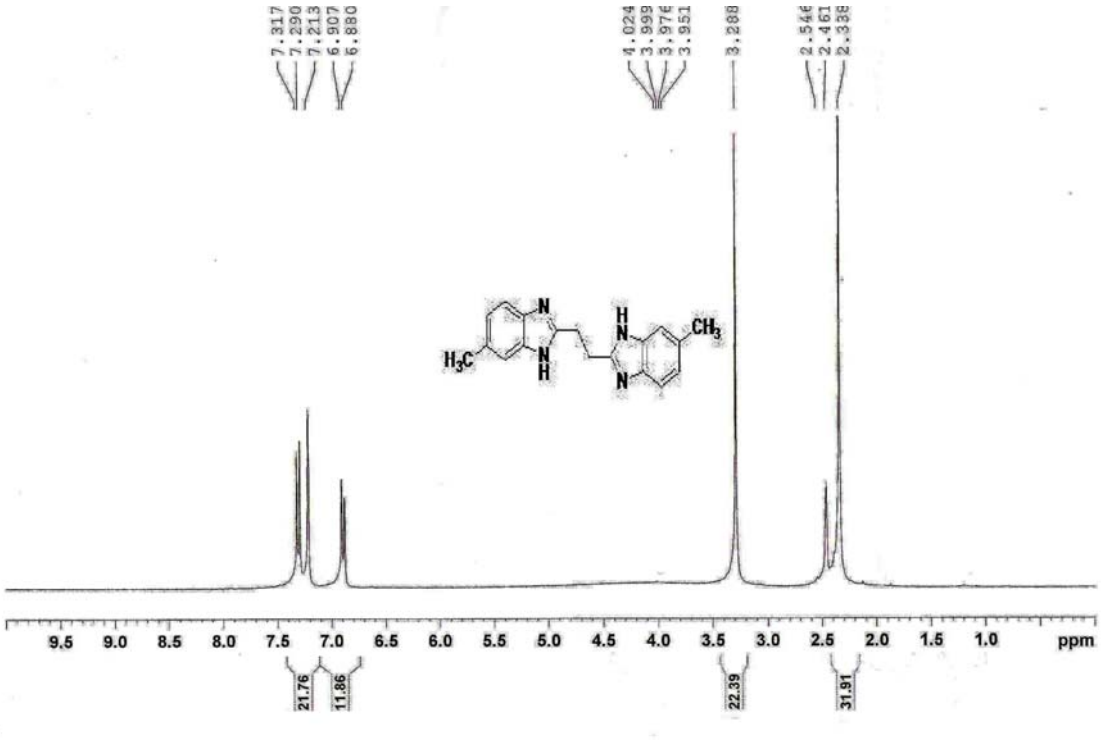


Each individual peak has been assigned both in ^{1}H and in ^{13}C NMR (please see the details of assignment).

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.



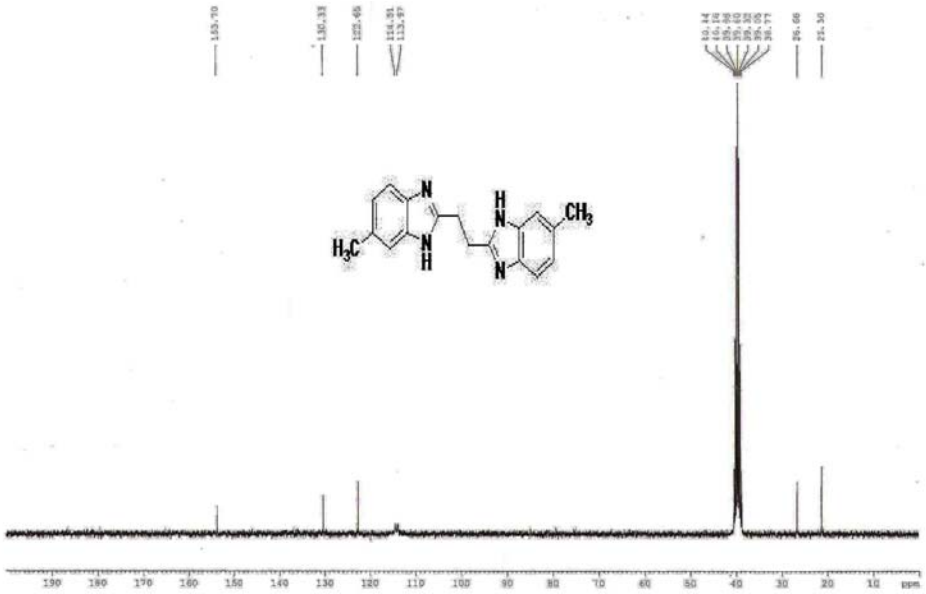
Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4h:



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

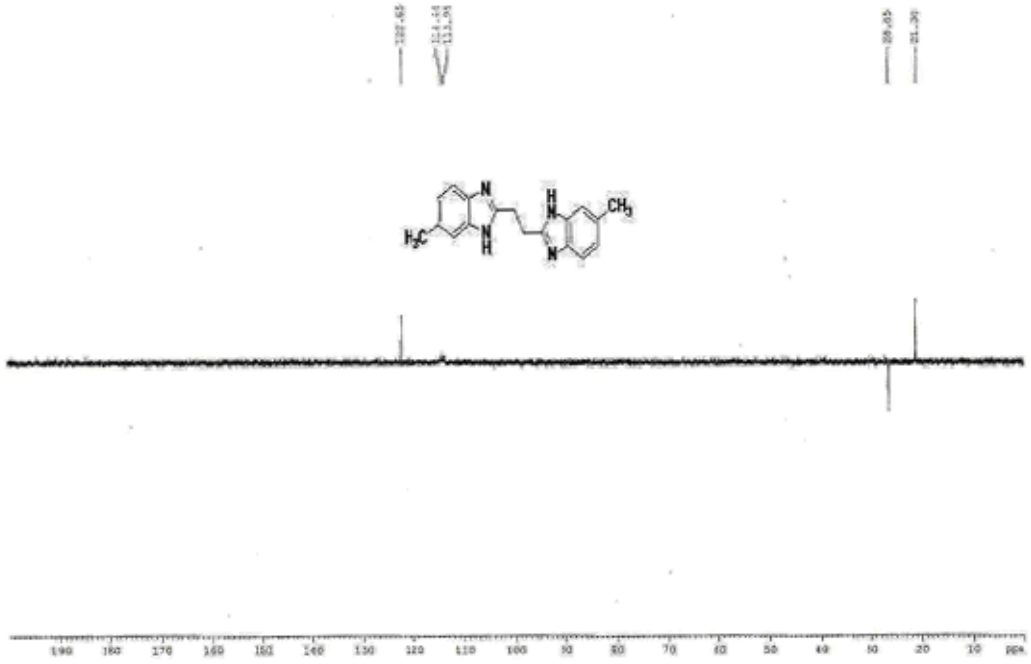
Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure simple bis-benzimidazole. Integration of the two methyl group protons and the two methylene group protons are also satisfactory.

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



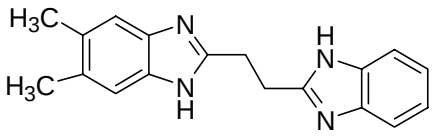
The left side two signals disappear in DEPT 135 experiment as they are quaternary carbons.

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

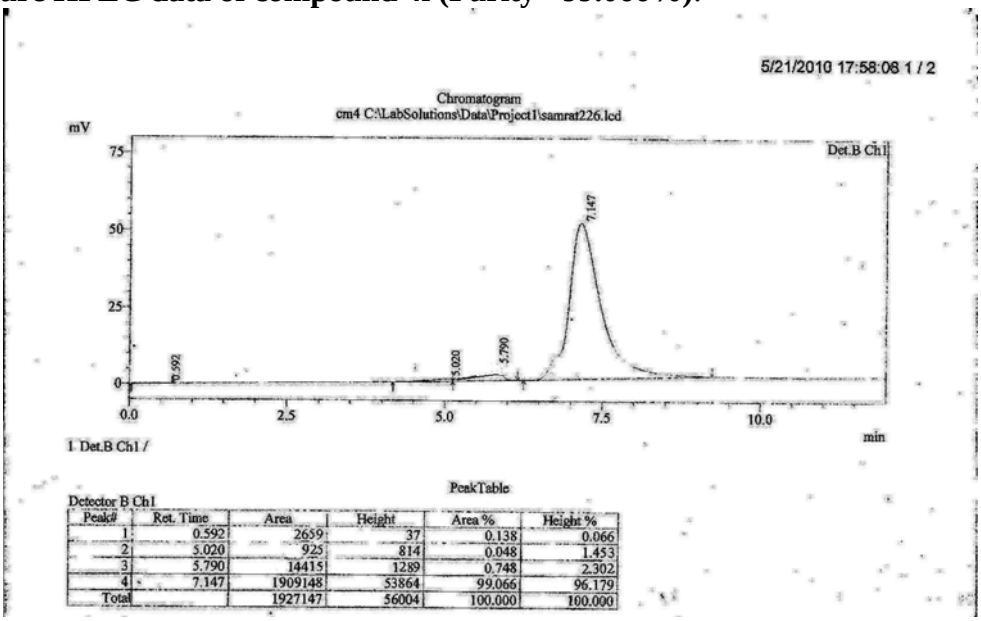


As stated earlier, the left side two signals disappear in DEPT 135 experiment as they are quaternary carbons while the right side five signals remain in DEPT 135 experiment as they are hydrogen bearing carbons. The second signal from the right side is inversed in DEPT-135 experiment showing the presence 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%):

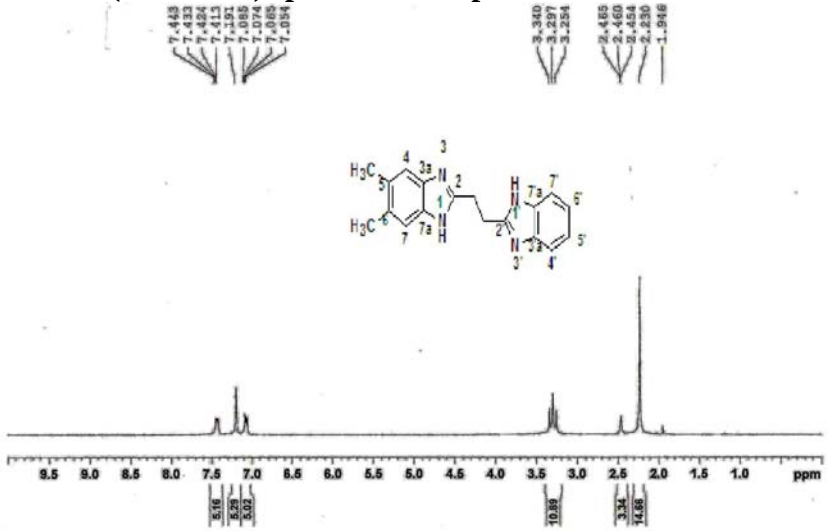


PeakTable

Detector B Ch1

Peak#	Ret. Time	Area	Height	Area %	Height %
1	0.592	2659	37	0.138	0.066
2	5.020	925	814	0.048	1.453
3	5.790	14415	1289	0.748	2.302
4	7.147	1909148	53864	99.066	96.179
Total		1927147	56004	100.000	100.000

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

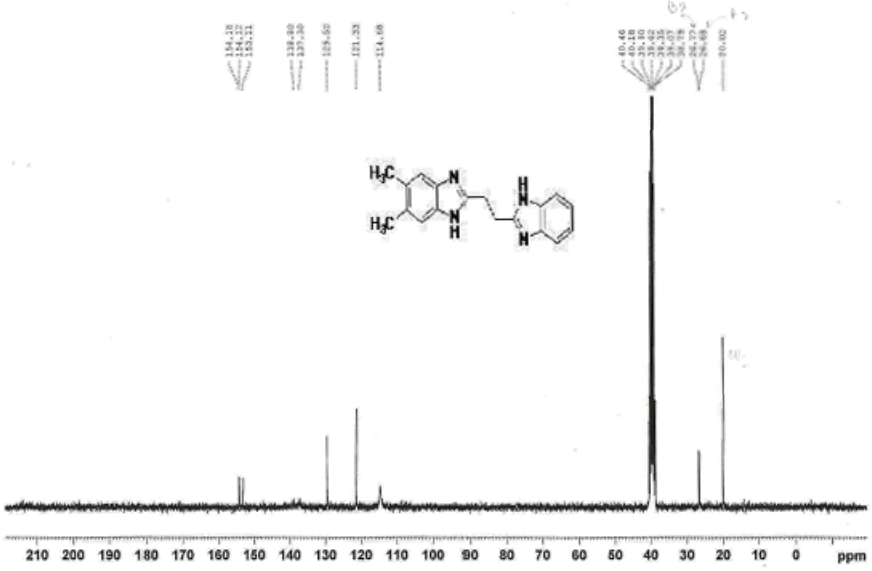


δ 2.23 (s, 6H, C_5-C<u>H</u>$_3$ and C_6-C<u>H</u>$_3$), 3.30 (t, *J*=12.9 Hz, 4H, C_2-C<u>H</u>$_2$ and $C_{2'}$-C<u>H</u>$_2$), 7.07 (dd, *J*=6.0 Hz, 3.3 Hz, 2H, $C_{5'}$-H and $C_{6'}$-H), 7.19 (s, 2H, C_4-H and C_7-H) and 7.43 (dd, *J*=6.0 Hz, 3.0 Hz, 2H, $C_{4'}$-H and $C_{7'}$-H)

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

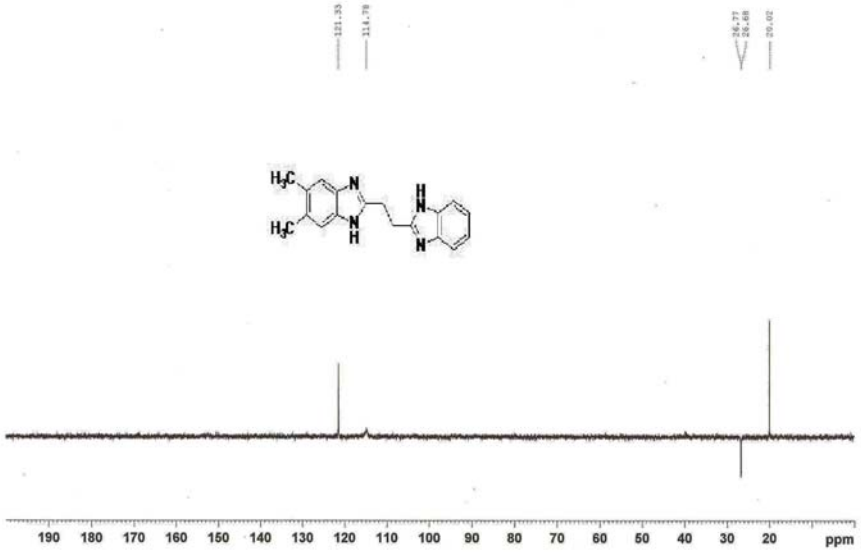
Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the two methyl group protons and the methylene group protons are also satisfactory.

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

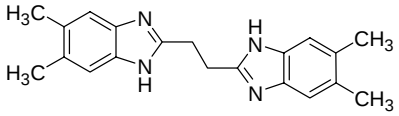


The five signals from the left side are the quarternary carbons and they disappear in DEPT-135 experiment.

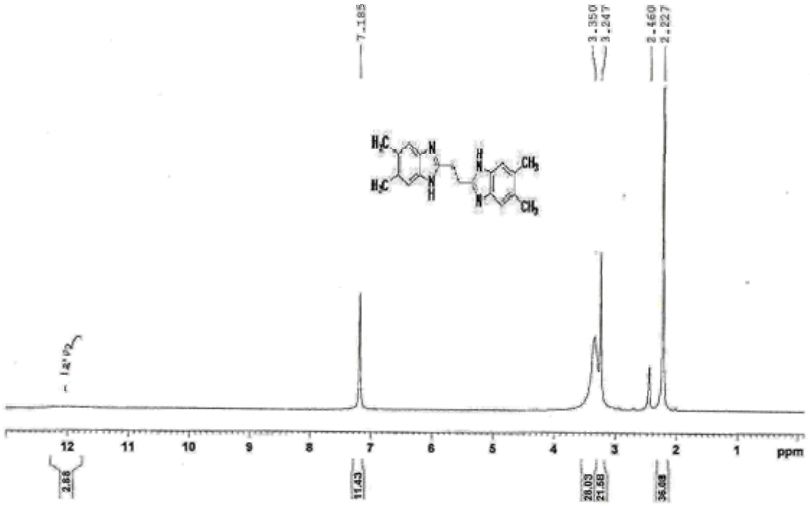
Copy of pure DEPT-135 spectra of compound 4i:



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 inversed indicates the presence of the carbon atoms of the methylene groups.

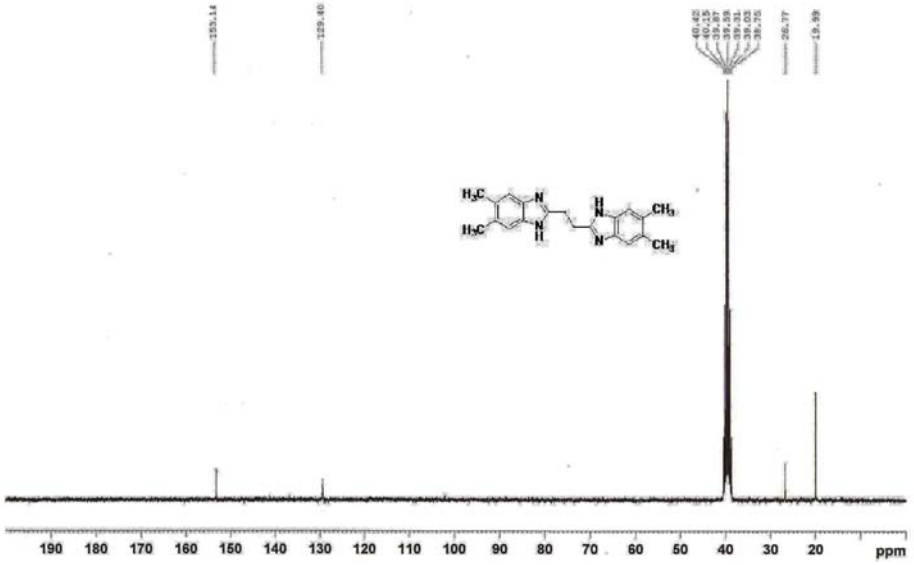


Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4j:

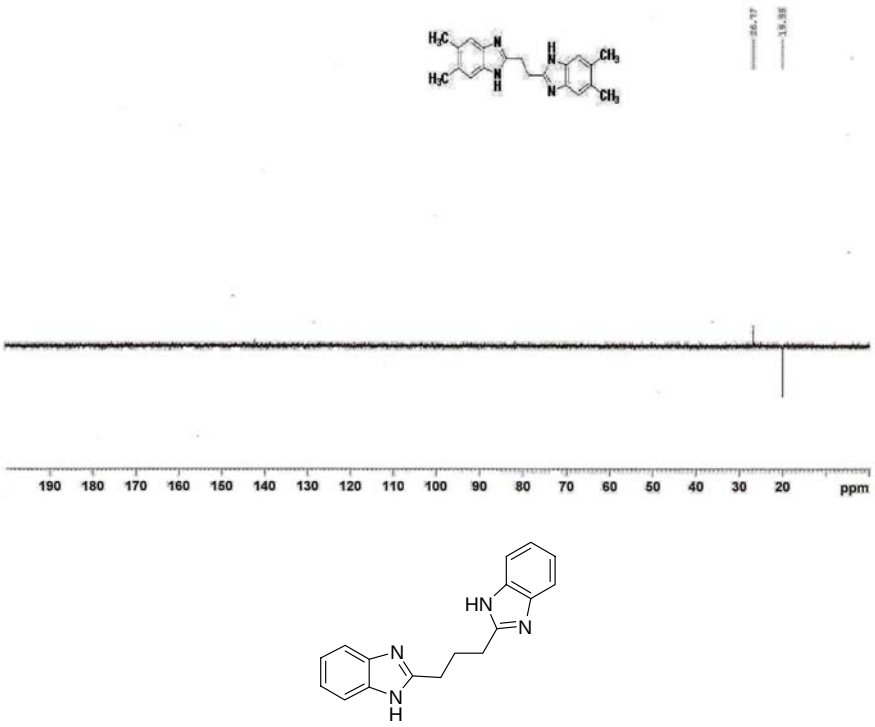


Each individual peak has been assigned both in ^{1}H and in ^{13}C NMR (please see the details of assignment).

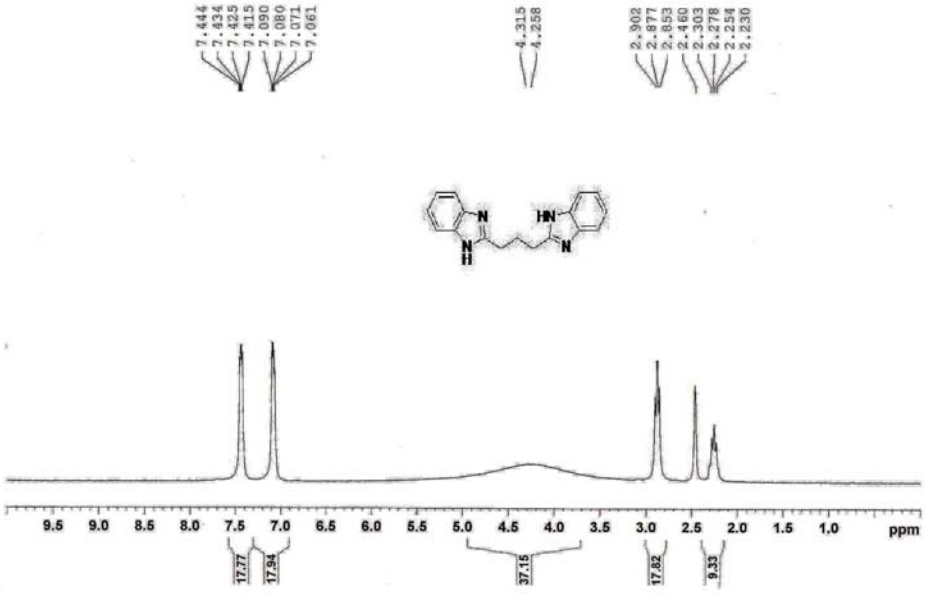
Copy of pure ^{13}C-NMR (75 MHz, DMSO-d_6) spectra of compound 4j:



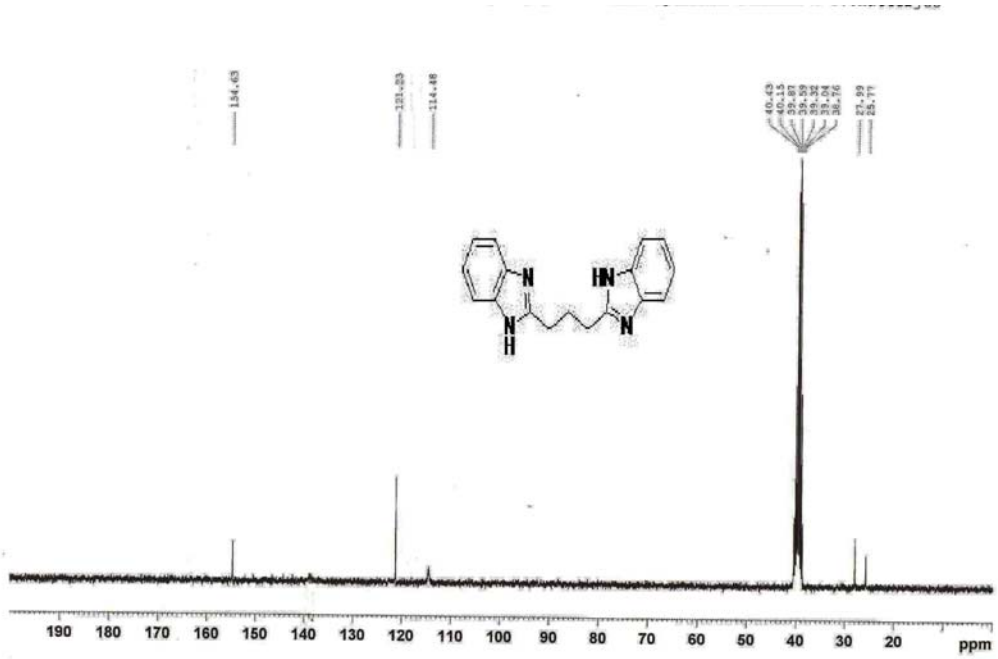
Copy of pure DEPT-135 spectra of compound 4j: no remaining signal in the aromatic region due to possible scrambling of the methyl groups; the inversed signal shows the presence of carbon atoms of the methylene groups.



Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4k:

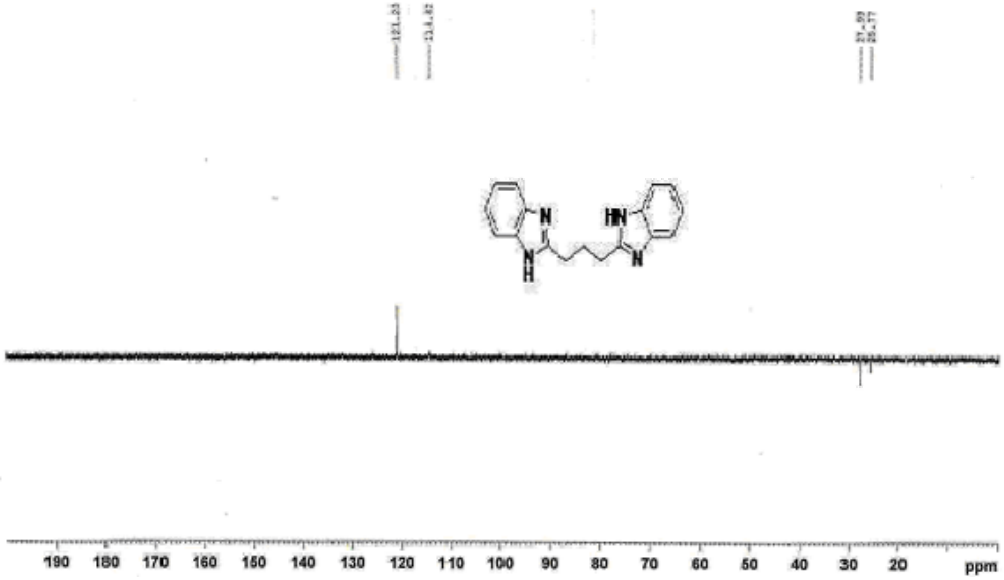


Copy of pure ^{13}C-NMR (75 MHz, DMSO-d_6) spectra of compound 4k:



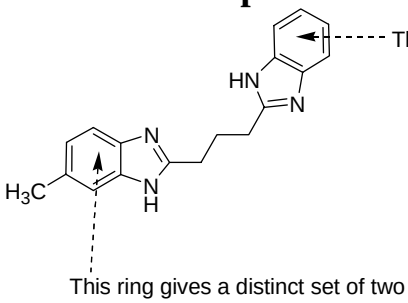
The two signals from left are due to quarternary carbons; the remaing four signals are due to hydrogen bearing carbon atoms.

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

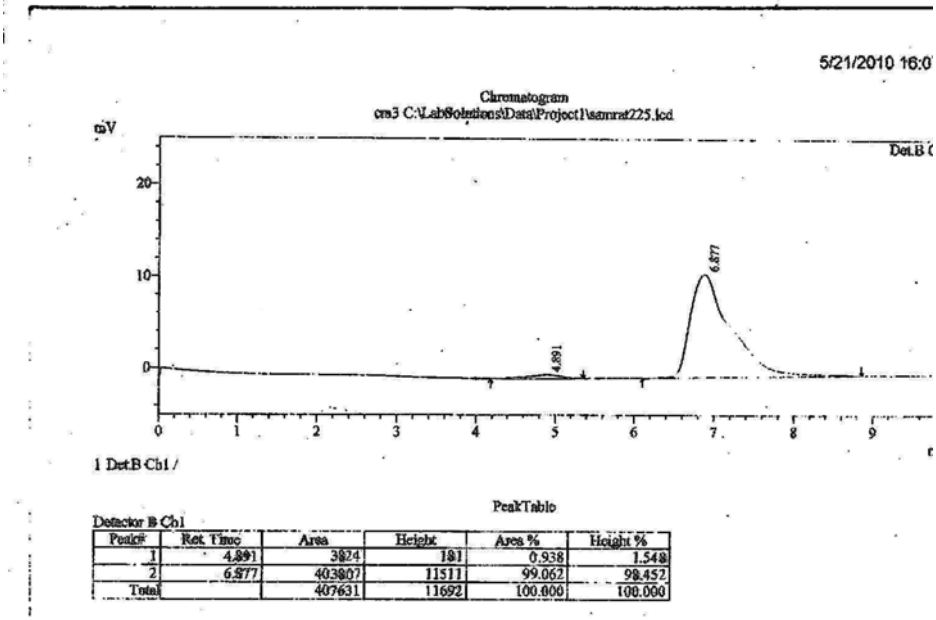


The signals due to quarternary carbon atoms disappear and the two inversed signals are due to the the two types of carbon atoms from the three methylene groups present.

4. HPLC data for compound 4l

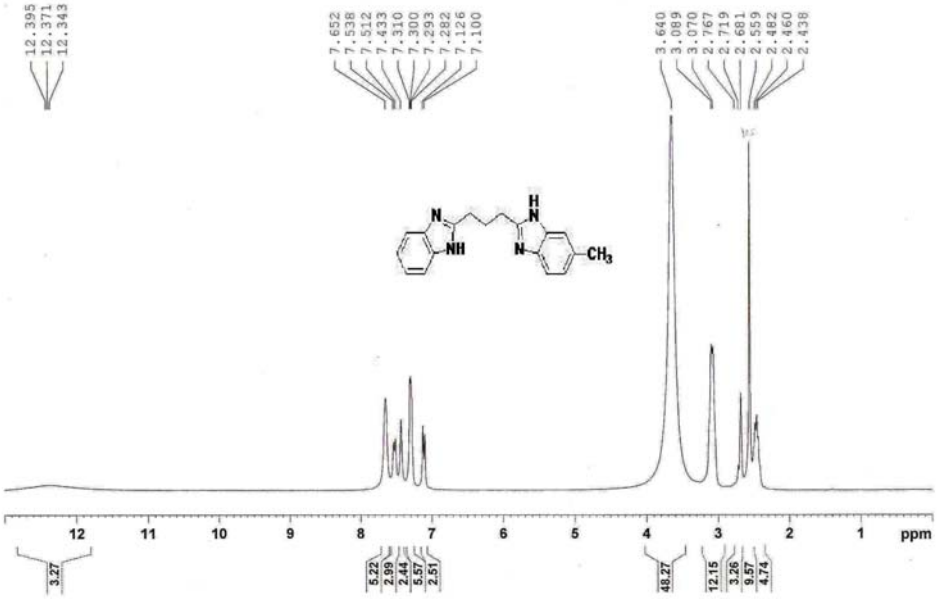


Copy of crude HPLC data of compound 4l (Purity= 99.062%):



Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.891	3824	181	0.938	1.548
2	6.877	403807	11511	99.062	98.452
Total		407631	11692	100.000	100.000

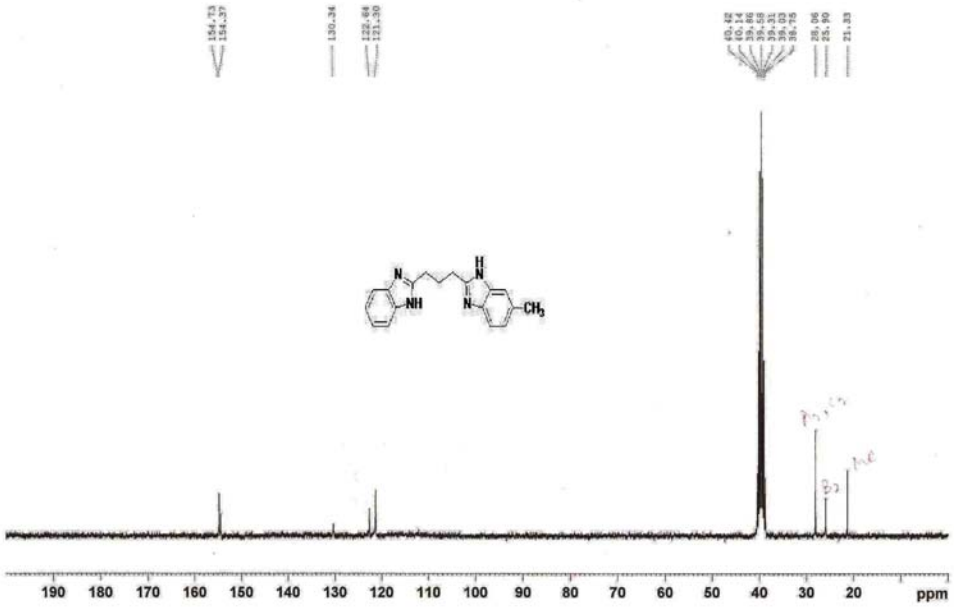
Copy of crude ^{1}H-NMR (DMSO-d_6) spectra of compound 4l:



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

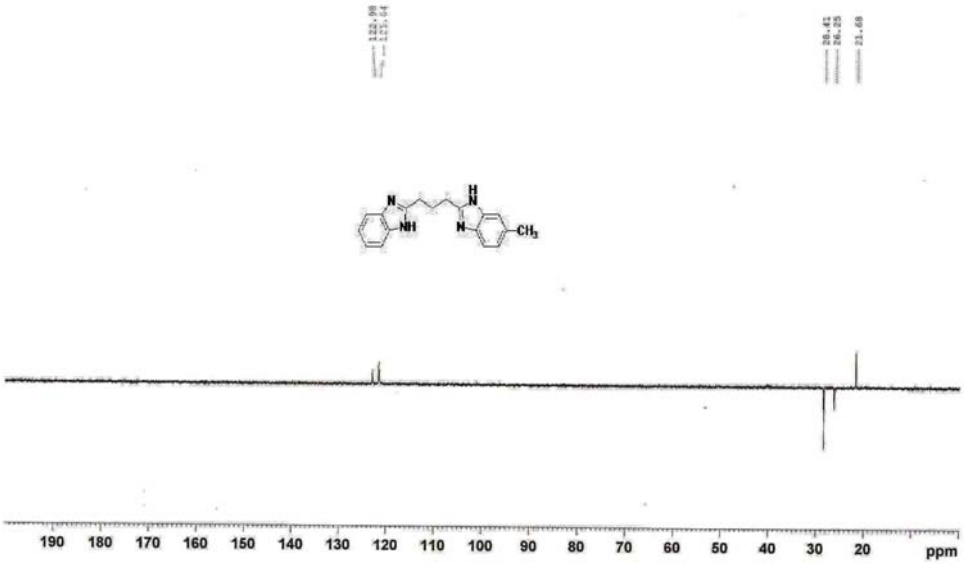
Ratio of the aromatic protons (from left to right): 2: 1: 1: 2: 1 (total 7 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the methyl group protons and the methylene group protons are also satisfactory.

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



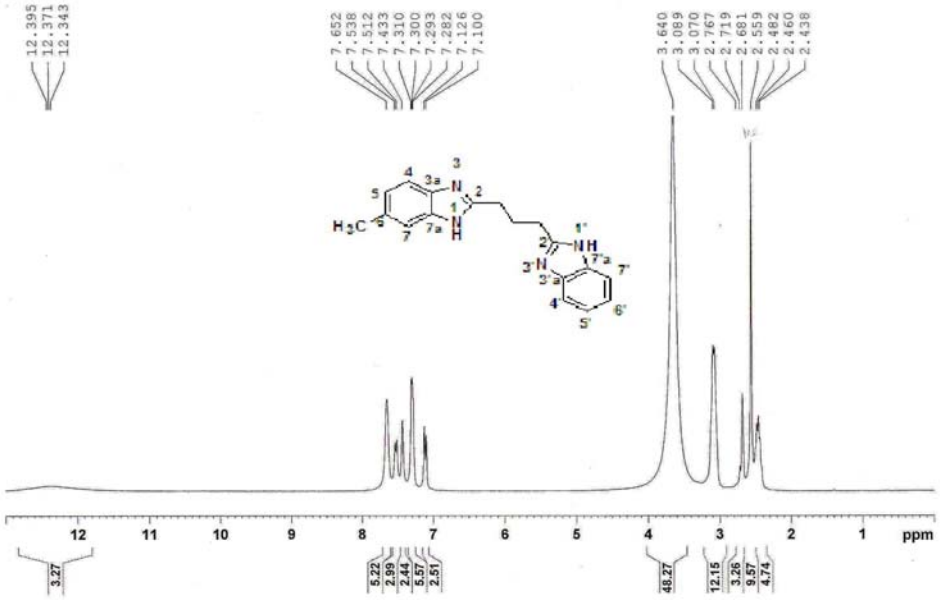
The signals beyond δ 130.0 are for the quarternary carbon atoms, the remaining five signals are for the hydrogen bearing carbon atoms.

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



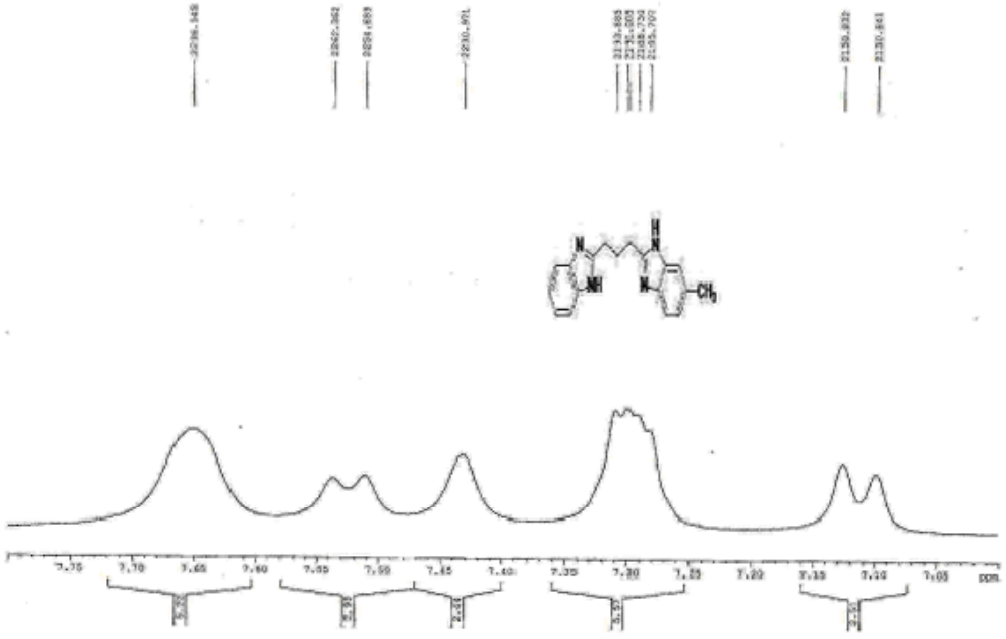
The hydrogen bearing carbon atoms remain in DEPT-135 experiment, the two inversed signals are for the methylene group carbon atoms of two different types.

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

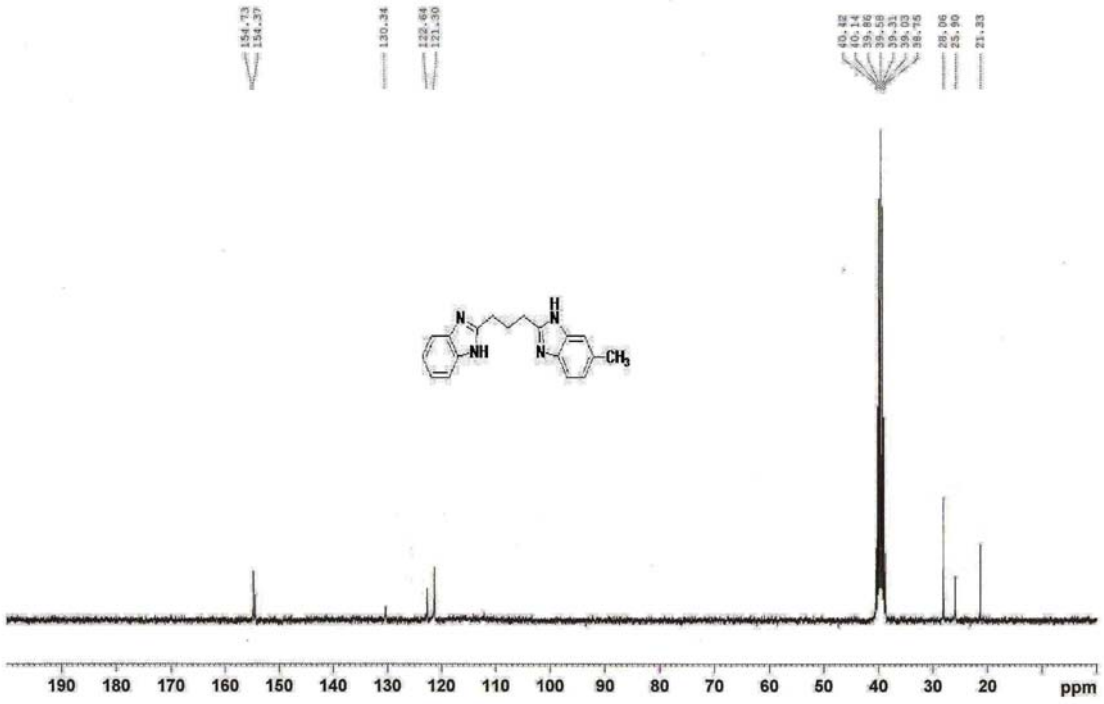


δ 2.44-2.48 (m, 2H, C_2-CH_2-C$\underline{H}_2$), 2.56 (s, 3H, C_6-C$\underline{H}_3$), 3.08 (d, *J*=5.7 Hz, 4H, C_2-C$\underline{H}_2$ and $C_{2'}$-C$\underline{H}_2$), 7.11(d, *J*=7.8 Hz, 1H, C_5-H), 7.28-7.31 (m, 2H, $C_{5'}$-H and $C_{6'}$-H), 7.43 (s, 1H, C_7-H), 7.53 (d, *J*=7.8 Hz, 1H, C_4-H), 7.65 (br s, 2H, $C_{4'}$-H and $C_{7'}$-H) and 12.37 (br s, 2H, N_1-H and $N_{1'}$-H)

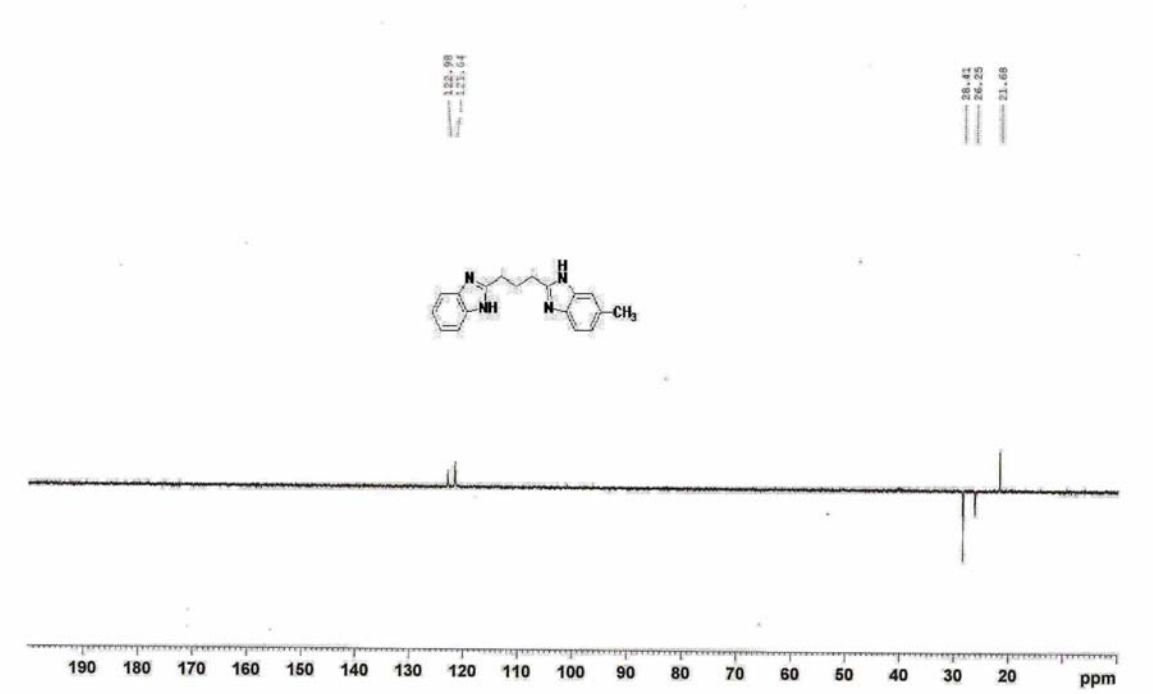
Expanded portion of the aromatic region of pure compound 4l showing the doublet-singlet-doublet(right-hand side ring) and multiplet patterns(left-hand side ring) of the two different halves of the heterodimeric compound.

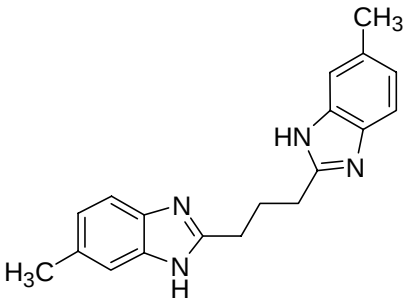


Copy of pure ^{13}C-NMR (75 MHz, DMSO-d_6) spectra of compound 4l:

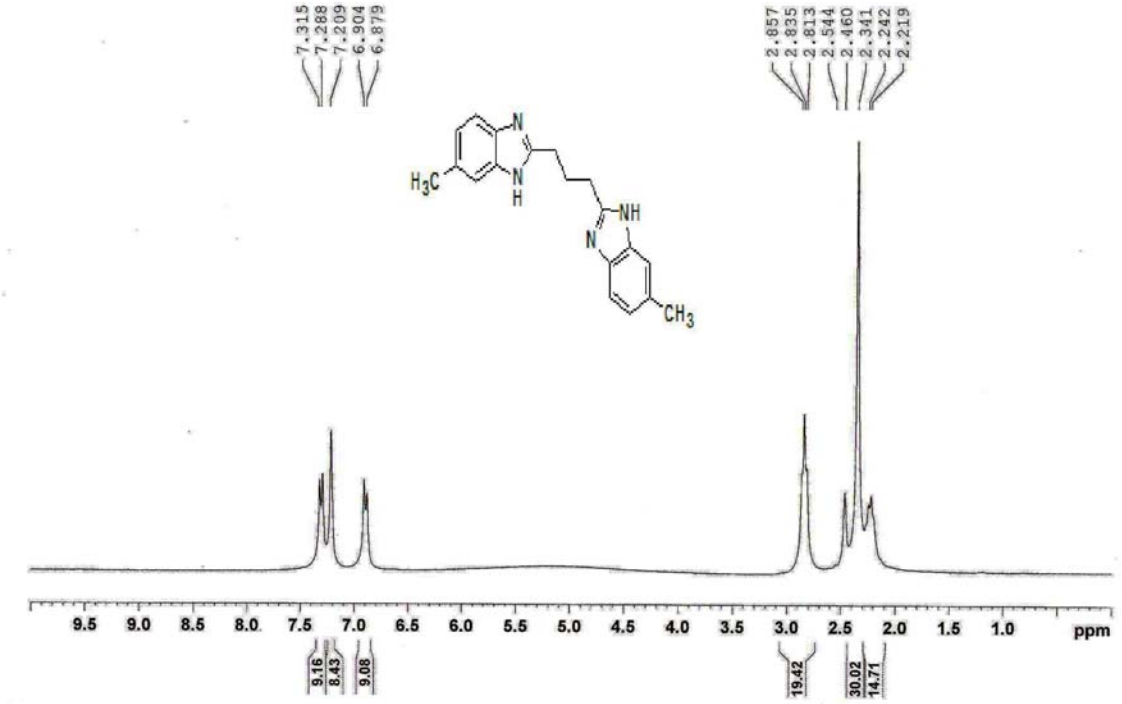


Copy of pure DEPT-135 spectra of compound 4l:





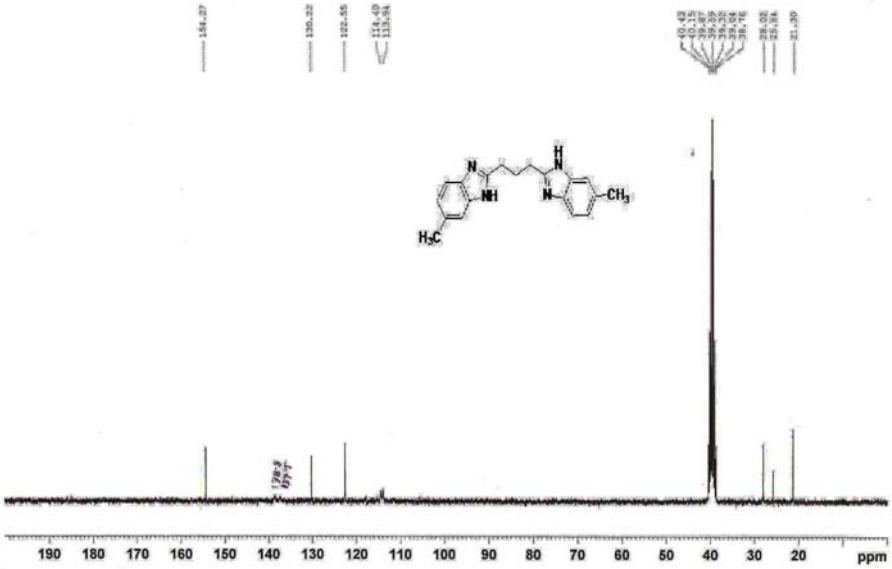
Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4m:



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

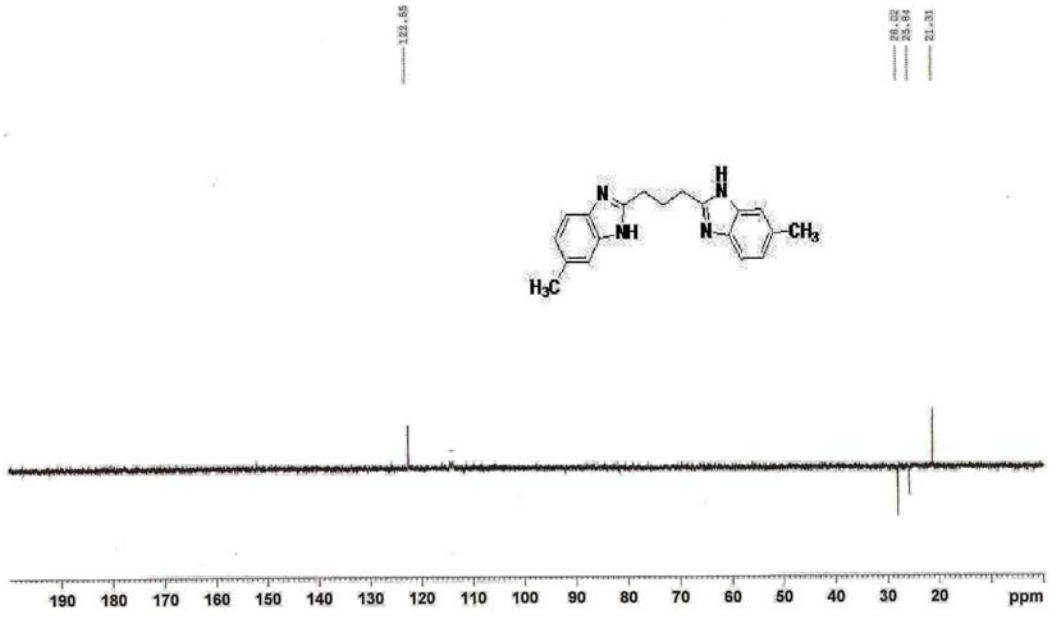
Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure simple bis-benzimidazole. Integration of the two methyl group protons and the methylene group protons are also satisfactory.

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

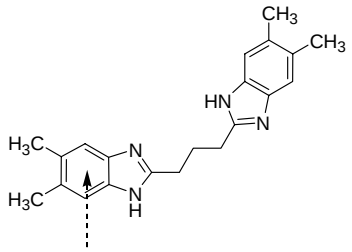


All the seven carbons of one half of the molecule have come separately, the left side four signals disappear in DEPT 135 experiment as they are quaternary carbons while the right side six signals remain in DEPT 135 experiment as they are hydrogen bearing carbons along with the two inversed signals for 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:

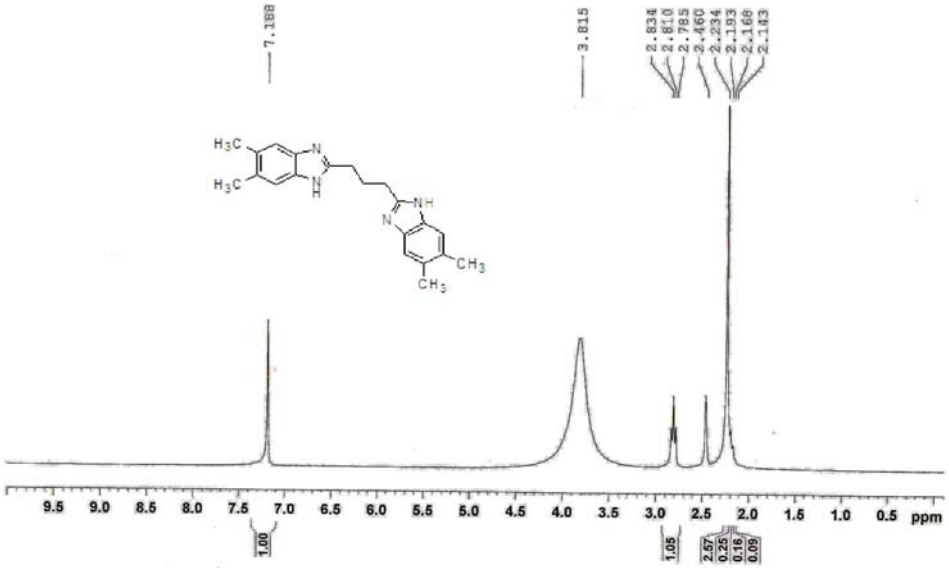


As stated earlier, the disappearance and inversion of signals is seen clearly in DEPT-135 experiment.



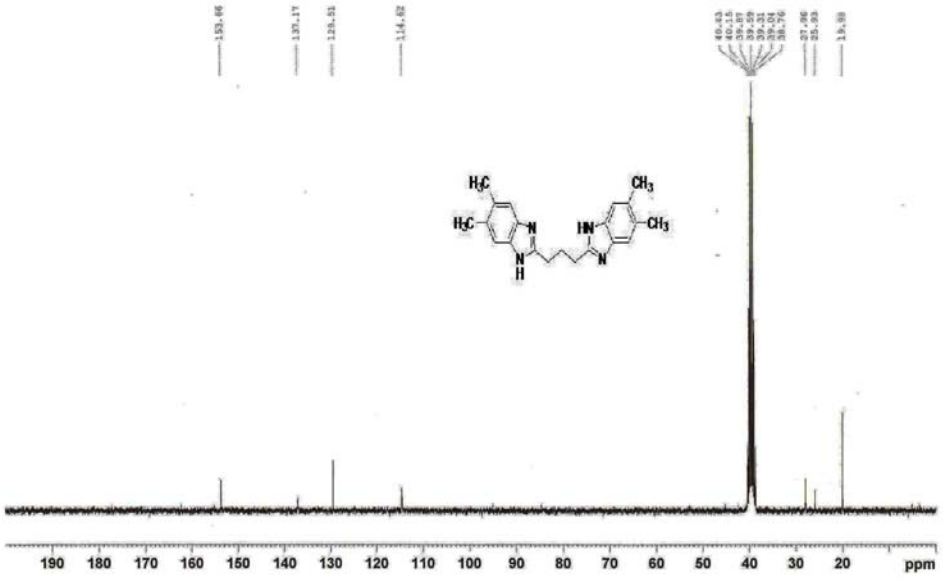
This ring gives a sharp singlet in ^{1}H-NMR spectra.

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



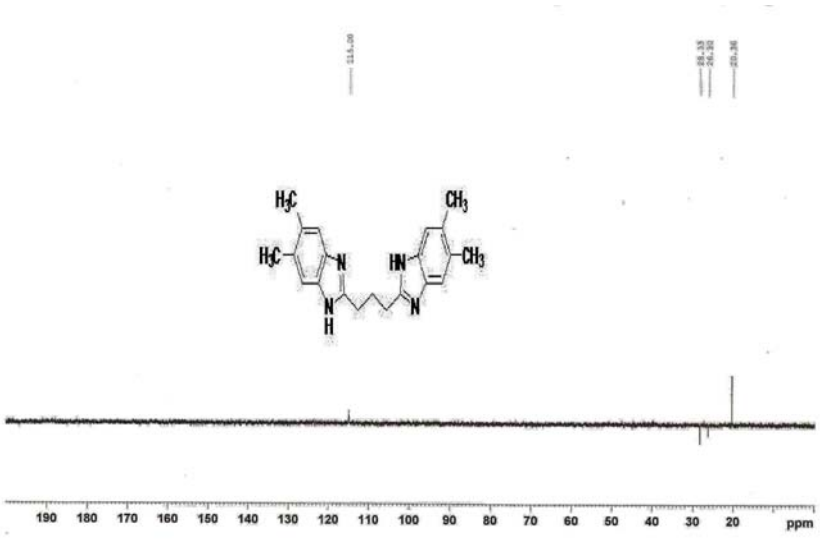
Each individual peak has been assigned both in ^{1}H and in ^{13}C NMR (please see the details of assignment).

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

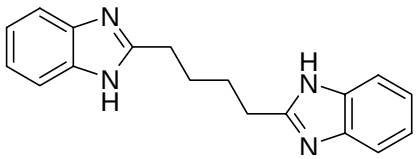


The three signals from left are due to the quarternary carbons.

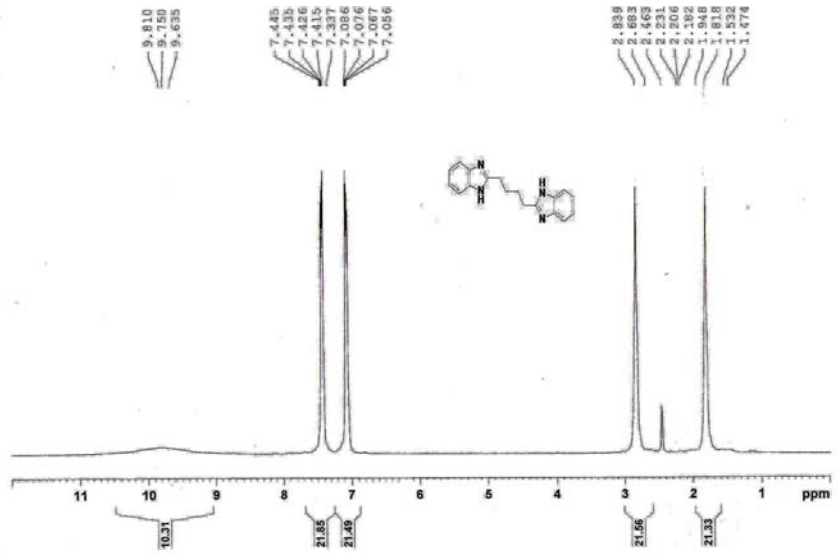
Copy of pure DEPT-135 spectra of compound 4n:



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

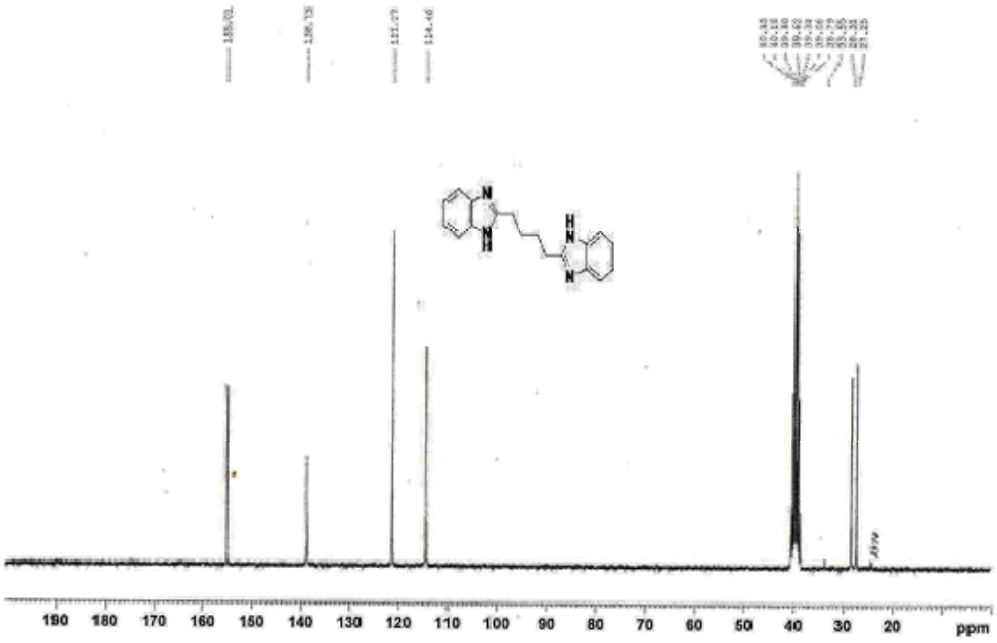


Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4o:



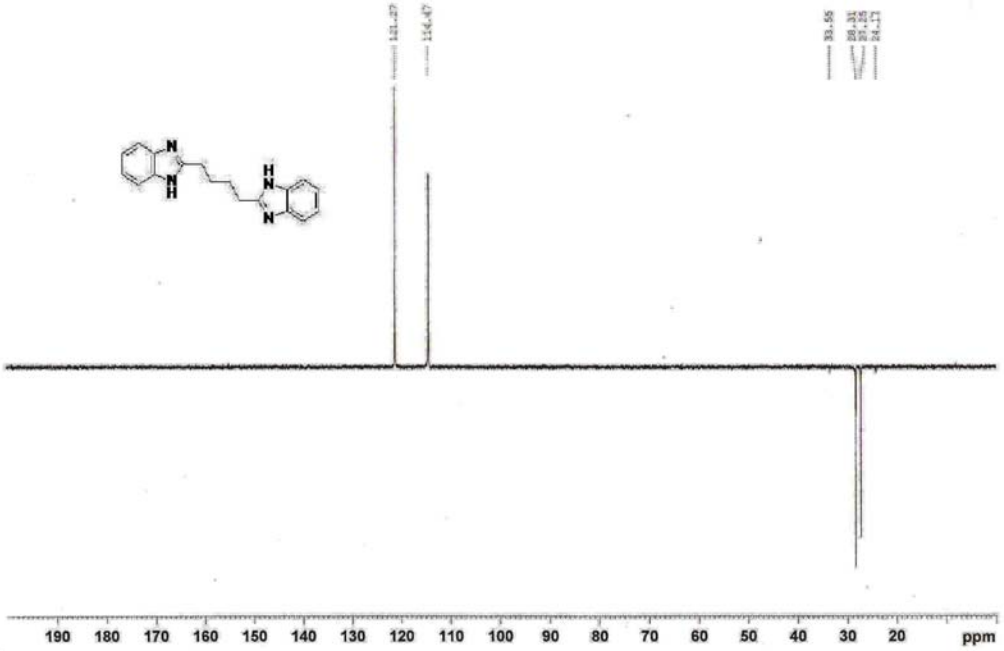
Each individual peak has been assigned both in ^{1}H and in ^{13}C NMR (please see the details of assignment).

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

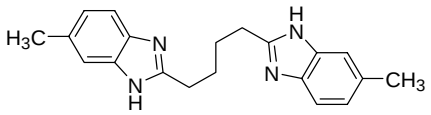


The two signals from the left are the quarternary carbon atoms, the rest are the hydrogen bearing carbon atoms.

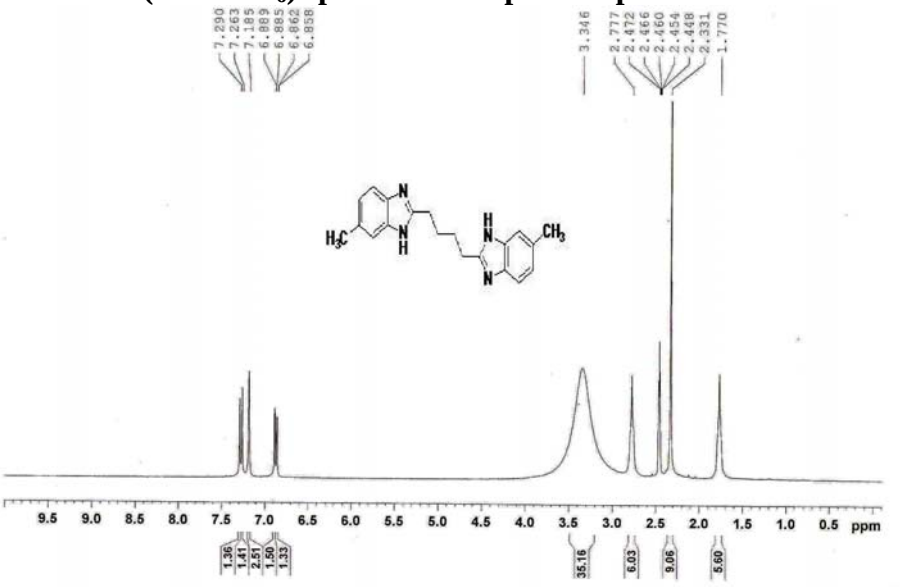
Copy of pure DEPT-135 spectra of compound 4o:



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



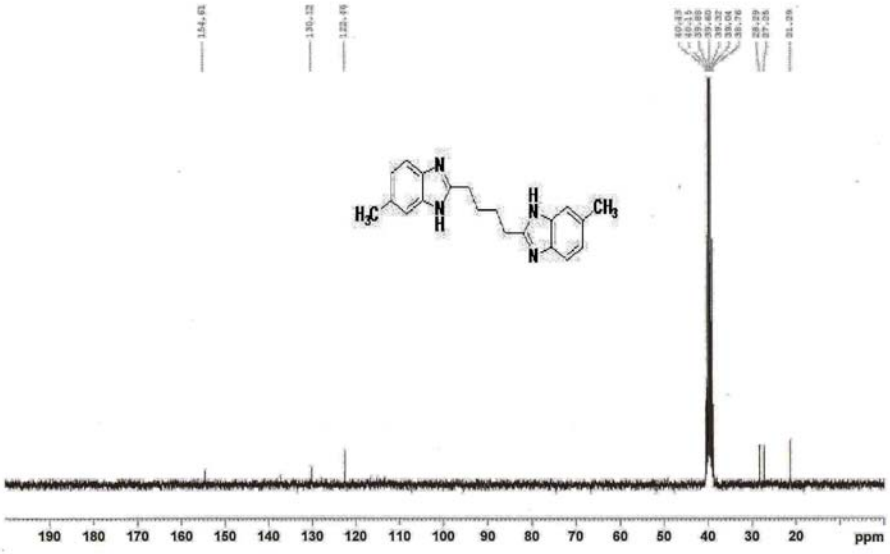
Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4p:



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

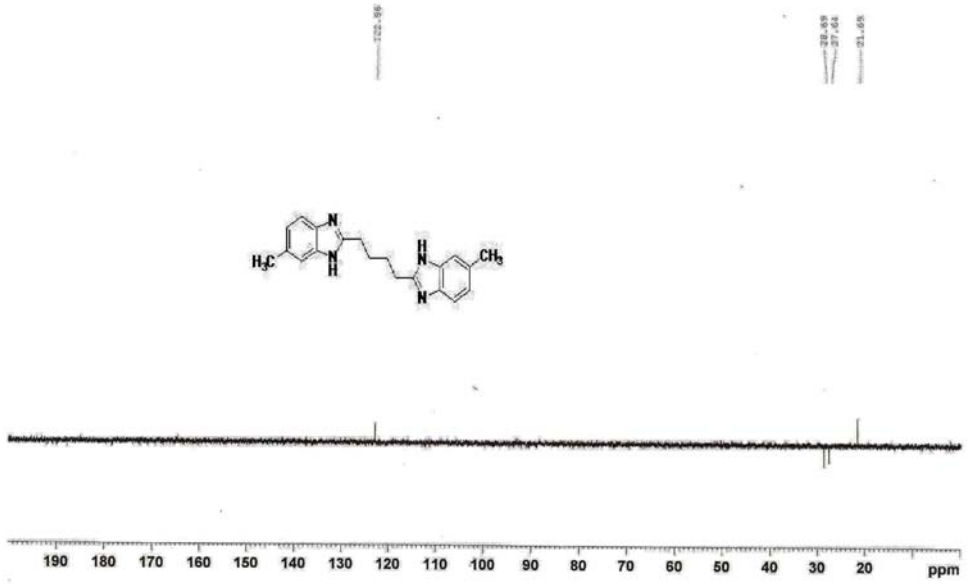
Ratio of the aromatic protons (from left to right): 2: 2: 2 (total 6 protons) indicating the presence of pure mixed bis-benzimidazole. Integration of the methylene group protons is also satisfactory.

Copy of pure ^{13}C-NMR (75 MHz, DMSO-d_6) spectra of compound 4p:

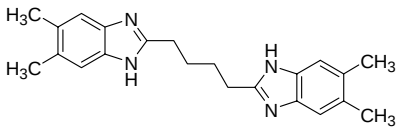


The two signals from left are for the quarternary carbon atoms, the rest are the hydrogen bearing carbon atoms.

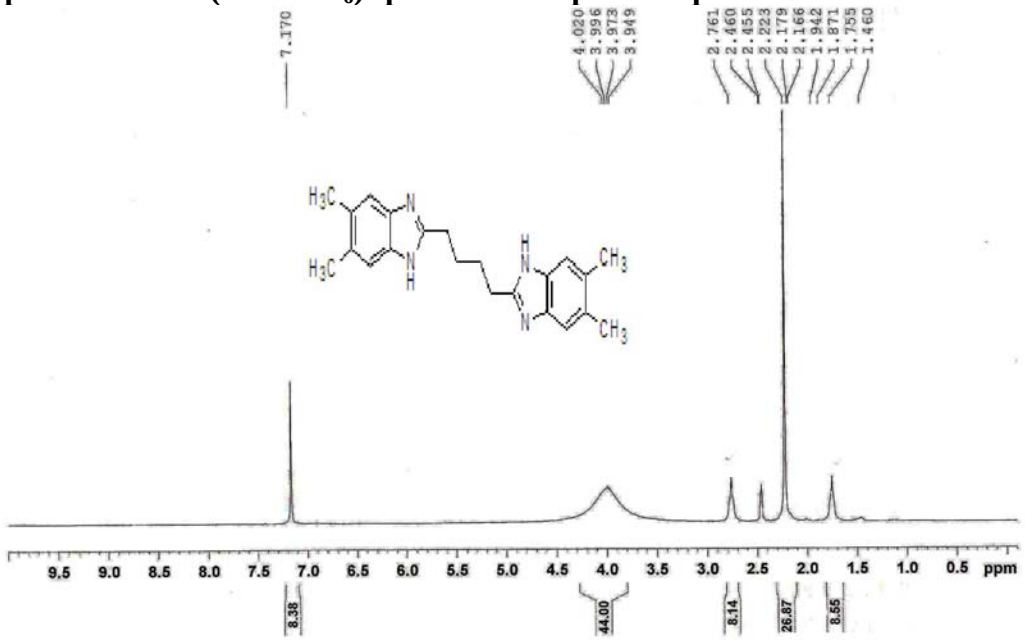
Copy of pure DEPT-135 spectra of compound 4p:



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

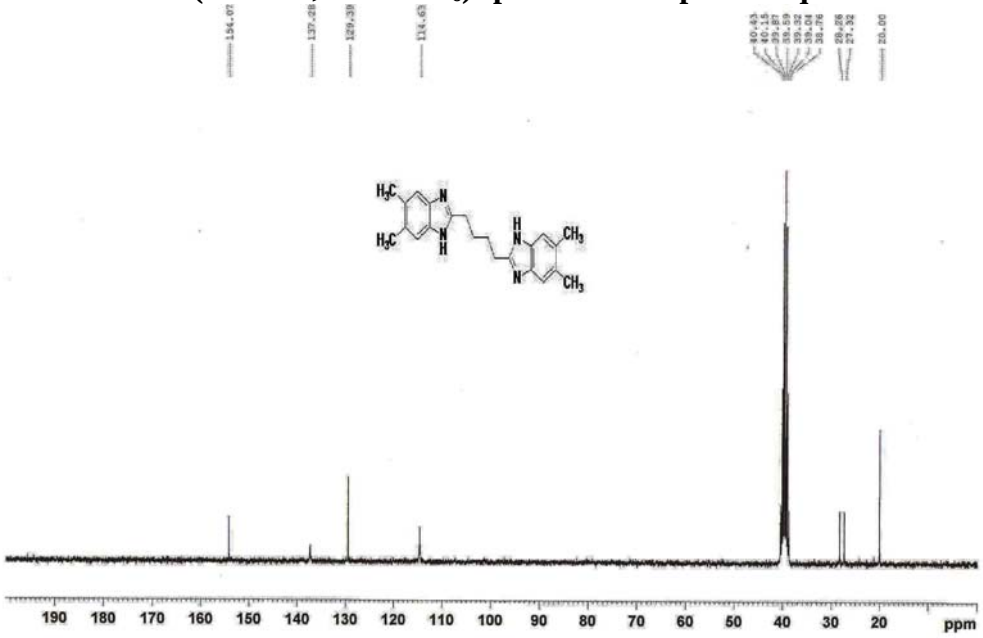


Copy of pure ^{1}H-NMR (DMSO-d_6) spectra of compound 4q:



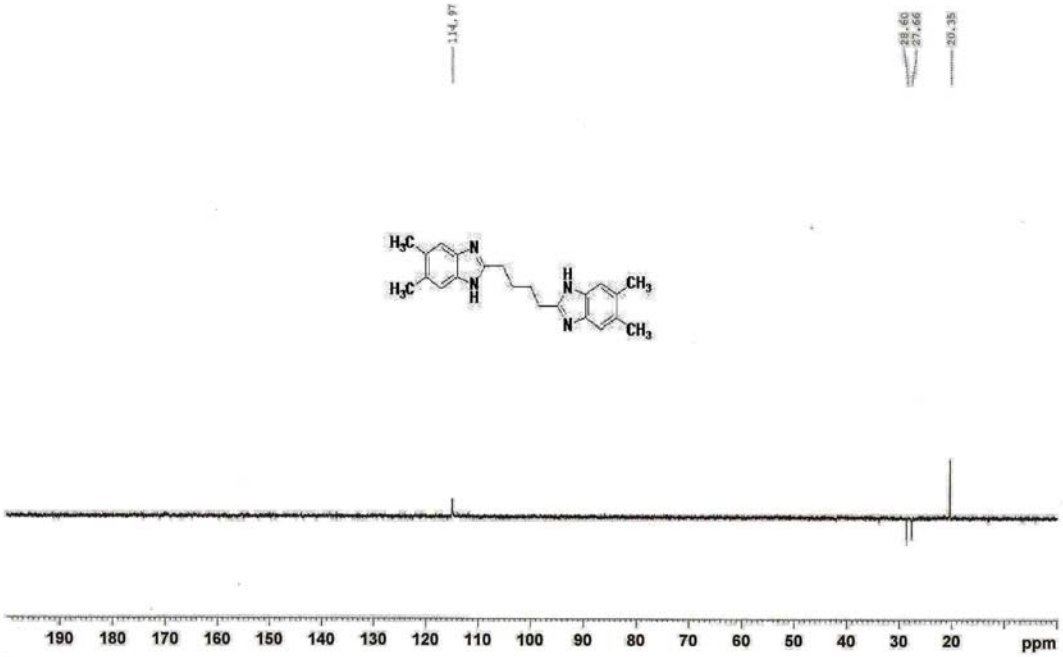
Each individual peak has been assigned both in ^{1}H and in ^{13}C NMR (please see the details of assignment).

Copy of pure ^{13}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:



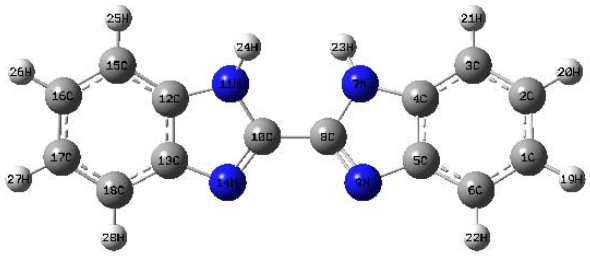
The signals for the quarternary carbon atoms disappear and the methylene carbon atom signals are inversed.

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

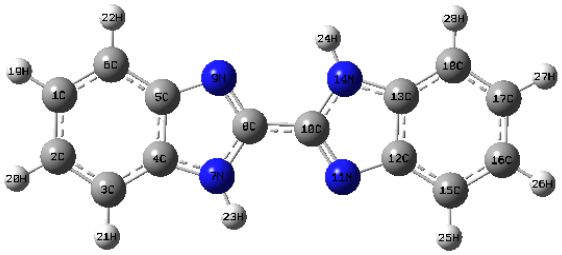


HF=-758.5611264

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

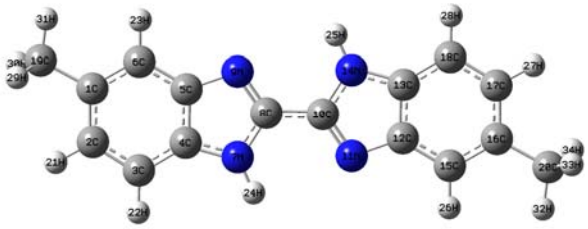


HF=-758.5796288

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



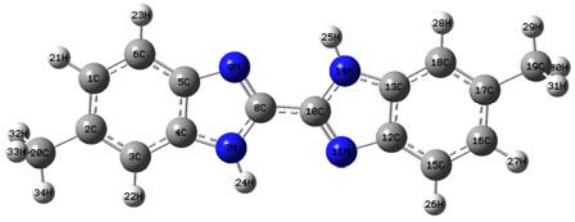
HF=-837.2195299

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



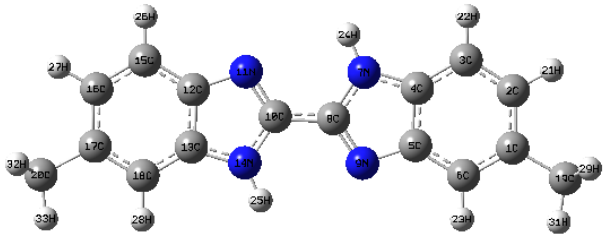
HF=-837.2201707

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) 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



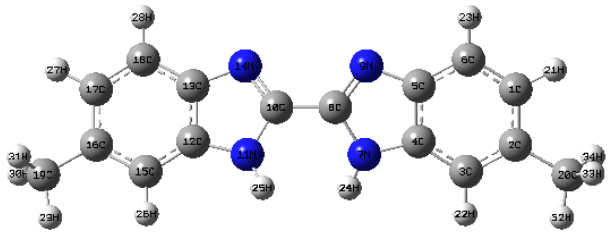
HF=-837.2198856

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



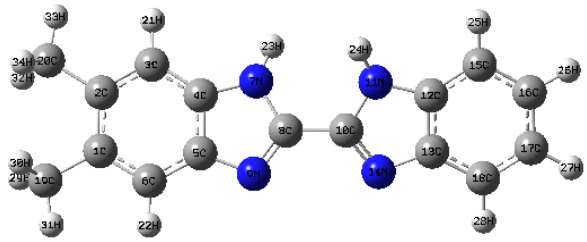
HF=-837.2017569

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



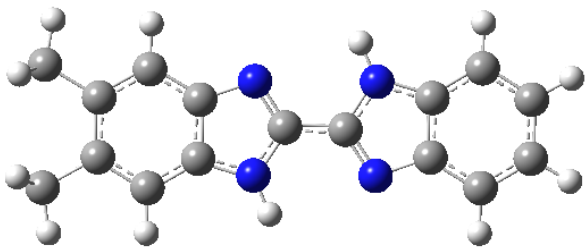
HF=-837.2006823

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.428236	-0.677528	0.148577
2	6	0	-4.398587	0.719959	-0.146317
3	6	0	-3.182746	1.388795	-0.290539
4	6	0	-2.007172	0.653205	-0.142574
5	6	0	-2.016641	-0.730308	0.138495
6	6	0	-3.242016	-1.391956	0.290794

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

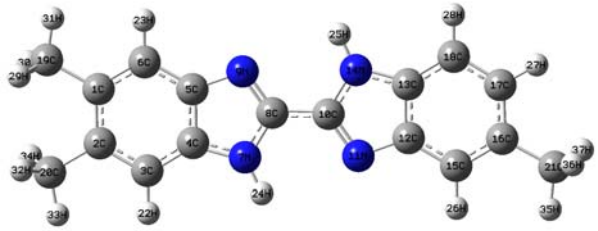


HF=-837.2191376

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



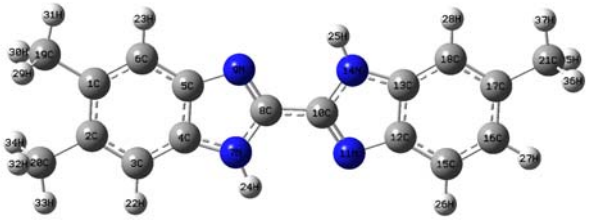
HF=-876.5390786

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



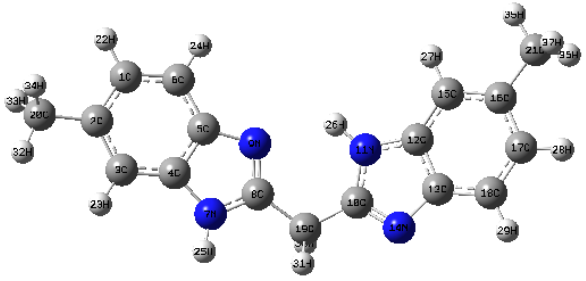
HF=-876.5393751

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

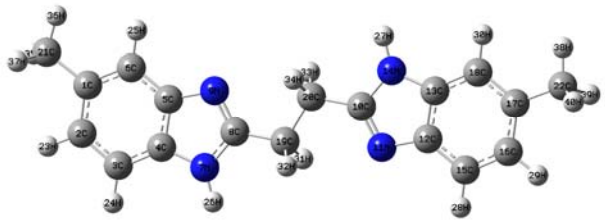
HF=-915.8443704

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



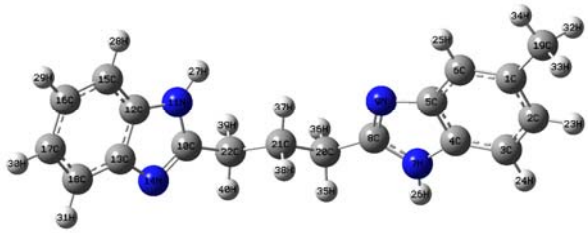
HF=-915.8440751

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



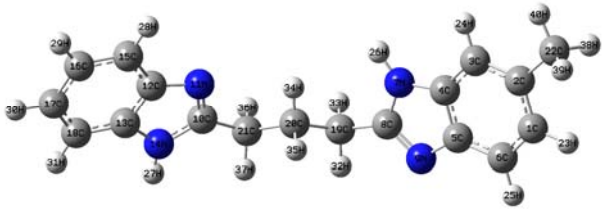
HF=-915.8386045

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



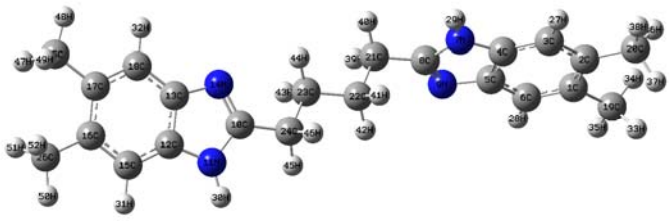
HF=-915.8388506

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	Atomic Type	Coordinates (Angstroms) 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.

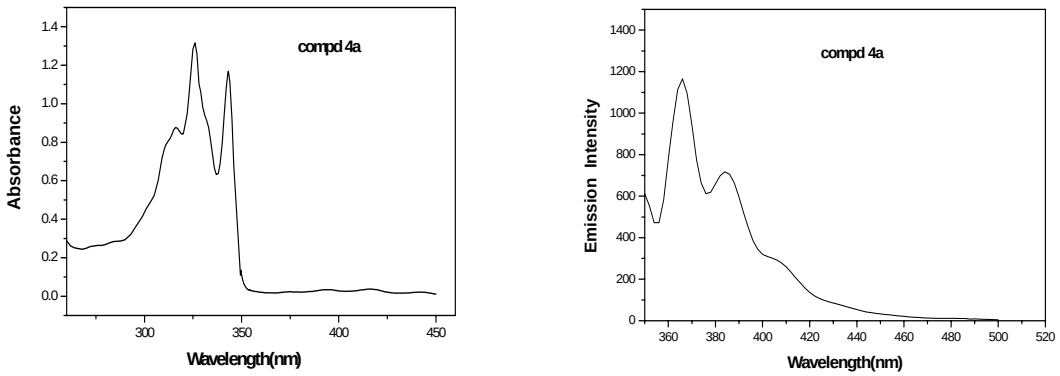


Figure 9. Absorption and Emission graphs of compound **4a**.

Absorption Spectra plot details of a representative compound: Compound **4d**	**Emission Spectra plot details of a representative compound:** Compound **4d**
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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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